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# Making the right link to theranostics: the photophysical and biological properties of dinuclear Ru(II)-Re(I) dppz complexes depend on their tether.

## Supplementary information

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## S1. MATERIALS AND METHODS

### S1.1. Linker synthesis: N,N'-bis(4-pyridylmethyl)-1,6-hexanediamine (L1)

A solution of 4-pyridinecarboxaldehyde (18.5 g, 173 mmol) in ethanol (100 mL) was added to a solution of 1,6-hexanediamine (10.0 g, 86.6 mmol) in ethanol (200 mL) and then heated to reflux for 2 h. The reaction solution was allowed to cool to room temperature.  $\text{NaBH}_4$  (8.0 g, 211 mmol) was carefully added in small portions and then the mixture was heated to reflux for 2 h and then stirred at room temperature overnight. Aqueous  $\text{NaOH}$  (2.0M, 200 mL) was added to the solution. The aqueous solution was extracted with  $\text{CH}_2\text{Cl}_2$  (3V200 mL), the organic fractions combined and dried over anhydrous  $\text{MgSO}_4$ . Filtration and concentration under reduced pressure yielded pale coloured viscous oil. Upon shaking with diethyl ether, a cream coloured solid precipitated, which was collected by filtration, washed with copious amounts of diethyl ether and dried in vacuo (20.2 g, 74%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{H}}$ =8.49 (dd,  $J$ =8.0, 2.8 Hz, 4H), 7.50 (d,  $J$ =8.0 Hz, 4H), 3.82 (s, 4H), 2.64 (t,  $J$ =6.72 Hz, 4H), 1.81 (t,  $J$ =8.4 Hz, 4H), 1.45 ppm (m, 4H).  $^{13}\text{C}$  NMR (63 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 27.1, 30.0, 49.4, 52.7, 122.9, 149.6, 149.8 ppm; ES-MS  $m/z$ =299  $[\text{M}+\text{H}^+]$ .

### S1.2. $[\text{Ru}(\text{tpm})\text{dppz-L1-Re}(\text{CO})_3\text{dppz}]\text{Cl}_3$

$[\text{Re}(\text{CO})_3\text{Cl}]\text{dppz}$  (80 mg, 0.131 mmol) and  $\text{AgCF}_3\text{SO}_3$  (2.1eq, 45 mg, 0.175 mmol) were placed in ethanol (50 mL) and heated to reflux overnight. The solution was allowed to cool and filtered through celite to remove the  $\text{AgCl}$  precipitate. The yellow coloured filtrate was returned to the reaction vessel.  $[(\text{tpm})\text{Ru}(\text{dppz})(\text{L1})]\text{Cl}_2$  (40 mg, 0.041 mmol) was added and the solution was refluxed overnight again. The solution was allowed to cool to room temperature and then evaporated to obtain a red-brown precipitate. The product was then purified by anion metathesis (38%);  $^1\text{H}$  NMR (400 MHz,  $\text{D}_2\text{O}$ ):  $\delta_{\text{H}}$  = 9.79 (s, 1H), 9.59 (d,  $J$  = 9.0 Hz, 4H), 9.02 (d,  $J$  = 5.3 Hz, 4H), 8.55 (d, 4H), 8.20 (m,  $J$  = 2.8 Hz, 4H), 8.08 (m, 4H), 7.85 (dd,  $J$  = 8.2, 5.4 Hz, 4H), 7.50 (d,  $J$  = 6.2 Hz, 4H), 7.31 (d,  $J$  = 5.9 Hz, 4H), 6.92 (d,  $J$  = 5.9 Hz, 2H), 6.70 (m, 2H), 6.24 (m, 1H), 3.98 (s, 4H), 3.86 (m, 4H), 2.62 (m, 4H), 1.39 (m, 4H);  $m/z$  (ES-MS) 744.0 (100%,  $[\text{M}-2\text{Cl}_2]^{2+}$ ). Elemental analysis of chloride calcd (%) for  $\text{C}_{67}\text{H}_{59}\text{Cl}_3\text{N}_{18}\text{O}_3\text{ReRu}\cdot\text{H}_2\text{O}$ : C 51.65, H 3.82, N 16.18; found: C 51.04, H 3.90, N 16.00.

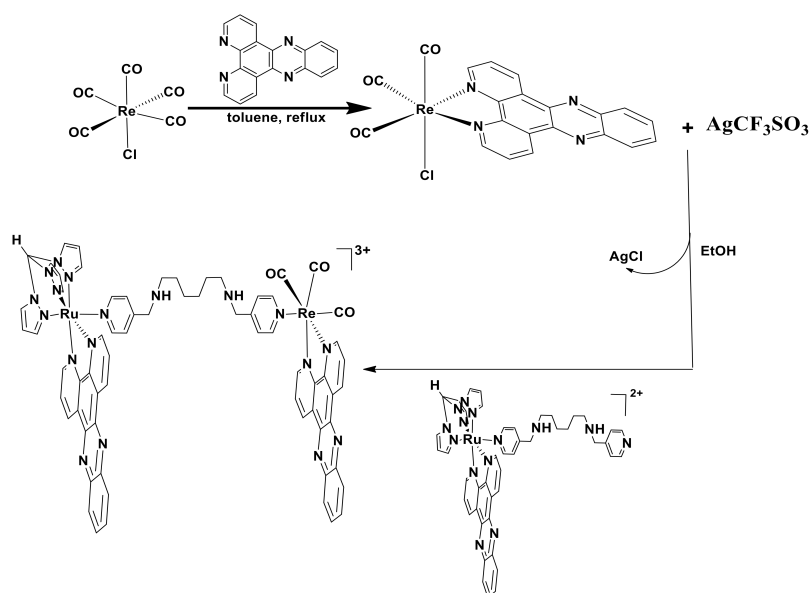


FIG. S1. Synthesis route of dinuclear complex  $2^{3+}$

### S1.3. UV-vis titration of complex 2 with CT-DNA

UV-Visible titrations were performed on a thermoregulated Varian-Carey 50 UV-Visible spectrometer at 25 °C. 3 ml of buffer was loaded into a 10 mm path length cuvette and allowed to equilibrate inside the spectrometer before a baseline reading was taken. A volume of buffer was removed with a Gilson pipette and replaced with the same volume of a stock solution of complex to give a final concentration of around 50  $\mu\text{M}$  complex inside the cuvette. After equilibration the spectrum was recorded between 200-600 nm. 5  $\mu\text{L}$  of a concentrated stock solution of CT-DNA was added to the cuvette and mixed 10 times with a pipette to ensure homogeneity. The spectrum was recorded after leaving the sample to equilibrate for 5 minutes, checking no bubbles were present. This procedure was continued until the absorbance became constant indicating saturation binding had occurred or the increase of CT-DNA concentration only caused small changes in the absorption spectra.

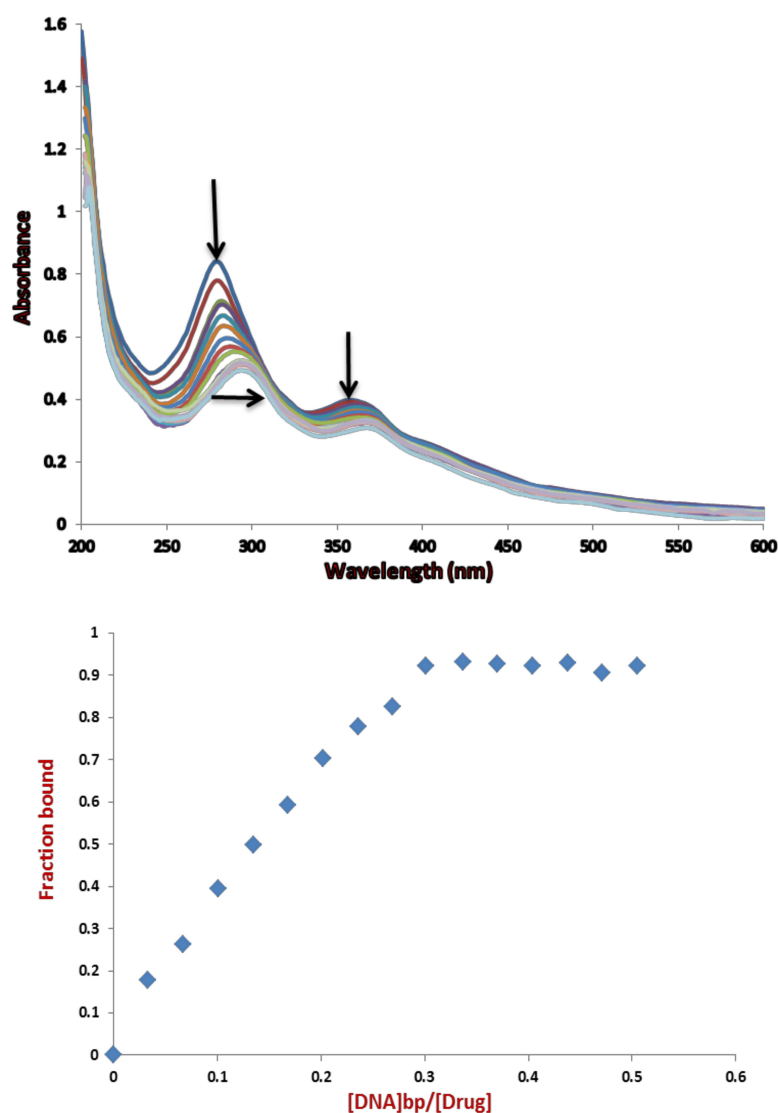


FIG. S2. UV-Vis titration and binding curve of 1.01 mM  $\text{bp}^{-1}$  CT-DNA into a solution of 50  $\mu\text{M}$   $[\mathbf{2}]\text{Cl}_3$  in 5 mM tris buffer, 25 mM NaCl, pH 7.4 at 25 °C.

### S1.4. Luminescence titrations

Luminescence titrations were carried out in a thermoregulated Horiba Jobin-Yvon FluoroMax-3 spectrophotometer in a procedure similar to the UV-Visible titrations. 3 mL of buffer was loaded into 10 mm path length luminescence cuvette and allowed to equilibrate inside the spectrophotometer at 25 °C before a background reading was taken. A volume of buffer was removed and replaced with the same volume of a stock solution of complex to give a final concentration of around 50  $\mu\text{M}$  complex inside the cuvette. After equilibration, the emission spectrum of the solution was recorded using the excitation wavelength characteristic of the complex. 2.5  $\mu\text{L}$  of a concentrated stock solution of CT-DNA was added to the cuvette and mixed 10 times to ensure homogeneity. After leaving the sample to equilibrate for 3 minutes and checking no bubbles were present, the emission spectrum was recorded, showing an enhancement in emission. The procedure was continued until the emission became constant.

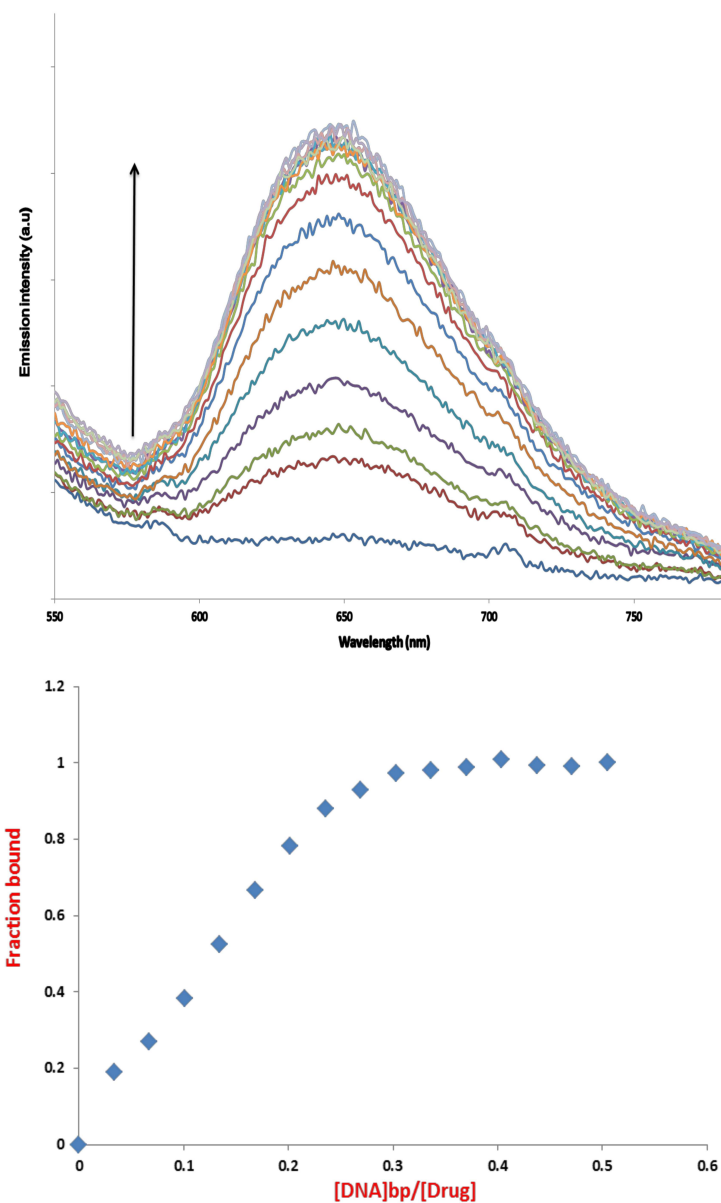


FIG. S3. Luminescence titration and binding curve of complex  $[2]\text{Cl}_3$  in 5 mM tris buffer, with CT-DNA

### S1.5. Ultrafast Transient Absorption

Our ultrafast Transient Absorption setup comprises of a commercial detection instrument (Helios, Ultrafast Systems) as well as the following light sources: a 84 MHz Ti:Sapphire 25 fs 800 nm seed laser (Mai Tai Spectra Physics), a Ti:Sapphire chirped-pulse amplifier with a repetition rate of 10 KHz, 12W average power and a nominal pulse duration of 40 fs (Spitfire Ace PA-40) both from Spectra-Physics; frequency doubling and tripling achieved by a commercial instrument utilising beta-Barium-Borate crystals (TimePlate, by Photop Technologies); UV-Vis-NIR generation has been done by means of Optical Parametric Amplification (Topas Prime, by Light Conversion). The latter two served as quasi monochromatic excitation pump sources, selectable from 235 nm to 1600 nm. The probe beam is a white light supercontinuum generated in-situ and optimised for the UV (340-750 nm), Vis (450-950 nm) and NIR (800-1600 nm) regions. Detection was performed by virtue of CMOS and InGaAs sensors for UV/Vis and NIR grating-dispersed spectra, respectively. Sample concentration for  $1^{3+}$  and  $2^{3+}$  was approximately  $5 \mu\text{M}$ , CT-DNA was added at approximately  $25 \mu\text{M bp}^{-1}$ . Dynamics were fitted using global analysis in Glotaran 1.5.1.

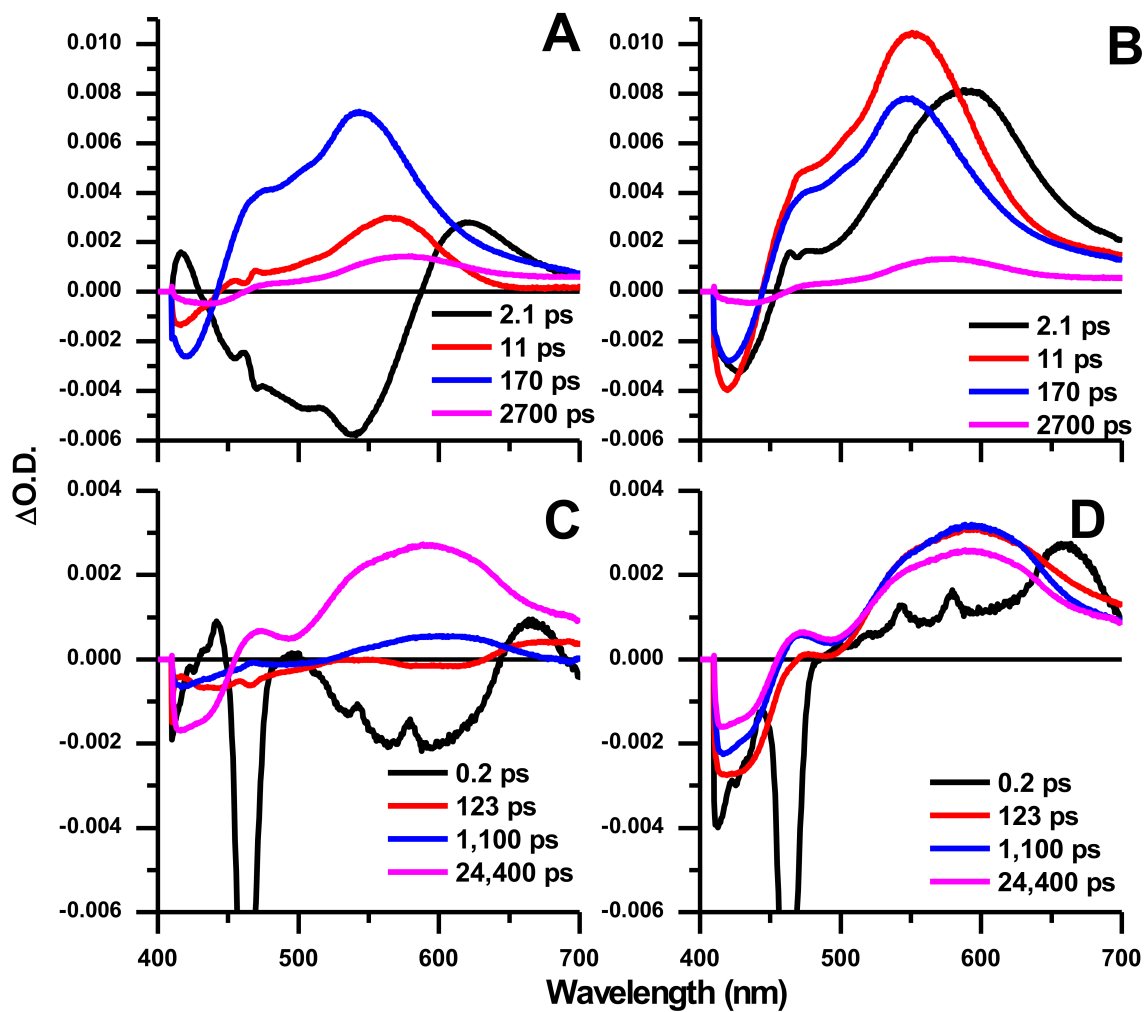


FIG. S4. A— Decay Associated Spectra for  $2^{3+}$  in TRIS buffer. B— Signal Associated Spectra for  $2^{3+}$  in TRIS buffer. C— Decay Associated Spectra for  $2^{3+}$  in TRIS buffer with  $25 \mu\text{M bp}^{-1}$  CT-DNA. D— Signal Associated Spectra for  $2^{3+}$  in TRIS buffer with  $25 \mu\text{M bp}^{-1}$  CT-DNA.

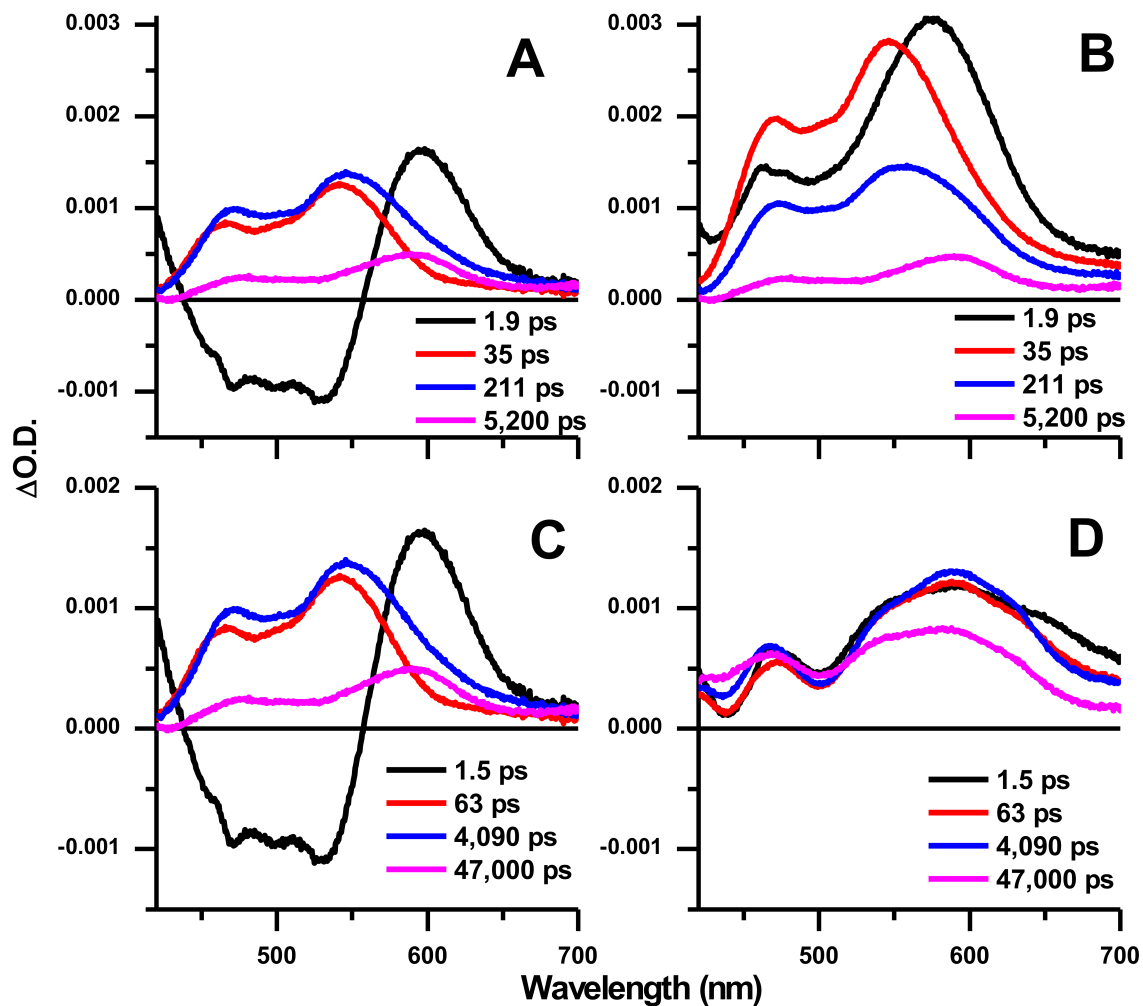


FIG. S5. A– Decay Associated Spectra for  $1^{3+}$  in TRIS buffer. B– Signal Associated Spectra for  $1^{3+}$  in TRIS buffer. C– Decay Associated Spectra for  $1^{3+}$  in TRIS buffer with  $25 \mu\text{M bp}^{-1}$  CT-DNA. D– Signal Associated Spectra for  $1^{3+}$  in TRIS buffer with  $25 \mu\text{M bp}^{-1}$  CT-DNA.

#### S1.6. Agarose Gel Electrophoresis of DNA

Photoinduced cleavage of supercoiled pBR322 and pUC57 DNA by the complexes was studied by agarose gel electrophoresis. The reactions were performed under illuminated conditions using 470 nm using FLUOstar OPTIMA microplate reader. The sample was prepared in a dark room at room temperature using supercoiled DNA ( $0.1 \mu\text{g}/\mu\text{L}$ ) in 50 mM Tris-HCL buffer and varying concentrations of the complex. After photoexposure, the sample was incubated followed by the addition of the loading buffer containing 25% bromophenol blue, 0.25% xylene cyanol and 30% glycerol ( $2 \mu\text{L}$ ), and the solution was finally loaded on an 0.8% agarose gel containing  $1.0 \mu\text{g}/\text{mL}$  ethidium bromide. Electrophoresis was carried out for an hour at 100 mW in TAE (Tris-acetate-EDTA) buffer. The gel was visualised using a UVP transilluminator and photographed for analysis.

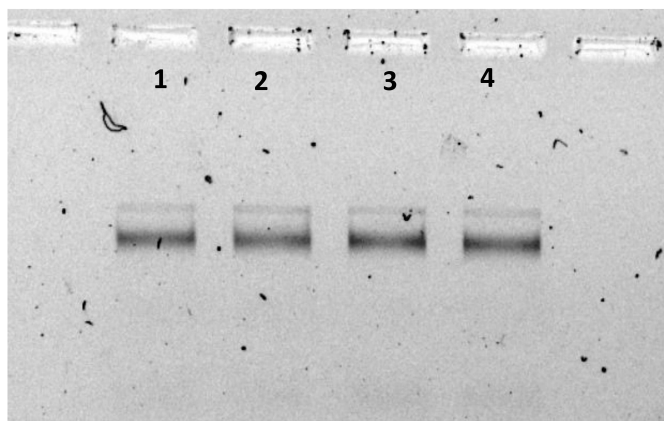


FIG. S6. Photocleavage of supercoiled pBR322 DNA ( $0.1 \mu\text{g}/\mu\text{L}$ ) by [2] under illuminated condition (470 nm, 100 mW, 60 minutes exposure) in 50 mM Tris-HCL buffer. Lane 1, DNA control; lane 2, DNA + 2 ( $10 \mu\text{M}$ ); lane 3, DNA + 2 ( $20 \mu\text{M}$ ); lane 4, DNA + 2 ( $40 \mu\text{M}$ ). No nicking was observed.

### S1.7. Structured Illumination Microscopy and Wide Field Fluorescence Microscopy

#### S1.7.1. Structured Illumination Microscopy (SIM): General Description

Structured Illumination Microscopy (SIM) offers unique features compared to traditional optical microscopy techniques, such as wide field microscopy (WF). Multiple images are obtained by adjusting the fringe pattern and by slicing through the sample with respect to different focal planes in a Z-stack. Each frame of the Z-stack is reconstructed to provide definitive information of the details of the imaged sample and thereby improving the resolution close to two fold in comparison to traditional optical microscopy techniques. The resolution improvement achieved along the axial plane is 350 nm and along the lateral plane is 120 nm. Single colour SIM and Wide field experiments were performed for both complexes 1 and 2, which were bright photostable probes able to withstand the SIM imaging conditions.

#### S1.7.2. Sample preparation (SIM and WF)

A2780 cells were seeded on cover slips (22 mm X 22 mm,  $170 \pm 5 \mu\text{m}$  square cover glasses) placed in 6 well plates in RPMI culture medium containing 10% FBS and 1% Penicillin Streptomycin for 24 h at  $37^\circ\text{C}$ , 5%  $\text{CO}_2$ . After 24 h when 70% confluency was achieved the cells were washed with RPMI culture medium then cells were treated with complexes 1 and 2 ( $100 \mu\text{M}$ ) for 7 h. Cells were then washed thrice with culture medium and washed again with phosphate buffer saline (PBS). After carrying out the live cell uptake of the complexes 1 and 2, the cells were fixed with 4% paraformaldehyde (PFA) for 15 min, washed thrice with PBS and then the cover slips were mounted using mounting medium (Vectashield, h-1000). The coverslips were then sealed using nail varnish before imaging.

#### S1.7.3. Data acquisition and processing

**S1.7.3.1. Structured Illumination Microscopy (SIM)** Resolution improvement is achieved based on the reconstruction of the acquired Z stacks using the software programme SoftWoRx. Complexes 1 and 2 were excited at 488 nm and the emission was collected  $>650 \text{ nm}$  (Cy5 Channel of the Delta Vision OMX). The Structured Illumination (SI) parameters employed for running the single colour SI experiment depended on the thickness of the Z stack (number of sections 50 - 80), section spacing (0.125 - 0.150) and thickness of the sample (8 - 12). Exposure and %T was varied, but ranges used were an exposure time of 50 - 100 and the %T of 10 - 50.

**S1.7.3.2. Wide Field Fluorescence Microscopy (WF)** The WF technique involves improvement in resolution only after post processing the Z-stacks acquired. Post processing of acquired data is done by using SoftWoRx software provided in the Delta Vision OMX. Offline image processing for the manuscript was carried out by using FIJI software.

Complexes 1 and 2 were excited at 488 nm and the emission was collected at 650 nm (Cy5 Channel of the Delta Vision OMX). The WF imaging conditions employed were thickness of the Z stack (Number of sections 30 - 60), section spacing (0.25 - 0.50) and thickness of the sample (8 - 12). Exposure and %T was varied, but ranges used were an exposure time of 50 - 100 and %T of 10 - 50.

*S1.7.3.3. Deconvoluted Wide Field Microscopy* The Deconvolution procedure involves the processing of the raw WF images obtained from the Delta Vision OMX. This Image processing is carried out by using the SoftWoRx software which is used for carrying out the post processing of the SIM data. Deconvolution is a computationally intensive image processing technique which helps in improving the contrast and axial resolution of the images post acquisition from 400 nm to 350 nm. The deconvolution procedure removes the out of focus blur from the Z-stack of acquired images. This improves the quasi random disarrangement, signal to noise ratio and the point spread function, and thereby gives greater resolution and retrieves more information from the post processed wide field image.

#### *S1.7.4. Comparative SIM and WF intensity profiles*

A comparison between SIM and WF techniques is essential to understand the effectiveness of the complexes 1 and 2 as super-resolution microscopy DNA imaging probes. Intensity v distance plots were generated by using FIJI software to give a comparison of the region of interest using the two different techniques of SIM and WF. The extent of improvement of resolution and sharpness is directly proportional to the extent of retrievable biological information from these images. The intensity profiles obtained for both SIM and WF deconvoluted images of A2780 cells stained with complex 2 indicate localisation in the cytosol. The SIM and WF Images obtained for A2780 cells stained with complex 1 indicate localisation mainly in the nucleus. The improvement in resolution is evident from the comparative SIM and Wide field images in the main paper.

#### *S1.7.5. HyVolution, deconvoluted Laser scanning confocal microscopy (d-LSCM)*

This methodology developed by Leica microsystems utilises for the image acquisition a reduced size of pinhole right in front of the HyD detectors, and then employs a deconvolution software developed by SVI (Huygens) in Netherlands. The deconvolution software uses the raw data information from the Leica acquisition files for an optimal deconvolution. This software can use either a theoretical PSF or a calculated one. The single plane images were deconvolved with a theoretical calculated PSF provided by the software and by an experimentally calculated PSF from fluorescent beads, in both case no apparent difference was observed.

#### *S1.7.6. STED nanoscopy*

STED images were taken in a commercial LEICA SP8 3X gSTED SMD confocal microscope (Leica Microsystems, Mannheim, Germany). The microscope is equipped with 3 depletion lines and it is also equipped with a 3D STED additional vortex to obtain higher spatially resolved images in XY and Z. The excitation laser beam consisted of a pulsed (80MHz) super-continuum white light laser (WLL). For a cleaner emission the excitation lines had a clean-up notch filter (NF) in the optical pathway. The gSTED imaging was taken with a continuous wavelength 660nm nm depletion laser, and the pulsed STED images with a pulsed 775 nm laser, again in every case the respective NF were in place. The best results were obtained with the pulsed 775nm laser. The objective employed was a Leica 100x/1.4 NA oil objective. The pinhole was set at one Airy unit. The gated HyD detectors were set with the gated option on and the temporal gated selected was from 2 to 6.5ns when depleting at 660nm. For the 3D STED images the depletion lasers were split in two, the second vortex was set at 50%. Live images and videos of cells were taken at 37 °C and 5% CO<sub>2</sub>. The dye was excited with a WLL at 470 nm, and STED depleted at 775 nm; the emission was collected from 620 to 710 nm and a gating between 2 and 6.5 ns was used.

### **S1.8. Image analysis and deconvolution**

gSTED nanoscopy resolved the localisation and of the mitochondria and Lysosomes with high resolution. To enhance the signal to noise ratio obtained when employing either a continuous wavelength or a pulsed depletion laser deconvolution was applied. Deconvolution was carried out with the software package Huygens (SVI, Netherlands). To quantify the background level of noise we used either an automated quantification provided by the software or a manual by means of computing the averaged background intensity from regions outside the cell. For the deconvolution we used

40 iterations, a signal to noise ratio of 13, and the classical maximum likelihood estimation method. Colocalisation analysis was performed using the Huygens software package and the Pearson colocalisation coefficient was quantified. The software allows obtaining the 2D colocalisation map of the regions that colocalise. Lines profiles were drawn at regions of interest, the intensity profile over the distance drawn was plotted as normalized intensity employing Origin Pro (OriginLab Corporation, Northampton, MA, U.S.A.). The figures in this paper have been made using the free open source software Inkscape ([www.inkscape.org](http://www.inkscape.org)). The surface rendered images, and intensity images have been processed using Huygens Professional, LAX software (Leica SP8) and the kymographs using a plugin specially designed in Fiji (ImageJ; NIH)

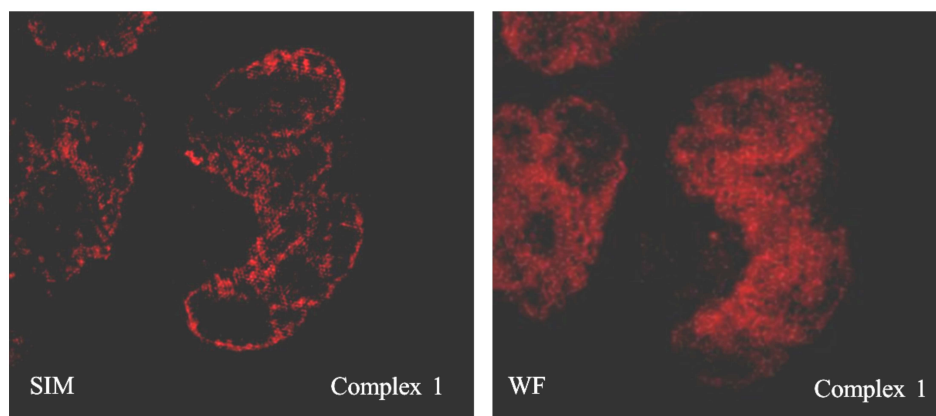


FIG. S7. SIM and WF images of complex 1

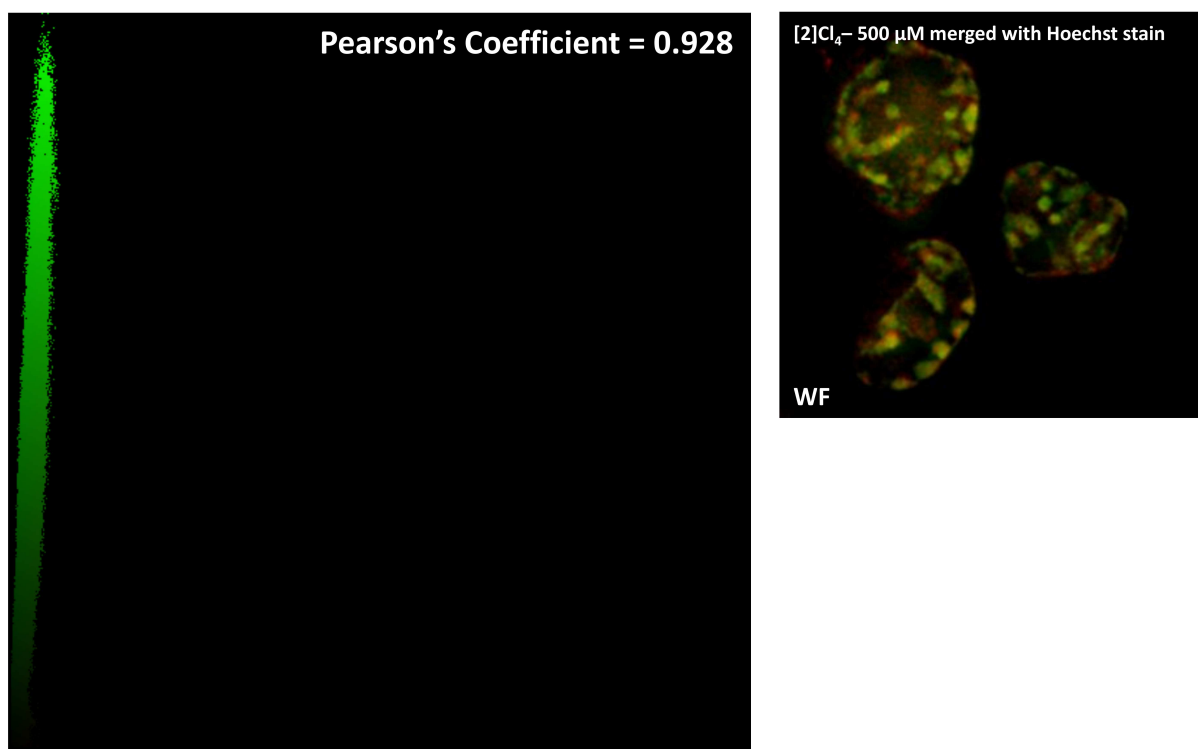


FIG. S8. Colocalization of **2** and H33342



### S1.9. Intracellular ruthenium analysis - Inductively Coupled Mass Spectrometry (ICP-MS)

A2780 or A2780cis cells were seeded in 6 well plates ( $2 \times 10^5$  cells/well) and incubated for 24 h ( $37^\circ\text{C}$ , 5%  $\text{CO}_2$ ) in regular RPMI culture medium (RPMI 1640 supplemented with 10% FBS, 2 mM glutamine and penicillin/streptomycin). All media was removed before 200  $\mu\text{M}$  complex  $1^{3+}$  or  $2^{3+}$  (2 mM stock in PBS, diluted in regular RPMI culture medium, 10% PBS maintained throughout all solutions) or control media was added and cells incubated for 24 h. All complex solutions (or control medium) were removed, cells washed with ice cold PBS and 200  $\mu\text{L}$  PBS added. Cells were detached by scraping and samples collected in microcentrifuge tubes and centrifuged (4000 rpm, 3 min). The supernatant was removed, pellet resuspended in 100  $\mu\text{L}$  Nuclei EZ lysis buffer (Sigma cat no. N3408) and samples put on ice for 5 mins. The nuclear fraction was collected by centrifugation ( $500 \times g$ , 5 min,  $4^\circ\text{C}$ ) and the cytoplasmic supernatant transferred to microcentrifuge tubes. The nuclear pellets on ice were washed briefly with EZ lysis buffer, then 100  $\mu\text{L}$  EZ lysis buffer added and samples vortexed to resuspend. All samples were then subjected to 3 freeze-thaw cycles and 10  $\mu\text{L}$  of each sample preserved for the determination of protein concentration before the remainder was transferred to a glass sample tube, 2 mL concentrated  $\text{HNO}_3$  added, heated to  $60^\circ\text{C}$  overnight, diluted to 10 mL total volume with ultrapure Milli-Q  $\text{H}_2\text{O}$  and analysed for ruthenium content by ICP-MS. The protein concentration of each sample was determined by Bradford assay with a BSA standard curve, and the data normalised to total protein content.

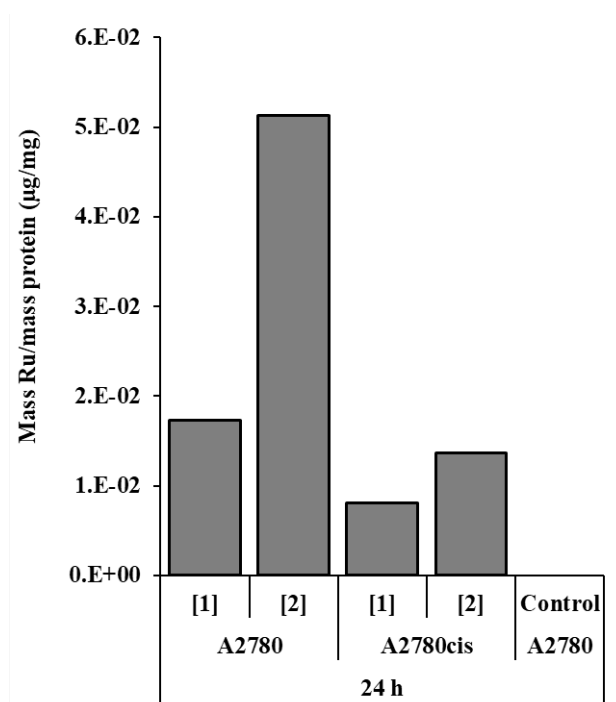


FIG. S9. A2780 and A2780cis intracellular ruthenium (normalised to protein content) after 24 h treatment with complexes  $1^{3+}$  and  $2^{3+}$ ; combined nuclear and cytoplasmic data.

### S1.10. Cytotoxicity

$\text{IC}_{50}$  determination by MTT assay: Cells were maintained in RPMI 1640 medium supplemented with 10% FBS, 100  $\text{mg ml}^{-1}$  streptomycin, 100 units  $\text{ml}^{-1}$  penicillin, and 2 mM glutamine, at  $37^\circ\text{C}$  in a humidified atmosphere containing 5%  $\text{CO}_2$ . Experimental cultures were grown on 48 well plates at a seeding density of  $5 \times 10^4$  cells/well and incubated for 24 h. The cells were then treated with complex (solubilised in and maintained at 10% PBS/ $\text{H}_2\text{O}$ : 90% medium throughout all solutions) of a 1–200  $\mu\text{M}$  concentration range, in triplicate, and incubated for 48 h. All medium was then removed and cells incubated with MTT (0.5  $\text{mg ml}^{-1}$  dissolved in PBS) for 40 min. The MTT was removed and formazan product eluted using 120  $\mu\text{L}$ /well acidified isopropanol, 100  $\mu\text{L}$  of which was transferred to a 96 well plate for the absorbance to be quantified by spectrophotometer (595 nm, referenced at 640 nm). An average absorbance for

each concentration was calculated and cell viability was determined as a percentage of the untreated negative control wells (10% PBS/H<sub>2</sub>O: 90% medium, average of triplicate). Data were plotted in a graph of concentration against cell viability to produce a curve from which the IC<sub>50</sub> value (half maximal inhibitory concentration) could be derived by interpolation.

### S1.11. Photocytotoxicity (phototoxicity)

#### S1.11.1. Light Irradiation Source Apparatus (LISA)

The apparatus used to irradiate the samples was a custom-made device featuring a broadband illumination source fully contained in an empty computer base unit, referred to as the Light Irradiation Source Apparatus (LISA). The technical specifications of the bulb contained within are as follows (Table S1).

TABLE S1. Specification of the bulb contained within the irradiation apparatus

|                                |                                    |
|--------------------------------|------------------------------------|
| Product Code                   | 871691                             |
| International Model Number     | HC01080i                           |
| Description                    | CFL 80W E40 Integrated Clusterlite |
| Watts                          | 80 W                               |
| Cap                            | E40                                |
| Operating Hours                | 15000                              |
| Colour Temp                    | 4000 K                             |
| Lumens                         | 5400 lm                            |
| Dimming                        | No                                 |
| Dimensions (length x diameter) | 256mm x 80mm                       |

#### S1.11.2. Light irradiation protocol

The 48 hour IC<sub>50</sub> determination protocol was used except four separate plates were employed and after 24 h each had the complex removed prior to irradiation for a varying length of time. All complex solution (and control medium) was removed from the cells and replaced with regular growth medium 30 min prior to irradiation. Of the four prepared well plates, one remained in the incubator whilst the other three were exposed to the LISA for the duration of 5, 15 or 30 min (corresponding to light doses of 8, 24 or 48 J cm<sup>-2</sup>) before being incubated for a further 24 h after culmination of light treatment. To provide a comparison in assessing any phototoxicity upon irradiation, the dark control plate was essential. Untreated control wells served both the usual purpose of delineating maximum cell viability to make curves showing the effect of increasing compound concentration on cell viability, and - through inclusion in each plate individually - they also acted as a control for any damaging effects of the radiation alone. This internal control for each variable prevented any false positive results in which increased exposure to the irradiation increased toxicity independent of compound treatment. Cell viability and IC<sub>50</sub> values were determined by MTT assay, as described above for cytotoxicity.

TABLE S2. 24 h IC<sub>50</sub> (μM) for A2780cis cells exposed to complexes **1**<sup>3+</sup> and **2**<sup>3+</sup> as chloride salts upon photoirradiation

| Fluence (J cm <sup>-2</sup> ) | 24 h                   | IC <sub>50</sub> con. (μM) |
|-------------------------------|------------------------|----------------------------|
|                               | <b>1</b> <sup>3+</sup> | <b>2</b> <sup>3+</sup>     |
| 0                             | >100                   | 110                        |
| 12 (*8)                       | 93                     | 83*                        |
| 24                            | 93                     | 56                         |
| 48                            | 85                     | 56                         |

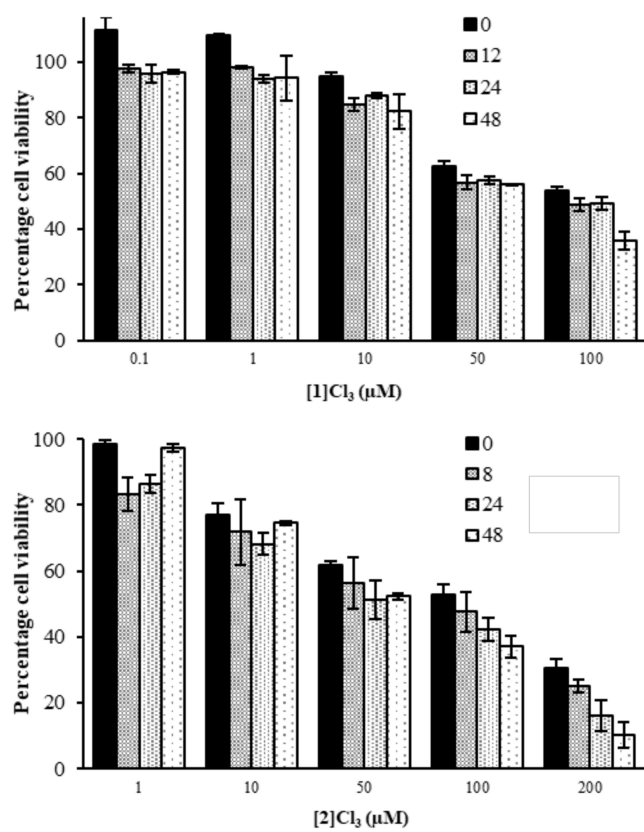


FIG. S10. 24 h A2780cis cell viability data for complexes  $1^{3+}$  and  $2^{3+}$  upon irradiation.

## S2. COMPUTATIONAL METHODS

All calculations were performed with Gaussian 09 v. D.01<sup>55</sup> using density-functional theory. The functional used was B3LYP<sup>56</sup> with empirical dispersion corrections.<sup>57</sup> The basis set used consisted of SDD<sup>66</sup> on Ru/Re and 6-311G(d,p)<sup>67,68</sup> on all other atoms. All bulk solvent was described using the PCM method<sup>69,70</sup> as implemented in Gaussian using the provided parameters for water. Two sets of calculations were performed. In the first one, no additional waters were included to simulate hydrogen bonding. In the second one, waters were placed in hydrogen-bonding positions near available nitrogen atoms. The number of additional hydrogens varied from four for all conformers of **1** to five for the closed isomer of **2** to six for the extended conformer of **2**. In this second set of calculations, PCM was still used to describe the bulk solvent.

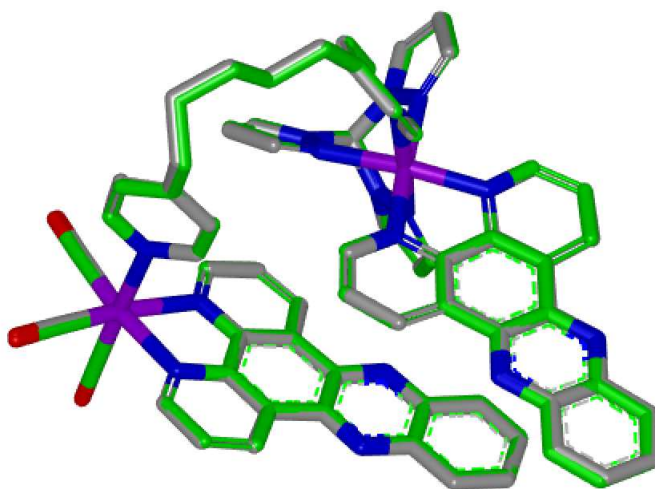
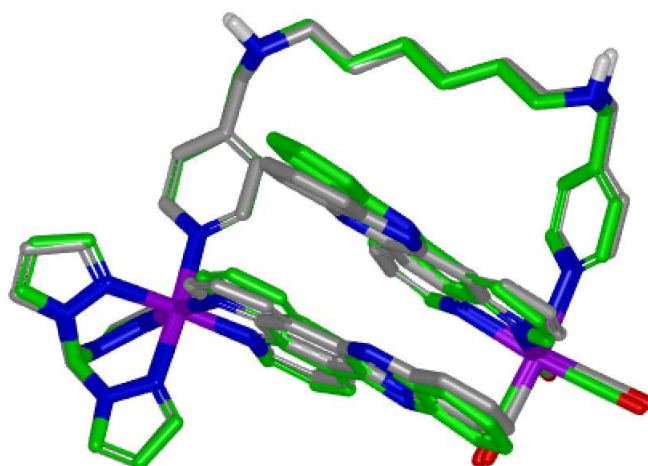
For both complex **1** and complex **2** calculations were done in three different ways. Firstly, optimized structures were calculated with an extended chain, i.e. with the dppz units as far away from each other as possible for both the lowest singlet and triplet states. Secondly, a series of calculations were done, where the overlap of the two dppz units was maximized for both singlet and triplet states as well as for the two relative orderings of the dppz units with respect to the backbone. Starting points for these calculations were made using manual manipulation of the structures. An extensive conformational search for these systems was outside the scope of the work presented here. In the third set of calculations we took the optimized structures of all previously generated species and added water molecules to all available nitrogen lone pairs, chosen using chemical intuition. These structures were subsequently re-optimized.

For all optimised structures frequencies were calculated in the harmonic approximation. Only small imaginary frequencies ( $< 15\text{ cm}^{-1}$ ) were found. These molecules were considered to be true minima, since such small imaginary values are commonly associated with errors in the integration grids used.

All absorption spectra were calculated with the TD-DFT method<sup>71</sup> as implemented. Additional keywords were used to perform the wavefunction analysis using the TheoDORE 1.7.2 program.<sup>58</sup> Briefly, this involves partition of the one-particle transition density matrices into atomic contributions using a Löwdin partitioning.<sup>72,73</sup> The atomic contributions are collected into molecular fragments, in this case corresponding to the metals and ligands of the system, as well as water molecules if present. From this, a map of the excited states in terms of electron transfer between fragments can be generated, known as electron-hole correlation plots.<sup>74</sup> The resulting plots are created using in-house developed software, obtainable online. [1]

All images were created with in-house developed software, which is available upon request. The computational ESI was created using in-house developed software based on the Open Eye Toolkit.<sup>75</sup>

## S2.1. Additional Computational Figures

FIG. S11. Calculated overlay for  $[1]^{3+}$  ( $S_0$ ) and  $[1]^{3+}$  ( $T_1$ ).FIG. S12. Calculated overlay for  $[2]^{3+}$  ( $S_0$ ) and  $[2]^{3+}$  ( $T_1$ ).

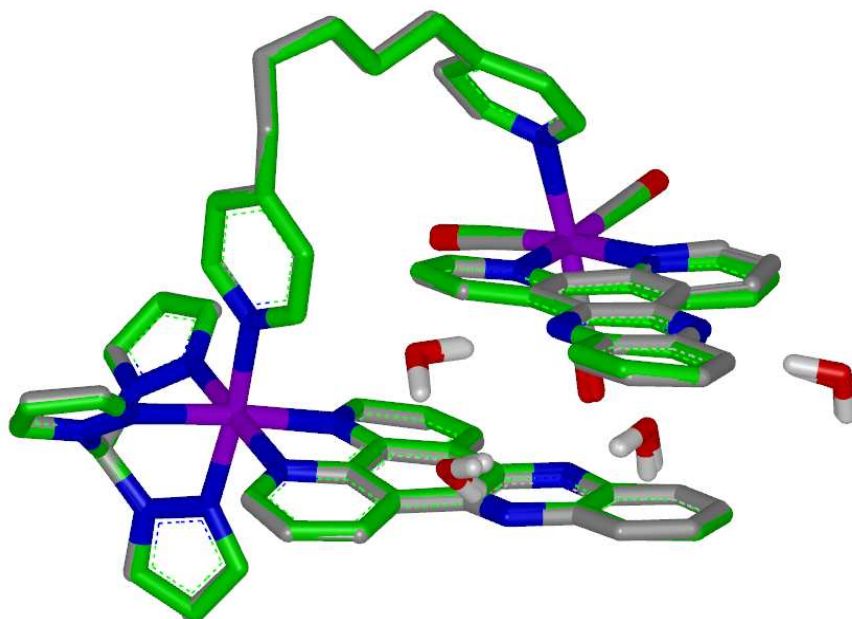


FIG. S13. Calculated overlay for  $[1\mathbf{w}]^{3+}$  ( $S_0$ ) and  $[1\mathbf{w}]^{3+}$  ( $T_1$ ).

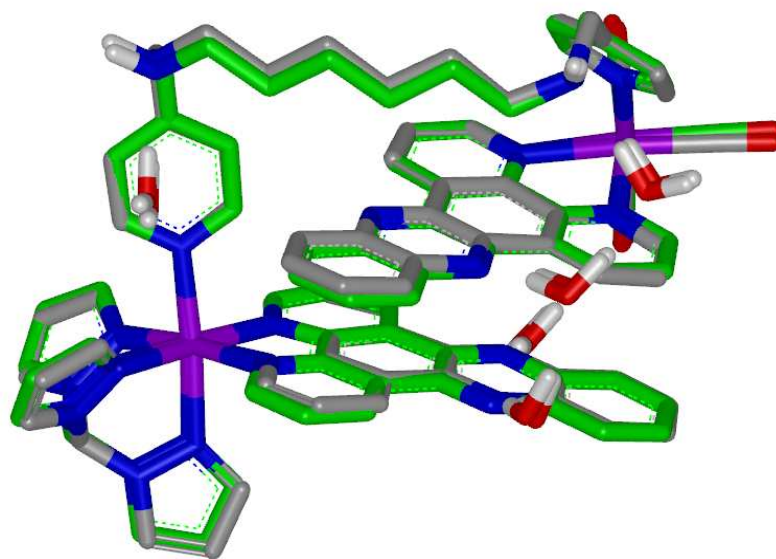


FIG. S14. Calculated overlay for  $[2\mathbf{w}]^{3+}$  ( $S_0$ ) and  $[2\mathbf{w}]^{3+}$  ( $T_1$ ).

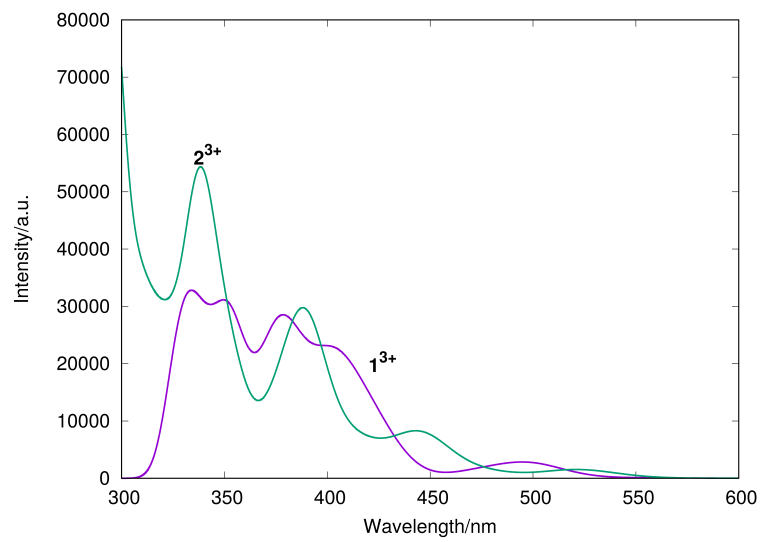


FIG. S15. Calculated UV-VIS spectra for  $[1]^{3+}$  (purple trace) and  $[2]^{3+}$  (green trace).

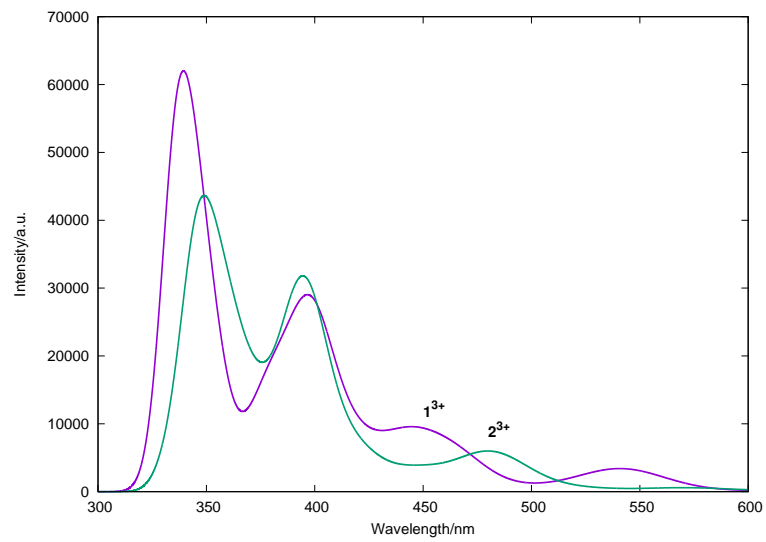


FIG. S16. Calculated UV-VIS spectra for  $[1w]^{3+}$  (purple trace) and  $[2w]^{3+}$  (green trace).

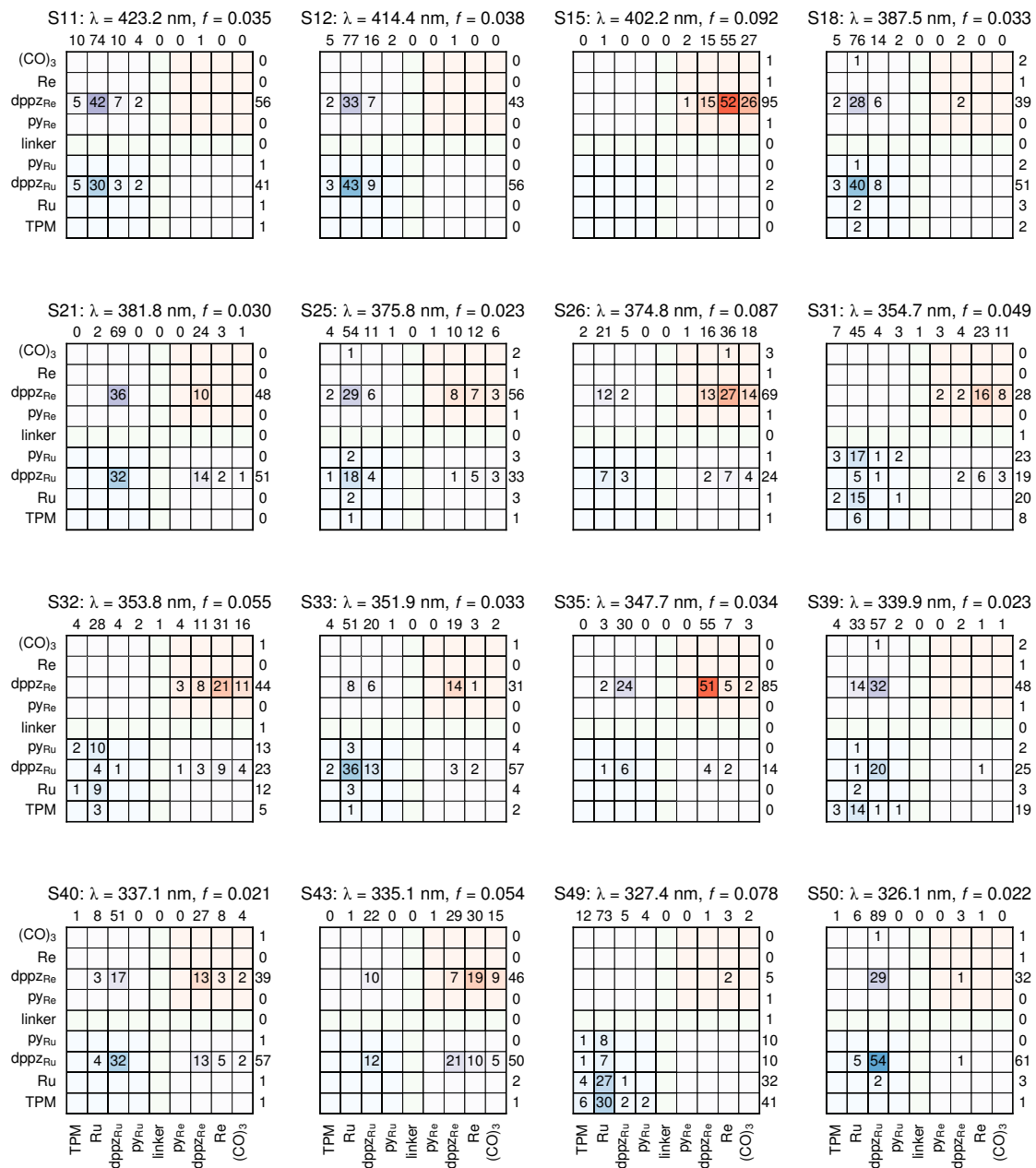


FIG. S17. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **1** in water (PCM).



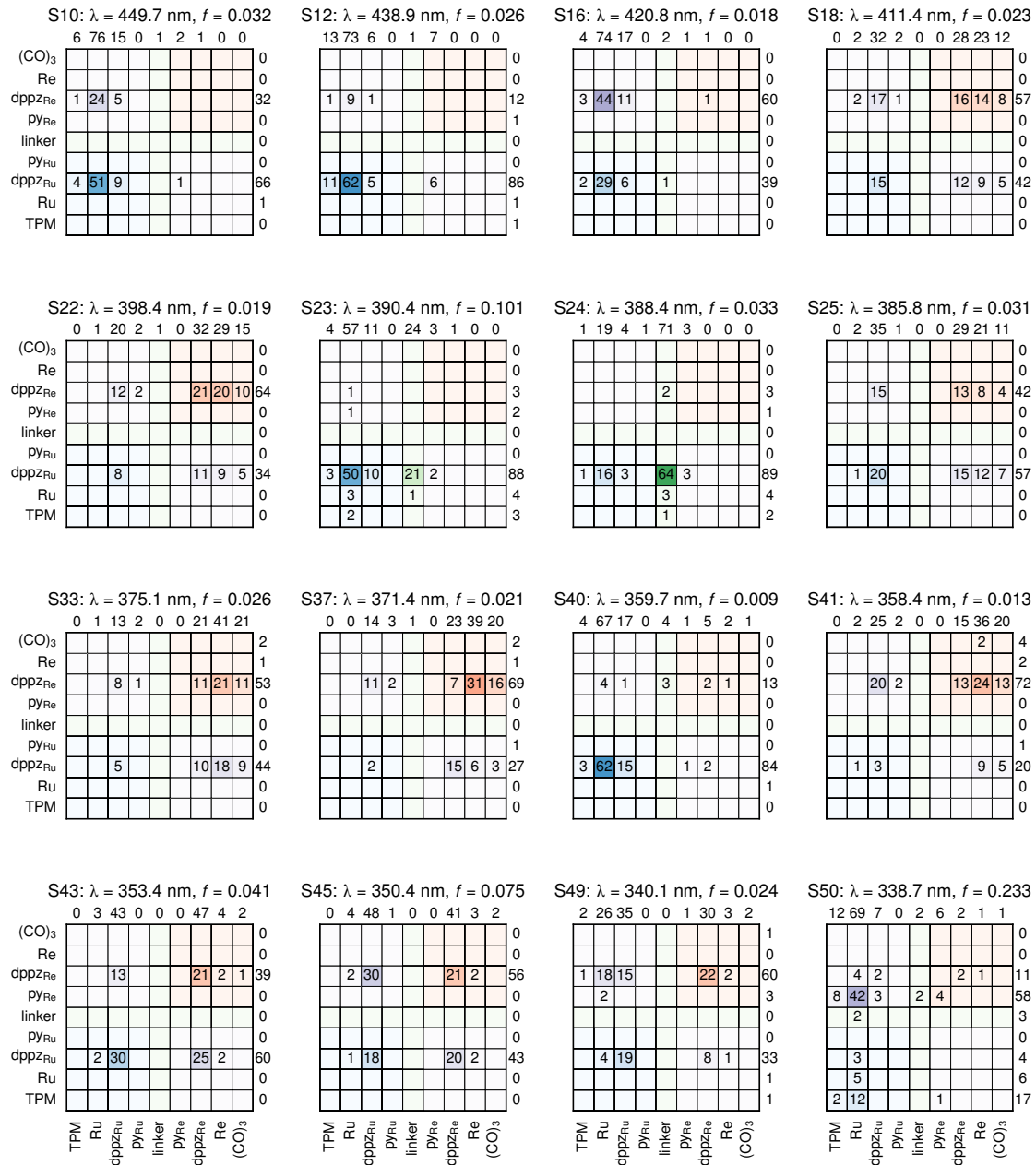


FIG. S18. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **2** in water (PCM).

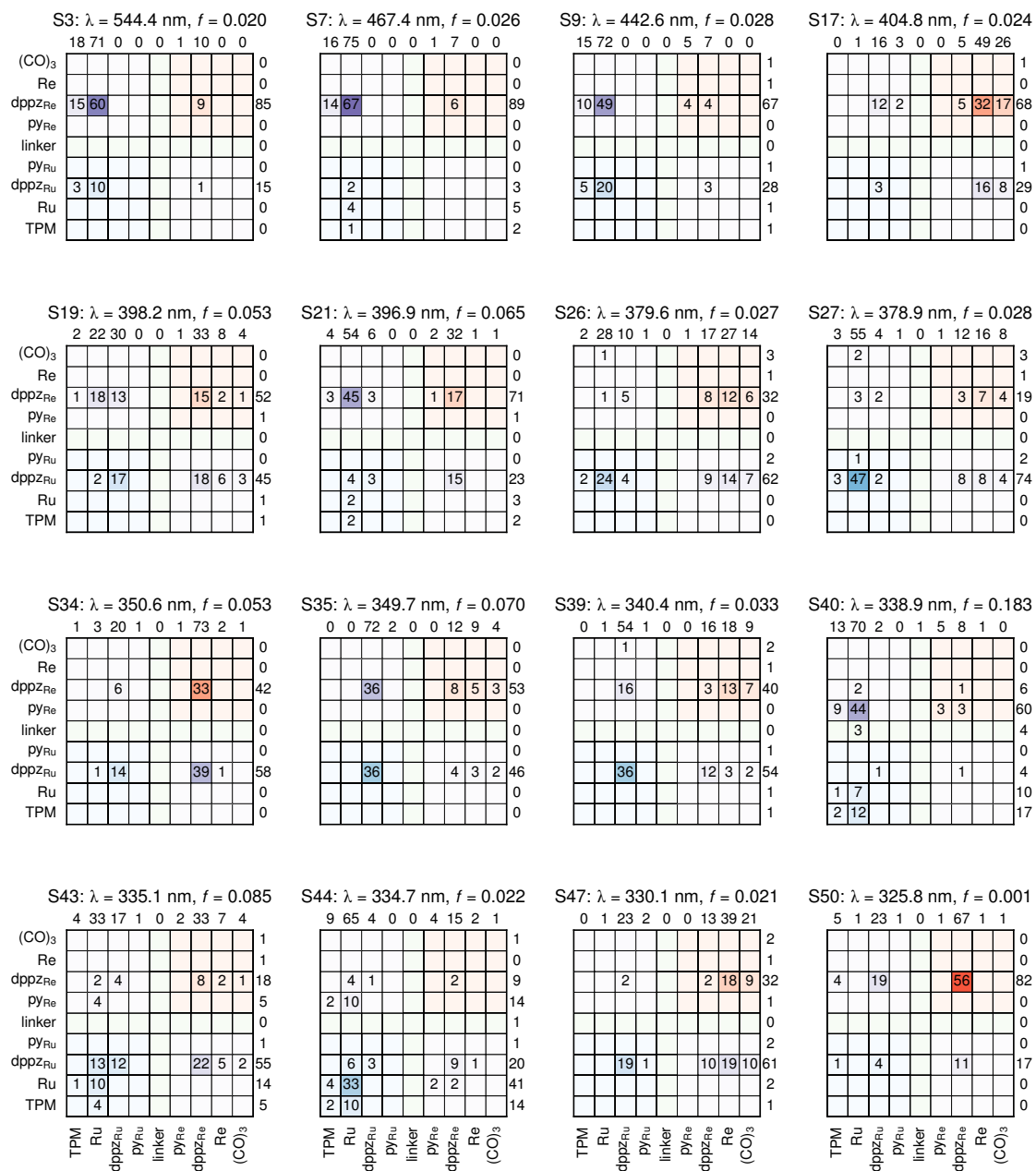


FIG. S19. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **1w** in water (PCM).

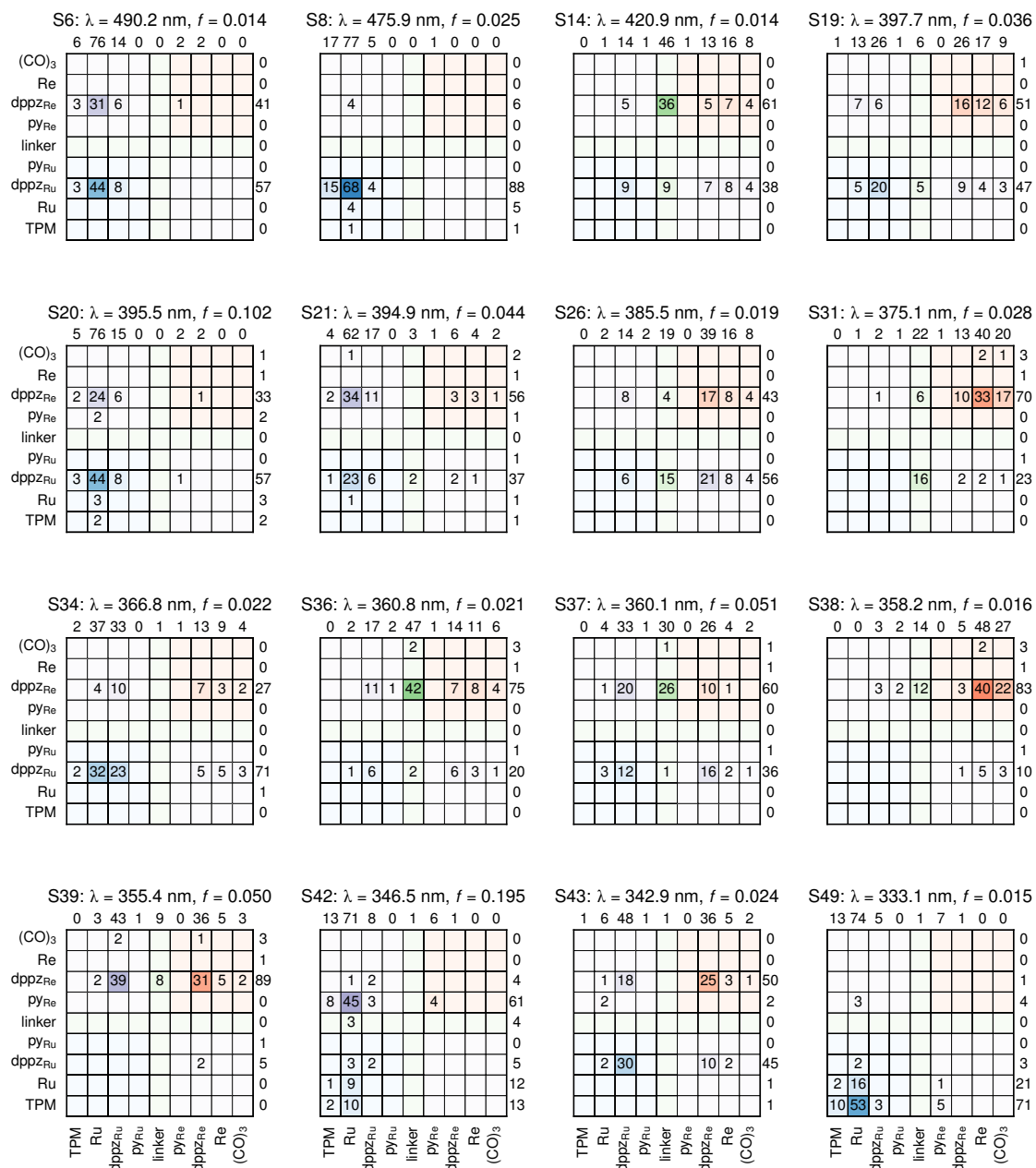


FIG. S20. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **2w** in water (PCM).

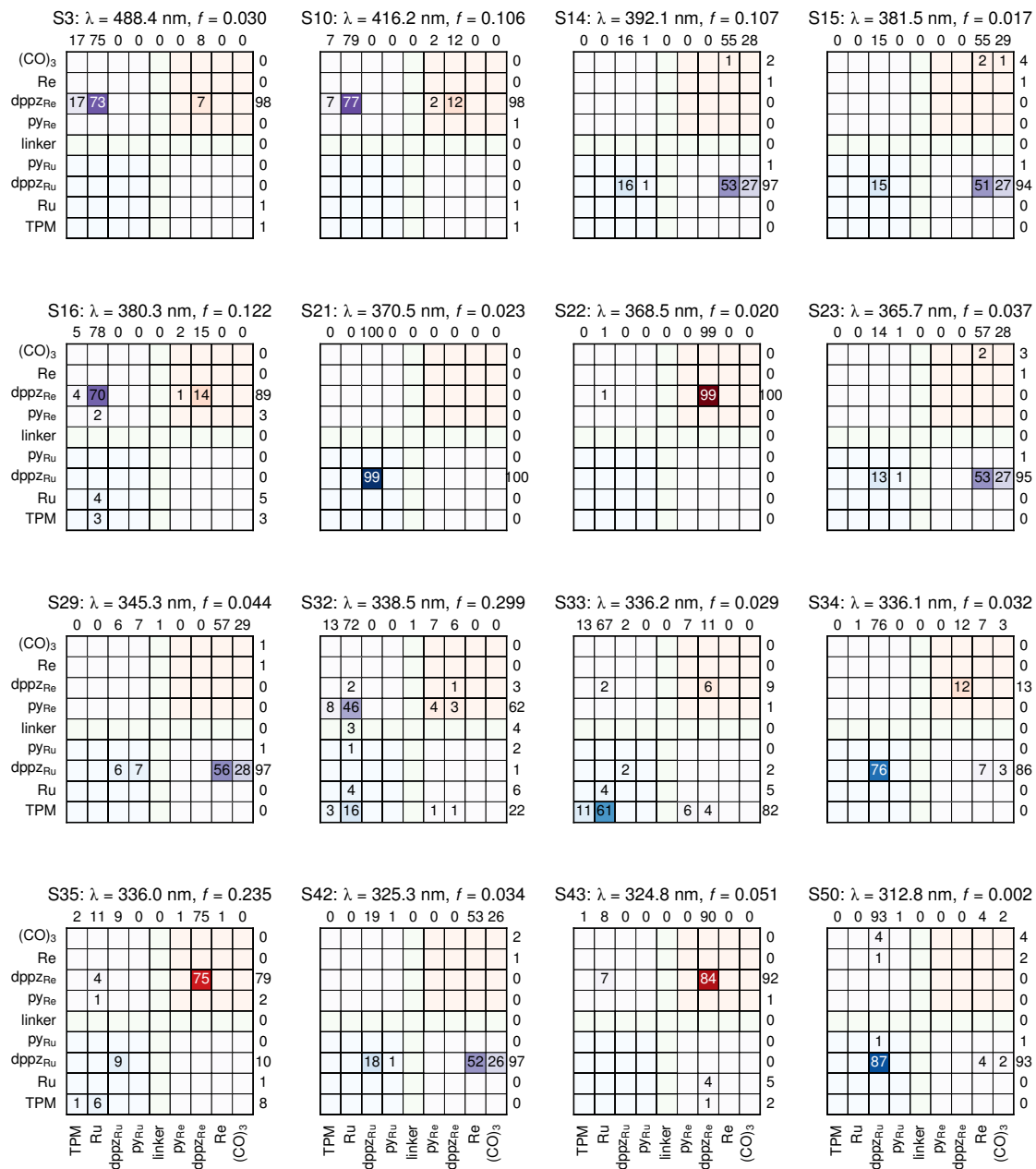


FIG. S21. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound 1 in water (PCM; extended conformer).

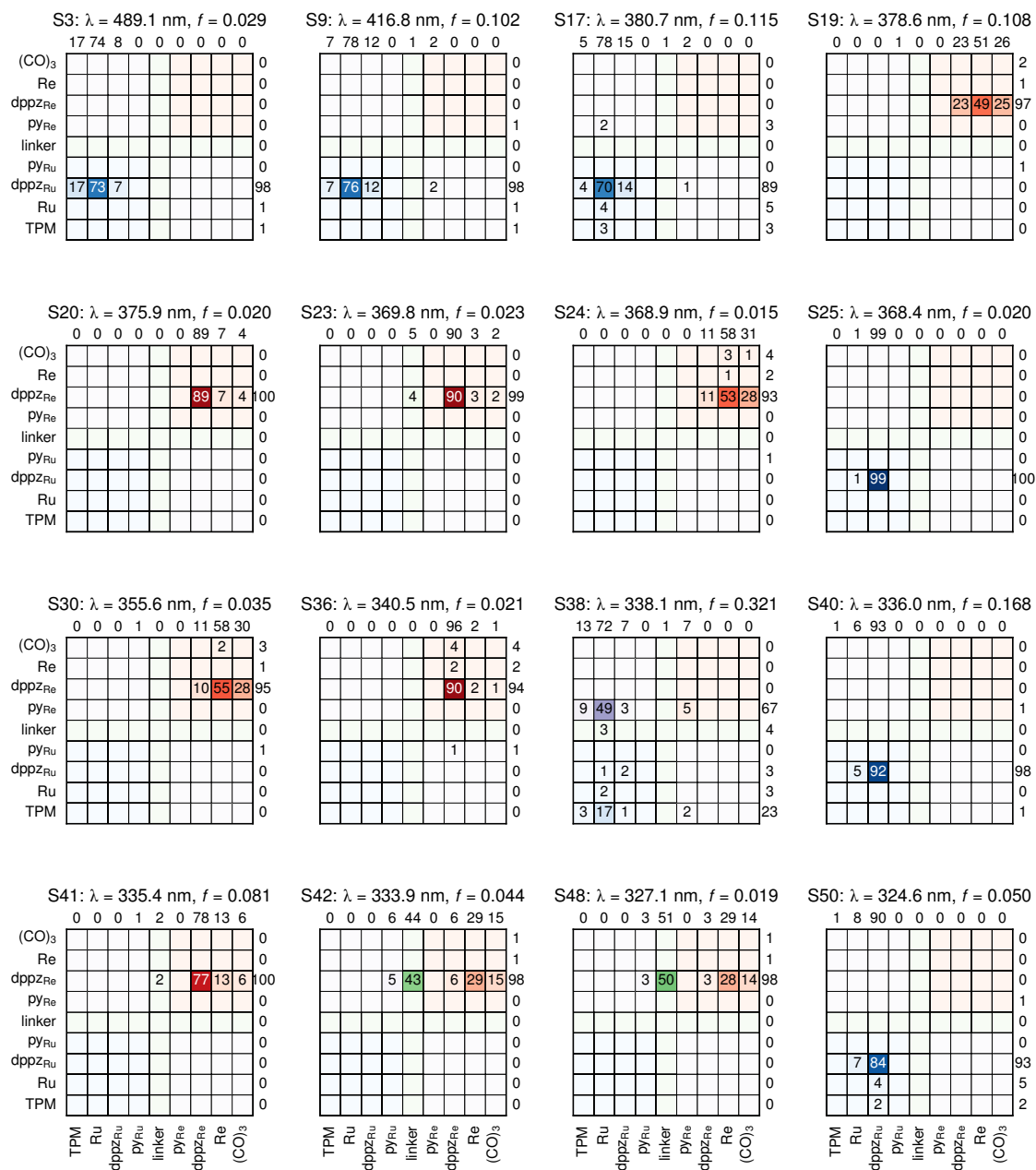


FIG. S22. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **2** in water (PCM; extended conformer).

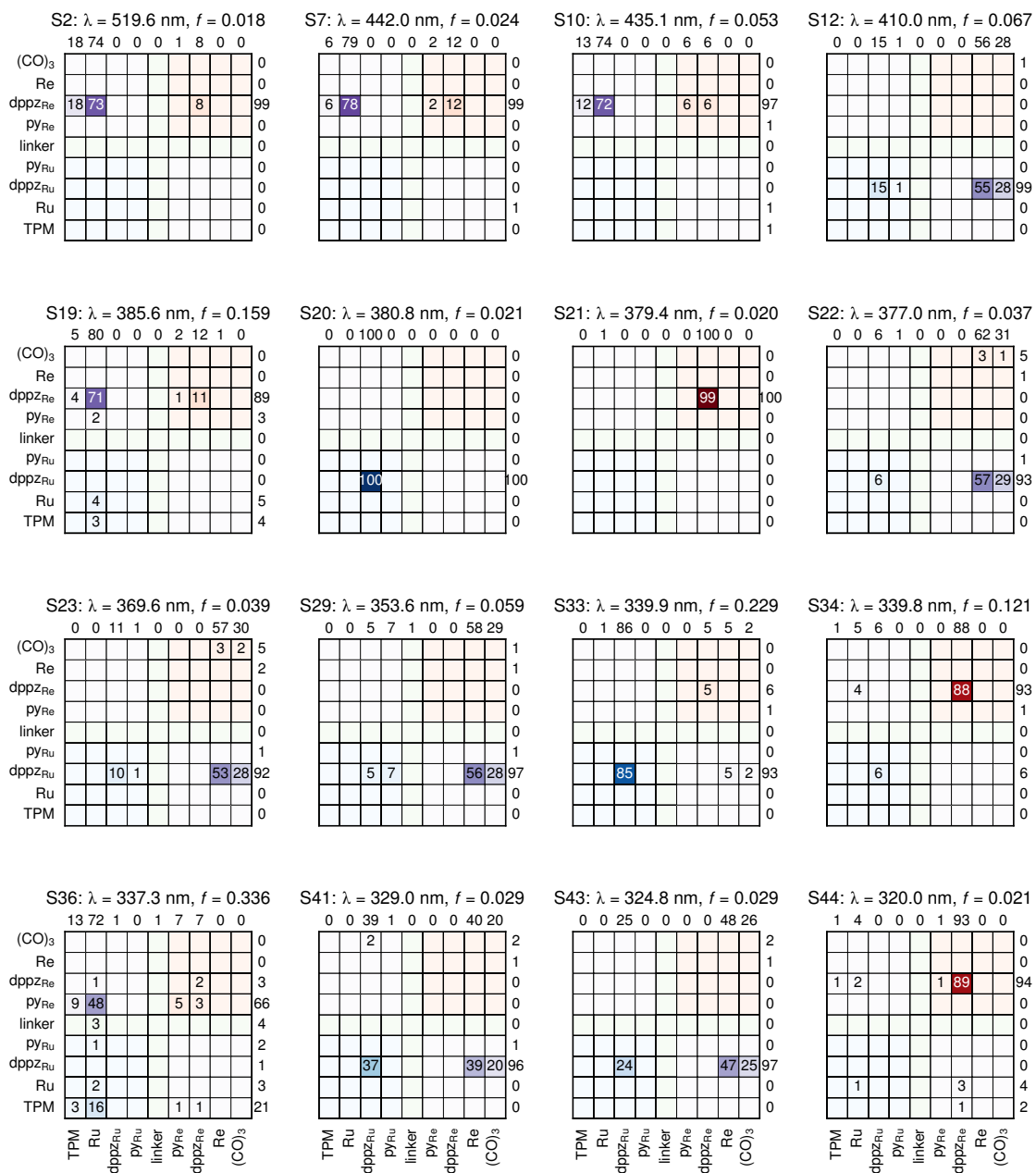


FIG. S23. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **1w** in water (PCM; extended conformer).

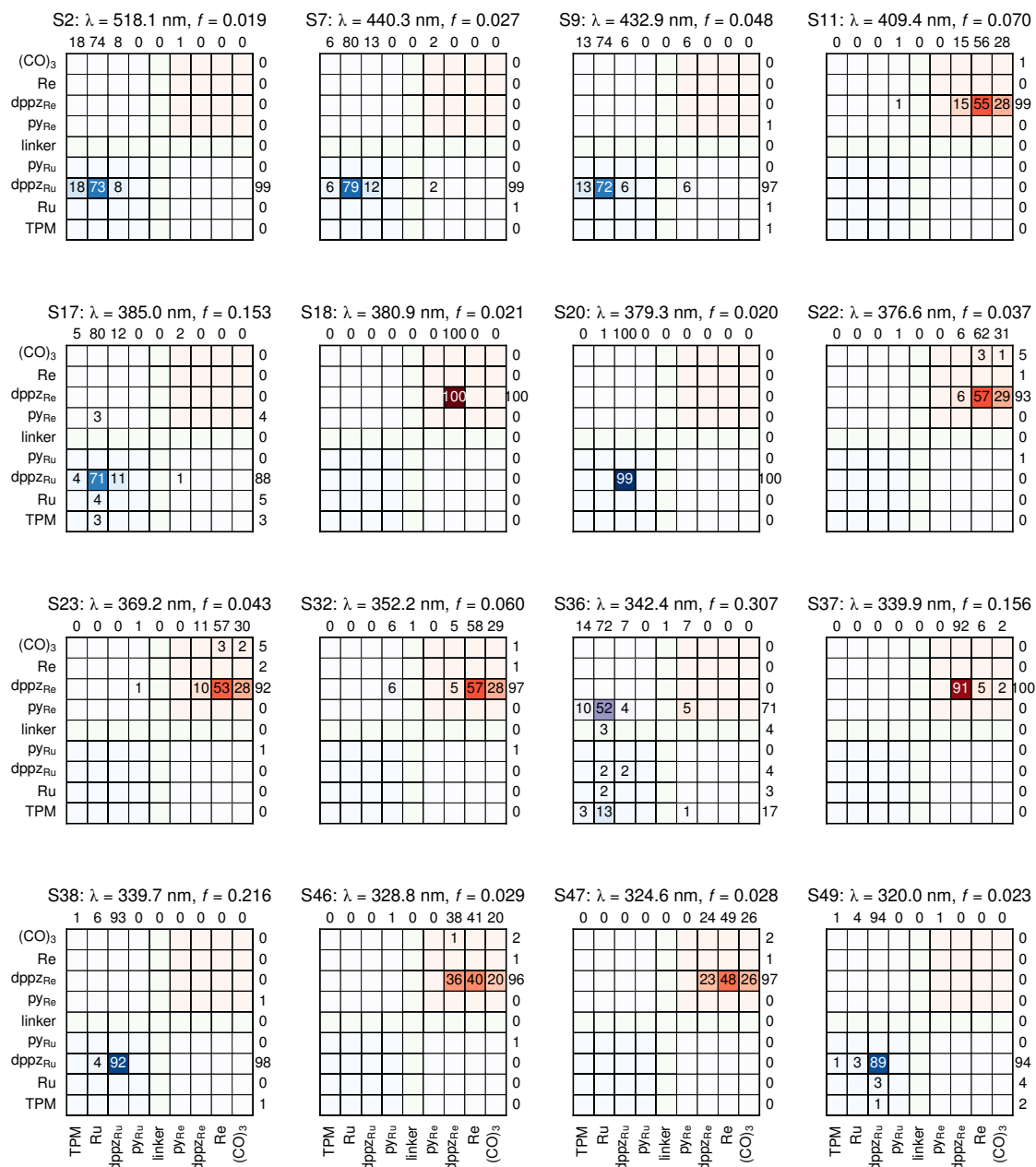
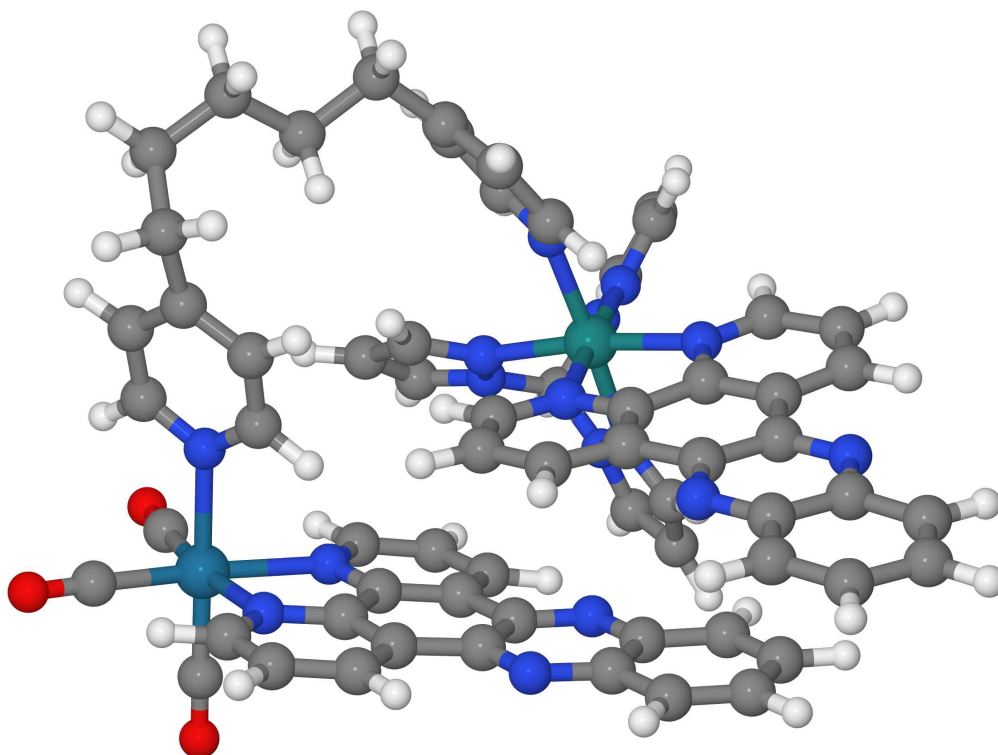


FIG. S24. Wave function analysis on the sixteen strongest transitions in the TD-DFT calculations for compound **2w** in water (PCM; extended conformer).

### S3. CALCULATIONS ON $1^{3+}$ ( $^1A$ )



|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](c6[Ru]578(n9ccc[n+](c9C([n+]<br>1n7ccc1)[n+](n8ccc1)[n+](c1ccc(cc1)CCCCC1cc[n+](cc1)[Re]1([n+]<br>2cccc3c2c2[n+](c1ccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 1  |      |
| Energy                          | : -3743.86674759   | a.u. |
| Gibbs Energy                    | : -3742.94382700   | a.u. |
| Number of imaginary frequencies | : 0  |      |

#### S3.1. Cartesian Co-ordinates (XYZ format)

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|   |            |             |            |
|---|------------|-------------|------------|
| C | 0.90324599 | -3.94991398 | 5.08219385 |
| H | 1.19759297 | -4.98287821 | 5.28588676 |
| H | 0.40386701 | -3.56011200 | 5.97281313 |
| C | 2.15583897 | -3.10148907 | 4.77446508 |
| H | 1.82523704 | -2.10274911 | 4.47351503 |
| H | 2.67042089 | -3.52919793 | 3.90685105 |
| C | 3.12296200 | -2.99749398 | 5.94988012 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.41810489  | -4.00275803 | 6.26966190  |
| H | 2.60801196  | -2.53836608 | 6.80199909  |
| C | 4.10539579  | -0.71955299 | 5.22733402  |
| H | 4.86789703  | -0.08050200 | 5.68402290  |
| H | 3.14865494  | -0.39291301 | 5.64193821  |
| C | -0.55028200 | -3.83704591 | -3.04086304 |
| N | -1.37287700 | -4.84503317 | -2.40575194 |
| N | -1.34373498 | -2.68124390 | -3.40030003 |
| N | 0.54686201  | -3.46153498 | -2.17025399 |
| N | -1.98563802 | -4.55114603 | -1.22781396 |
| C | -1.58449900 | -6.14062977 | -2.76353407 |
| N | -1.99765205 | -1.99255598 | -2.42542291 |
| C | -1.69742095 | -2.23543096 | -4.63853407 |
| N | 0.28466401  | -2.91693091 | -0.94910198 |
| C | 1.87707400  | -3.70165491 | -2.33006001 |
| C | -2.59114408 | -5.67349720 | -0.84050202 |
| C | -2.36919999 | -6.69880009 | -1.77882099 |
| H | -1.17062294 | -6.54734993 | -3.67089605 |
| C | -2.75704408 | -1.09782696 | -3.05222201 |
| C | -2.59633303 | -1.20978796 | -4.44697618 |
| H | -1.28148603 | -2.67375803 | -5.52989483 |
| C | 1.46773100  | -2.80112195 | -0.34436700 |
| C | 2.49766397  | -3.27548695 | -1.17707801 |
| H | 2.26234388  | -4.13494110 | -3.23766398 |
| N | 2.83021092  | 0.89659899  | -1.68948805 |
| N | 3.35265398  | 3.04714608  | -0.17060301 |
| H | -3.14354610 | -5.69636679 | 0.08451100  |
| H | -2.73546410 | -7.70994282 | -1.73869705 |
| H | -3.36002302 | -0.40999299 | -2.48638701 |
| H | -3.06919098 | -0.61263299 | -5.20722198 |
| H | 1.53735101  | -2.40965104 | 0.65632701  |
| H | 3.55153799  | -3.29898906 | -0.96026897 |
| C | 2.62573695  | -0.14474700 | -2.50272989 |
| C | 1.79461896  | 1.73984098  | -1.43565702 |
| C | 2.07361889  | 2.89493895  | -0.60880500 |
| C | 3.64419508  | 4.09619188  | 0.60587901  |
| C | 1.39443696  | -0.38403100 | -3.10991311 |
| H | 3.47157693  | -0.78911799 | -2.68854809 |
| C | 0.51327199  | 1.52765203  | -1.96189702 |
| C | 1.05919003  | 3.80732703  | -0.28766200 |
| C | 2.68520188  | 5.03878784  | 0.97707701  |
| H | 4.66876507  | 4.18394613  | 0.93717802  |
| C | 0.32794899  | 0.44758800  | -2.83432889 |
| H | 1.29988897  | -1.21203303 | -3.79613304 |
| C | -0.57324600 | 2.42983007  | -1.59325695 |
| C | 1.38635004  | 4.90001583  | 0.52743399  |
| C | -0.29665601 | 3.57871103  | -0.78239900 |
| H | 2.97504807  | 5.86647987  | 1.60922098  |
| H | -0.64165401 | 0.29860100  | -3.28388906 |
| N | -1.80322003 | 2.14119291  | -1.98692000 |
| H | 0.61403197  | 5.60969687  | 0.78954500  |
| N | -1.25206602 | 4.42453909  | -0.43532199 |
| C | -2.79356790 | 2.98062706  | -1.61914098 |
| C | -2.50876999 | 4.15845919  | -0.84690100 |
| C | -4.13501596 | 2.70009398  | -1.98428702 |
| C | -3.56775594 | 5.03387690  | -0.49623799 |
| C | -5.13666105 | 3.56142402  | -1.61675704 |
| H | -4.33871508 | 1.80595696  | -2.55831003 |
| C | -4.85001087 | 4.74015284  | -0.87845802 |
| H | -3.33148289 | 5.91368580  | 0.08788900  |
| H | -6.16187906 | 3.34517288  | -1.88926995 |
| H | -5.66259718 | 5.39879322  | -0.59971398 |
| N | -3.75296807 | -2.17383790 | -0.15983100 |
| N | -1.60415101 | -0.70051003 | 0.35144901  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.80567884 | -2.92426491 | -0.49990001 |
| C  | -3.97824597 | -0.90734702 | 0.28521001  |
| C  | -2.80964589 | -0.12823001 | 0.61639798  |
| C  | -0.49949700 | -0.05474300 | 0.73714101  |
| C  | -6.11647701 | -2.45540309 | -0.40356600 |
| H  | -4.59274817 | -3.91658592 | -0.86820298 |
| C  | -5.26520109 | -0.37233001 | 0.42361000  |
| C  | -2.93228889 | 1.13038695  | 1.21916699  |
| C  | -0.54636401 | 1.16950297  | 1.40152299  |
| H  | 0.44011000  | -0.53403401 | 0.51275998  |
| C  | -6.35491180 | -1.17486203 | 0.06091500  |
| H  | -6.93016005 | -3.10545993 | -0.69446099 |
| C  | -5.41708612 | 0.98448497  | 0.94531000  |
| C  | -1.76462901 | 1.78012097  | 1.63348806  |
| C  | -4.26106119 | 1.71044695  | 1.38694406  |
| H  | 0.36945099  | 1.64071095  | 1.72640097  |
| H  | -7.35676098 | -0.77919400 | 0.15290400  |
| N  | -6.62765121 | 1.51050901  | 1.01492596  |
| H  | -1.83546901 | 2.74305511  | 2.11881495  |
| N  | -4.36227512 | 2.91276002  | 1.92596495  |
| C  | -6.74319315 | 2.75466800  | 1.52520299  |
| C  | -5.59142685 | 3.46011901  | 2.01090097  |
| C  | -8.01530075 | 3.37952089  | 1.58245301  |
| C  | -5.74803209 | 4.76098394  | 2.55281091  |
| C  | -8.13077545 | 4.64272499  | 2.10207009  |
| H  | -8.87085819 | 2.83299398  | 1.20663404  |
| C  | -6.99127722 | 5.33621216  | 2.59289002  |
| H  | -4.86533117 | 5.27555513  | 2.91018701  |
| H  | -9.09991837 | 5.12418318  | 2.14342189  |
| H  | -7.11395216 | 6.33292913  | 2.99811101  |
| H  | -0.13116799 | -4.25814486 | -3.94888711 |
| C  | -0.01349700 | -3.88291001 | 3.89741397  |
| C  | -1.01326096 | -2.91252208 | 3.79946303  |
| C  | 0.19780700  | -4.68588400 | 2.77446389  |
| C  | -1.64669204 | -2.69525695 | 2.58942389  |
| H  | -1.26729500 | -2.28862309 | 4.64704418  |
| C  | -0.46526000 | -4.40739584 | 1.59477496  |
| H  | 0.92153603  | -5.49089718 | 2.79454398  |
| N  | -1.33030498 | -3.37822294 | 1.47093999  |
| H  | -2.39670300 | -1.92452896 | 2.49446011  |
| H  | -0.26670399 | -4.97871017 | 0.70078999  |
| C  | 4.14083099  | -0.41682899 | 3.75091290  |
| C  | 3.08316994  | 0.20687699  | 3.08587503  |
| C  | 5.28805685  | -0.67045802 | 2.99007511  |
| C  | 3.23483109  | 0.61501402  | 1.76993096  |
| H  | 2.15155196  | 0.41246799  | 3.59718990  |
| C  | 5.36665487  | -0.23628300 | 1.68126500  |
| H  | 6.14557123  | -1.16862297 | 3.42365003  |
| N  | 4.36863422  | 0.43958700  | 1.06908500  |
| H  | 2.43507195  | 1.13360596  | 1.26509798  |
| H  | 6.26607513  | -0.39610001 | 1.10434699  |
| C  | 4.38614321  | -2.18904209 | 5.63296700  |
| H  | 4.95315886  | -2.69134998 | 4.84307718  |
| H  | 5.02773809  | -2.18999910 | 6.51701307  |
| Re | 4.79322815  | 1.51668501  | -0.87836099 |
| Ru | -1.73999703 | -2.62533903 | -0.45838499 |
| C  | 5.13402796  | 2.51693606  | -2.50701404 |
| O  | 5.32968998  | 3.11534405  | -3.47092295 |
| C  | 5.81980896  | 0.02103500  | -1.56453502 |
| O  | 6.39760017  | -0.88432801 | -1.98421395 |
| C  | 6.39335299  | 2.27069592  | -0.07786100 |
| O  | 7.32732201  | 2.74338102  | 0.40391299  |

### S3.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 7.82960000   | 1.73350000   | 0.00000000      |
| 2    | 13.43990000  | 0.47130000   | 0.00000000      |
| 3    | 19.13250000  | 0.20000000   | 0.00000000      |
| 4    | 21.30250000  | 0.75430000   | 0.00000000      |
| 5    | 28.97920000  | 0.35010000   | 0.00000000      |
| 6    | 31.42220000  | 0.29230000   | 0.00000000      |
| 7    | 34.97770000  | 0.32130000   | 0.00000000      |
| 8    | 36.61350000  | 0.50340000   | 0.00000000      |
| 9    | 41.44690000  | 1.80290000   | 0.00000000      |
| 10   | 45.70380000  | 1.06010000   | 0.00000000      |
| 11   | 50.15230000  | 0.40040000   | 0.00000000      |
| 12   | 55.59400000  | 0.85960000   | 0.00000000      |
| 13   | 61.99800000  | 0.41400000   | 0.00000000      |
| 14   | 63.13620000  | 0.80820000   | 0.00000000      |
| 15   | 64.59600000  | 1.06780000   | 0.00000000      |
| 16   | 67.73660000  | 0.48580000   | 0.00000000      |
| 17   | 69.62560000  | 1.93840000   | 0.00000000      |
| 18   | 77.40320000  | 2.51980000   | 0.00000000      |
| 19   | 79.66830000  | 2.89960000   | 0.00000000      |
| 20   | 86.31170000  | 1.21100000   | 0.00000000      |
| 21   | 89.60590000  | 2.82390000   | 0.00000000      |
| 22   | 92.48400000  | 0.88860000   | 0.00000000      |
| 23   | 92.93900000  | 0.80450000   | 0.00000000      |
| 24   | 94.10690000  | 0.65590000   | 0.00000000      |
| 25   | 96.36470000  | 0.44200000   | 0.00000000      |
| 26   | 97.08090000  | 0.94210000   | 0.00000000      |
| 27   | 103.71200000 | 0.38240000   | 0.00000000      |
| 28   | 107.71050000 | 0.76650000   | 0.00000000      |
| 29   | 115.03460000 | 0.50780000   | 0.00000000      |
| 30   | 119.74980000 | 0.29420000   | 0.00000000      |
| 31   | 124.74240000 | 0.83590000   | 0.00000000      |
| 32   | 136.51200000 | 1.41400000   | 0.00000000      |
| 33   | 138.05470000 | 0.74750000   | 0.00000000      |
| 34   | 140.57570000 | 6.77840000   | 0.00000000      |
| 35   | 146.45990000 | 1.80820000   | 0.00000000      |
| 36   | 154.02540000 | 0.21350000   | 0.00000000      |
| 37   | 155.50880000 | 0.12510000   | 0.00000000      |
| 38   | 165.05740000 | 0.27330000   | 0.00000000      |
| 39   | 175.37980000 | 0.40660000   | 0.00000000      |
| 40   | 177.41120000 | 0.07510000   | 0.00000000      |
| 41   | 178.74370000 | 0.38570000   | 0.00000000      |
| 42   | 180.27790000 | 0.32890000   | 0.00000000      |
| 43   | 182.91200000 | 1.28440000   | 0.00000000      |
| 44   | 188.27440000 | 0.09190000   | 0.00000000      |
| 45   | 190.43020000 | 0.62770000   | 0.00000000      |
| 46   | 193.76870000 | 0.50620000   | 0.00000000      |
| 47   | 195.97520000 | 0.45510000   | 0.00000000      |
| 48   | 204.63650000 | 0.79280000   | 0.00000000      |
| 49   | 205.72700000 | 1.18900000   | 0.00000000      |
| 50   | 209.73380000 | 0.29360000   | 0.00000000      |
| 51   | 212.67950000 | 1.03460000   | 0.00000000      |
| 52   | 217.96790000 | 1.46300000   | 0.00000000      |
| 53   | 225.26560000 | 1.36010000   | 0.00000000      |
| 54   | 237.68850000 | 0.33540000   | 0.00000000      |
| 55   | 243.74780000 | 0.49860000   | 0.00000000      |
| 56   | 254.94690000 | 0.37690000   | 0.00000000      |
| 57   | 259.71070000 | 0.49250000   | 0.00000000      |
| 58   | 274.32910000 | 0.89740000   | 0.00000000      |
| 59   | 274.82240000 | 2.01250000   | 0.00000000      |
| 60   | 276.24850000 | 6.98840000   | 0.00000000      |

|     |              |             |            |
|-----|--------------|-------------|------------|
| 61  | 305.69290000 | 0.61800000  | 0.00000000 |
| 62  | 315.67450000 | 4.17020000  | 0.00000000 |
| 63  | 319.71590000 | 0.87750000  | 0.00000000 |
| 64  | 324.25260000 | 1.19140000  | 0.00000000 |
| 65  | 328.64910000 | 4.29400000  | 0.00000000 |
| 66  | 332.88920000 | 3.11580000  | 0.00000000 |
| 67  | 335.08340000 | 0.27520000  | 0.00000000 |
| 68  | 337.77940000 | 5.28440000  | 0.00000000 |
| 69  | 338.74280000 | 1.59040000  | 0.00000000 |
| 70  | 340.20370000 | 0.60570000  | 0.00000000 |
| 71  | 353.61080000 | 0.42920000  | 0.00000000 |
| 72  | 359.17740000 | 2.15750000  | 0.00000000 |
| 73  | 364.60130000 | 4.67210000  | 0.00000000 |
| 74  | 370.71200000 | 2.44840000  | 0.00000000 |
| 75  | 376.71230000 | 4.06640000  | 0.00000000 |
| 76  | 382.03830000 | 1.48580000  | 0.00000000 |
| 77  | 387.42880000 | 0.36600000  | 0.00000000 |
| 78  | 395.25370000 | 4.08540000  | 0.00000000 |
| 79  | 404.75160000 | 4.30340000  | 0.00000000 |
| 80  | 407.57060000 | 0.95720000  | 0.00000000 |
| 81  | 411.24550000 | 0.29120000  | 0.00000000 |
| 82  | 430.30130000 | 0.69880000  | 0.00000000 |
| 83  | 437.51720000 | 7.38960000  | 0.00000000 |
| 84  | 443.25270000 | 7.66150000  | 0.00000000 |
| 85  | 444.34560000 | 30.59740000 | 0.00000000 |
| 86  | 445.37790000 | 9.54610000  | 0.00000000 |
| 87  | 456.68150000 | 6.56630000  | 0.00000000 |
| 88  | 457.53180000 | 2.96880000  | 0.00000000 |
| 89  | 473.85600000 | 35.30500000 | 0.00000000 |
| 90  | 476.09730000 | 28.10660000 | 0.00000000 |
| 91  | 478.47690000 | 0.69160000  | 0.00000000 |
| 92  | 482.29860000 | 8.08170000  | 0.00000000 |
| 93  | 487.22990000 | 4.53720000  | 0.00000000 |
| 94  | 494.17320000 | 4.51420000  | 0.00000000 |
| 95  | 495.80390000 | 0.15680000  | 0.00000000 |
| 96  | 497.47370000 | 0.44080000  | 0.00000000 |
| 97  | 500.43260000 | 0.10690000  | 0.00000000 |
| 98  | 505.00590000 | 0.31750000  | 0.00000000 |
| 99  | 513.66910000 | 9.05070000  | 0.00000000 |
| 100 | 520.49670000 | 7.78020000  | 0.00000000 |
| 101 | 532.14970000 | 14.39820000 | 0.00000000 |
| 102 | 536.16470000 | 10.79010000 | 0.00000000 |
| 103 | 563.37210000 | 0.28180000  | 0.00000000 |
| 104 | 565.80030000 | 3.02990000  | 0.00000000 |
| 105 | 568.82380000 | 31.20140000 | 0.00000000 |
| 106 | 575.98110000 | 0.69530000  | 0.00000000 |
| 107 | 576.76350000 | 1.85870000  | 0.00000000 |
| 108 | 581.29980000 | 3.18720000  | 0.00000000 |
| 109 | 582.98340000 | 0.33210000  | 0.00000000 |
| 110 | 595.17940000 | 34.10580000 | 0.00000000 |
| 111 | 595.48680000 | 17.34420000 | 0.00000000 |
| 112 | 599.51350000 | 11.29210000 | 0.00000000 |
| 113 | 604.05070000 | 5.53780000  | 0.00000000 |
| 114 | 604.82770000 | 3.48050000  | 0.00000000 |
| 115 | 609.09720000 | 11.25180000 | 0.00000000 |
| 116 | 611.57010000 | 4.15880000  | 0.00000000 |
| 117 | 616.26720000 | 25.50100000 | 0.00000000 |
| 118 | 622.15970000 | 34.98740000 | 0.00000000 |
| 119 | 626.34720000 | 16.74580000 | 0.00000000 |
| 120 | 633.61760000 | 36.44740000 | 0.00000000 |
| 121 | 638.93450000 | 2.33400000  | 0.00000000 |
| 122 | 639.67950000 | 1.12390000  | 0.00000000 |
| 123 | 646.22210000 | 81.97960000 | 0.00000000 |
| 124 | 654.47770000 | 2.36110000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 655.57620000 | 1.09110000   | 0.00000000 |
| 126 | 658.10730000 | 1.01420000   | 0.00000000 |
| 127 | 667.80550000 | 2.58160000   | 0.00000000 |
| 128 | 672.13030000 | 5.91960000   | 0.00000000 |
| 129 | 677.02410000 | 4.35750000   | 0.00000000 |
| 130 | 684.14910000 | 0.03440000   | 0.00000000 |
| 131 | 685.44330000 | 0.16170000   | 0.00000000 |
| 132 | 686.89880000 | 0.37290000   | 0.00000000 |
| 133 | 739.83000000 | 10.40660000  | 0.00000000 |
| 134 | 740.40440000 | 2.73370000   | 0.00000000 |
| 135 | 741.24550000 | 2.73410000   | 0.00000000 |
| 136 | 742.06170000 | 3.63090000   | 0.00000000 |
| 137 | 744.49430000 | 6.69650000   | 0.00000000 |
| 138 | 748.86300000 | 0.54920000   | 0.00000000 |
| 139 | 749.95830000 | 0.31710000   | 0.00000000 |
| 140 | 752.09830000 | 6.76360000   | 0.00000000 |
| 141 | 754.38590000 | 83.60620000  | 0.00000000 |
| 142 | 756.50900000 | 106.14870000 | 0.00000000 |
| 143 | 760.55490000 | 133.33460000 | 0.00000000 |
| 144 | 761.05450000 | 21.11600000  | 0.00000000 |
| 145 | 765.69840000 | 106.76770000 | 0.00000000 |
| 146 | 768.71310000 | 104.67810000 | 0.00000000 |
| 147 | 778.85070000 | 92.92600000  | 0.00000000 |
| 148 | 782.61360000 | 37.83830000  | 0.00000000 |
| 149 | 783.27300000 | 2.18890000   | 0.00000000 |
| 150 | 784.19260000 | 51.84170000  | 0.00000000 |
| 151 | 784.88730000 | 8.65700000   | 0.00000000 |
| 152 | 797.13940000 | 106.86690000 | 0.00000000 |
| 153 | 801.39080000 | 125.21350000 | 0.00000000 |
| 154 | 815.31770000 | 0.00940000   | 0.00000000 |
| 155 | 817.33600000 | 4.30050000   | 0.00000000 |
| 156 | 819.69760000 | 0.73490000   | 0.00000000 |
| 157 | 823.47170000 | 75.65050000  | 0.00000000 |
| 158 | 826.25520000 | 0.43370000   | 0.00000000 |
| 159 | 839.55350000 | 94.66670000  | 0.00000000 |
| 160 | 840.56900000 | 2.14180000   | 0.00000000 |
| 161 | 843.72720000 | 73.39840000  | 0.00000000 |
| 162 | 844.23730000 | 15.30190000  | 0.00000000 |
| 163 | 858.31200000 | 5.17820000   | 0.00000000 |
| 164 | 860.50760000 | 6.74700000   | 0.00000000 |
| 165 | 861.23430000 | 25.07920000  | 0.00000000 |
| 166 | 867.31270000 | 11.23230000  | 0.00000000 |
| 167 | 867.95490000 | 11.27710000  | 0.00000000 |
| 168 | 870.24880000 | 33.81230000  | 0.00000000 |
| 169 | 872.87200000 | 0.33620000   | 0.00000000 |
| 170 | 873.46410000 | 21.77930000  | 0.00000000 |
| 171 | 876.77770000 | 2.08140000   | 0.00000000 |
| 172 | 877.98720000 | 3.86600000   | 0.00000000 |
| 173 | 879.86840000 | 33.93840000  | 0.00000000 |
| 174 | 889.99860000 | 1.79330000   | 0.00000000 |
| 175 | 894.12610000 | 0.23480000   | 0.00000000 |
| 176 | 895.29460000 | 0.35340000   | 0.00000000 |
| 177 | 910.15560000 | 1.55730000   | 0.00000000 |
| 178 | 921.24950000 | 0.40610000   | 0.00000000 |
| 179 | 921.32010000 | 1.46370000   | 0.00000000 |
| 180 | 926.33670000 | 4.11980000   | 0.00000000 |
| 181 | 930.31440000 | 3.97000000   | 0.00000000 |
| 182 | 937.56230000 | 18.60890000  | 0.00000000 |
| 183 | 947.70100000 | 0.11260000   | 0.00000000 |
| 184 | 949.84100000 | 0.16330000   | 0.00000000 |
| 185 | 955.45380000 | 0.70000000   | 0.00000000 |
| 186 | 958.22190000 | 2.65910000   | 0.00000000 |
| 187 | 977.94990000 | 0.11920000   | 0.00000000 |
| 188 | 980.43630000 | 3.19570000   | 0.00000000 |

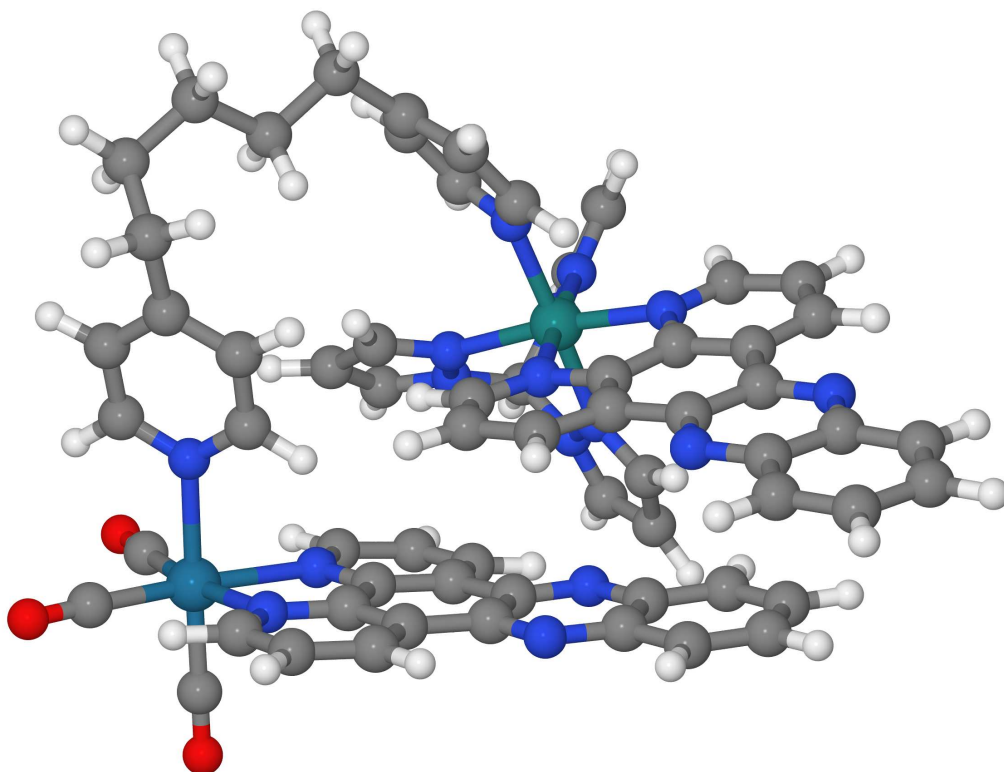
|     |               |             |            |
|-----|---------------|-------------|------------|
| 189 | 983.30900000  | 1.98050000  | 0.00000000 |
| 190 | 986.17260000  | 0.72730000  | 0.00000000 |
| 191 | 987.07750000  | 1.19440000  | 0.00000000 |
| 192 | 990.26030000  | 0.50650000  | 0.00000000 |
| 193 | 992.33200000  | 2.28850000  | 0.00000000 |
| 194 | 993.60520000  | 1.91070000  | 0.00000000 |
| 195 | 1006.66330000 | 2.78990000  | 0.00000000 |
| 196 | 1008.04800000 | 1.20040000  | 0.00000000 |
| 197 | 1008.35230000 | 0.39850000  | 0.00000000 |
| 198 | 1009.24590000 | 5.98210000  | 0.00000000 |
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| 200 | 1011.57240000 | 8.68220000  | 0.00000000 |
| 201 | 1014.65690000 | 11.46940000 | 0.00000000 |
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| 205 | 1024.56200000 | 0.34910000  | 0.00000000 |
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| 208 | 1032.38780000 | 2.60720000  | 0.00000000 |
| 209 | 1034.07570000 | 0.15880000  | 0.00000000 |
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| 211 | 1046.00060000 | 27.54030000 | 0.00000000 |
| 212 | 1052.01590000 | 4.08150000  | 0.00000000 |
| 213 | 1054.73590000 | 4.65990000  | 0.00000000 |
| 214 | 1070.25350000 | 4.10990000  | 0.00000000 |
| 215 | 1070.70800000 | 2.55610000  | 0.00000000 |
| 216 | 1072.51510000 | 38.94690000 | 0.00000000 |
| 217 | 1076.48900000 | 47.49070000 | 0.00000000 |
| 218 | 1077.59760000 | 4.69000000  | 0.00000000 |
| 219 | 1078.14770000 | 14.83560000 | 0.00000000 |
| 220 | 1081.21680000 | 75.90580000 | 0.00000000 |
| 221 | 1087.42530000 | 1.88980000  | 0.00000000 |
| 222 | 1090.14410000 | 7.18840000  | 0.00000000 |
| 223 | 1093.70390000 | 2.79220000  | 0.00000000 |
| 224 | 1098.07150000 | 17.67100000 | 0.00000000 |
| 225 | 1105.25550000 | 38.17370000 | 0.00000000 |
| 226 | 1110.31800000 | 35.13100000 | 0.00000000 |
| 227 | 1117.57250000 | 10.22760000 | 0.00000000 |
| 228 | 1119.71800000 | 76.54370000 | 0.00000000 |
| 229 | 1125.90700000 | 7.81470000  | 0.00000000 |
| 230 | 1126.15480000 | 12.84960000 | 0.00000000 |
| 231 | 1126.96710000 | 80.07510000 | 0.00000000 |
| 232 | 1129.01000000 | 56.04390000 | 0.00000000 |
| 233 | 1144.96900000 | 22.63720000 | 0.00000000 |
| 234 | 1146.35520000 | 25.80390000 | 0.00000000 |
| 235 | 1148.11710000 | 12.96920000 | 0.00000000 |
| 236 | 1151.11840000 | 2.69390000  | 0.00000000 |
| 237 | 1156.61290000 | 1.88170000  | 0.00000000 |
| 238 | 1159.80640000 | 15.90790000 | 0.00000000 |
| 239 | 1164.29120000 | 7.26890000  | 0.00000000 |
| 240 | 1164.51590000 | 17.59810000 | 0.00000000 |
| 241 | 1173.18650000 | 0.43490000  | 0.00000000 |
| 242 | 1176.75850000 | 0.71930000  | 0.00000000 |
| 243 | 1212.44790000 | 3.75400000  | 0.00000000 |
| 244 | 1213.47080000 | 0.97080000  | 0.00000000 |
| 245 | 1216.57890000 | 1.98570000  | 0.00000000 |
| 246 | 1218.80020000 | 3.69870000  | 0.00000000 |
| 247 | 1221.99270000 | 1.73920000  | 0.00000000 |
| 248 | 1234.14850000 | 15.49080000 | 0.00000000 |
| 249 | 1238.43720000 | 5.75400000  | 0.00000000 |
| 250 | 1239.31920000 | 8.43530000  | 0.00000000 |
| 251 | 1241.76860000 | 21.14400000 | 0.00000000 |
| 252 | 1246.92240000 | 1.33690000  | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1257.32630000 | 3.26720000   | 0.00000000 |
| 254 | 1259.33600000 | 33.53600000  | 0.00000000 |
| 255 | 1263.55670000 | 2.23360000   | 0.00000000 |
| 256 | 1264.79860000 | 16.00410000  | 0.00000000 |
| 257 | 1265.39720000 | 4.26380000   | 0.00000000 |
| 258 | 1269.19150000 | 92.68030000  | 0.00000000 |
| 259 | 1274.56870000 | 0.93400000   | 0.00000000 |
| 260 | 1275.28740000 | 117.31760000 | 0.00000000 |
| 261 | 1275.80120000 | 2.84840000   | 0.00000000 |
| 262 | 1281.04170000 | 2.66530000   | 0.00000000 |
| 263 | 1297.85980000 | 9.33660000   | 0.00000000 |
| 264 | 1304.38210000 | 8.36410000   | 0.00000000 |
| 265 | 1307.79660000 | 0.56470000   | 0.00000000 |
| 266 | 1308.28500000 | 0.90450000   | 0.00000000 |
| 267 | 1309.43200000 | 7.47540000   | 0.00000000 |
| 268 | 1312.49930000 | 1.09410000   | 0.00000000 |
| 269 | 1317.63000000 | 40.58870000  | 0.00000000 |
| 270 | 1317.88620000 | 41.70620000  | 0.00000000 |
| 271 | 1320.01350000 | 45.02650000  | 0.00000000 |
| 272 | 1326.92280000 | 90.88600000  | 0.00000000 |
| 273 | 1329.96420000 | 0.40210000   | 0.00000000 |
| 274 | 1334.30140000 | 0.79560000   | 0.00000000 |
| 275 | 1338.57750000 | 2.88080000   | 0.00000000 |
| 276 | 1348.16070000 | 6.30450000   | 0.00000000 |
| 277 | 1351.74630000 | 0.70680000   | 0.00000000 |
| 278 | 1354.72070000 | 0.87730000   | 0.00000000 |
| 279 | 1360.46210000 | 3.93300000   | 0.00000000 |
| 280 | 1371.59080000 | 5.54610000   | 0.00000000 |
| 281 | 1372.04910000 | 37.75020000  | 0.00000000 |
| 282 | 1373.17790000 | 12.33190000  | 0.00000000 |
| 283 | 1373.76510000 | 17.26440000  | 0.00000000 |
| 284 | 1374.27710000 | 186.07360000 | 0.00000000 |
| 285 | 1374.59260000 | 32.32580000  | 0.00000000 |
| 286 | 1375.35960000 | 57.82210000  | 0.00000000 |
| 287 | 1380.90800000 | 8.98570000   | 0.00000000 |
| 288 | 1381.58250000 | 5.47500000   | 0.00000000 |
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| 290 | 1404.33980000 | 3.90610000   | 0.00000000 |
| 291 | 1409.65970000 | 2.19140000   | 0.00000000 |
| 292 | 1421.31350000 | 9.21720000   | 0.00000000 |
| 293 | 1427.53230000 | 11.70830000  | 0.00000000 |
| 294 | 1428.36910000 | 1.58810000   | 0.00000000 |
| 295 | 1435.16530000 | 76.72820000  | 0.00000000 |
| 296 | 1438.84610000 | 52.79740000  | 0.00000000 |
| 297 | 1444.13840000 | 151.15620000 | 0.00000000 |
| 298 | 1453.58580000 | 114.44180000 | 0.00000000 |
| 299 | 1455.57120000 | 122.14520000 | 0.00000000 |
| 300 | 1461.92230000 | 30.88080000  | 0.00000000 |
| 301 | 1465.52370000 | 42.86390000  | 0.00000000 |
| 302 | 1472.26000000 | 71.12340000  | 0.00000000 |
| 303 | 1472.86170000 | 62.01430000  | 0.00000000 |
| 304 | 1473.84770000 | 15.56400000  | 0.00000000 |
| 305 | 1474.55570000 | 33.54180000  | 0.00000000 |
| 306 | 1475.68390000 | 2.91060000   | 0.00000000 |
| 307 | 1485.63650000 | 9.96170000   | 0.00000000 |
| 308 | 1488.60280000 | 8.72590000   | 0.00000000 |
| 309 | 1490.04540000 | 3.79880000   | 0.00000000 |
| 310 | 1491.68660000 | 8.48670000   | 0.00000000 |
| 311 | 1501.27770000 | 11.54040000  | 0.00000000 |
| 312 | 1503.22730000 | 13.27800000  | 0.00000000 |
| 313 | 1505.01110000 | 10.62830000  | 0.00000000 |
| 314 | 1506.48030000 | 6.75730000   | 0.00000000 |
| 315 | 1506.51570000 | 7.50880000   | 0.00000000 |
| 316 | 1524.98560000 | 25.53940000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1525.71350000 | 16.59540000   | 0.00000000 |
| 318 | 1527.83660000 | 49.82210000   | 0.00000000 |
| 319 | 1530.41720000 | 130.94500000  | 0.00000000 |
| 320 | 1535.47010000 | 36.56090000   | 0.00000000 |
| 321 | 1540.54470000 | 27.47270000   | 0.00000000 |
| 322 | 1551.02350000 | 10.28110000   | 0.00000000 |
| 323 | 1553.57500000 | 10.98620000   | 0.00000000 |
| 324 | 1557.89640000 | 10.81350000   | 0.00000000 |
| 325 | 1575.70090000 | 3.35900000    | 0.00000000 |
| 326 | 1578.79420000 | 6.85260000    | 0.00000000 |
| 327 | 1582.03910000 | 17.44270000   | 0.00000000 |
| 328 | 1582.84250000 | 27.38230000   | 0.00000000 |
| 329 | 1590.48380000 | 14.49060000   | 0.00000000 |
| 330 | 1591.93480000 | 10.67950000   | 0.00000000 |
| 331 | 1610.57740000 | 1.03180000    | 0.00000000 |
| 332 | 1614.15950000 | 8.41180000    | 0.00000000 |
| 333 | 1624.33050000 | 2.93240000    | 0.00000000 |
| 334 | 1624.55520000 | 0.55040000    | 0.00000000 |
| 335 | 1627.69840000 | 6.47210000    | 0.00000000 |
| 336 | 1628.11620000 | 3.50570000    | 0.00000000 |
| 337 | 1636.67170000 | 0.78000000    | 0.00000000 |
| 338 | 1639.09450000 | 3.85590000    | 0.00000000 |
| 339 | 1658.33830000 | 126.42770000  | 0.00000000 |
| 340 | 1660.14110000 | 108.13670000  | 0.00000000 |
| 341 | 1661.01700000 | 1.23640000    | 0.00000000 |
| 342 | 1661.27930000 | 0.75590000    | 0.00000000 |
| 343 | 1965.86920000 | 2401.36540000 | 0.00000000 |
| 344 | 1972.82960000 | 2282.61720000 | 0.00000000 |
| 345 | 2086.34110000 | 2085.87600000 | 0.00000000 |
| 346 | 3010.19890000 | 28.61970000   | 0.00000000 |
| 347 | 3021.66700000 | 53.70850000   | 0.00000000 |
| 348 | 3030.46180000 | 16.57800000   | 0.00000000 |
| 349 | 3033.32820000 | 16.18640000   | 0.00000000 |
| 350 | 3042.36250000 | 73.84690000   | 0.00000000 |
| 351 | 3044.65510000 | 26.49140000   | 0.00000000 |
| 352 | 3062.14590000 | 66.15390000   | 0.00000000 |
| 353 | 3076.30890000 | 85.63440000   | 0.00000000 |
| 354 | 3077.33690000 | 39.25820000   | 0.00000000 |
| 355 | 3090.49030000 | 69.49110000   | 0.00000000 |
| 356 | 3170.52490000 | 1.54900000    | 0.00000000 |
| 357 | 3184.31980000 | 0.93580000    | 0.00000000 |
| 358 | 3188.64900000 | 0.24870000    | 0.00000000 |
| 359 | 3192.79660000 | 2.92660000    | 0.00000000 |
| 360 | 3194.01700000 | 3.94480000    | 0.00000000 |
| 361 | 3194.85290000 | 6.15190000    | 0.00000000 |
| 362 | 3197.09580000 | 0.82210000    | 0.00000000 |
| 363 | 3197.38020000 | 3.06190000    | 0.00000000 |
| 364 | 3197.63620000 | 1.93510000    | 0.00000000 |
| 365 | 3202.07630000 | 15.42170000   | 0.00000000 |
| 366 | 3206.45030000 | 10.94070000   | 0.00000000 |
| 367 | 3207.68100000 | 40.52670000   | 0.00000000 |
| 368 | 3211.78950000 | 25.96680000   | 0.00000000 |
| 369 | 3211.84960000 | 0.39380000    | 0.00000000 |
| 370 | 3214.28570000 | 0.18720000    | 0.00000000 |
| 371 | 3221.47130000 | 4.47450000    | 0.00000000 |
| 372 | 3222.70890000 | 7.51670000    | 0.00000000 |
| 373 | 3224.64200000 | 3.47560000    | 0.00000000 |
| 374 | 3224.65880000 | 2.91240000    | 0.00000000 |
| 375 | 3230.26440000 | 0.54930000    | 0.00000000 |
| 376 | 3230.36310000 | 9.69260000    | 0.00000000 |
| 377 | 3231.74400000 | 4.20030000    | 0.00000000 |
| 378 | 3231.89840000 | 8.04210000    | 0.00000000 |
| 379 | 3235.71160000 | 3.30870000    | 0.00000000 |
| 380 | 3236.55460000 | 7.17870000    | 0.00000000 |



|     |               |             |            |
|-----|---------------|-------------|------------|
| 381 | 3236.80310000 | 4.08550000  | 0.00000000 |
| 382 | 3239.76260000 | 18.16640000 | 0.00000000 |
| 383 | 3247.11910000 | 7.59790000  | 0.00000000 |
| 384 | 3252.55800000 | 9.83890000  | 0.00000000 |
| 385 | 3260.54720000 | 0.92390000  | 0.00000000 |
| 386 | 3264.13780000 | 3.57600000  | 0.00000000 |
| 387 | 3267.62480000 | 5.47920000  | 0.00000000 |
| 388 | 3269.35990000 | 7.21930000  | 0.00000000 |
| 389 | 3271.05860000 | 8.55310000  | 0.00000000 |
| 390 | 3279.56960000 | 7.40260000  | 0.00000000 |
| 391 | 3284.57850000 | 6.14390000  | 0.00000000 |
| 392 | 3285.37370000 | 5.37780000  | 0.00000000 |
| 393 | 3290.09340000 | 2.26590000  | 0.00000000 |

S4. CALCULATIONS ON  $1^{3+}$  ( $^3A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](c6[Ru]578(n9ccc[n+](c9C([n+]<br>1n7ccc1)[n+](n8ccc1)[n+](c1ccc(cc1)CCCCc1cc[n+](cc1)[Re]<br>1([n+](c2ccc3c2c2[n+](c1ccc2c1c3nc2cccc2n1)([C][O])([C][O])([C][O]) |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -3743.79575197   | a.u. |
| Gibbs Energy                    | : -3742.87613400   | a.u. |
| Number of imaginary frequencies | : 0  |      |

## S4.1. Cartesian Co-ordinates (XYZ format)

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|   |             |            |            |
|---|-------------|------------|------------|
| C | -0.68550599 | 3.86019492 | 5.14828300 |
| H | -0.95449299 | 4.89363909 | 5.37977409 |
| H | -0.18731099 | 3.43243194 | 6.02118587 |
| C | -1.96078598 | 3.04774189 | 4.82473993 |
| H | -1.65488195 | 2.05108809 | 4.49370909 |
| H | -2.47289991 | 3.51192188 | 3.97501898 |
| C | -2.91805196 | 2.93406200 | 6.00760794 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.19483709 | 3.93678403  | 6.35020781  |
| H | -2.40258908 | 2.44916201  | 6.84472418  |
| C | -3.93790793 | 0.68155700  | 5.25515985  |
| H | -4.67632008 | 0.04022000  | 5.74567080  |
| H | -2.96116710 | 0.35144901  | 5.61647081  |
| C | 0.69955200  | 3.90104604  | -3.02587605 |
| N | 1.54791796  | 4.87400293  | -2.37402797 |
| N | 1.45585501  | 2.71002102  | -3.36253595 |
| N | -0.42638999 | 3.56828308  | -2.17543411 |
| N | 2.13256693  | 4.55581093  | -1.18972504 |
| C | 1.82944906  | 6.15420198  | -2.73084307 |
| N | 2.05497098  | 1.98956597  | -2.37137008 |
| C | 1.80297196  | 2.22783589  | -4.58001900 |
| N | -0.20992400 | 3.00097990  | -0.95584100 |
| C | -1.74172699 | 3.85336995  | -2.35549998 |
| C | 2.79137397  | 5.64687920  | -0.79625601 |
| C | 2.62844491  | 6.67694712  | -1.73697305 |
| H | 1.44751406  | 6.57813406  | -3.64456701 |
| C | 2.77697706  | 1.04162300  | -2.97582293 |
| C | 2.64436197  | 1.15096998  | -4.36450911 |
| H | 1.42744505  | 2.67397904  | -5.48572302 |
| C | -1.40876901 | 2.91705894  | -0.37341300 |
| C | -2.40035009 | 3.43823099  | -1.21747100 |
| H | -2.09697104 | 4.30681086  | -3.26564908 |
| N | -2.89441705 | -0.79989201 | -1.69378304 |
| N | -3.42306805 | -2.96812296 | -0.20236100 |
| H | 3.33835602  | 5.64643812  | 0.13246000  |
| H | 3.04234695  | 7.66920805  | -1.69385695 |
| H | 3.32849908  | 0.32967600  | -2.38805509 |
| H | 3.09396100  | 0.52313298  | -5.11375713 |
| H | -1.51350200 | 2.51363111  | 0.61957800  |
| H | -3.45656395 | 3.49767303  | -1.02081501 |
| C | -2.68823910 | 0.25159699  | -2.49471807 |
| C | -1.86460805 | -1.65558004 | -1.45993102 |
| C | -2.14592195 | -2.81772804 | -0.64584798 |
| C | -3.71492696 | -4.02084112 | 0.56900299  |
| C | -1.46022606 | 0.48500100  | -3.11122799 |
| H | -3.52997088 | 0.90614498  | -2.66406393 |
| C | -0.58263898 | -1.44583499 | -1.98812401 |
| C | -1.13198805 | -3.73543596 | -0.33687800 |
| C | -2.75705600 | -4.96947813 | 0.92806900  |
| H | -4.73804188 | -4.10702610 | 0.90510201  |
| C | -0.39872101 | -0.35920301 | -2.85351110 |
| H | -1.36617506 | 1.31629205  | -3.79437304 |
| C | 0.50059003  | -2.35779810 | -1.63891006 |
| C | -1.46030796 | -4.83305597 | 0.47163001  |
| C | 0.22151400  | -3.51265597 | -0.83987999 |
| H | -3.04649997 | -5.80042887 | 1.55624199  |
| H | 0.56599700  | -0.22074300 | -3.31607699 |
| N | 1.72944295  | -2.07770395 | -2.04697394 |
| H | -0.68931299 | -5.54778004 | 0.72368002  |
| N | 1.17048705  | -4.37516212 | -0.51522601 |
| C | 2.71488905  | -2.93945599 | -1.70877099 |
| C | 2.42551804  | -4.12412977 | -0.94998401 |
| C | 4.05390120  | -2.67645192 | -2.08980393 |
| C | 3.47377300  | -5.02089500 | -0.63285798 |
| C | 5.05010986  | -3.55925488 | -1.75071800 |
| H | 4.26757812  | -1.77930105 | -2.65548110 |
| C | 4.75782013  | -4.74323082 | -1.02910995 |
| H | 3.23276210  | -5.90401077 | -0.05558300 |
| H | 6.07393217  | -3.35162711 | -2.03529596 |
| H | 5.56278610  | -5.41956282 | -0.77144599 |
| N | 3.78389001  | 2.09846902  | -0.11964300 |
| N | 1.56763804  | 0.69093001  | 0.32148299  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.87196207  | 2.81517196  | -0.43636799 |
| C  | 3.94204998  | 0.79427499  | 0.32745600  |
| C  | 2.78118396  | 0.07164800  | 0.59965301  |
| C  | 0.43514600  | 0.07998300  | 0.69931698  |
| C  | 6.15663385  | 2.31158209  | -0.30413499 |
| H  | 4.70069790  | 3.81312299  | -0.81225199 |
| C  | 5.23846817  | 0.22621800  | 0.48970300  |
| C  | 2.82933307  | -1.22360599 | 1.18828297  |
| C  | 0.42810801  | -1.14888501 | 1.33473504  |
| H  | -0.48523101 | 0.59778303  | 0.47831601  |
| C  | 6.33880186  | 1.00228500  | 0.16670001  |
| H  | 6.99908876  | 2.93472099  | -0.56767398 |
| C  | 5.33390808  | -1.14925003 | 0.97184098  |
| C  | 1.64355302  | -1.81756997 | 1.57070601  |
| C  | 4.13670015  | -1.85469401 | 1.36271596  |
| H  | -0.50392199 | -1.59316599 | 1.64650500  |
| H  | 7.32910919  | 0.58124602  | 0.27718300  |
| N  | 6.52280998  | -1.72340202 | 1.04789698  |
| H  | 1.66277897  | -2.79375792 | 2.03406811  |
| N  | 4.18929005  | -3.07668090 | 1.86103404  |
| C  | 6.58296490  | -2.99442291 | 1.51153696  |
| C  | 5.40131283  | -3.67311406 | 1.94798398  |
| C  | 7.82761621  | -3.66850591 | 1.56523705  |
| C  | 5.50059414  | -4.99652004 | 2.43983006  |
| C  | 7.89133406  | -4.95759296 | 2.03704596  |
| H  | 8.70978928  | -3.14025211 | 1.22544396  |
| C  | 6.72191286  | -5.62457991 | 2.47998095  |
| H  | 4.59254694  | -5.49125385 | 2.76107693  |
| H  | 8.84290504  | -5.47376680 | 2.07381511  |
| H  | 6.79704380  | -6.64049101 | 2.84796810  |
| H  | 0.31907600  | 4.33423901  | -3.94485593 |
| C  | 0.21193200  | 3.80156803  | 3.95245600  |
| C  | 1.18442202  | 2.80417204  | 3.81771302  |
| C  | 0.00536100  | 4.64669323  | 2.85688901  |
| C  | 1.79047596  | 2.59584689  | 2.59677291  |
| H  | 1.43022597  | 2.15301108  | 4.64623213  |
| C  | 0.63898897  | 4.38362312  | 1.66225004  |
| H  | -0.69277400 | 5.47144079  | 2.91355610  |
| N  | 1.47426403  | 3.33034492  | 1.50702202  |
| H  | 2.50943804  | 1.80276895  | 2.45844507  |
| H  | 0.44909400  | 4.98342514  | 0.78546703  |
| C  | -4.04835987 | 0.39929301  | 3.77886510  |
| C  | -3.00179505 | -0.14568800 | 3.03271604  |
| C  | -5.25399017 | 0.60680199  | 3.09801793  |
| C  | -3.21282792 | -0.52181000 | 1.71542799  |
| H  | -2.02877092 | -0.31293800 | 3.47674394  |
| C  | -5.39118099 | 0.20486400  | 1.78374600  |
| H  | -6.10724688 | 1.04467201  | 3.59995604  |
| N  | -4.39577818 | -0.39254001 | 1.09118795  |
| H  | -2.41812205 | -0.97240603 | 1.14292800  |
| H  | -6.33199787 | 0.32829601  | 1.26684701  |
| C  | -4.19538689 | 2.15081191  | 5.68335915  |
| H  | -4.75634384 | 2.67243409  | 4.90173006  |
| H  | -4.83368921 | 2.15091896  | 6.56959581  |
| Re | -4.85666084 | -1.41596603 | -0.87359601 |
| Ru | 1.81010401  | 2.61195397  | -0.42154801 |
| C  | -5.21957016 | -2.37116790 | -2.52449203 |
| O  | -5.42727709 | -2.94206190 | -3.50259304 |
| C  | -5.87485504 | 0.11023700  | -1.50363100 |
| O  | -6.44690800 | 1.03631306  | -1.88423097 |
| C  | -6.45474005 | -2.18058300 | -0.08124900 |
| O  | -7.38790178 | -2.66381788 | 0.39234200  |

**S4.2. Frequencies**

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 11.91810000  | 2.20910000   | 0.00000000      |
| 2    | 12.93760000  | 0.87550000   | 0.00000000      |
| 3    | 18.24110000  | 0.25900000   | 0.00000000      |
| 4    | 21.45540000  | 1.19610000   | 0.00000000      |
| 5    | 31.89970000  | 0.23220000   | 0.00000000      |
| 6    | 33.25660000  | 1.96130000   | 0.00000000      |
| 7    | 36.13360000  | 1.37320000   | 0.00000000      |
| 8    | 38.04570000  | 0.43870000   | 0.00000000      |
| 9    | 43.90960000  | 1.98250000   | 0.00000000      |
| 10   | 47.24090000  | 1.13100000   | 0.00000000      |
| 11   | 49.75360000  | 0.63240000   | 0.00000000      |
| 12   | 57.56880000  | 0.64330000   | 0.00000000      |
| 13   | 60.76970000  | 0.28080000   | 0.00000000      |
| 14   | 62.63640000  | 3.25190000   | 0.00000000      |
| 15   | 64.73920000  | 0.81610000   | 0.00000000      |
| 16   | 67.03220000  | 1.83210000   | 0.00000000      |
| 17   | 69.78710000  | 4.39790000   | 0.00000000      |
| 18   | 78.45050000  | 4.61660000   | 0.00000000      |
| 19   | 81.32480000  | 2.03780000   | 0.00000000      |
| 20   | 83.96360000  | 4.70170000   | 0.00000000      |
| 21   | 88.90210000  | 2.39440000   | 0.00000000      |
| 22   | 91.68140000  | 1.40570000   | 0.00000000      |
| 23   | 92.72650000  | 1.26890000   | 0.00000000      |
| 24   | 93.61320000  | 0.96320000   | 0.00000000      |
| 25   | 95.67160000  | 0.27910000   | 0.00000000      |
| 26   | 96.99180000  | 0.36800000   | 0.00000000      |
| 27   | 104.98900000 | 0.08610000   | 0.00000000      |
| 28   | 110.02230000 | 7.07490000   | 0.00000000      |
| 29   | 114.81600000 | 0.19920000   | 0.00000000      |
| 30   | 121.12370000 | 0.71330000   | 0.00000000      |
| 31   | 126.29940000 | 1.84140000   | 0.00000000      |
| 32   | 136.83790000 | 6.89220000   | 0.00000000      |
| 33   | 138.82280000 | 2.66270000   | 0.00000000      |
| 34   | 143.87790000 | 14.24380000  | 0.00000000      |
| 35   | 148.99960000 | 5.96890000   | 0.00000000      |
| 36   | 150.60730000 | 3.05400000   | 0.00000000      |
| 37   | 155.08220000 | 0.71520000   | 0.00000000      |
| 38   | 161.85840000 | 0.53590000   | 0.00000000      |
| 39   | 174.79850000 | 0.83780000   | 0.00000000      |
| 40   | 177.34640000 | 0.69130000   | 0.00000000      |
| 41   | 178.47260000 | 4.88130000   | 0.00000000      |
| 42   | 179.97970000 | 2.14140000   | 0.00000000      |
| 43   | 182.67800000 | 5.62340000   | 0.00000000      |
| 44   | 185.33260000 | 5.97800000   | 0.00000000      |
| 45   | 191.41980000 | 5.01500000   | 0.00000000      |
| 46   | 192.76430000 | 4.25830000   | 0.00000000      |
| 47   | 194.26020000 | 1.86580000   | 0.00000000      |
| 48   | 205.20320000 | 5.08990000   | 0.00000000      |
| 49   | 208.07750000 | 6.28820000   | 0.00000000      |
| 50   | 210.50170000 | 1.26010000   | 0.00000000      |
| 51   | 215.26960000 | 6.18900000   | 0.00000000      |
| 52   | 221.46880000 | 6.60380000   | 0.00000000      |
| 53   | 221.80660000 | 2.65620000   | 0.00000000      |
| 54   | 231.09520000 | 1.40570000   | 0.00000000      |
| 55   | 239.27900000 | 22.75630000  | 0.00000000      |
| 56   | 250.28300000 | 10.45480000  | 0.00000000      |
| 57   | 257.45610000 | 3.52890000   | 0.00000000      |
| 58   | 274.08750000 | 8.61680000   | 0.00000000      |
| 59   | 274.69150000 | 8.88150000   | 0.00000000      |
| 60   | 282.20570000 | 34.87940000  | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 286.60080000 | 41.90180000  | 0.00000000 |
| 62  | 307.71880000 | 20.60780000  | 0.00000000 |
| 63  | 314.98280000 | 30.17380000  | 0.00000000 |
| 64  | 320.89240000 | 23.82550000  | 0.00000000 |
| 65  | 327.01860000 | 0.13580000   | 0.00000000 |
| 66  | 327.80060000 | 2.22400000   | 0.00000000 |
| 67  | 328.61200000 | 21.35700000  | 0.00000000 |
| 68  | 333.64150000 | 1.99900000   | 0.00000000 |
| 69  | 334.99000000 | 12.12110000  | 0.00000000 |
| 70  | 338.32020000 | 7.04900000   | 0.00000000 |
| 71  | 341.37700000 | 20.10830000  | 0.00000000 |
| 72  | 356.33640000 | 4.25410000   | 0.00000000 |
| 73  | 358.23780000 | 9.31080000   | 0.00000000 |
| 74  | 368.09940000 | 0.74010000   | 0.00000000 |
| 75  | 375.17200000 | 1.73790000   | 0.00000000 |
| 76  | 379.52680000 | 51.14280000  | 0.00000000 |
| 77  | 384.90240000 | 4.43370000   | 0.00000000 |
| 78  | 391.68540000 | 20.28970000  | 0.00000000 |
| 79  | 399.93120000 | 29.37010000  | 0.00000000 |
| 80  | 408.91850000 | 14.81860000  | 0.00000000 |
| 81  | 410.78590000 | 7.56650000   | 0.00000000 |
| 82  | 427.16020000 | 11.53000000  | 0.00000000 |
| 83  | 431.92100000 | 17.33860000  | 0.00000000 |
| 84  | 436.50220000 | 47.15290000  | 0.00000000 |
| 85  | 437.91730000 | 25.50710000  | 0.00000000 |
| 86  | 441.36050000 | 12.70950000  | 0.00000000 |
| 87  | 449.25700000 | 16.34880000  | 0.00000000 |
| 88  | 453.17110000 | 5.18900000   | 0.00000000 |
| 89  | 458.81640000 | 6.43420000   | 0.00000000 |
| 90  | 474.06190000 | 31.75850000  | 0.00000000 |
| 91  | 475.85640000 | 24.15590000  | 0.00000000 |
| 92  | 482.96090000 | 16.27530000  | 0.00000000 |
| 93  | 485.35620000 | 34.95420000  | 0.00000000 |
| 94  | 487.28560000 | 6.78990000   | 0.00000000 |
| 95  | 490.94720000 | 11.07800000  | 0.00000000 |
| 96  | 494.21410000 | 5.60490000   | 0.00000000 |
| 97  | 494.33360000 | 6.49110000   | 0.00000000 |
| 98  | 495.57640000 | 7.78200000   | 0.00000000 |
| 99  | 515.40710000 | 7.62190000   | 0.00000000 |
| 100 | 521.80880000 | 8.71870000   | 0.00000000 |
| 101 | 530.59920000 | 17.79230000  | 0.00000000 |
| 102 | 536.56580000 | 10.61330000  | 0.00000000 |
| 103 | 540.29040000 | 7.08090000   | 0.00000000 |
| 104 | 565.25860000 | 3.13640000   | 0.00000000 |
| 105 | 565.93580000 | 42.36120000  | 0.00000000 |
| 106 | 571.09960000 | 25.03410000  | 0.00000000 |
| 107 | 573.42330000 | 3.88380000   | 0.00000000 |
| 108 | 577.07100000 | 0.36340000   | 0.00000000 |
| 109 | 581.82120000 | 6.57700000   | 0.00000000 |
| 110 | 588.08020000 | 22.99410000  | 0.00000000 |
| 111 | 593.67150000 | 172.67290000 | 0.00000000 |
| 112 | 594.22220000 | 42.29160000  | 0.00000000 |
| 113 | 600.86060000 | 7.54580000   | 0.00000000 |
| 114 | 601.26830000 | 0.86200000   | 0.00000000 |
| 115 | 602.87350000 | 5.98490000   | 0.00000000 |
| 116 | 610.17680000 | 31.94680000  | 0.00000000 |
| 117 | 616.84960000 | 51.39550000  | 0.00000000 |
| 118 | 620.28410000 | 39.95860000  | 0.00000000 |
| 119 | 626.03800000 | 19.39890000  | 0.00000000 |
| 120 | 630.54150000 | 254.08420000 | 0.00000000 |
| 121 | 633.37580000 | 53.56410000  | 0.00000000 |
| 122 | 637.67910000 | 73.34610000  | 0.00000000 |
| 123 | 645.53650000 | 85.68130000  | 0.00000000 |
| 124 | 647.08350000 | 0.82720000   | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 651.48620000 | 3.53600000   | 0.00000000 |
| 126 | 655.52050000 | 0.51350000   | 0.00000000 |
| 127 | 661.56330000 | 1.11180000   | 0.00000000 |
| 128 | 668.08340000 | 4.53810000   | 0.00000000 |
| 129 | 672.64710000 | 5.35470000   | 0.00000000 |
| 130 | 676.76260000 | 5.13770000   | 0.00000000 |
| 131 | 678.84370000 | 0.73650000   | 0.00000000 |
| 132 | 686.09840000 | 0.08730000   | 0.00000000 |
| 133 | 706.68490000 | 117.37730000 | 0.00000000 |
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| 135 | 739.72910000 | 10.96430000  | 0.00000000 |
| 136 | 740.36580000 | 104.14330000 | 0.00000000 |
| 137 | 741.33830000 | 25.28040000  | 0.00000000 |
| 138 | 745.83340000 | 5.73590000   | 0.00000000 |
| 139 | 746.03160000 | 3.14180000   | 0.00000000 |
| 140 | 747.66950000 | 8.75310000   | 0.00000000 |
| 141 | 754.07500000 | 14.72750000  | 0.00000000 |
| 142 | 754.78480000 | 39.03420000  | 0.00000000 |
| 143 | 759.63120000 | 9.61710000   | 0.00000000 |
| 144 | 767.42610000 | 44.09170000  | 0.00000000 |
| 145 | 774.26710000 | 75.59910000  | 0.00000000 |
| 146 | 774.57030000 | 85.68530000  | 0.00000000 |
| 147 | 775.77350000 | 126.82550000 | 0.00000000 |
| 148 | 777.39450000 | 27.71300000  | 0.00000000 |
| 149 | 778.79590000 | 78.22710000  | 0.00000000 |
| 150 | 780.36820000 | 220.32810000 | 0.00000000 |
| 151 | 783.48530000 | 19.29550000  | 0.00000000 |
| 152 | 785.98740000 | 2.83830000   | 0.00000000 |
| 153 | 790.22520000 | 150.72890000 | 0.00000000 |
| 154 | 792.51920000 | 14.13410000  | 0.00000000 |
| 155 | 793.49440000 | 70.29620000  | 0.00000000 |
| 156 | 800.05200000 | 115.15660000 | 0.00000000 |
| 157 | 813.28770000 | 8.38140000   | 0.00000000 |
| 158 | 823.70070000 | 14.10630000  | 0.00000000 |
| 159 | 825.79190000 | 53.66720000  | 0.00000000 |
| 160 | 838.57410000 | 4.35430000   | 0.00000000 |
| 161 | 842.91590000 | 99.61180000  | 0.00000000 |
| 162 | 843.38960000 | 4.13920000   | 0.00000000 |
| 163 | 847.98140000 | 18.10030000  | 0.00000000 |
| 164 | 862.10180000 | 20.07560000  | 0.00000000 |
| 165 | 862.32830000 | 24.07620000  | 0.00000000 |
| 166 | 867.73910000 | 29.44930000  | 0.00000000 |
| 167 | 871.58090000 | 209.45320000 | 0.00000000 |
| 168 | 873.36470000 | 14.08580000  | 0.00000000 |
| 169 | 874.18670000 | 74.27960000  | 0.00000000 |
| 170 | 879.28980000 | 3.43750000   | 0.00000000 |
| 171 | 883.43760000 | 3.80110000   | 0.00000000 |
| 172 | 887.44290000 | 1.31060000   | 0.00000000 |
| 173 | 889.02660000 | 0.40060000   | 0.00000000 |
| 174 | 889.93680000 | 4.70900000   | 0.00000000 |
| 175 | 890.19360000 | 10.31280000  | 0.00000000 |
| 176 | 897.10750000 | 15.23490000  | 0.00000000 |
| 177 | 917.92680000 | 11.05520000  | 0.00000000 |
| 178 | 920.20760000 | 13.07060000  | 0.00000000 |
| 179 | 928.66950000 | 0.27390000   | 0.00000000 |
| 180 | 939.03770000 | 18.72380000  | 0.00000000 |
| 181 | 939.47560000 | 3.04310000   | 0.00000000 |
| 182 | 945.62810000 | 0.45680000   | 0.00000000 |
| 183 | 946.56470000 | 1.63820000   | 0.00000000 |
| 184 | 952.94300000 | 5.28970000   | 0.00000000 |
| 185 | 956.95640000 | 1.35930000   | 0.00000000 |
| 186 | 959.09870000 | 12.39320000  | 0.00000000 |
| 187 | 962.46800000 | 6.49470000   | 0.00000000 |
| 188 | 969.02540000 | 9.68480000   | 0.00000000 |

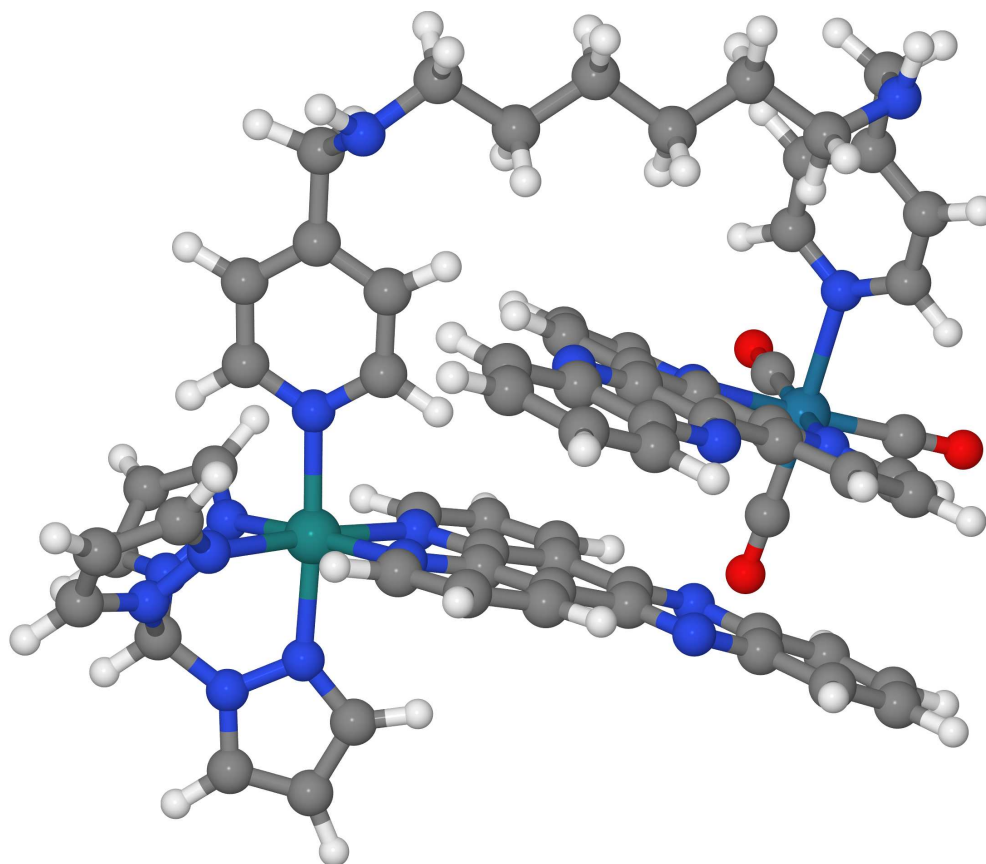
|     |               |               |            |
|-----|---------------|---------------|------------|
| 189 | 977.44790000  | 4.11810000    | 0.00000000 |
| 190 | 981.54470000  | 3.51330000    | 0.00000000 |
| 191 | 982.47790000  | 1.12250000    | 0.00000000 |
| 192 | 983.23030000  | 1.83810000    | 0.00000000 |
| 193 | 985.10410000  | 4.71860000    | 0.00000000 |
| 194 | 989.20550000  | 19.46010000   | 0.00000000 |
| 195 | 989.96470000  | 14.24870000   | 0.00000000 |
| 196 | 998.43970000  | 105.06320000  | 0.00000000 |
| 197 | 1003.22300000 | 25.68130000   | 0.00000000 |
| 198 | 1007.02620000 | 1.35960000    | 0.00000000 |
| 199 | 1009.30130000 | 3.37620000    | 0.00000000 |
| 200 | 1010.38830000 | 0.45300000    | 0.00000000 |
| 201 | 1011.91050000 | 4.69520000    | 0.00000000 |
| 202 | 1014.01560000 | 12.22670000   | 0.00000000 |
| 203 | 1014.68490000 | 13.90440000   | 0.00000000 |
| 204 | 1016.12510000 | 67.37310000   | 0.00000000 |
| 205 | 1020.64720000 | 31.44680000   | 0.00000000 |
| 206 | 1022.97720000 | 46.92830000   | 0.00000000 |
| 207 | 1031.35220000 | 15.50740000   | 0.00000000 |
| 208 | 1032.93450000 | 0.46730000    | 0.00000000 |
| 209 | 1033.41780000 | 5.53930000    | 0.00000000 |
| 210 | 1034.67690000 | 11.92050000   | 0.00000000 |
| 211 | 1044.84410000 | 315.73710000  | 0.00000000 |
| 212 | 1048.24810000 | 802.99880000  | 0.00000000 |
| 213 | 1052.63320000 | 609.08060000  | 0.00000000 |
| 214 | 1053.42930000 | 791.68190000  | 0.00000000 |
| 215 | 1056.04230000 | 358.97430000  | 0.00000000 |
| 216 | 1069.59420000 | 3.26410000    | 0.00000000 |
| 217 | 1075.19410000 | 85.50130000   | 0.00000000 |
| 218 | 1079.08280000 | 7.04570000    | 0.00000000 |
| 219 | 1081.81830000 | 101.47300000  | 0.00000000 |
| 220 | 1084.47240000 | 130.58390000  | 0.00000000 |
| 221 | 1085.44720000 | 13.00270000   | 0.00000000 |
| 222 | 1087.83090000 | 3.88630000    | 0.00000000 |
| 223 | 1092.82790000 | 160.20620000  | 0.00000000 |
| 224 | 1097.05880000 | 18.68380000   | 0.00000000 |
| 225 | 1099.69150000 | 73.00480000   | 0.00000000 |
| 226 | 1100.88350000 | 50.20630000   | 0.00000000 |
| 227 | 1109.25970000 | 32.98280000   | 0.00000000 |
| 228 | 1122.25700000 | 155.53150000  | 0.00000000 |
| 229 | 1124.42350000 | 16.33500000   | 0.00000000 |
| 230 | 1126.88730000 | 2.86520000    | 0.00000000 |
| 231 | 1132.50900000 | 231.05520000  | 0.00000000 |
| 232 | 1134.63520000 | 171.36480000  | 0.00000000 |
| 233 | 1137.04740000 | 46.95970000   | 0.00000000 |
| 234 | 1146.59660000 | 25.59120000   | 0.00000000 |
| 235 | 1147.62780000 | 11.68730000   | 0.00000000 |
| 236 | 1148.16830000 | 5.29370000    | 0.00000000 |
| 237 | 1153.58130000 | 4.30840000    | 0.00000000 |
| 238 | 1154.71870000 | 270.89090000  | 0.00000000 |
| 239 | 1163.07690000 | 1722.16310000 | 0.00000000 |
| 240 | 1163.65760000 | 685.17510000  | 0.00000000 |
| 241 | 1166.10840000 | 16.53980000   | 0.00000000 |
| 242 | 1167.79060000 | 823.77030000  | 0.00000000 |
| 243 | 1175.20570000 | 618.50790000  | 0.00000000 |
| 244 | 1209.46620000 | 99.44750000   | 0.00000000 |
| 245 | 1213.68400000 | 17.34820000   | 0.00000000 |
| 246 | 1215.02910000 | 5.79860000    | 0.00000000 |
| 247 | 1215.22730000 | 5.42990000    | 0.00000000 |
| 248 | 1218.84230000 | 192.72450000  | 0.00000000 |
| 249 | 1233.40810000 | 86.76450000   | 0.00000000 |
| 250 | 1237.94370000 | 11.06490000   | 0.00000000 |
| 251 | 1241.31350000 | 54.25630000   | 0.00000000 |
| 252 | 1245.44420000 | 5.51450000    | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1250.28000000 | 2130.91950000 | 0.00000000 |
| 254 | 1258.64060000 | 72.93200000   | 0.00000000 |
| 255 | 1260.03010000 | 41.00830000   | 0.00000000 |
| 256 | 1261.47010000 | 78.54480000   | 0.00000000 |
| 257 | 1263.76670000 | 5.98880000    | 0.00000000 |
| 258 | 1264.73970000 | 16.46060000   | 0.00000000 |
| 259 | 1272.95060000 | 572.44360000  | 0.00000000 |
| 260 | 1275.12890000 | 109.71600000  | 0.00000000 |
| 261 | 1275.73690000 | 44.10890000   | 0.00000000 |
| 262 | 1280.65950000 | 535.78650000  | 0.00000000 |
| 263 | 1283.03220000 | 3.73870000    | 0.00000000 |
| 264 | 1294.99830000 | 843.50250000  | 0.00000000 |
| 265 | 1299.32660000 | 14.14920000   | 0.00000000 |
| 266 | 1301.52210000 | 638.61190000  | 0.00000000 |
| 267 | 1309.21720000 | 87.80050000   | 0.00000000 |
| 268 | 1309.46380000 | 13.98210000   | 0.00000000 |
| 269 | 1318.25420000 | 11.25830000   | 0.00000000 |
| 270 | 1318.41820000 | 18.21070000   | 0.00000000 |
| 271 | 1318.65180000 | 48.34880000   | 0.00000000 |
| 272 | 1321.53900000 | 116.13600000  | 0.00000000 |
| 273 | 1325.17820000 | 121.32070000  | 0.00000000 |
| 274 | 1332.02610000 | 11.06320000   | 0.00000000 |
| 275 | 1337.98350000 | 1.45080000    | 0.00000000 |
| 276 | 1341.40650000 | 502.22810000  | 0.00000000 |
| 277 | 1346.76660000 | 211.05170000  | 0.00000000 |
| 278 | 1353.87730000 | 1.86410000    | 0.00000000 |
| 279 | 1358.07750000 | 335.60280000  | 0.00000000 |
| 280 | 1358.71310000 | 46.39540000   | 0.00000000 |
| 281 | 1363.49100000 | 1.91070000    | 0.00000000 |
| 282 | 1370.21670000 | 12.50940000   | 0.00000000 |
| 283 | 1371.24820000 | 3.38070000    | 0.00000000 |
| 284 | 1372.68610000 | 196.58060000  | 0.00000000 |
| 285 | 1375.56410000 | 2.50040000    | 0.00000000 |
| 286 | 1378.26860000 | 19.92230000   | 0.00000000 |
| 287 | 1379.25240000 | 36.34020000   | 0.00000000 |
| 288 | 1390.91230000 | 59.23170000   | 0.00000000 |
| 289 | 1392.23870000 | 230.71130000  | 0.00000000 |
| 290 | 1401.36550000 | 1.06070000    | 0.00000000 |
| 291 | 1403.21570000 | 4.58030000    | 0.00000000 |
| 292 | 1408.23410000 | 54.02500000   | 0.00000000 |
| 293 | 1414.02540000 | 360.16120000  | 0.00000000 |
| 294 | 1418.50560000 | 130.18970000  | 0.00000000 |
| 295 | 1429.41130000 | 134.78410000  | 0.00000000 |
| 296 | 1433.39960000 | 884.20350000  | 0.00000000 |
| 297 | 1435.45210000 | 27.96000000   | 0.00000000 |
| 298 | 1442.16050000 | 357.96230000  | 0.00000000 |
| 299 | 1449.47320000 | 682.65500000  | 0.00000000 |
| 300 | 1452.84870000 | 138.19300000  | 0.00000000 |
| 301 | 1466.55000000 | 13.45910000   | 0.00000000 |
| 302 | 1468.81660000 | 486.31320000  | 0.00000000 |
| 303 | 1471.19800000 | 47.34330000   | 0.00000000 |
| 304 | 1476.84630000 | 3.71310000    | 0.00000000 |
| 305 | 1480.18210000 | 40.52270000   | 0.00000000 |
| 306 | 1484.16830000 | 483.21090000  | 0.00000000 |
| 307 | 1484.99330000 | 45.15200000   | 0.00000000 |
| 308 | 1486.98170000 | 20.13950000   | 0.00000000 |
| 309 | 1490.03810000 | 11.86240000   | 0.00000000 |
| 310 | 1491.28520000 | 1353.62850000 | 0.00000000 |
| 311 | 1492.70720000 | 34.36090000   | 0.00000000 |
| 312 | 1497.38100000 | 7.07200000    | 0.00000000 |
| 313 | 1500.66050000 | 4.11140000    | 0.00000000 |
| 314 | 1506.50050000 | 167.27500000  | 0.00000000 |
| 315 | 1507.13370000 | 15.08460000   | 0.00000000 |
| 316 | 1512.61450000 | 21.56010000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1517.42480000 | 649.40140000  | 0.00000000 |
| 318 | 1523.11840000 | 75.03490000   | 0.00000000 |
| 319 | 1524.77780000 | 122.16860000  | 0.00000000 |
| 320 | 1529.79490000 | 298.51530000  | 0.00000000 |
| 321 | 1533.86770000 | 13.98870000   | 0.00000000 |
| 322 | 1540.30610000 | 30.37160000   | 0.00000000 |
| 323 | 1547.42520000 | 381.06300000  | 0.00000000 |
| 324 | 1548.67830000 | 188.87320000  | 0.00000000 |
| 325 | 1551.86460000 | 89.78890000   | 0.00000000 |
| 326 | 1557.04340000 | 6.28470000    | 0.00000000 |
| 327 | 1558.42730000 | 66.97010000   | 0.00000000 |
| 328 | 1565.78040000 | 26.44310000   | 0.00000000 |
| 329 | 1575.99160000 | 177.05420000  | 0.00000000 |
| 330 | 1582.32960000 | 107.78600000  | 0.00000000 |
| 331 | 1584.75060000 | 14.91870000   | 0.00000000 |
| 332 | 1591.38140000 | 16.04430000   | 0.00000000 |
| 333 | 1600.20340000 | 595.28320000  | 0.00000000 |
| 334 | 1613.21160000 | 186.18410000  | 0.00000000 |
| 335 | 1621.46500000 | 318.39560000  | 0.00000000 |
| 336 | 1622.26150000 | 9.48500000    | 0.00000000 |
| 337 | 1624.85680000 | 87.01790000   | 0.00000000 |
| 338 | 1635.11760000 | 11.12990000   | 0.00000000 |
| 339 | 1652.51900000 | 1.86420000    | 0.00000000 |
| 340 | 1654.90520000 | 313.90950000  | 0.00000000 |
| 341 | 1656.49160000 | 1.71790000    | 0.00000000 |
| 342 | 1658.61870000 | 191.40880000  | 0.00000000 |
| 343 | 1964.72520000 | 2402.51690000 | 0.00000000 |
| 344 | 1971.61620000 | 2281.36860000 | 0.00000000 |
| 345 | 2085.23610000 | 2512.01920000 | 0.00000000 |
| 346 | 3013.02610000 | 33.95110000   | 0.00000000 |
| 347 | 3025.81560000 | 47.41990000   | 0.00000000 |
| 348 | 3032.39570000 | 18.36220000   | 0.00000000 |
| 349 | 3037.18920000 | 16.39080000   | 0.00000000 |
| 350 | 3047.25780000 | 38.66130000   | 0.00000000 |
| 351 | 3049.52350000 | 44.86530000   | 0.00000000 |
| 352 | 3067.10420000 | 63.87530000   | 0.00000000 |
| 353 | 3077.67920000 | 81.74300000   | 0.00000000 |
| 354 | 3080.12020000 | 42.87080000   | 0.00000000 |
| 355 | 3098.86530000 | 51.75970000   | 0.00000000 |
| 356 | 3178.79800000 | 0.14390000    | 0.00000000 |
| 357 | 3180.53920000 | 5.45470000    | 0.00000000 |
| 358 | 3186.23840000 | 0.55940000    | 0.00000000 |
| 359 | 3187.10200000 | 2.05250000    | 0.00000000 |
| 360 | 3194.76540000 | 3.93430000    | 0.00000000 |
| 361 | 3195.30730000 | 2.32710000    | 0.00000000 |
| 362 | 3196.05510000 | 26.38850000   | 0.00000000 |
| 363 | 3197.70030000 | 2.14590000    | 0.00000000 |
| 364 | 3202.70950000 | 90.35140000   | 0.00000000 |
| 365 | 3203.19010000 | 0.86340000    | 0.00000000 |
| 366 | 3204.01330000 | 19.05190000   | 0.00000000 |
| 367 | 3204.67460000 | 1.81860000    | 0.00000000 |
| 368 | 3208.44760000 | 10.00900000   | 0.00000000 |
| 369 | 3209.67390000 | 22.56150000   | 0.00000000 |
| 370 | 3213.23610000 | 1.53090000    | 0.00000000 |
| 371 | 3218.97180000 | 6.78990000    | 0.00000000 |
| 372 | 3219.52040000 | 39.34590000   | 0.00000000 |
| 373 | 3221.04740000 | 5.99110000    | 0.00000000 |
| 374 | 3224.29170000 | 2.39320000    | 0.00000000 |
| 375 | 3227.66500000 | 6.10400000    | 0.00000000 |
| 376 | 3231.16800000 | 4.35290000    | 0.00000000 |
| 377 | 3232.32180000 | 21.65940000   | 0.00000000 |
| 378 | 3232.59480000 | 23.73710000   | 0.00000000 |
| 379 | 3234.31840000 | 1.06640000    | 0.00000000 |
| 380 | 3238.72790000 | 10.18600000   | 0.00000000 |

|     |               |             |            |
|-----|---------------|-------------|------------|
| 381 | 3241.68640000 | 9.23460000  | 0.00000000 |
| 382 | 3244.65500000 | 12.65310000 | 0.00000000 |
| 383 | 3248.13940000 | 1.48250000  | 0.00000000 |
| 384 | 3248.30320000 | 4.73550000  | 0.00000000 |
| 385 | 3261.79370000 | 1.40200000  | 0.00000000 |
| 386 | 3267.91570000 | 4.71100000  | 0.00000000 |
| 387 | 3272.22700000 | 6.96130000  | 0.00000000 |
| 388 | 3272.41000000 | 6.65240000  | 0.00000000 |
| 389 | 3272.76880000 | 19.96000000 | 0.00000000 |
| 390 | 3283.57560000 | 22.72780000 | 0.00000000 |
| 391 | 3287.62760000 | 9.03040000  | 0.00000000 |
| 392 | 3287.99100000 | 9.24530000  | 0.00000000 |
| 393 | 3294.35500000 | 10.30460000 | 0.00000000 |

S5. CALCULATIONS ON  $2^{3+}$  ( $^1A$ )

|                                 |   |      |
|---------------------------------|---|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular   |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]<br>1n7ccc1)[n+](n8ccc1)[n+](1ccc(cc1)CNC(CCCCCNCc1cc[n+](cc1)[Re]<br>1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+</sup>   |      |
| Charge                          | : 3   |      |
| Multiplicity                    | : 1   |      |
| Energy                          | : -3972.59369652  | a.u. |
| Gibbs Energy                    | : -3971.55445000  | a.u. |
| Number of imaginary frequencies | : 1   |      |

## S5.1. Cartesian Co-ordinates (XYZ format)

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|   |            |            |             |
|---|------------|------------|-------------|
| C | 4.64906120 | 4.72182083 | 0.60845500  |
| H | 4.52120781 | 4.86268902 | 1.68592298  |
| H | 4.36520720 | 3.68425012 | 0.40257999  |
| C | 3.69652510 | 5.66175413 | -0.14223801 |
| H | 3.94720888 | 5.68009615 | -1.20788002 |
| H | 3.83328509 | 6.68489504 | 0.22766000  |
| C | 2.23504400 | 5.23608303 | 0.00801600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.99953699  | 5.08148193  | 1.06848395  |
| H  | 2.10075903  | 4.26044893  | -0.47604400 |
| C  | 1.23774004  | 6.23688602  | -0.58252800 |
| H  | 1.54522598  | 6.50649977  | -1.60007799 |
| H  | 1.26547396  | 7.16283894  | 0.00455100  |
| C  | -1.25446606 | 6.69849300  | -0.99411899 |
| H  | -1.01774204 | 7.12835884  | -1.98132205 |
| H  | -1.23016000 | 7.52234983  | -0.27536300 |
| N  | 6.08117199  | 4.85589314  | 0.31252301  |
| C  | -3.02551198 | 5.36115503  | -2.13268900 |
| H  | -2.20724106 | 5.32031202  | -2.86230707 |
| H  | -3.86510110 | 5.84407377  | -2.63995910 |
| N  | -2.60627007 | 6.12598610  | -0.95297801 |
| C  | 6.45280886  | 4.51365519  | -1.06210101 |
| H  | 5.93266487  | 5.09770823  | -1.83336401 |
| H  | 7.52239323  | 4.71180391  | -1.17870903 |
| C  | -7.30616617 | -1.97757995 | -0.87069100 |
| N  | -6.73130989 | -1.69225705 | -2.17025495 |
| N  | -6.46814394 | -2.88980293 | -0.12708800 |
| N  | -7.51167822 | -0.74506801 | -0.13667899 |
| N  | -5.52947712 | -1.05893397 | -2.24565101 |
| C  | -7.27488518 | -1.87173903 | -3.40397191 |
| N  | -5.19502020 | -2.52965593 | 0.17997000  |
| C  | -6.75670290 | -4.13503122 | 0.33925501  |
| N  | -6.44249201 | 0.04697500  | 0.14744100  |
| C  | -8.67937660 | -0.14800900 | 0.22671001  |
| Ru | -4.55621386 | -0.63841099 | -0.44012201 |
| C  | -5.31445217 | -0.84245801 | -3.54348111 |
| C  | -6.38381004 | -1.34116602 | -4.31012297 |
| H  | -8.22956371 | -2.35401392 | -3.52914190 |
| C  | -4.67483807 | -3.55698299 | 0.84841299  |
| C  | -5.62226105 | -4.59114504 | 0.97262901  |
| H  | -7.72492981 | -4.57990980 | 0.18342499  |
| C  | -6.94335222 | 1.15032995  | 0.70168298  |
| C  | -8.34650517 | 1.06943202  | 0.77728301  |
| H  | -9.62852192 | -0.63192099 | 0.06872900  |
| N  | -2.67963290 | -1.43267596 | -0.91311997 |
| N  | -3.53296304 | -0.37739301 | 1.36966598  |
| H  | -4.42180920 | -0.33308899 | -3.86710000 |
| H  | -6.48702097 | -1.31428695 | -5.38098383 |
| H  | -3.66022205 | -3.51598001 | 1.20793104  |
| H  | -5.49047804 | -5.54132509 | 1.46052504  |
| H  | -6.28774786 | 1.94936001  | 1.00587797  |
| H  | -9.02130508 | 1.80413198  | 1.18109298  |
| C  | -2.28569794 | -1.94717300 | -2.08233500 |
| C  | -1.83274901 | -1.52288103 | 0.14902800  |
| C  | -2.29269600 | -0.94085699 | 1.38834500  |
| C  | -3.97939301 | 0.20793700  | 2.48488402  |
| C  | -1.04862702 | -2.57134700 | -2.24648309 |
| H  | -2.98342991 | -1.87390304 | -2.90227604 |
| C  | -0.58744103 | -2.16166711 | 0.06877300  |
| C  | -1.49511302 | -0.97005600 | 2.53992701  |
| C  | -3.22096109 | 0.26401201  | 3.65543389  |
| H  | -4.96934080 | 0.63636202  | 2.44216704  |
| C  | -0.19539399 | -2.69533110 | -1.16583705 |
| H  | -0.78138399 | -2.96485901 | -3.21747494 |
| C  | 0.21661600  | -2.29940701 | 1.28069496  |
| C  | -1.97772098 | -0.33899501 | 3.69473791  |
| C  | -0.22945499 | -1.70073998 | 2.50590205  |
| H  | -3.62442398 | 0.76958197  | 4.52141714  |
| H  | 0.75462401  | -3.20357490 | -1.24677801 |
| N  | 1.32759702  | -3.01681495 | 1.22769296  |
| H  | -1.37444401 | -0.34198099 | 4.59132814  |
| N  | 0.45914400  | -1.83353996 | 3.62811708  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.01668811  | -3.19735599 | 2.37273908  |
| C  | 1.57864702  | -2.58437800 | 3.59590006  |
| C  | 3.17893100  | -4.01106024 | 2.37999701  |
| C  | 2.32649708  | -2.79047704 | 4.78387022  |
| C  | 3.86562800  | -4.20584917 | 3.55052209  |
| H  | 3.48964691  | -4.47117996 | 1.45171404  |
| C  | 3.44056392  | -3.58851004 | 4.75695419  |
| H  | 1.98424006  | -2.31170893 | 5.69228697  |
| H  | 4.74948978  | -4.83122683 | 3.55950403  |
| H  | 4.00936508  | -3.75358701 | 5.66336012  |
| N  | 4.19453382  | -1.15335095 | 0.64338201  |
| N  | 2.66531110  | -0.61390501 | -1.53364599 |
| C  | 4.95622921  | -1.44647300 | 1.70140398  |
| C  | 3.13300896  | -0.32128799 | 0.80719799  |
| C  | 2.31869698  | -0.02669400 | -0.35857800 |
| C  | 1.92710805  | -0.37755501 | -2.62283492 |
| C  | 4.71648693  | -0.91393501 | 2.96740603  |
| H  | 5.77963686  | -2.12548709 | 1.53299701  |
| C  | 2.81586504  | 0.23114000  | 2.05487990  |
| C  | 1.21548998  | 0.83547598  | -0.26106101 |
| C  | 0.83411801  | 0.48662901  | -2.60824394 |
| H  | 2.22330809  | -0.88691097 | -3.52891397 |
| C  | 3.63771510  | -0.07446600 | 3.14953208  |
| H  | 5.36626720  | -1.18272305 | 3.78753400  |
| C  | 1.63532901  | 1.07677698  | 2.19154811  |
| C  | 0.48520699  | 1.10800397  | -1.42632902 |
| C  | 0.84926599  | 1.39303100  | 1.03848398  |
| H  | 0.27766100  | 0.65753400  | -3.51894999 |
| H  | 3.40030098  | 0.34685901  | 4.11614418  |
| N  | 1.29811502  | 1.50428200  | 3.39700389  |
| H  | -0.34903401 | 1.78974104  | -1.38261294 |
| N  | -0.23550899 | 2.14694190  | 1.13183403  |
| C  | 0.18122000  | 2.24865198  | 3.51219893  |
| C  | -0.59653598 | 2.59082508  | 2.35334110  |
| C  | -0.24642400 | 2.68252802  | 4.79347181  |
| C  | -1.76966703 | 3.37375903  | 2.51264906  |
| C  | -1.39233601 | 3.42385197  | 4.91260481  |
| H  | 0.35138601  | 2.40475893  | 5.65197420  |
| C  | -2.15388489 | 3.77466297  | 3.76541495  |
| H  | -2.34591007 | 3.63649106  | 1.63702297  |
| H  | -1.72667098 | 3.75120592  | 5.88905287  |
| H  | -3.05319595 | 4.36484814  | 3.88935089  |
| H  | -8.27046013 | -2.45165896 | -1.02115297 |
| C  | 6.19183016  | 3.04696107  | -1.30424905 |
| C  | 5.37812281  | 2.60417199  | -2.34390092 |
| C  | 6.71276712  | 2.08347011  | -0.43778601 |
| C  | 5.06749392  | 1.25708699  | -2.44548798 |
| H  | 4.95112324  | 3.30203509  | -3.05258393 |
| C  | 6.36675978  | 0.75718802  | -0.60500902 |
| H  | 7.34942913  | 2.37525702  | 0.38621601  |
| N  | 5.52662277  | 0.34237000  | -1.57490098 |
| H  | 4.40946579  | 0.90154600  | -3.22601891 |
| H  | 6.74685192  | -0.00097100 | 0.06463800  |
| C  | -3.40966511 | 3.93928003  | -1.78259301 |
| C  | -2.57188296 | 3.16216707  | -0.98296499 |
| C  | -4.59041023 | 3.34097004  | -2.21892905 |
| C  | -2.91749310 | 1.86760795  | -0.66599399 |
| H  | -1.65189505 | 3.55877304  | -0.58596998 |
| C  | -4.88753414 | 2.03669810  | -1.84637105 |
| H  | -5.29673910 | 3.88334799  | -2.83514595 |
| N  | -4.06413507 | 1.29424000  | -1.07959497 |
| H  | -2.26653004 | 1.27507997  | -0.04555100 |
| H  | -5.81049109 | 1.56816399  | -2.15469694 |
| Re | 4.60467577  | -1.83028901 | -1.50036895 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.70878196  | -3.53417993 | -1.34005499 |
| O | 3.17170596  | -4.55164814 | -1.25822306 |
| C | 4.81153679  | -2.11246395 | -3.40478110 |
| O | 4.91806984  | -2.25437498 | -4.54391479 |
| C | 6.31717300  | -2.68496704 | -1.21095896 |
| O | 7.33818007  | -3.18190098 | -1.01148701 |
| H | -3.28150511 | 6.85582018  | -0.77182502 |
| C | -0.18466100 | 5.67857122  | -0.60816997 |
| H | -0.43820101 | 5.27532816  | 0.37831399  |
| H | -0.20825800 | 4.83691692  | -1.30915999 |
| H | 6.39467382  | 5.79836893  | 0.51920998  |

## S5.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -6.35860000  | 0.56110000   | 0.00000000      |
| 2    | 7.82540000   | 0.08660000   | 0.00000000      |
| 3    | 17.10430000  | 0.87350000   | 0.00000000      |
| 4    | 18.67260000  | 0.81870000   | 0.00000000      |
| 5    | 21.17930000  | 0.53160000   | 0.00000000      |
| 6    | 30.20090000  | 0.40420000   | 0.00000000      |
| 7    | 32.64400000  | 0.71670000   | 0.00000000      |
| 8    | 34.84560000  | 0.52530000   | 0.00000000      |
| 9    | 37.70480000  | 0.25730000   | 0.00000000      |
| 10   | 39.64890000  | 0.20580000   | 0.00000000      |
| 11   | 45.00110000  | 0.08010000   | 0.00000000      |
| 12   | 45.56220000  | 0.61560000   | 0.00000000      |
| 13   | 53.01890000  | 1.37240000   | 0.00000000      |
| 14   | 58.29950000  | 1.52070000   | 0.00000000      |
| 15   | 60.51650000  | 0.39800000   | 0.00000000      |
| 16   | 63.59780000  | 2.77750000   | 0.00000000      |
| 17   | 69.83510000  | 0.51220000   | 0.00000000      |
| 18   | 71.06320000  | 0.85310000   | 0.00000000      |
| 19   | 71.44400000  | 1.57110000   | 0.00000000      |
| 20   | 72.01660000  | 1.21450000   | 0.00000000      |
| 21   | 73.93150000  | 1.08550000   | 0.00000000      |
| 22   | 76.10700000  | 0.54630000   | 0.00000000      |
| 23   | 80.46710000  | 3.01450000   | 0.00000000      |
| 24   | 88.99370000  | 0.07610000   | 0.00000000      |
| 25   | 91.49960000  | 1.36390000   | 0.00000000      |
| 26   | 93.15780000  | 0.34450000   | 0.00000000      |
| 27   | 94.91830000  | 1.53600000   | 0.00000000      |
| 28   | 96.89660000  | 3.40020000   | 0.00000000      |
| 29   | 101.84490000 | 0.13390000   | 0.00000000      |
| 30   | 104.42350000 | 1.43500000   | 0.00000000      |
| 31   | 106.24050000 | 0.91320000   | 0.00000000      |
| 32   | 108.48750000 | 3.01770000   | 0.00000000      |
| 33   | 110.97920000 | 0.73270000   | 0.00000000      |
| 34   | 115.10670000 | 1.21210000   | 0.00000000      |
| 35   | 124.12450000 | 0.62440000   | 0.00000000      |
| 36   | 127.62630000 | 5.97270000   | 0.00000000      |
| 37   | 131.56240000 | 1.69880000   | 0.00000000      |
| 38   | 135.80500000 | 0.05010000   | 0.00000000      |
| 39   | 142.52820000 | 0.32590000   | 0.00000000      |
| 40   | 144.14740000 | 0.90500000   | 0.00000000      |
| 41   | 150.21150000 | 2.24020000   | 0.00000000      |
| 42   | 155.58830000 | 0.02780000   | 0.00000000      |
| 43   | 156.25700000 | 0.50310000   | 0.00000000      |
| 44   | 167.38020000 | 0.37730000   | 0.00000000      |
| 45   | 176.18000000 | 1.04240000   | 0.00000000      |
| 46   | 177.97560000 | 0.09870000   | 0.00000000      |
| 47   | 180.41900000 | 0.81420000   | 0.00000000      |
| 48   | 182.61850000 | 0.53560000   | 0.00000000      |
| 49   | 185.79310000 | 0.72230000   | 0.00000000      |
| 50   | 188.55280000 | 2.56690000   | 0.00000000      |
| 51   | 191.29360000 | 0.69120000   | 0.00000000      |
| 52   | 193.04760000 | 1.85800000   | 0.00000000      |
| 53   | 197.11040000 | 1.82590000   | 0.00000000      |
| 54   | 199.68900000 | 0.42990000   | 0.00000000      |
| 55   | 201.72710000 | 0.25110000   | 0.00000000      |
| 56   | 205.76710000 | 2.46520000   | 0.00000000      |
| 57   | 209.22860000 | 2.15830000   | 0.00000000      |
| 58   | 225.62150000 | 6.13580000   | 0.00000000      |
| 59   | 230.56110000 | 1.86610000   | 0.00000000      |
| 60   | 242.25210000 | 0.33190000   | 0.00000000      |



|     |              |             |            |
|-----|--------------|-------------|------------|
| 61  | 244.71760000 | 1.31780000  | 0.00000000 |
| 62  | 252.46400000 | 0.36430000  | 0.00000000 |
| 63  | 258.53200000 | 3.96350000  | 0.00000000 |
| 64  | 260.64300000 | 0.53630000  | 0.00000000 |
| 65  | 273.63800000 | 6.55640000  | 0.00000000 |
| 66  | 280.21810000 | 1.32360000  | 0.00000000 |
| 67  | 292.96090000 | 2.26040000  | 0.00000000 |
| 68  | 306.69260000 | 0.43110000  | 0.00000000 |
| 69  | 324.96630000 | 1.23840000  | 0.00000000 |
| 70  | 328.15530000 | 0.98500000  | 0.00000000 |
| 71  | 330.05720000 | 1.79360000  | 0.00000000 |
| 72  | 330.45490000 | 0.41230000  | 0.00000000 |
| 73  | 331.64270000 | 3.07100000  | 0.00000000 |
| 74  | 334.89840000 | 3.53570000  | 0.00000000 |
| 75  | 336.19750000 | 4.38770000  | 0.00000000 |
| 76  | 340.96710000 | 3.78610000  | 0.00000000 |
| 77  | 344.04260000 | 6.34450000  | 0.00000000 |
| 78  | 350.69100000 | 7.46730000  | 0.00000000 |
| 79  | 364.18790000 | 5.10110000  | 0.00000000 |
| 80  | 367.74120000 | 3.53850000  | 0.00000000 |
| 81  | 373.60160000 | 6.13980000  | 0.00000000 |
| 82  | 380.81810000 | 1.58770000  | 0.00000000 |
| 83  | 387.45240000 | 0.84660000  | 0.00000000 |
| 84  | 388.89660000 | 0.97630000  | 0.00000000 |
| 85  | 391.80920000 | 6.13530000  | 0.00000000 |
| 86  | 404.19790000 | 4.80130000  | 0.00000000 |
| 87  | 404.69340000 | 6.81920000  | 0.00000000 |
| 88  | 409.88930000 | 8.07710000  | 0.00000000 |
| 89  | 413.10670000 | 12.04740000 | 0.00000000 |
| 90  | 421.56600000 | 0.37590000  | 0.00000000 |
| 91  | 423.38060000 | 13.17750000 | 0.00000000 |
| 92  | 440.12270000 | 23.87610000 | 0.00000000 |
| 93  | 441.35210000 | 24.92910000 | 0.00000000 |
| 94  | 444.46910000 | 4.00250000  | 0.00000000 |
| 95  | 457.46160000 | 0.53410000  | 0.00000000 |
| 96  | 473.92830000 | 21.59340000 | 0.00000000 |
| 97  | 477.71500000 | 19.83160000 | 0.00000000 |
| 98  | 478.91990000 | 0.22380000  | 0.00000000 |
| 99  | 481.16010000 | 3.59370000  | 0.00000000 |
| 100 | 486.53500000 | 14.88910000 | 0.00000000 |
| 101 | 487.21890000 | 17.26020000 | 0.00000000 |
| 102 | 492.97280000 | 12.34600000 | 0.00000000 |
| 103 | 493.98770000 | 0.91260000  | 0.00000000 |
| 104 | 495.56410000 | 1.60600000  | 0.00000000 |
| 105 | 497.93600000 | 0.40530000  | 0.00000000 |
| 106 | 501.85550000 | 0.32650000  | 0.00000000 |
| 107 | 505.00280000 | 0.25830000  | 0.00000000 |
| 108 | 511.35220000 | 0.24230000  | 0.00000000 |
| 109 | 516.52280000 | 31.08800000 | 0.00000000 |
| 110 | 522.83110000 | 9.07950000  | 0.00000000 |
| 111 | 528.29300000 | 16.45050000 | 0.00000000 |
| 112 | 532.89300000 | 2.37460000  | 0.00000000 |
| 113 | 558.61640000 | 31.28660000 | 0.00000000 |
| 114 | 563.74300000 | 0.25290000  | 0.00000000 |
| 115 | 564.54480000 | 0.86160000  | 0.00000000 |
| 116 | 575.36950000 | 1.58600000  | 0.00000000 |
| 117 | 576.24580000 | 2.00790000  | 0.00000000 |
| 118 | 578.93340000 | 0.12560000  | 0.00000000 |
| 119 | 581.39610000 | 0.46250000  | 0.00000000 |
| 120 | 594.17970000 | 28.14080000 | 0.00000000 |
| 121 | 595.01400000 | 16.44180000 | 0.00000000 |
| 122 | 597.38540000 | 2.48360000  | 0.00000000 |
| 123 | 605.53310000 | 0.47540000  | 0.00000000 |
| 124 | 607.43530000 | 8.52490000  | 0.00000000 |

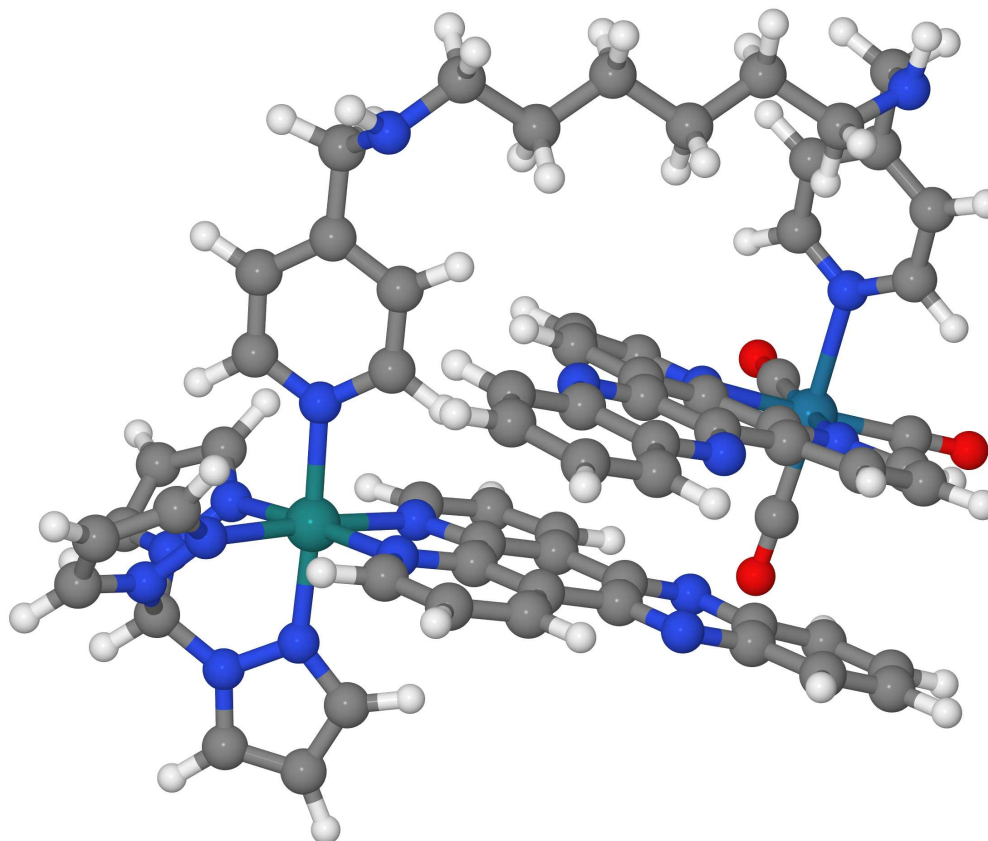
|     |              |              |            |
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| 125 | 617.27590000 | 19.44440000  | 0.00000000 |
| 126 | 618.82430000 | 6.06110000   | 0.00000000 |
| 127 | 623.09410000 | 32.63910000  | 0.00000000 |
| 128 | 623.12810000 | 50.30660000  | 0.00000000 |
| 129 | 630.86330000 | 17.94800000  | 0.00000000 |
| 130 | 633.88700000 | 32.44600000  | 0.00000000 |
| 131 | 639.56630000 | 0.84160000   | 0.00000000 |
| 132 | 650.77630000 | 72.38630000  | 0.00000000 |
| 133 | 652.04200000 | 4.18000000   | 0.00000000 |
| 134 | 653.45190000 | 0.30360000   | 0.00000000 |
| 135 | 656.26280000 | 13.79570000  | 0.00000000 |
| 136 | 658.73690000 | 0.33180000   | 0.00000000 |
| 137 | 663.68190000 | 12.99320000  | 0.00000000 |
| 138 | 665.88360000 | 1.03410000   | 0.00000000 |
| 139 | 677.27680000 | 1.93900000   | 0.00000000 |
| 140 | 683.52830000 | 0.52590000   | 0.00000000 |
| 141 | 686.03740000 | 3.25300000   | 0.00000000 |
| 142 | 686.55550000 | 0.80710000   | 0.00000000 |
| 143 | 699.36420000 | 103.31060000 | 0.00000000 |
| 144 | 724.39460000 | 28.80480000  | 0.00000000 |
| 145 | 733.78270000 | 8.48270000   | 0.00000000 |
| 146 | 737.91640000 | 67.76190000  | 0.00000000 |
| 147 | 739.46250000 | 4.31630000   | 0.00000000 |
| 148 | 740.20180000 | 5.02680000   | 0.00000000 |
| 149 | 746.97310000 | 1.23540000   | 0.00000000 |
| 150 | 747.57820000 | 0.83640000   | 0.00000000 |
| 151 | 752.31310000 | 128.10390000 | 0.00000000 |
| 152 | 756.15680000 | 24.75540000  | 0.00000000 |
| 153 | 758.18280000 | 43.86040000  | 0.00000000 |
| 154 | 759.94370000 | 67.88570000  | 0.00000000 |
| 155 | 761.04510000 | 141.24950000 | 0.00000000 |
| 156 | 761.75080000 | 24.92140000  | 0.00000000 |
| 157 | 765.31890000 | 124.12830000 | 0.00000000 |
| 158 | 767.64300000 | 10.27830000  | 0.00000000 |
| 159 | 776.90130000 | 68.43090000  | 0.00000000 |
| 160 | 780.74630000 | 94.99810000  | 0.00000000 |
| 161 | 781.37970000 | 11.59100000  | 0.00000000 |
| 162 | 782.20010000 | 18.54370000  | 0.00000000 |
| 163 | 795.90740000 | 87.05150000  | 0.00000000 |
| 164 | 799.19120000 | 9.14800000   | 0.00000000 |
| 165 | 800.67650000 | 117.22990000 | 0.00000000 |
| 166 | 805.57150000 | 31.92990000  | 0.00000000 |
| 167 | 813.44490000 | 4.82460000   | 0.00000000 |
| 168 | 815.15440000 | 1.49940000   | 0.00000000 |
| 169 | 819.45190000 | 2.02360000   | 0.00000000 |
| 170 | 827.17560000 | 3.31120000   | 0.00000000 |
| 171 | 833.70410000 | 19.70780000  | 0.00000000 |
| 172 | 835.26050000 | 75.75930000  | 0.00000000 |
| 173 | 838.24340000 | 22.06540000  | 0.00000000 |
| 174 | 840.64630000 | 78.83890000  | 0.00000000 |
| 175 | 853.56370000 | 0.10940000   | 0.00000000 |
| 176 | 864.31270000 | 0.65260000   | 0.00000000 |
| 177 | 866.20140000 | 4.90760000   | 0.00000000 |
| 178 | 868.39970000 | 17.83510000  | 0.00000000 |
| 179 | 868.94640000 | 70.62320000  | 0.00000000 |
| 180 | 869.85610000 | 9.78870000   | 0.00000000 |
| 181 | 871.42150000 | 14.91520000  | 0.00000000 |
| 182 | 874.22590000 | 29.62010000  | 0.00000000 |
| 183 | 878.75980000 | 33.26450000  | 0.00000000 |
| 184 | 884.21860000 | 2.86910000   | 0.00000000 |
| 185 | 885.15060000 | 7.33490000   | 0.00000000 |
| 186 | 890.96930000 | 0.03440000   | 0.00000000 |
| 187 | 895.32590000 | 0.64130000   | 0.00000000 |
| 188 | 899.94180000 | 0.11670000   | 0.00000000 |

|     |               |             |            |
|-----|---------------|-------------|------------|
| 189 | 911.51730000  | 27.23480000 | 0.00000000 |
| 190 | 916.93580000  | 1.81240000  | 0.00000000 |
| 191 | 918.03960000  | 2.12410000  | 0.00000000 |
| 192 | 921.27410000  | 0.49730000  | 0.00000000 |
| 193 | 924.36620000  | 3.27700000  | 0.00000000 |
| 194 | 924.81220000  | 3.28980000  | 0.00000000 |
| 195 | 938.17570000  | 23.86820000 | 0.00000000 |
| 196 | 946.74360000  | 0.08380000  | 0.00000000 |
| 197 | 947.89230000  | 0.09650000  | 0.00000000 |
| 198 | 953.56550000  | 0.45990000  | 0.00000000 |
| 199 | 965.17740000  | 6.07670000  | 0.00000000 |
| 200 | 975.80290000  | 1.37530000  | 0.00000000 |
| 201 | 978.89020000  | 1.23260000  | 0.00000000 |
| 202 | 982.49570000  | 7.61050000  | 0.00000000 |
| 203 | 989.82910000  | 1.29830000  | 0.00000000 |
| 204 | 991.34880000  | 1.63060000  | 0.00000000 |
| 205 | 993.16660000  | 1.43480000  | 0.00000000 |
| 206 | 993.85130000  | 0.81810000  | 0.00000000 |
| 207 | 995.32250000  | 1.71430000  | 0.00000000 |
| 208 | 998.25470000  | 1.38960000  | 0.00000000 |
| 209 | 1000.84600000 | 2.38040000  | 0.00000000 |
| 210 | 1003.67300000 | 1.26790000  | 0.00000000 |
| 211 | 1006.90180000 | 0.81370000  | 0.00000000 |
| 212 | 1009.80550000 | 13.63350000 | 0.00000000 |
| 213 | 1010.10480000 | 8.87960000  | 0.00000000 |
| 214 | 1011.55840000 | 0.76470000  | 0.00000000 |
| 215 | 1013.80110000 | 3.07340000  | 0.00000000 |
| 216 | 1013.83410000 | 26.09700000 | 0.00000000 |
| 217 | 1019.48800000 | 2.01500000  | 0.00000000 |
| 218 | 1021.31950000 | 1.04890000  | 0.00000000 |
| 219 | 1021.37380000 | 0.02430000  | 0.00000000 |
| 220 | 1023.00100000 | 15.43510000 | 0.00000000 |
| 221 | 1024.21360000 | 1.06820000  | 0.00000000 |
| 222 | 1026.54300000 | 0.72260000  | 0.00000000 |
| 223 | 1029.66660000 | 4.63430000  | 0.00000000 |
| 224 | 1030.83920000 | 0.80880000  | 0.00000000 |
| 225 | 1033.17350000 | 0.68900000  | 0.00000000 |
| 226 | 1034.24770000 | 3.21590000  | 0.00000000 |
| 227 | 1048.05380000 | 0.32810000  | 0.00000000 |
| 228 | 1057.46110000 | 0.09960000  | 0.00000000 |
| 229 | 1060.28300000 | 55.91210000 | 0.00000000 |
| 230 | 1066.04810000 | 9.28870000  | 0.00000000 |
| 231 | 1070.17770000 | 0.19270000  | 0.00000000 |
| 232 | 1071.80510000 | 4.15990000  | 0.00000000 |
| 233 | 1072.25650000 | 43.85830000 | 0.00000000 |
| 234 | 1072.57330000 | 7.42300000  | 0.00000000 |
| 235 | 1075.66630000 | 48.16910000 | 0.00000000 |
| 236 | 1076.89600000 | 10.98330000 | 0.00000000 |
| 237 | 1086.80790000 | 16.52580000 | 0.00000000 |
| 238 | 1090.11890000 | 5.46200000  | 0.00000000 |
| 239 | 1092.88340000 | 5.64250000  | 0.00000000 |
| 240 | 1104.08580000 | 5.29940000  | 0.00000000 |
| 241 | 1105.79060000 | 40.27680000 | 0.00000000 |
| 242 | 1109.70650000 | 9.23880000  | 0.00000000 |
| 243 | 1117.40150000 | 20.94550000 | 0.00000000 |
| 244 | 1120.43870000 | 50.87380000 | 0.00000000 |
| 245 | 1122.73420000 | 6.55570000  | 0.00000000 |
| 246 | 1122.82500000 | 93.23190000 | 0.00000000 |
| 247 | 1123.46570000 | 52.26200000 | 0.00000000 |
| 248 | 1128.05280000 | 56.87440000 | 0.00000000 |
| 249 | 1134.17080000 | 56.08580000 | 0.00000000 |
| 250 | 1135.50440000 | 4.14840000  | 0.00000000 |
| 251 | 1138.80610000 | 39.05970000 | 0.00000000 |
| 252 | 1143.86060000 | 30.49330000 | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1149.89760000 | 36.68880000  | 0.00000000 |
| 254 | 1152.47740000 | 1.51940000   | 0.00000000 |
| 255 | 1154.00430000 | 4.76450000   | 0.00000000 |
| 256 | 1159.83300000 | 15.01690000  | 0.00000000 |
| 257 | 1162.17470000 | 22.41610000  | 0.00000000 |
| 258 | 1167.96000000 | 7.67210000   | 0.00000000 |
| 259 | 1174.20710000 | 2.09390000   | 0.00000000 |
| 260 | 1177.05330000 | 1.92350000   | 0.00000000 |
| 261 | 1196.67520000 | 6.24750000   | 0.00000000 |
| 262 | 1212.45520000 | 2.47080000   | 0.00000000 |
| 263 | 1213.87040000 | 1.50980000   | 0.00000000 |
| 264 | 1215.03360000 | 0.96360000   | 0.00000000 |
| 265 | 1215.09310000 | 1.47990000   | 0.00000000 |
| 266 | 1228.55840000 | 16.22830000  | 0.00000000 |
| 267 | 1230.24250000 | 1.36490000   | 0.00000000 |
| 268 | 1237.39520000 | 2.18760000   | 0.00000000 |
| 269 | 1239.01340000 | 0.05440000   | 0.00000000 |
| 270 | 1245.12420000 | 1.62570000   | 0.00000000 |
| 271 | 1248.72020000 | 9.29540000   | 0.00000000 |
| 272 | 1254.86830000 | 2.15410000   | 0.00000000 |
| 273 | 1257.19560000 | 55.78090000  | 0.00000000 |
| 274 | 1258.11780000 | 5.88130000   | 0.00000000 |
| 275 | 1264.01910000 | 2.25520000   | 0.00000000 |
| 276 | 1264.58900000 | 1.51200000   | 0.00000000 |
| 277 | 1268.70760000 | 0.39680000   | 0.00000000 |
| 278 | 1269.25480000 | 91.04150000  | 0.00000000 |
| 279 | 1273.40200000 | 4.02070000   | 0.00000000 |
| 280 | 1274.68810000 | 13.73060000  | 0.00000000 |
| 281 | 1275.51930000 | 104.83810000 | 0.00000000 |
| 282 | 1280.07030000 | 10.40810000  | 0.00000000 |
| 283 | 1295.99690000 | 1.89240000   | 0.00000000 |
| 284 | 1302.34690000 | 1.14590000   | 0.00000000 |
| 285 | 1304.53400000 | 0.78600000   | 0.00000000 |
| 286 | 1305.44930000 | 0.70230000   | 0.00000000 |
| 287 | 1307.60650000 | 11.67820000  | 0.00000000 |
| 288 | 1310.84160000 | 11.77780000  | 0.00000000 |
| 289 | 1316.26000000 | 33.81020000  | 0.00000000 |
| 290 | 1319.64160000 | 7.31230000   | 0.00000000 |
| 291 | 1320.99870000 | 67.88980000  | 0.00000000 |
| 292 | 1324.22930000 | 107.97530000 | 0.00000000 |
| 293 | 1326.09890000 | 8.29470000   | 0.00000000 |
| 294 | 1328.63000000 | 0.94430000   | 0.00000000 |
| 295 | 1331.12270000 | 1.11100000   | 0.00000000 |
| 296 | 1333.80970000 | 0.32630000   | 0.00000000 |
| 297 | 1334.86690000 | 8.91200000   | 0.00000000 |
| 298 | 1340.15290000 | 4.84130000   | 0.00000000 |
| 299 | 1347.09370000 | 10.18930000  | 0.00000000 |
| 300 | 1347.90110000 | 4.98420000   | 0.00000000 |
| 301 | 1358.12420000 | 28.09370000  | 0.00000000 |
| 302 | 1361.59090000 | 13.82250000  | 0.00000000 |
| 303 | 1366.71650000 | 2.73930000   | 0.00000000 |
| 304 | 1371.25870000 | 181.75870000 | 0.00000000 |
| 305 | 1372.69920000 | 16.39340000  | 0.00000000 |
| 306 | 1373.50870000 | 48.49210000  | 0.00000000 |
| 307 | 1375.78570000 | 1.30840000   | 0.00000000 |
| 308 | 1378.14240000 | 69.43820000  | 0.00000000 |
| 309 | 1378.33020000 | 18.89790000  | 0.00000000 |
| 310 | 1379.78590000 | 34.64420000  | 0.00000000 |
| 311 | 1387.70960000 | 24.88770000  | 0.00000000 |
| 312 | 1394.89970000 | 7.95510000   | 0.00000000 |
| 313 | 1399.04560000 | 8.69280000   | 0.00000000 |
| 314 | 1403.94220000 | 12.32910000  | 0.00000000 |
| 315 | 1411.43550000 | 4.75360000   | 0.00000000 |
| 316 | 1414.18850000 | 14.72460000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1417.62740000 | 5.97620000    | 0.00000000 |
| 318 | 1427.05270000 | 4.24190000    | 0.00000000 |
| 319 | 1430.18070000 | 11.10670000   | 0.00000000 |
| 320 | 1436.54530000 | 64.27380000   | 0.00000000 |
| 321 | 1437.73940000 | 58.27890000   | 0.00000000 |
| 322 | 1443.88380000 | 158.66010000  | 0.00000000 |
| 323 | 1451.49800000 | 86.90350000   | 0.00000000 |
| 324 | 1454.13950000 | 90.64970000   | 0.00000000 |
| 325 | 1460.71750000 | 52.80130000   | 0.00000000 |
| 326 | 1461.71590000 | 92.29330000   | 0.00000000 |
| 327 | 1468.45610000 | 23.48150000   | 0.00000000 |
| 328 | 1469.76880000 | 20.19580000   | 0.00000000 |
| 329 | 1471.89230000 | 25.29210000   | 0.00000000 |
| 330 | 1473.39800000 | 55.08350000   | 0.00000000 |
| 331 | 1474.93020000 | 0.92020000    | 0.00000000 |
| 332 | 1475.25500000 | 82.04780000   | 0.00000000 |
| 333 | 1480.47980000 | 1.73260000    | 0.00000000 |
| 334 | 1485.49970000 | 1.75240000    | 0.00000000 |
| 335 | 1491.52460000 | 0.29890000    | 0.00000000 |
| 336 | 1492.00290000 | 5.67460000    | 0.00000000 |
| 337 | 1493.17230000 | 7.27720000    | 0.00000000 |
| 338 | 1494.15450000 | 23.88430000   | 0.00000000 |
| 339 | 1500.30700000 | 11.00730000   | 0.00000000 |
| 340 | 1501.59910000 | 4.40670000    | 0.00000000 |
| 341 | 1501.98930000 | 8.06810000    | 0.00000000 |
| 342 | 1503.15950000 | 7.12030000    | 0.00000000 |
| 343 | 1503.48030000 | 4.68920000    | 0.00000000 |
| 344 | 1505.83450000 | 8.65570000    | 0.00000000 |
| 345 | 1513.06980000 | 20.69470000   | 0.00000000 |
| 346 | 1521.98650000 | 28.03140000   | 0.00000000 |
| 347 | 1523.90630000 | 22.67770000   | 0.00000000 |
| 348 | 1525.88790000 | 7.02760000    | 0.00000000 |
| 349 | 1526.05050000 | 77.12720000   | 0.00000000 |
| 350 | 1532.26580000 | 123.78620000  | 0.00000000 |
| 351 | 1537.76850000 | 35.51860000   | 0.00000000 |
| 352 | 1551.06130000 | 10.10260000   | 0.00000000 |
| 353 | 1553.41030000 | 14.02380000   | 0.00000000 |
| 354 | 1557.18110000 | 12.29730000   | 0.00000000 |
| 355 | 1575.54300000 | 3.88660000    | 0.00000000 |
| 356 | 1576.68250000 | 4.27190000    | 0.00000000 |
| 357 | 1579.75100000 | 27.57400000   | 0.00000000 |
| 358 | 1582.38340000 | 4.87420000    | 0.00000000 |
| 359 | 1598.92270000 | 7.08250000    | 0.00000000 |
| 360 | 1602.47820000 | 4.02710000    | 0.00000000 |
| 361 | 1609.52050000 | 3.38840000    | 0.00000000 |
| 362 | 1613.56880000 | 15.50800000   | 0.00000000 |
| 363 | 1619.20170000 | 3.00420000    | 0.00000000 |
| 364 | 1622.83180000 | 1.84390000    | 0.00000000 |
| 365 | 1623.23510000 | 3.60500000    | 0.00000000 |
| 366 | 1626.53670000 | 9.75610000    | 0.00000000 |
| 367 | 1635.04120000 | 0.33330000    | 0.00000000 |
| 368 | 1639.33100000 | 4.61860000    | 0.00000000 |
| 369 | 1654.23080000 | 87.11780000   | 0.00000000 |
| 370 | 1659.26290000 | 2.44890000    | 0.00000000 |
| 371 | 1661.25260000 | 3.85040000    | 0.00000000 |
| 372 | 1664.68170000 | 45.50050000   | 0.00000000 |
| 373 | 1899.99750000 | 57.47870000   | 0.00000000 |
| 374 | 1963.62040000 | 2418.98210000 | 0.00000000 |
| 375 | 1964.97540000 | 2258.92290000 | 0.00000000 |
| 376 | 2084.81170000 | 1897.60860000 | 0.00000000 |
| 377 | 2938.70900000 | 147.92670000  | 0.00000000 |
| 378 | 2982.25240000 | 92.30830000   | 0.00000000 |
| 379 | 2996.16480000 | 8.61150000    | 0.00000000 |
| 380 | 3002.86780000 | 24.52950000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 3007.18420000 | 47.44960000  | 0.00000000 |
| 382 | 3011.29470000 | 29.23300000  | 0.00000000 |
| 383 | 3014.64760000 | 150.99090000 | 0.00000000 |
| 384 | 3016.78730000 | 8.65810000   | 0.00000000 |
| 385 | 3024.28560000 | 99.71440000  | 0.00000000 |
| 386 | 3033.14900000 | 33.00090000  | 0.00000000 |
| 387 | 3045.65600000 | 4.01910000   | 0.00000000 |
| 388 | 3051.36660000 | 33.45350000  | 0.00000000 |
| 389 | 3056.45160000 | 25.89340000  | 0.00000000 |
| 390 | 3061.20990000 | 56.98140000  | 0.00000000 |
| 391 | 3066.21530000 | 1.31120000   | 0.00000000 |
| 392 | 3067.74030000 | 327.13810000 | 0.00000000 |
| 393 | 3181.16070000 | 1.27290000   | 0.00000000 |
| 394 | 3186.91660000 | 2.25650000   | 0.00000000 |
| 395 | 3187.26990000 | 2.65260000   | 0.00000000 |
| 396 | 3191.42760000 | 8.51730000   | 0.00000000 |
| 397 | 3196.16310000 | 1.66800000   | 0.00000000 |
| 398 | 3196.54370000 | 6.94040000   | 0.00000000 |
| 399 | 3197.18100000 | 8.21040000   | 0.00000000 |
| 400 | 3206.56690000 | 18.84410000  | 0.00000000 |
| 401 | 3207.19160000 | 24.12420000  | 0.00000000 |
| 402 | 3208.29500000 | 0.99240000   | 0.00000000 |
| 403 | 3213.44150000 | 1.20910000   | 0.00000000 |
| 404 | 3214.52760000 | 17.73540000  | 0.00000000 |
| 405 | 3214.66500000 | 8.67710000   | 0.00000000 |
| 406 | 3215.31010000 | 0.77470000   | 0.00000000 |
| 407 | 3215.85400000 | 3.41410000   | 0.00000000 |
| 408 | 3217.99960000 | 1.83480000   | 0.00000000 |
| 409 | 3222.44360000 | 6.46620000   | 0.00000000 |
| 410 | 3222.66510000 | 10.44440000  | 0.00000000 |
| 411 | 3224.88830000 | 3.99680000   | 0.00000000 |
| 412 | 3226.72510000 | 6.30200000   | 0.00000000 |
| 413 | 3227.34490000 | 4.61070000   | 0.00000000 |
| 414 | 3227.51340000 | 2.12780000   | 0.00000000 |
| 415 | 3230.88010000 | 9.65580000   | 0.00000000 |
| 416 | 3234.01910000 | 1.86990000   | 0.00000000 |
| 417 | 3239.00780000 | 5.92210000   | 0.00000000 |
| 418 | 3242.87610000 | 6.28690000   | 0.00000000 |
| 419 | 3251.44660000 | 7.86100000   | 0.00000000 |
| 420 | 3256.97360000 | 21.59010000  | 0.00000000 |
| 421 | 3258.96770000 | 1.22880000   | 0.00000000 |
| 422 | 3260.14010000 | 0.82920000   | 0.00000000 |
| 423 | 3262.74100000 | 0.94670000   | 0.00000000 |
| 424 | 3263.80590000 | 0.31900000   | 0.00000000 |
| 425 | 3269.09690000 | 4.46660000   | 0.00000000 |
| 426 | 3269.52570000 | 9.26740000   | 0.00000000 |
| 427 | 3272.34950000 | 6.78820000   | 0.00000000 |
| 428 | 3284.37170000 | 3.74660000   | 0.00000000 |
| 429 | 3284.54420000 | 4.34070000   | 0.00000000 |
| 430 | 3285.73590000 | 3.90830000   | 0.00000000 |
| 431 | 3527.04100000 | 1.18110000   | 0.00000000 |
| 432 | 3570.33320000 | 6.72820000   | 0.00000000 |

S6. CALCULATIONS ON  $2^{3+}$  ( $^3A$ )

|                                 |   |      |
|---------------------------------|---|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular   |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](c6[Re]578(n9ccc[n+](c9C([n+]<br>1n7ccc1)[n+](c1n8ccc1)[n+](c1ccc(cc1)CNC(CCCCNCc1cc[n+](c1cc1)[Re]<br>1([n+](c2ccc3c2c2[n+](c1ccc2c1c3nc2cccc2n1)([C]([O])([C]([O])([C]([O]) |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>   |      |
| Charge                          | : 3   |      |
| Multiplicity                    | : 3   |      |
| Energy                          | : -3972.52740052  | a.u. |
| Gibbs Energy                    | : -3971.49286700  | a.u. |
| Number of imaginary frequencies | : 1   |      |

## S6.1. Cartesian Co-ordinates (XYZ format)

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|   |            |            |             |
|---|------------|------------|-------------|
| C | 4.93306780 | 4.70662308 | 0.70535702  |
| H | 4.84602499 | 4.84579611 | 1.78708398  |
| H | 4.65414286 | 3.66581202 | 0.51004702  |
| C | 3.93924308 | 5.63392591 | -0.00592200 |
| H | 4.14510202 | 5.65516376 | -1.08104205 |
| H | 4.07836008 | 6.65893412 | 0.35799399  |
| C | 2.48993897 | 5.19139624 | 0.20542701  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 2.30608392  | 5.02011490  | 1.27347803  |
| H  | 2.33981299  | 4.22223377  | -0.28725201 |
| C  | 1.46211898  | 6.19643116  | -0.31977600 |
| H  | 1.71859097  | 6.48324919  | -1.34669101 |
| H  | 1.52025104  | 7.11326313  | 0.27946100  |
| C  | -1.03290701 | 6.70258713  | -0.56375802 |
| H  | -0.82540798 | 7.19645786  | -1.52681994 |
| H  | -0.97201198 | 7.47478724  | 0.20775500  |
| N  | 6.35084295  | 4.85836792  | 0.35465699  |
| C  | -2.86905289 | 5.50343323  | -1.74030101 |
| H  | -2.06421208 | 5.46103477  | -2.48430490 |
| H  | -3.68490005 | 6.06584883  | -2.20279503 |
| N  | -2.38905096 | 6.14434814  | -0.51719302 |
| C  | 6.67159224  | 4.53843498  | -1.03828299 |
| H  | 6.13023901  | 5.14119720  | -1.78003705 |
| H  | 7.73822594  | 4.73040485  | -1.18830204 |
| C  | -7.40154886 | -1.78334796 | -1.27629399 |
| N  | -6.74856997 | -1.36889100 | -2.50077391 |
| N  | -6.58852386 | -2.75498796 | -0.57217002 |
| N  | -7.66085577 | -0.63127798 | -0.43964100 |
| N  | -5.54746819 | -0.73413002 | -2.43776798 |
| C  | -7.19249201 | -1.44737196 | -3.78052497 |
| N  | -5.34131813 | -2.40714788 | -0.14801501 |
| C  | -6.86484480 | -4.03852177 | -0.24884500 |
| N  | -6.62000322 | 0.12977600  | -0.00883100 |
| C  | -8.84796429 | -0.09225400 | -0.06208400 |
| Ru | -4.67897892 | -0.49203199 | -0.53153902 |
| C  | -5.23339081 | -0.41158599 | -3.69447207 |
| C  | -6.23958015 | -0.84209698 | -4.57203484 |
| H  | -8.12962818 | -1.92200994 | -4.01836300 |
| C  | -4.83229208 | -3.49084806 | 0.45186201  |
| C  | -5.75529099 | -4.53858614 | 0.41088799  |
| H  | -7.80826378 | -4.49172688 | -0.50445300 |
| C  | -7.15833521 | 1.15622497  | 0.65209299  |
| C  | -8.55817413 | 1.05584800  | 0.64445698  |
| H  | -9.78227139 | -0.56313002 | -0.31866699 |
| N  | -2.78308201 | -1.23439598 | -0.96354598 |
| N  | -3.81167412 | -0.43326601 | 1.36240399  |
| H  | -4.32192612 | 0.11953000  | -3.91359997 |
| H  | -6.26415205 | -0.72565198 | -5.64135218 |
| H  | -3.84282899 | -3.46353698 | 0.87668699  |
| H  | -5.63462496 | -5.53097916 | 0.80868602  |
| H  | -6.52937508 | 1.91584694  | 1.08635402  |
| H  | -9.26147842 | 1.73272204  | 1.09705997  |
| C  | -2.32497692 | -1.65200698 | -2.14222002 |
| C  | -1.99579406 | -1.38237906 | 0.15430500  |
| C  | -2.54061508 | -0.95998001 | 1.38746095  |
| C  | -4.38077784 | -0.05692200 | 2.50842690  |
| C  | -1.06084895 | -2.23165894 | -2.28386211 |
| H  | -2.98146105 | -1.53922796 | -2.99111891 |
| C  | -0.72092402 | -1.99276400 | 0.08816500  |
| C  | -1.82693601 | -1.12548900 | 2.59703588  |
| C  | -3.72440600 | -0.17129000 | 3.73452091  |
| H  | -5.38577080 | 0.33263701  | 2.44979596  |
| C  | -0.26692799 | -2.41682696 | -1.16510606 |
| H  | -0.73300201 | -2.54567599 | -3.26448894 |
| C  | 0.03086700  | -2.20643592 | 1.31232798  |
| C  | -2.44784403 | -0.71266001 | 3.77865410  |
| C  | -0.51245201 | -1.75829506 | 2.56774402  |
| H  | -4.22610188 | 0.15766200  | 4.63284588  |
| H  | 0.70323998  | -2.88953495 | -1.23430598 |
| N  | 1.19215405  | -2.84937906 | 1.24173498  |
| H  | -1.91834199 | -0.82944399 | 4.71356678  |
| N  | 0.14050101  | -1.92998898 | 3.70852089  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.85283899  | -3.06813598 | 2.40938807  |
| C  | 1.33577204  | -2.57740903 | 3.65266991  |
| C  | 3.06592798  | -3.79158711 | 2.40429497  |
| C  | 2.07588196  | -2.78729010 | 4.83693218  |
| C  | 3.75741792  | -3.99428797 | 3.57905889  |
| H  | 3.43185091  | -4.16897583 | 1.45851898  |
| C  | 3.26686001  | -3.48033595 | 4.79829216  |
| H  | 1.67624497  | -2.39322805 | 5.76322889  |
| H  | 4.69141579  | -4.54274511 | 3.56737590  |
| H  | 3.83069301  | -3.63768911 | 5.70965719  |
| N  | 4.37877703  | -1.18230999 | 0.61040199  |
| N  | 2.80783606  | -0.59996003 | -1.53568494 |
| C  | 5.17942476  | -1.44943905 | 1.64322305  |
| C  | 3.25050306  | -0.44517201 | 0.82076597  |
| C  | 2.42130804  | -0.13391900 | -0.31408101 |
| C  | 2.07818508  | -0.29972199 | -2.61151195 |
| C  | 4.91963720  | -0.99115199 | 2.93578792  |
| H  | 6.05263519  | -2.05249095 | 1.43618500  |
| C  | 2.89759493  | 0.00521000  | 2.10530710  |
| C  | 1.25475800  | 0.64421898  | -0.15987000 |
| C  | 0.93829203  | 0.50354600  | -2.54169297 |
| H  | 2.41198993  | -0.70987099 | -3.55432010 |
| C  | 3.76590896  | -0.27163801 | 3.17033005  |
| H  | 5.60812283  | -1.23141694 | 3.73295999  |
| C  | 1.63962495  | 0.71379602  | 2.30279207  |
| C  | 0.53075498  | 0.97974598  | -1.31280994 |
| C  | 0.83030403  | 1.05522597  | 1.17047405  |
| H  | 0.39151499  | 0.73289800  | -3.44532704 |
| H  | 3.50319290  | 0.07516900  | 4.15947580  |
| N  | 1.25995004  | 0.99581599  | 3.54099393  |
| H  | -0.34707001 | 1.60028100  | -1.22132397 |
| N  | -0.31288499 | 1.72153699  | 1.30867100  |
| C  | 0.07230500  | 1.62330794  | 3.70257211  |
| C  | -0.71326202 | 2.02106404  | 2.57044792  |
| C  | -0.40794799 | 1.88457096  | 5.00875902  |
| C  | -1.93005395 | 2.71100497  | 2.78983498  |
| C  | -1.61015606 | 2.52551699  | 5.18712282  |
| H  | 0.19674399  | 1.55913699  | 5.84592199  |
| C  | -2.36970711 | 2.94815612  | 4.07034492  |
| H  | -2.51034999 | 3.03387308  | 1.93778503  |
| H  | -1.98065901 | 2.71572590  | 6.18680906  |
| H  | -3.30939102 | 3.46243906  | 4.22959805  |
| H  | -8.34875774 | -2.24772692 | -1.52843797 |
| C  | 6.38840294  | 3.07904696  | -1.29853201 |
| C  | 5.54270887  | 2.66367006  | -2.32385898 |
| C  | 6.91908979  | 2.09509397  | -0.46147099 |
| C  | 5.21463394  | 1.32169604  | -2.44074392 |
| H  | 5.10558319  | 3.37867403  | -3.00898194 |
| C  | 6.55198908  | 0.77600598  | -0.64165699 |
| H  | 7.57903099  | 2.36576390  | 0.35140499  |
| N  | 5.68554020  | 0.38763401  | -1.59843397 |
| H  | 4.53399277  | 0.98571002  | -3.21043611 |
| H  | 6.93580723  | 0.00197700  | 0.00726900  |
| C  | -3.32436299 | 4.08579206  | -1.47977197 |
| C  | -2.52639389 | 3.22208691  | -0.72576600 |
| C  | -4.53696299 | 3.58373809  | -1.95799005 |
| C  | -2.93283796 | 1.92932904  | -0.49790001 |
| H  | -1.59192204 | 3.55086994  | -0.29874301 |
| C  | -4.90459013 | 2.28187108  | -1.67273903 |
| H  | -5.20839691 | 4.20394182  | -2.53745699 |
| N  | -4.11140585 | 1.45435500  | -0.95591497 |
| H  | -2.30906296 | 1.26340997  | 0.07566400  |
| H  | -5.84781981 | 1.87883699  | -2.00904202 |
| Re | 4.76043081  | -1.78979599 | -1.55486798 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.85857701  | -3.49015093 | -1.40047503 |
| O | 3.31044507  | -4.50147200 | -1.31018901 |
| C | 4.93013811  | -2.03096509 | -3.46852493 |
| O | 5.01294899  | -2.14860797 | -4.61346388 |
| C | 6.47805691  | -2.64706898 | -1.30853701 |
| O | 7.50331497  | -3.14690495 | -1.13395905 |
| H | -3.05028105 | 6.84892321  | -0.22168200 |
| C | 0.03608500  | 5.64644623  | -0.28598499 |
| H | -0.16882700 | 5.20216894  | 0.69476497  |
| H | -0.04178000 | 4.83633614  | -1.02045000 |
| H | 6.66398716  | 5.80086994  | 0.56184298  |

## S6.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -5.11250000  | 2.31290000   | 0.00000000      |
| 2    | 9.96410000   | 0.08480000   | 0.00000000      |
| 3    | 15.01730000  | 2.42340000   | 0.00000000      |
| 4    | 18.00920000  | 0.04440000   | 0.00000000      |
| 5    | 21.40940000  | 0.65410000   | 0.00000000      |
| 6    | 28.40340000  | 0.93860000   | 0.00000000      |
| 7    | 31.86400000  | 0.16690000   | 0.00000000      |
| 8    | 36.45820000  | 0.18800000   | 0.00000000      |
| 9    | 39.33610000  | 7.35000000   | 0.00000000      |
| 10   | 42.18780000  | 0.19310000   | 0.00000000      |
| 11   | 43.61690000  | 0.19840000   | 0.00000000      |
| 12   | 46.89690000  | 0.18870000   | 0.00000000      |
| 13   | 51.61920000  | 0.96700000   | 0.00000000      |
| 14   | 55.90720000  | 2.07930000   | 0.00000000      |
| 15   | 60.35240000  | 1.74720000   | 0.00000000      |
| 16   | 62.34240000  | 2.64210000   | 0.00000000      |
| 17   | 65.48490000  | 1.32710000   | 0.00000000      |
| 18   | 68.12460000  | 0.73750000   | 0.00000000      |
| 19   | 69.14710000  | 0.11070000   | 0.00000000      |
| 20   | 69.66390000  | 0.51410000   | 0.00000000      |
| 21   | 78.38200000  | 0.81020000   | 0.00000000      |
| 22   | 81.42110000  | 2.40130000   | 0.00000000      |
| 23   | 82.37670000  | 11.95860000  | 0.00000000      |
| 24   | 84.30610000  | 0.39230000   | 0.00000000      |
| 25   | 89.84700000  | 0.02950000   | 0.00000000      |
| 26   | 92.59490000  | 0.41810000   | 0.00000000      |
| 27   | 93.47710000  | 0.60880000   | 0.00000000      |
| 28   | 101.05800000 | 0.56220000   | 0.00000000      |
| 29   | 105.30860000 | 1.92900000   | 0.00000000      |
| 30   | 105.37840000 | 2.47760000   | 0.00000000      |
| 31   | 109.23410000 | 2.13560000   | 0.00000000      |
| 32   | 114.85710000 | 1.18660000   | 0.00000000      |
| 33   | 116.49370000 | 5.44310000   | 0.00000000      |
| 34   | 119.44350000 | 18.14450000  | 0.00000000      |
| 35   | 122.95540000 | 4.09600000   | 0.00000000      |
| 36   | 127.88300000 | 1.20930000   | 0.00000000      |
| 37   | 135.10550000 | 1.90650000   | 0.00000000      |
| 38   | 136.53920000 | 0.69100000   | 0.00000000      |
| 39   | 141.03260000 | 0.10000000   | 0.00000000      |
| 40   | 145.53820000 | 2.07130000   | 0.00000000      |
| 41   | 147.32320000 | 1.05660000   | 0.00000000      |
| 42   | 153.16540000 | 4.87700000   | 0.00000000      |
| 43   | 157.79200000 | 0.54790000   | 0.00000000      |
| 44   | 164.47130000 | 1.07030000   | 0.00000000      |
| 45   | 165.96790000 | 0.65170000   | 0.00000000      |
| 46   | 176.00800000 | 2.13380000   | 0.00000000      |
| 47   | 176.65290000 | 1.68240000   | 0.00000000      |
| 48   | 180.59240000 | 3.40440000   | 0.00000000      |
| 49   | 183.47250000 | 24.60310000  | 0.00000000      |
| 50   | 187.26990000 | 2.31390000   | 0.00000000      |
| 51   | 188.35410000 | 1.72850000   | 0.00000000      |
| 52   | 191.55790000 | 1.60930000   | 0.00000000      |
| 53   | 196.45360000 | 0.67750000   | 0.00000000      |
| 54   | 198.32150000 | 6.99120000   | 0.00000000      |
| 55   | 200.14030000 | 7.79710000   | 0.00000000      |
| 56   | 205.11010000 | 7.16200000   | 0.00000000      |
| 57   | 209.24480000 | 4.05670000   | 0.00000000      |
| 58   | 222.53430000 | 20.88270000  | 0.00000000      |
| 59   | 231.19130000 | 2.83270000   | 0.00000000      |
| 60   | 240.13020000 | 30.22230000  | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 242.21640000 | 6.44790000   | 0.00000000 |
| 62  | 249.05400000 | 4.31820000   | 0.00000000 |
| 63  | 251.57350000 | 1.15920000   | 0.00000000 |
| 64  | 256.87220000 | 3.60990000   | 0.00000000 |
| 65  | 275.36580000 | 4.17620000   | 0.00000000 |
| 66  | 277.73160000 | 28.74200000  | 0.00000000 |
| 67  | 288.39640000 | 17.36370000  | 0.00000000 |
| 68  | 296.45530000 | 69.37070000  | 0.00000000 |
| 69  | 308.63080000 | 6.58310000   | 0.00000000 |
| 70  | 321.48730000 | 16.05330000  | 0.00000000 |
| 71  | 324.79580000 | 2.37990000   | 0.00000000 |
| 72  | 327.42200000 | 13.50050000  | 0.00000000 |
| 73  | 330.35090000 | 12.64920000  | 0.00000000 |
| 74  | 332.48660000 | 3.73300000   | 0.00000000 |
| 75  | 334.71340000 | 1.12070000   | 0.00000000 |
| 76  | 336.23370000 | 34.01970000  | 0.00000000 |
| 77  | 338.93630000 | 6.38430000   | 0.00000000 |
| 78  | 349.38230000 | 3.58460000   | 0.00000000 |
| 79  | 359.84450000 | 3.13570000   | 0.00000000 |
| 80  | 369.95140000 | 1.25490000   | 0.00000000 |
| 81  | 374.12070000 | 22.22190000  | 0.00000000 |
| 82  | 378.08130000 | 74.13860000  | 0.00000000 |
| 83  | 386.79610000 | 0.47860000   | 0.00000000 |
| 84  | 389.57970000 | 8.20060000   | 0.00000000 |
| 85  | 391.12210000 | 5.99840000   | 0.00000000 |
| 86  | 399.20960000 | 18.30740000  | 0.00000000 |
| 87  | 401.55370000 | 22.09050000  | 0.00000000 |
| 88  | 406.34220000 | 8.98930000   | 0.00000000 |
| 89  | 414.19160000 | 68.65650000  | 0.00000000 |
| 90  | 416.30480000 | 29.21090000  | 0.00000000 |
| 91  | 422.37850000 | 15.39230000  | 0.00000000 |
| 92  | 425.99630000 | 3.91820000   | 0.00000000 |
| 93  | 435.73090000 | 18.91800000  | 0.00000000 |
| 94  | 444.59830000 | 67.58060000  | 0.00000000 |
| 95  | 453.25530000 | 6.90620000   | 0.00000000 |
| 96  | 461.52440000 | 8.60720000   | 0.00000000 |
| 97  | 474.18390000 | 17.65950000  | 0.00000000 |
| 98  | 476.51580000 | 29.42400000  | 0.00000000 |
| 99  | 481.26640000 | 10.08020000  | 0.00000000 |
| 100 | 486.88210000 | 29.91620000  | 0.00000000 |
| 101 | 487.56530000 | 15.98450000  | 0.00000000 |
| 102 | 492.49610000 | 13.15640000  | 0.00000000 |
| 103 | 494.20140000 | 2.04570000   | 0.00000000 |
| 104 | 495.05910000 | 0.98070000   | 0.00000000 |
| 105 | 496.25530000 | 3.38750000   | 0.00000000 |
| 106 | 501.94510000 | 0.22750000   | 0.00000000 |
| 107 | 502.18100000 | 2.67570000   | 0.00000000 |
| 108 | 512.55600000 | 0.81800000   | 0.00000000 |
| 109 | 516.58280000 | 22.73400000  | 0.00000000 |
| 110 | 523.78790000 | 11.27550000  | 0.00000000 |
| 111 | 528.80000000 | 13.71500000  | 0.00000000 |
| 112 | 529.98600000 | 7.34650000   | 0.00000000 |
| 113 | 547.47210000 | 2.67170000   | 0.00000000 |
| 114 | 555.85950000 | 31.48810000  | 0.00000000 |
| 115 | 558.95240000 | 21.79980000  | 0.00000000 |
| 116 | 571.93910000 | 3.63560000   | 0.00000000 |
| 117 | 575.22360000 | 2.07350000   | 0.00000000 |
| 118 | 576.29890000 | 2.46700000   | 0.00000000 |
| 119 | 577.33480000 | 7.55090000   | 0.00000000 |
| 120 | 592.02130000 | 114.13080000 | 0.00000000 |
| 121 | 592.79320000 | 97.66040000  | 0.00000000 |
| 122 | 593.75080000 | 172.66710000 | 0.00000000 |
| 123 | 596.95990000 | 16.55620000  | 0.00000000 |
| 124 | 600.14280000 | 0.26430000   | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 609.43920000 | 30.65830000  | 0.00000000 |
| 126 | 617.00450000 | 17.52710000  | 0.00000000 |
| 127 | 617.40950000 | 100.16440000 | 0.00000000 |
| 128 | 621.56980000 | 72.75420000  | 0.00000000 |
| 129 | 626.53650000 | 168.34900000 | 0.00000000 |
| 130 | 629.54380000 | 58.56500000  | 0.00000000 |
| 131 | 631.96700000 | 74.98360000  | 0.00000000 |
| 132 | 646.15190000 | 0.26200000   | 0.00000000 |
| 133 | 648.77230000 | 164.01060000 | 0.00000000 |
| 134 | 651.14080000 | 9.41830000   | 0.00000000 |
| 135 | 652.86800000 | 3.47940000   | 0.00000000 |
| 136 | 655.05170000 | 21.41860000  | 0.00000000 |
| 137 | 658.72690000 | 134.60270000 | 0.00000000 |
| 138 | 666.32270000 | 7.31150000   | 0.00000000 |
| 139 | 669.19000000 | 2.67750000   | 0.00000000 |
| 140 | 674.03760000 | 3.16690000   | 0.00000000 |
| 141 | 678.74050000 | 15.05180000  | 0.00000000 |
| 142 | 683.71500000 | 0.59700000   | 0.00000000 |
| 143 | 686.27810000 | 97.65100000  | 0.00000000 |
| 144 | 723.60520000 | 25.50150000  | 0.00000000 |
| 145 | 725.25850000 | 74.53550000  | 0.00000000 |
| 146 | 732.95480000 | 11.91940000  | 0.00000000 |
| 147 | 737.70310000 | 51.46860000  | 0.00000000 |
| 148 | 738.56270000 | 12.49890000  | 0.00000000 |
| 149 | 742.94910000 | 271.51020000 | 0.00000000 |
| 150 | 743.36620000 | 20.60060000  | 0.00000000 |
| 151 | 744.47380000 | 64.03980000  | 0.00000000 |
| 152 | 746.83820000 | 11.62910000  | 0.00000000 |
| 153 | 754.58320000 | 1.56340000   | 0.00000000 |
| 154 | 756.50400000 | 14.30330000  | 0.00000000 |
| 155 | 765.78920000 | 14.42930000  | 0.00000000 |
| 156 | 771.30990000 | 34.95570000  | 0.00000000 |
| 157 | 771.82820000 | 78.24520000  | 0.00000000 |
| 158 | 772.98260000 | 124.19680000 | 0.00000000 |
| 159 | 773.04420000 | 142.44300000 | 0.00000000 |
| 160 | 774.98240000 | 286.48210000 | 0.00000000 |
| 161 | 779.49820000 | 109.76030000 | 0.00000000 |
| 162 | 780.46170000 | 14.72480000  | 0.00000000 |
| 163 | 784.63610000 | 4.92090000   | 0.00000000 |
| 164 | 792.42130000 | 92.80390000  | 0.00000000 |
| 165 | 794.87720000 | 92.78140000  | 0.00000000 |
| 166 | 796.90470000 | 9.71570000   | 0.00000000 |
| 167 | 799.44290000 | 7.44960000   | 0.00000000 |
| 168 | 803.71200000 | 1.75130000   | 0.00000000 |
| 169 | 804.89250000 | 37.07220000  | 0.00000000 |
| 170 | 812.60320000 | 3.58340000   | 0.00000000 |
| 171 | 814.70770000 | 63.89330000  | 0.00000000 |
| 172 | 826.18740000 | 64.40290000  | 0.00000000 |
| 173 | 834.66900000 | 17.91370000  | 0.00000000 |
| 174 | 836.93280000 | 2.11090000   | 0.00000000 |
| 175 | 839.03400000 | 6.09000000   | 0.00000000 |
| 176 | 855.93710000 | 4.14230000   | 0.00000000 |
| 177 | 865.59650000 | 183.36870000 | 0.00000000 |
| 178 | 868.85060000 | 7.56780000   | 0.00000000 |
| 179 | 870.46760000 | 383.31010000 | 0.00000000 |
| 180 | 875.40360000 | 159.30060000 | 0.00000000 |
| 181 | 881.04160000 | 0.29850000   | 0.00000000 |
| 182 | 881.33680000 | 1.64650000   | 0.00000000 |
| 183 | 881.44930000 | 2.78340000   | 0.00000000 |
| 184 | 883.85690000 | 8.37080000   | 0.00000000 |
| 185 | 886.85460000 | 3.53660000   | 0.00000000 |
| 186 | 888.90150000 | 4.44210000   | 0.00000000 |
| 187 | 893.44480000 | 1.30110000   | 0.00000000 |
| 188 | 897.52960000 | 0.47650000   | 0.00000000 |

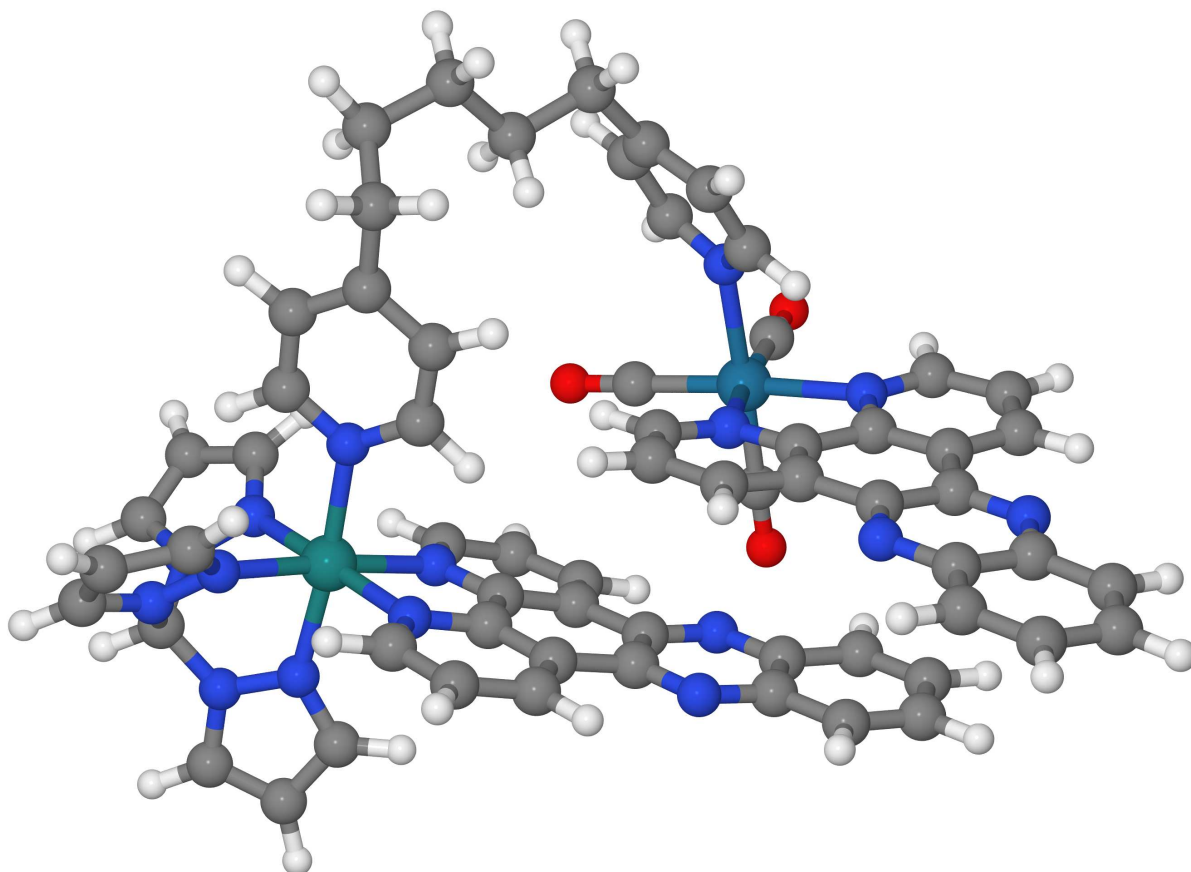
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|-----|---------------|---------------|------------|
| 189 | 915.62380000  | 4.18820000    | 0.00000000 |
| 190 | 916.10100000  | 30.49180000   | 0.00000000 |
| 191 | 918.63820000  | 2.77570000    | 0.00000000 |
| 192 | 937.03320000  | 38.33740000   | 0.00000000 |
| 193 | 937.18680000  | 6.67230000    | 0.00000000 |
| 194 | 940.05740000  | 0.26570000    | 0.00000000 |
| 195 | 940.38970000  | 3.06040000    | 0.00000000 |
| 196 | 943.66110000  | 1.59580000    | 0.00000000 |
| 197 | 946.95700000  | 0.21710000    | 0.00000000 |
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| 212 | 1005.73470000 | 26.23550000   | 0.00000000 |
| 213 | 1006.05400000 | 0.11180000    | 0.00000000 |
| 214 | 1006.88270000 | 1.66100000    | 0.00000000 |
| 215 | 1009.72740000 | 61.18180000   | 0.00000000 |
| 216 | 1014.24770000 | 17.04500000   | 0.00000000 |
| 217 | 1014.97260000 | 3.63800000    | 0.00000000 |
| 218 | 1016.41240000 | 1.85450000    | 0.00000000 |
| 219 | 1018.48330000 | 8.94190000    | 0.00000000 |
| 220 | 1019.92450000 | 48.15840000   | 0.00000000 |
| 221 | 1020.56250000 | 130.74940000  | 0.00000000 |
| 222 | 1021.62040000 | 15.46170000   | 0.00000000 |
| 223 | 1022.38270000 | 97.85320000   | 0.00000000 |
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| 225 | 1038.18480000 | 45.79010000   | 0.00000000 |
| 226 | 1038.80560000 | 0.69790000    | 0.00000000 |
| 227 | 1046.80140000 | 1.60750000    | 0.00000000 |
| 228 | 1056.38920000 | 526.66290000  | 0.00000000 |
| 229 | 1058.14080000 | 168.51490000  | 0.00000000 |
| 230 | 1061.87180000 | 116.43050000  | 0.00000000 |
| 231 | 1065.76900000 | 295.53380000  | 0.00000000 |
| 232 | 1066.73080000 | 235.32220000  | 0.00000000 |
| 233 | 1068.36320000 | 1066.74910000 | 0.00000000 |
| 234 | 1072.72920000 | 4.38690000    | 0.00000000 |
| 235 | 1084.13460000 | 93.74330000   | 0.00000000 |
| 236 | 1085.55340000 | 106.36600000  | 0.00000000 |
| 237 | 1086.50730000 | 40.45930000   | 0.00000000 |
| 238 | 1088.80420000 | 86.91580000   | 0.00000000 |
| 239 | 1096.85410000 | 919.99280000  | 0.00000000 |
| 240 | 1103.28850000 | 1.42100000    | 0.00000000 |
| 241 | 1103.59240000 | 18.16420000   | 0.00000000 |
| 242 | 1104.66000000 | 19.90200000   | 0.00000000 |
| 243 | 1110.02970000 | 24.46910000   | 0.00000000 |
| 244 | 1116.90990000 | 44.14010000   | 0.00000000 |
| 245 | 1125.78350000 | 93.54860000   | 0.00000000 |
| 246 | 1128.85610000 | 57.38800000   | 0.00000000 |
| 247 | 1129.76750000 | 125.38480000  | 0.00000000 |
| 248 | 1132.06320000 | 917.30390000  | 0.00000000 |
| 249 | 1134.21750000 | 24.89660000   | 0.00000000 |
| 250 | 1136.40100000 | 50.56700000   | 0.00000000 |
| 251 | 1139.47130000 | 19.23500000   | 0.00000000 |
| 252 | 1140.36680000 | 252.62680000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1143.80150000 | 28.61990000   | 0.00000000 |
| 254 | 1149.10430000 | 21.33530000   | 0.00000000 |
| 255 | 1153.80750000 | 183.29320000  | 0.00000000 |
| 256 | 1154.76090000 | 113.72950000  | 0.00000000 |
| 257 | 1157.40910000 | 61.75390000   | 0.00000000 |
| 258 | 1163.59230000 | 1652.79460000 | 0.00000000 |
| 259 | 1165.98250000 | 1741.45800000 | 0.00000000 |
| 260 | 1167.67510000 | 31.99340000   | 0.00000000 |
| 261 | 1175.05540000 | 618.91150000  | 0.00000000 |
| 262 | 1197.14130000 | 5.94060000    | 0.00000000 |
| 263 | 1205.10390000 | 60.14010000   | 0.00000000 |
| 264 | 1206.39170000 | 363.19370000  | 0.00000000 |
| 265 | 1207.67750000 | 38.13380000   | 0.00000000 |
| 266 | 1224.33380000 | 43.75150000   | 0.00000000 |
| 267 | 1226.92440000 | 4.40770000    | 0.00000000 |
| 268 | 1228.19330000 | 30.18810000   | 0.00000000 |
| 269 | 1237.32950000 | 5.46160000    | 0.00000000 |
| 270 | 1239.92920000 | 61.90610000   | 0.00000000 |
| 271 | 1248.57320000 | 625.79970000  | 0.00000000 |
| 272 | 1249.72960000 | 952.16050000  | 0.00000000 |
| 273 | 1255.28330000 | 15.19700000   | 0.00000000 |
| 274 | 1256.13090000 | 58.49890000   | 0.00000000 |
| 275 | 1259.97260000 | 582.85870000  | 0.00000000 |
| 276 | 1261.68820000 | 58.09840000   | 0.00000000 |
| 277 | 1264.67350000 | 384.92120000  | 0.00000000 |
| 278 | 1266.95840000 | 339.12770000  | 0.00000000 |
| 279 | 1273.55010000 | 238.49760000  | 0.00000000 |
| 280 | 1275.67840000 | 739.16030000  | 0.00000000 |
| 281 | 1276.90860000 | 119.29510000  | 0.00000000 |
| 282 | 1281.84520000 | 9.29600000    | 0.00000000 |
| 283 | 1291.34520000 | 1132.13260000 | 0.00000000 |
| 284 | 1295.08680000 | 12.97530000   | 0.00000000 |
| 285 | 1295.88080000 | 98.89600000   | 0.00000000 |
| 286 | 1303.35780000 | 1445.05520000 | 0.00000000 |
| 287 | 1305.17430000 | 29.31190000   | 0.00000000 |
| 288 | 1306.50440000 | 489.80700000  | 0.00000000 |
| 289 | 1312.50050000 | 37.49980000   | 0.00000000 |
| 290 | 1314.05430000 | 110.59550000  | 0.00000000 |
| 291 | 1314.27240000 | 23.03390000   | 0.00000000 |
| 292 | 1316.97820000 | 165.02630000  | 0.00000000 |
| 293 | 1322.53050000 | 40.86810000   | 0.00000000 |
| 294 | 1327.47050000 | 17.14410000   | 0.00000000 |
| 295 | 1329.18710000 | 4.71520000    | 0.00000000 |
| 296 | 1330.99980000 | 1.28360000    | 0.00000000 |
| 297 | 1331.88620000 | 958.65180000  | 0.00000000 |
| 298 | 1336.26120000 | 16.33690000   | 0.00000000 |
| 299 | 1339.17550000 | 7.25820000    | 0.00000000 |
| 300 | 1350.34750000 | 96.40510000   | 0.00000000 |
| 301 | 1356.53690000 | 145.60250000  | 0.00000000 |
| 302 | 1359.28400000 | 9.81220000    | 0.00000000 |
| 303 | 1362.00600000 | 72.51020000   | 0.00000000 |
| 304 | 1362.66210000 | 14.10060000   | 0.00000000 |
| 305 | 1365.86640000 | 3.34130000    | 0.00000000 |
| 306 | 1366.41600000 | 45.00930000   | 0.00000000 |
| 307 | 1369.32170000 | 20.90010000   | 0.00000000 |
| 308 | 1375.50640000 | 669.28330000  | 0.00000000 |
| 309 | 1381.65360000 | 45.91160000   | 0.00000000 |
| 310 | 1386.12140000 | 596.45330000  | 0.00000000 |
| 311 | 1388.15810000 | 7.32350000    | 0.00000000 |
| 312 | 1388.68410000 | 59.59110000   | 0.00000000 |
| 313 | 1395.06620000 | 6.54760000    | 0.00000000 |
| 314 | 1399.58730000 | 5.80290000    | 0.00000000 |
| 315 | 1404.03800000 | 14.41660000   | 0.00000000 |
| 316 | 1404.17710000 | 13.55100000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1406.79330000 | 114.46920000  | 0.00000000 |
| 318 | 1408.29100000 | 19.61000000   | 0.00000000 |
| 319 | 1412.95060000 | 17.73410000   | 0.00000000 |
| 320 | 1423.68220000 | 73.24990000   | 0.00000000 |
| 321 | 1426.68260000 | 113.28110000  | 0.00000000 |
| 322 | 1429.10660000 | 163.25870000  | 0.00000000 |
| 323 | 1441.27560000 | 1569.29370000 | 0.00000000 |
| 324 | 1442.62910000 | 423.67110000  | 0.00000000 |
| 325 | 1444.01970000 | 692.64150000  | 0.00000000 |
| 326 | 1448.46290000 | 1050.96670000 | 0.00000000 |
| 327 | 1459.83930000 | 45.76290000   | 0.00000000 |
| 328 | 1462.67540000 | 193.27840000  | 0.00000000 |
| 329 | 1464.72490000 | 54.08210000   | 0.00000000 |
| 330 | 1469.81020000 | 214.42120000  | 0.00000000 |
| 331 | 1475.27360000 | 1.08880000    | 0.00000000 |
| 332 | 1475.92370000 | 106.85080000  | 0.00000000 |
| 333 | 1478.86710000 | 46.62260000   | 0.00000000 |
| 334 | 1479.92560000 | 1.86660000    | 0.00000000 |
| 335 | 1484.73310000 | 3.18010000    | 0.00000000 |
| 336 | 1485.36430000 | 44.70700000   | 0.00000000 |
| 337 | 1487.61300000 | 399.59770000  | 0.00000000 |
| 338 | 1491.28560000 | 0.13810000    | 0.00000000 |
| 339 | 1493.22600000 | 8.17700000    | 0.00000000 |
| 340 | 1494.52350000 | 22.77290000   | 0.00000000 |
| 341 | 1495.02880000 | 45.26700000   | 0.00000000 |
| 342 | 1500.74190000 | 1.72130000    | 0.00000000 |
| 343 | 1501.97690000 | 7.93350000    | 0.00000000 |
| 344 | 1503.34250000 | 86.00770000   | 0.00000000 |
| 345 | 1505.09290000 | 15.32480000   | 0.00000000 |
| 346 | 1509.30100000 | 757.00650000  | 0.00000000 |
| 347 | 1512.20400000 | 12.29660000   | 0.00000000 |
| 348 | 1516.53570000 | 106.91710000  | 0.00000000 |
| 349 | 1519.24740000 | 44.83730000   | 0.00000000 |
| 350 | 1519.95420000 | 39.59900000   | 0.00000000 |
| 351 | 1527.99060000 | 166.55060000  | 0.00000000 |
| 352 | 1529.78790000 | 65.85340000   | 0.00000000 |
| 353 | 1534.68160000 | 3.66900000    | 0.00000000 |
| 354 | 1546.78290000 | 66.25500000   | 0.00000000 |
| 355 | 1553.65740000 | 37.08980000   | 0.00000000 |
| 356 | 1557.56660000 | 2.62570000    | 0.00000000 |
| 357 | 1564.82910000 | 376.59060000  | 0.00000000 |
| 358 | 1572.84020000 | 345.32460000  | 0.00000000 |
| 359 | 1573.97980000 | 133.90280000  | 0.00000000 |
| 360 | 1581.26560000 | 47.42880000   | 0.00000000 |
| 361 | 1587.65680000 | 346.97930000  | 0.00000000 |
| 362 | 1590.41860000 | 23.44070000   | 0.00000000 |
| 363 | 1594.93000000 | 639.54690000  | 0.00000000 |
| 364 | 1603.03750000 | 22.50480000   | 0.00000000 |
| 365 | 1615.52810000 | 5.28120000    | 0.00000000 |
| 366 | 1616.30730000 | 128.87240000  | 0.00000000 |
| 367 | 1619.16530000 | 108.30080000  | 0.00000000 |
| 368 | 1623.43930000 | 1.52610000    | 0.00000000 |
| 369 | 1642.04640000 | 4.17200000    | 0.00000000 |
| 370 | 1650.77920000 | 30.70640000   | 0.00000000 |
| 371 | 1653.76830000 | 75.09800000   | 0.00000000 |
| 372 | 1657.69200000 | 387.89330000  | 0.00000000 |
| 373 | 1913.42790000 | 65.88190000   | 0.00000000 |
| 374 | 1956.98270000 | 2270.80770000 | 0.00000000 |
| 375 | 1958.18790000 | 2402.57390000 | 0.00000000 |
| 376 | 2079.96920000 | 1776.28100000 | 0.00000000 |
| 377 | 2944.52670000 | 135.47450000  | 0.00000000 |
| 378 | 2981.83510000 | 93.55890000   | 0.00000000 |
| 379 | 2995.53740000 | 8.42910000    | 0.00000000 |
| 380 | 3001.77180000 | 13.12060000   | 0.00000000 |



|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 3009.20300000 | 58.55940000  | 0.00000000 |
| 382 | 3011.81130000 | 154.27850000 | 0.00000000 |
| 383 | 3012.38900000 | 31.31670000  | 0.00000000 |
| 384 | 3016.11640000 | 18.82270000  | 0.00000000 |
| 385 | 3025.87880000 | 84.33740000  | 0.00000000 |
| 386 | 3031.03770000 | 30.62150000  | 0.00000000 |
| 387 | 3044.50770000 | 1.14500000   | 0.00000000 |
| 388 | 3050.63710000 | 69.01750000  | 0.00000000 |
| 389 | 3055.62110000 | 26.01420000  | 0.00000000 |
| 390 | 3060.99940000 | 51.06600000  | 0.00000000 |
| 391 | 3066.87710000 | 4.76680000   | 0.00000000 |
| 392 | 3067.89760000 | 305.37860000 | 0.00000000 |
| 393 | 3176.84600000 | 1.30460000   | 0.00000000 |
| 394 | 3181.50100000 | 1.85900000   | 0.00000000 |
| 395 | 3186.49890000 | 10.88250000  | 0.00000000 |
| 396 | 3187.30880000 | 5.22700000   | 0.00000000 |
| 397 | 3191.38170000 | 11.96770000  | 0.00000000 |
| 398 | 3195.71380000 | 2.12830000   | 0.00000000 |
| 399 | 3196.90970000 | 57.05670000  | 0.00000000 |
| 400 | 3201.79130000 | 55.24690000  | 0.00000000 |
| 401 | 3202.15690000 | 2.58020000   | 0.00000000 |
| 402 | 3206.82340000 | 33.73330000  | 0.00000000 |
| 403 | 3207.09160000 | 23.84490000  | 0.00000000 |
| 404 | 3209.39170000 | 8.54010000   | 0.00000000 |
| 405 | 3210.43000000 | 5.32860000   | 0.00000000 |
| 406 | 3213.37400000 | 17.68500000  | 0.00000000 |
| 407 | 3216.26500000 | 12.38000000  | 0.00000000 |
| 408 | 3218.52150000 | 11.04640000  | 0.00000000 |
| 409 | 3220.36000000 | 2.45940000   | 0.00000000 |
| 410 | 3223.49950000 | 1.69170000   | 0.00000000 |
| 411 | 3223.79310000 | 0.05050000   | 0.00000000 |
| 412 | 3223.80720000 | 6.28020000   | 0.00000000 |
| 413 | 3224.40520000 | 18.93530000  | 0.00000000 |
| 414 | 3227.79730000 | 7.17590000   | 0.00000000 |
| 415 | 3230.53960000 | 0.75770000   | 0.00000000 |
| 416 | 3235.71510000 | 1.51790000   | 0.00000000 |
| 417 | 3238.40430000 | 5.14570000   | 0.00000000 |
| 418 | 3241.86490000 | 22.48730000  | 0.00000000 |
| 419 | 3245.10690000 | 6.76830000   | 0.00000000 |
| 420 | 3246.58400000 | 10.91340000  | 0.00000000 |
| 421 | 3248.24140000 | 59.11600000  | 0.00000000 |
| 422 | 3264.41370000 | 0.62170000   | 0.00000000 |
| 423 | 3265.07910000 | 0.21800000   | 0.00000000 |
| 424 | 3268.61740000 | 8.02190000   | 0.00000000 |
| 425 | 3272.19590000 | 14.56280000  | 0.00000000 |
| 426 | 3274.35360000 | 10.59930000  | 0.00000000 |
| 427 | 3274.84780000 | 40.10850000  | 0.00000000 |
| 428 | 3288.42780000 | 7.74380000   | 0.00000000 |
| 429 | 3288.74710000 | 9.03320000   | 0.00000000 |
| 430 | 3289.23560000 | 5.20830000   | 0.00000000 |
| 431 | 3527.31960000 | 1.02190000   | 0.00000000 |
| 432 | 3576.85300000 | 12.66830000  | 0.00000000 |

S7. CALCULATIONS ON ALTERNATIVE CONFORMER OF  $1^{3+}$  ( $^1A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]<br>1n7ccc1)[n+](n8ccc1)[n+](1ccc(cc1)CCCCC1cc[n+](cc1)[Re]<br>1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 1  |      |
| Energy                          | : -3743.86298345   | a.u. |
| Gibbs Energy                    | : -3742.93905300   | a.u. |
| Number of imaginary frequencies | : 1  |      |

## S7.1. Cartesian Co-ordinates (XYZ format)

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|   |             |             |            |
|---|-------------|-------------|------------|
| C | -0.68395400 | -5.26784086 | 3.68999600 |
| H | -0.52974403 | -6.35050392 | 3.67964411 |
| H | -1.22020197 | -5.01548719 | 4.60798407 |
| C | 0.68692601  | -4.55647278 | 3.67439389 |
| H | 0.51680702  | -3.47558904 | 3.66129398 |
| H | 1.20467901  | -4.79976797 | 2.74018788 |
| C | 1.56614494  | -4.94365692 | 4.86213589 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 1.67644703  | -6.03346014 | 4.88333797  |
| H  | 1.06086397  | -4.66550016 | 5.79457188  |
| C  | 2.96431303  | -2.76344705 | 4.95186520  |
| H  | 3.73506594  | -2.46427608 | 5.66785192  |
| H  | 2.01280403  | -2.41977692 | 5.36462307  |
| C  | 7.36454296  | 1.10734904  | -1.17877996 |
| N  | 6.93450308  | -0.25516200 | -1.42227197 |
| N  | 6.53447819  | 2.04414105  | -1.90283203 |
| N  | 7.34435987  | 1.39164805  | 0.24226700  |
| N  | 5.69051218  | -0.64219803 | -1.03073800 |
| C  | 7.63525295  | -1.29753304 | -1.94424403 |
| N  | 5.20342302  | 2.09940696  | -1.63633394 |
| C  | 6.88209391  | 2.93871307  | -2.86771798 |
| N  | 6.17068911  | 1.30181003  | 0.92469901  |
| C  | 8.38231754  | 1.66408396  | 1.07865906  |
| Ru | 4.45946789  | 0.81546402  | -0.17609701 |
| C  | 5.60846090  | -1.94298196 | -1.31109798 |
| C  | 6.80745077  | -2.39721894 | -1.89070904 |
| H  | 8.64235306  | -1.17149699 | -2.30450797 |
| C  | 4.70564604  | 3.03735495  | -2.43929291 |
| C  | 5.72688389  | 3.59309506  | -3.23347402 |
| H  | 7.90067482  | 3.03091502  | -3.20495892 |
| C  | 6.47451782  | 1.52199495  | 2.20341802  |
| C  | 7.85416985  | 1.75935996  | 2.34701395  |
| H  | 9.38830853  | 1.76758003  | 0.70816302  |
| N  | 2.76272392  | 0.48409599  | -1.34251201 |
| N  | 3.18249202  | 2.31309295  | 0.53181100  |
| H  | 4.70979118  | -2.49018002 | -1.07832599 |
| H  | 7.03419781  | -3.39522910 | -2.22349596 |
| H  | 3.65436697  | 3.27197003  | -2.41556501 |
| H  | 5.62884378  | 4.36831093  | -3.97355890 |
| H  | 5.70370817  | 1.48972297  | 2.95560789  |
| H  | 8.38860321  | 1.97153997  | 3.25671911  |
| C  | 2.63312197  | -0.38158101 | -2.35330701 |
| C  | 1.72749305  | 1.32735705  | -1.07825398 |
| C  | 1.95188403  | 2.31848693  | -0.05283700 |
| C  | 3.45459294  | 3.24875593  | 1.44617200  |
| C  | 1.47506106  | -0.45746899 | -3.12693310 |
| H  | 3.48101807  | -1.01850402 | -2.55494404 |
| C  | 0.51806498  | 1.27948403  | -1.78272295 |
| C  | 0.95912600  | 3.24901891  | 0.28350201  |
| C  | 2.51621795  | 4.20540905  | 1.83649099  |
| H  | 4.44664001  | 3.23263001  | 1.87226200  |
| C  | 0.40279400  | 0.36573499  | -2.83797002 |
| H  | 1.42972302  | -1.17003906 | -3.93793297 |
| C  | -0.56796002 | 2.17055988  | -1.38487697 |
| C  | 1.25859904  | 4.20711708  | 1.26129496  |
| C  | -0.34278899 | 3.16807103  | -0.37753099 |
| H  | 2.78900409  | 4.93462610  | 2.58688402  |
| H  | -0.51314402 | 0.32995400  | -3.40896297 |
| N  | -1.75750506 | 2.00182509  | -1.93654597 |
| H  | 0.50493598  | 4.92956018  | 1.54207397  |
| N  | -1.30387998 | 3.99597192  | -0.00291700 |
| C  | -2.75830007 | 2.81305003  | -1.53605795 |
| C  | -2.52012110 | 3.84793591  | -0.56938702 |
| C  | -4.06617880 | 2.62787390  | -2.05209708 |
| C  | -3.59055805 | 4.69327402  | -0.18043301 |
| C  | -5.08222723 | 3.45029211  | -1.63695300 |
| H  | -4.22909594 | 1.82833397  | -2.76328611 |
| C  | -4.84080410 | 4.49565506  | -0.70576799 |
| H  | -3.39266491 | 5.46596813  | 0.55088699  |
| H  | -6.08544922 | 3.30343390  | -2.01669407 |
| H  | -5.66336918 | 5.12861204  | -0.39768299 |
| N  | -4.72120810 | -1.68400097 | -1.08448398 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -2.32512093 | -0.86278999 | -0.19739200 |
| C  | -5.89874792 | -2.13052702 | -1.53425300 |
| C  | -4.69848490 | -0.56346703 | -0.31568801 |
| C  | -3.41148901 | -0.15083000 | 0.20147499  |
| C  | -1.14465404 | -0.60950899 | 0.37665600  |
| C  | -7.09839296 | -1.47407699 | -1.25989199 |
| H  | -5.87919378 | -3.02877998 | -2.13416791 |
| C  | -5.86294603 | 0.14438701  | 0.00954200  |
| C  | -3.31915092 | 0.90021801  | 1.12316203  |
| C  | -0.99114501 | 0.38239700  | 1.34318399  |
| H  | -0.30914900 | -1.21600795 | 0.05841400  |
| C  | -7.08423805 | -0.32556799 | -0.49178001 |
| H  | -8.02200317 | -1.87574399 | -1.65293598 |
| C  | -5.76878595 | 1.32538295  | 0.86272699  |
| C  | -2.07247210 | 1.16182995  | 1.70307803  |
| C  | -4.50975180 | 1.67875004  | 1.44591796  |
| H  | -0.02741400 | 0.54430300  | 1.79945695  |
| H  | -7.99127817 | 0.21424900  | -0.25776601 |
| N  | -6.85854721 | 2.03931499  | 1.08913505  |
| H  | -1.98169506 | 1.96337497  | 2.42250705  |
| N  | -4.38755322 | 2.71579409  | 2.25660396  |
| C  | -6.74467516 | 3.12078810  | 1.88700402  |
| C  | -5.48658800 | 3.45896196  | 2.49247003  |
| C  | -7.87521505 | 3.94247293  | 2.12907505  |
| C  | -5.39875793 | 4.60509920  | 3.32304096  |
| C  | -7.75443888 | 5.04658604  | 2.93214393  |
| H  | -8.81346607 | 3.67205000  | 1.66179204  |
| C  | -6.50978899 | 5.37949514  | 3.53281593  |
| H  | -4.44021082 | 4.84342384  | 3.76600599  |
| H  | -8.61439228 | 5.67868185  | 3.11563110  |
| H  | -6.44591522 | 6.25906801  | 4.16126490  |
| H  | 8.38433361  | 1.21119905  | -1.53377199 |
| C  | -1.47957098 | -4.84923220 | 2.48920393  |
| C  | -2.42219305 | -3.82100010 | 2.54280400  |
| C  | -1.21986198 | -5.40160179 | 1.23106897  |
| C  | -2.95215011 | -3.31102395 | 1.36965597  |
| H  | -2.71388102 | -3.38175297 | 3.48817897  |
| C  | -1.78164303 | -4.83816195 | 0.10356800  |
| H  | -0.54107898 | -6.23774481 | 1.12054300  |
| N  | -2.59047794 | -3.75668001 | 0.15165600  |
| H  | -3.65652394 | -2.49285698 | 1.40157402  |
| H  | -1.55093396 | -5.22466087 | -0.87874001 |
| C  | 3.24803090  | -2.02285695 | 3.67055607  |
| C  | 2.31643295  | -1.17393100 | 3.07075906  |
| C  | 4.49843884  | -2.10981607 | 3.04850101  |
| C  | 2.66525507  | -0.44384399 | 1.94692194  |
| H  | 1.32491100  | -1.05556095 | 3.48864102  |
| C  | 4.77924013  | -1.34737504 | 1.92936802  |
| H  | 5.27432823  | -2.74884105 | 3.45095897  |
| N  | 3.88261008  | -0.50014502 | 1.37810004  |
| H  | 1.96481001  | 0.23748100  | 1.49332094  |
| H  | 5.75318003  | -1.38427997 | 1.46526098  |
| Re | -2.73030591 | -2.44825006 | -1.68666101 |
| C  | -2.78891706 | -1.24252105 | -3.20462799 |
| O  | -2.83832312 | -0.53716803 | -4.11450195 |
| C  | -0.89686298 | -2.91708589 | -2.10666490 |
| O  | 0.19800200  | -3.19290709 | -2.34109306 |
| C  | -3.35167599 | -3.90127110 | -2.81447792 |
| O  | -3.74667001 | -4.76683617 | -3.46412492 |
| C  | 2.96353793  | -4.31272078 | 4.84142494  |
| H  | 3.49055910  | -4.61913204 | 3.93225908  |
| H  | 3.53492904  | -4.72172785 | 5.67784214  |

## S7.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -5.88850000  | 0.56320000   | 0.00000000      |
| 2    | 10.52970000  | 0.48990000   | 0.00000000      |
| 3    | 17.34140000  | 1.06200000   | 0.00000000      |
| 4    | 19.46470000  | 1.54000000   | 0.00000000      |
| 5    | 22.74210000  | 0.46400000   | 0.00000000      |
| 6    | 26.42770000  | 0.64610000   | 0.00000000      |
| 7    | 29.71110000  | 0.07770000   | 0.00000000      |
| 8    | 38.13360000  | 0.80190000   | 0.00000000      |
| 9    | 40.14150000  | 1.07130000   | 0.00000000      |
| 10   | 46.78190000  | 0.21260000   | 0.00000000      |
| 11   | 50.07150000  | 0.18630000   | 0.00000000      |
| 12   | 50.93050000  | 1.00970000   | 0.00000000      |
| 13   | 57.39650000  | 0.14640000   | 0.00000000      |
| 14   | 58.66710000  | 1.73220000   | 0.00000000      |
| 15   | 62.22040000  | 0.90580000   | 0.00000000      |
| 16   | 67.18240000  | 1.88040000   | 0.00000000      |
| 17   | 68.93720000  | 1.70980000   | 0.00000000      |
| 18   | 70.72160000  | 0.81620000   | 0.00000000      |
| 19   | 74.54990000  | 1.49240000   | 0.00000000      |
| 20   | 77.37510000  | 0.90670000   | 0.00000000      |
| 21   | 83.05500000  | 0.44620000   | 0.00000000      |
| 22   | 88.36480000  | 0.33630000   | 0.00000000      |
| 23   | 91.54990000  | 2.75080000   | 0.00000000      |
| 24   | 93.85670000  | 0.93410000   | 0.00000000      |
| 25   | 95.49340000  | 0.67950000   | 0.00000000      |
| 26   | 96.41650000  | 0.22960000   | 0.00000000      |
| 27   | 104.05560000 | 1.33100000   | 0.00000000      |
| 28   | 110.25170000 | 0.76960000   | 0.00000000      |
| 29   | 115.20720000 | 0.35600000   | 0.00000000      |
| 30   | 118.75920000 | 0.27900000   | 0.00000000      |
| 31   | 124.60280000 | 5.25480000   | 0.00000000      |
| 32   | 135.78880000 | 0.49350000   | 0.00000000      |
| 33   | 136.91810000 | 2.59370000   | 0.00000000      |
| 34   | 141.43580000 | 7.30090000   | 0.00000000      |
| 35   | 143.19140000 | 0.08870000   | 0.00000000      |
| 36   | 147.69770000 | 0.23980000   | 0.00000000      |
| 37   | 151.88910000 | 0.57800000   | 0.00000000      |
| 38   | 163.40020000 | 0.12480000   | 0.00000000      |
| 39   | 165.63070000 | 0.74360000   | 0.00000000      |
| 40   | 174.27090000 | 0.59620000   | 0.00000000      |
| 41   | 174.80320000 | 0.76850000   | 0.00000000      |
| 42   | 179.91570000 | 0.06220000   | 0.00000000      |
| 43   | 181.62010000 | 0.05260000   | 0.00000000      |
| 44   | 184.56770000 | 0.06230000   | 0.00000000      |
| 45   | 185.58700000 | 1.12630000   | 0.00000000      |
| 46   | 193.07150000 | 1.91070000   | 0.00000000      |
| 47   | 194.63970000 | 0.03430000   | 0.00000000      |
| 48   | 196.49580000 | 0.38420000   | 0.00000000      |
| 49   | 202.36120000 | 0.06330000   | 0.00000000      |
| 50   | 209.35750000 | 1.32360000   | 0.00000000      |
| 51   | 209.91200000 | 1.38940000   | 0.00000000      |
| 52   | 218.11970000 | 0.08600000   | 0.00000000      |
| 53   | 223.46220000 | 2.32960000   | 0.00000000      |
| 54   | 236.57970000 | 0.30730000   | 0.00000000      |
| 55   | 242.28190000 | 0.31940000   | 0.00000000      |
| 56   | 252.29130000 | 0.39130000   | 0.00000000      |
| 57   | 261.98240000 | 0.13140000   | 0.00000000      |
| 58   | 272.35330000 | 0.63240000   | 0.00000000      |
| 59   | 275.47400000 | 7.59050000   | 0.00000000      |
| 60   | 276.56420000 | 1.64210000   | 0.00000000      |

|     |              |             |            |
|-----|--------------|-------------|------------|
| 61  | 308.27870000 | 1.98400000  | 0.00000000 |
| 62  | 315.12780000 | 2.28620000  | 0.00000000 |
| 63  | 319.38740000 | 1.82430000  | 0.00000000 |
| 64  | 326.90830000 | 0.15060000  | 0.00000000 |
| 65  | 328.82190000 | 4.05270000  | 0.00000000 |
| 66  | 331.31390000 | 2.13570000  | 0.00000000 |
| 67  | 333.72780000 | 5.07090000  | 0.00000000 |
| 68  | 337.68380000 | 1.51710000  | 0.00000000 |
| 69  | 341.33500000 | 0.08220000  | 0.00000000 |
| 70  | 341.51080000 | 2.33810000  | 0.00000000 |
| 71  | 348.73660000 | 1.98050000  | 0.00000000 |
| 72  | 356.10590000 | 0.78550000  | 0.00000000 |
| 73  | 365.11670000 | 4.96760000  | 0.00000000 |
| 74  | 372.95950000 | 6.37710000  | 0.00000000 |
| 75  | 377.51620000 | 4.29640000  | 0.00000000 |
| 76  | 381.87830000 | 1.10940000  | 0.00000000 |
| 77  | 391.74960000 | 1.04340000  | 0.00000000 |
| 78  | 394.17320000 | 0.34560000  | 0.00000000 |
| 79  | 401.70020000 | 3.57970000  | 0.00000000 |
| 80  | 408.62730000 | 0.13930000  | 0.00000000 |
| 81  | 415.14410000 | 0.52800000  | 0.00000000 |
| 82  | 417.77540000 | 0.05330000  | 0.00000000 |
| 83  | 438.57480000 | 13.63690000 | 0.00000000 |
| 84  | 443.06390000 | 20.93110000 | 0.00000000 |
| 85  | 443.48110000 | 8.72470000  | 0.00000000 |
| 86  | 445.95130000 | 14.48170000 | 0.00000000 |
| 87  | 450.06220000 | 3.01570000  | 0.00000000 |
| 88  | 456.38620000 | 2.17870000  | 0.00000000 |
| 89  | 475.36320000 | 43.77830000 | 0.00000000 |
| 90  | 477.78460000 | 8.12050000  | 0.00000000 |
| 91  | 479.78790000 | 6.34000000  | 0.00000000 |
| 92  | 481.64330000 | 11.56490000 | 0.00000000 |
| 93  | 487.37880000 | 4.24040000  | 0.00000000 |
| 94  | 493.99480000 | 0.18390000  | 0.00000000 |
| 95  | 496.45140000 | 1.49890000  | 0.00000000 |
| 96  | 497.18730000 | 1.65750000  | 0.00000000 |
| 97  | 500.00670000 | 0.79890000  | 0.00000000 |
| 98  | 506.65260000 | 0.19660000  | 0.00000000 |
| 99  | 515.64670000 | 2.16680000  | 0.00000000 |
| 100 | 527.02590000 | 5.23570000  | 0.00000000 |
| 101 | 529.83160000 | 32.03530000 | 0.00000000 |
| 102 | 534.75820000 | 19.51390000 | 0.00000000 |
| 103 | 562.23020000 | 27.31300000 | 0.00000000 |
| 104 | 563.39040000 | 0.12330000  | 0.00000000 |
| 105 | 565.02220000 | 1.43320000  | 0.00000000 |
| 106 | 576.25820000 | 1.08600000  | 0.00000000 |
| 107 | 576.42030000 | 1.25770000  | 0.00000000 |
| 108 | 579.88550000 | 0.63180000  | 0.00000000 |
| 109 | 583.71050000 | 1.27770000  | 0.00000000 |
| 110 | 594.51040000 | 30.17350000 | 0.00000000 |
| 111 | 595.11660000 | 19.32460000 | 0.00000000 |
| 112 | 603.08510000 | 9.59880000  | 0.00000000 |
| 113 | 604.67220000 | 3.84180000  | 0.00000000 |
| 114 | 605.61550000 | 0.09640000  | 0.00000000 |
| 115 | 608.77290000 | 21.86840000 | 0.00000000 |
| 116 | 609.56300000 | 11.19930000 | 0.00000000 |
| 117 | 618.44630000 | 21.19640000 | 0.00000000 |
| 118 | 622.51620000 | 33.29340000 | 0.00000000 |
| 119 | 626.77060000 | 31.38990000 | 0.00000000 |
| 120 | 633.33980000 | 28.60910000 | 0.00000000 |
| 121 | 639.08280000 | 1.68340000  | 0.00000000 |
| 122 | 639.60420000 | 1.48880000  | 0.00000000 |
| 123 | 646.80440000 | 78.25070000 | 0.00000000 |
| 124 | 654.10640000 | 1.21050000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 655.74470000 | 1.10720000   | 0.00000000 |
| 126 | 659.76950000 | 0.02580000   | 0.00000000 |
| 127 | 667.17080000 | 0.87910000   | 0.00000000 |
| 128 | 673.20100000 | 7.07390000   | 0.00000000 |
| 129 | 678.64550000 | 2.45910000   | 0.00000000 |
| 130 | 684.08070000 | 0.75040000   | 0.00000000 |
| 131 | 685.60330000 | 0.65710000   | 0.00000000 |
| 132 | 686.19950000 | 0.24030000   | 0.00000000 |
| 133 | 740.20930000 | 10.76810000  | 0.00000000 |
| 134 | 740.94840000 | 4.33880000   | 0.00000000 |
| 135 | 741.31900000 | 5.47860000   | 0.00000000 |
| 136 | 741.74250000 | 3.15410000   | 0.00000000 |
| 137 | 744.12920000 | 6.47280000   | 0.00000000 |
| 138 | 748.00250000 | 3.69820000   | 0.00000000 |
| 139 | 749.37930000 | 0.49460000   | 0.00000000 |
| 140 | 753.14940000 | 128.19030000 | 0.00000000 |
| 141 | 755.04050000 | 0.71800000   | 0.00000000 |
| 142 | 757.12850000 | 75.40550000  | 0.00000000 |
| 143 | 760.26220000 | 11.93460000  | 0.00000000 |
| 144 | 761.28220000 | 2.48750000   | 0.00000000 |
| 145 | 761.85320000 | 174.26020000 | 0.00000000 |
| 146 | 762.04220000 | 136.27600000 | 0.00000000 |
| 147 | 779.24250000 | 87.43250000  | 0.00000000 |
| 148 | 782.59460000 | 20.29130000  | 0.00000000 |
| 149 | 783.02250000 | 11.25330000  | 0.00000000 |
| 150 | 785.00640000 | 1.06110000   | 0.00000000 |
| 151 | 785.46860000 | 73.44080000  | 0.00000000 |
| 152 | 797.20390000 | 96.15710000  | 0.00000000 |
| 153 | 803.11160000 | 114.87250000 | 0.00000000 |
| 154 | 812.33850000 | 0.52590000   | 0.00000000 |
| 155 | 817.08750000 | 0.81880000   | 0.00000000 |
| 156 | 818.75020000 | 0.51410000   | 0.00000000 |
| 157 | 823.38880000 | 58.65980000  | 0.00000000 |
| 158 | 826.56080000 | 3.13770000   | 0.00000000 |
| 159 | 834.86710000 | 81.67440000  | 0.00000000 |
| 160 | 837.73850000 | 15.44960000  | 0.00000000 |
| 161 | 844.34320000 | 65.73710000  | 0.00000000 |
| 162 | 850.87870000 | 27.92570000  | 0.00000000 |
| 163 | 854.22610000 | 0.44740000   | 0.00000000 |
| 164 | 859.23410000 | 28.24080000  | 0.00000000 |
| 165 | 868.40200000 | 9.48370000   | 0.00000000 |
| 166 | 869.08880000 | 18.20200000  | 0.00000000 |
| 167 | 869.31320000 | 20.83230000  | 0.00000000 |
| 168 | 870.03040000 | 1.15860000   | 0.00000000 |
| 169 | 874.00630000 | 6.62430000   | 0.00000000 |
| 170 | 875.48440000 | 13.27770000  | 0.00000000 |
| 171 | 875.58220000 | 8.76440000   | 0.00000000 |
| 172 | 878.34930000 | 3.48770000   | 0.00000000 |
| 173 | 879.12060000 | 48.16040000  | 0.00000000 |
| 174 | 886.93560000 | 3.14090000   | 0.00000000 |
| 175 | 895.22180000 | 0.10790000   | 0.00000000 |
| 176 | 896.26570000 | 0.98310000   | 0.00000000 |
| 177 | 918.31340000 | 1.54460000   | 0.00000000 |
| 178 | 921.36310000 | 0.63490000   | 0.00000000 |
| 179 | 921.49410000 | 1.33630000   | 0.00000000 |
| 180 | 926.51500000 | 3.86490000   | 0.00000000 |
| 181 | 927.80370000 | 5.26280000   | 0.00000000 |
| 182 | 939.91920000 | 12.58440000  | 0.00000000 |
| 183 | 947.65700000 | 0.03480000   | 0.00000000 |
| 184 | 948.56380000 | 0.01230000   | 0.00000000 |
| 185 | 953.56090000 | 0.45350000   | 0.00000000 |
| 186 | 956.86140000 | 2.44900000   | 0.00000000 |
| 187 | 978.92490000 | 0.11990000   | 0.00000000 |
| 188 | 981.07400000 | 2.40160000   | 0.00000000 |

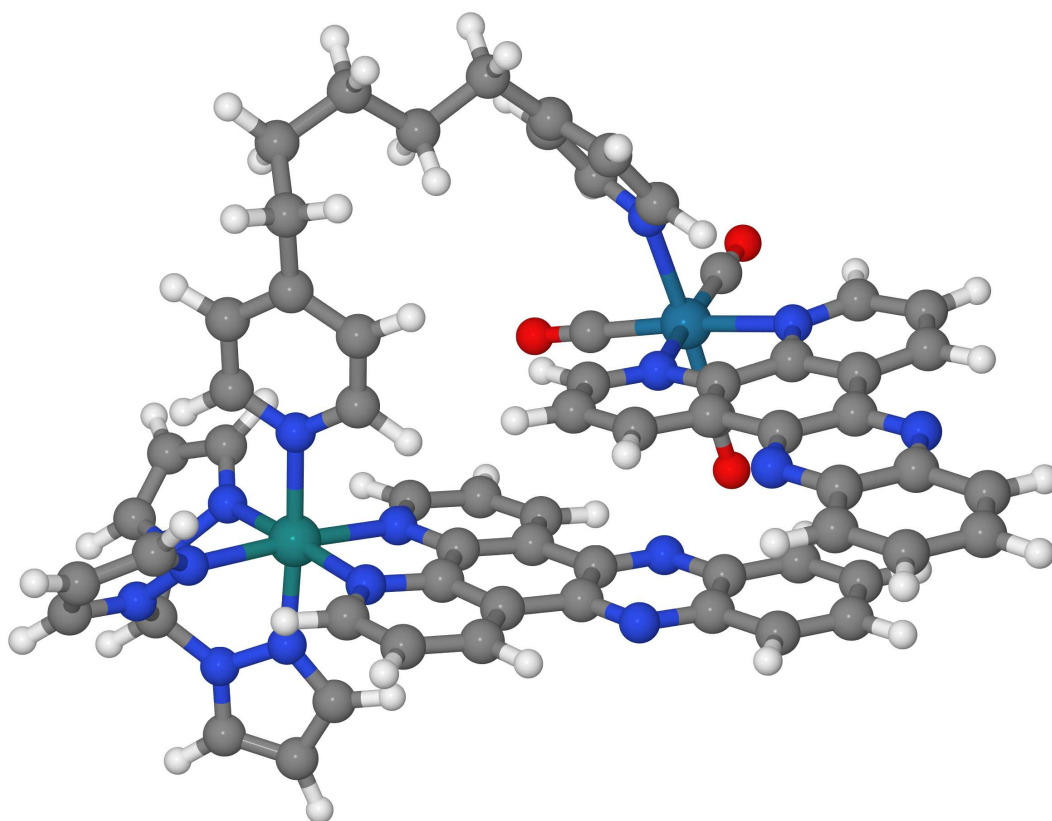
|     |               |             |            |
|-----|---------------|-------------|------------|
| 189 | 985.10440000  | 0.03780000  | 0.00000000 |
| 190 | 986.68350000  | 3.25740000  | 0.00000000 |
| 191 | 988.20070000  | 1.06070000  | 0.00000000 |
| 192 | 992.83330000  | 1.80330000  | 0.00000000 |
| 193 | 993.48650000  | 0.56020000  | 0.00000000 |
| 194 | 995.65490000  | 2.75780000  | 0.00000000 |
| 195 | 1004.87560000 | 0.91430000  | 0.00000000 |
| 196 | 1007.56430000 | 0.77440000  | 0.00000000 |
| 197 | 1007.95960000 | 0.05490000  | 0.00000000 |
| 198 | 1009.11860000 | 5.41920000  | 0.00000000 |
| 199 | 1009.74490000 | 19.68600000 | 0.00000000 |
| 200 | 1010.38280000 | 2.32100000  | 0.00000000 |
| 201 | 1013.38790000 | 12.37300000 | 0.00000000 |
| 202 | 1015.67290000 | 6.63380000  | 0.00000000 |
| 203 | 1020.74150000 | 0.40510000  | 0.00000000 |
| 204 | 1022.01050000 | 0.00270000  | 0.00000000 |
| 205 | 1025.51940000 | 0.30230000  | 0.00000000 |
| 206 | 1026.45080000 | 5.04290000  | 0.00000000 |
| 207 | 1027.60180000 | 3.21420000  | 0.00000000 |
| 208 | 1029.67870000 | 5.17620000  | 0.00000000 |
| 209 | 1031.99610000 | 0.10300000  | 0.00000000 |
| 210 | 1033.45570000 | 0.31990000  | 0.00000000 |
| 211 | 1046.26340000 | 27.15990000 | 0.00000000 |
| 212 | 1049.59420000 | 1.17560000  | 0.00000000 |
| 213 | 1057.43390000 | 8.22820000  | 0.00000000 |
| 214 | 1069.19030000 | 1.57790000  | 0.00000000 |
| 215 | 1070.40590000 | 0.62980000  | 0.00000000 |
| 216 | 1075.90510000 | 36.14630000 | 0.00000000 |
| 217 | 1076.33410000 | 35.98210000 | 0.00000000 |
| 218 | 1078.17800000 | 9.28550000  | 0.00000000 |
| 219 | 1079.36340000 | 30.79620000 | 0.00000000 |
| 220 | 1080.99210000 | 71.59790000 | 0.00000000 |
| 221 | 1086.09290000 | 7.69530000  | 0.00000000 |
| 222 | 1091.17160000 | 14.44340000 | 0.00000000 |
| 223 | 1093.91050000 | 3.82860000  | 0.00000000 |
| 224 | 1096.66830000 | 3.83920000  | 0.00000000 |
| 225 | 1105.57110000 | 38.93900000 | 0.00000000 |
| 226 | 1109.81750000 | 30.62260000 | 0.00000000 |
| 227 | 1118.01580000 | 31.59840000 | 0.00000000 |
| 228 | 1120.59680000 | 90.72550000 | 0.00000000 |
| 229 | 1121.18480000 | 72.61700000 | 0.00000000 |
| 230 | 1123.46680000 | 17.52100000 | 0.00000000 |
| 231 | 1123.76760000 | 27.43430000 | 0.00000000 |
| 232 | 1126.86810000 | 3.90400000  | 0.00000000 |
| 233 | 1143.95950000 | 35.55860000 | 0.00000000 |
| 234 | 1144.90410000 | 9.11030000  | 0.00000000 |
| 235 | 1148.09280000 | 17.61100000 | 0.00000000 |
| 236 | 1151.77720000 | 2.62680000  | 0.00000000 |
| 237 | 1153.44720000 | 3.73570000  | 0.00000000 |
| 238 | 1161.33080000 | 14.50350000 | 0.00000000 |
| 239 | 1162.18180000 | 18.69540000 | 0.00000000 |
| 240 | 1163.88400000 | 7.35430000  | 0.00000000 |
| 241 | 1174.05720000 | 0.25930000  | 0.00000000 |
| 242 | 1174.99400000 | 1.06090000  | 0.00000000 |
| 243 | 1212.69930000 | 0.63650000  | 0.00000000 |
| 244 | 1214.09930000 | 2.53970000  | 0.00000000 |
| 245 | 1214.96390000 | 2.48540000  | 0.00000000 |
| 246 | 1216.55010000 | 0.57340000  | 0.00000000 |
| 247 | 1221.18740000 | 1.65400000  | 0.00000000 |
| 248 | 1235.74720000 | 26.48130000 | 0.00000000 |
| 249 | 1237.59840000 | 5.09210000  | 0.00000000 |
| 250 | 1240.39290000 | 0.17880000  | 0.00000000 |
| 251 | 1243.40650000 | 18.90950000 | 0.00000000 |
| 252 | 1248.73860000 | 1.27940000  | 0.00000000 |



|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1256.56300000 | 40.01640000  | 0.00000000 |
| 254 | 1258.59340000 | 4.61800000   | 0.00000000 |
| 255 | 1259.98700000 | 8.56690000   | 0.00000000 |
| 256 | 1264.39700000 | 0.71790000   | 0.00000000 |
| 257 | 1264.54300000 | 1.93510000   | 0.00000000 |
| 258 | 1268.97570000 | 96.38140000  | 0.00000000 |
| 259 | 1273.56500000 | 1.71240000   | 0.00000000 |
| 260 | 1274.27640000 | 119.67630000 | 0.00000000 |
| 261 | 1276.07280000 | 6.14570000   | 0.00000000 |
| 262 | 1280.92970000 | 3.08600000   | 0.00000000 |
| 263 | 1300.16260000 | 9.28530000   | 0.00000000 |
| 264 | 1306.99260000 | 0.31750000   | 0.00000000 |
| 265 | 1307.20420000 | 6.38720000   | 0.00000000 |
| 266 | 1308.79700000 | 0.68630000   | 0.00000000 |
| 267 | 1310.97350000 | 6.38530000   | 0.00000000 |
| 268 | 1313.12680000 | 1.20390000   | 0.00000000 |
| 269 | 1317.21640000 | 34.66880000  | 0.00000000 |
| 270 | 1317.84840000 | 25.34370000  | 0.00000000 |
| 271 | 1321.50280000 | 67.07310000  | 0.00000000 |
| 272 | 1327.99280000 | 101.17460000 | 0.00000000 |
| 273 | 1329.67650000 | 1.41540000   | 0.00000000 |
| 274 | 1335.79740000 | 0.35230000   | 0.00000000 |
| 275 | 1336.97350000 | 1.84380000   | 0.00000000 |
| 276 | 1347.82230000 | 13.86640000  | 0.00000000 |
| 277 | 1353.07770000 | 0.82010000   | 0.00000000 |
| 278 | 1353.66380000 | 2.51120000   | 0.00000000 |
| 279 | 1359.45740000 | 6.24990000   | 0.00000000 |
| 280 | 1370.42760000 | 4.11540000   | 0.00000000 |
| 281 | 1371.08670000 | 126.18130000 | 0.00000000 |
| 282 | 1372.96040000 | 74.17570000  | 0.00000000 |
| 283 | 1374.18510000 | 19.44240000  | 0.00000000 |
| 284 | 1375.50860000 | 22.55160000  | 0.00000000 |
| 285 | 1376.42410000 | 94.96790000  | 0.00000000 |
| 286 | 1377.14470000 | 1.47130000   | 0.00000000 |
| 287 | 1379.90660000 | 5.72150000   | 0.00000000 |
| 288 | 1384.22140000 | 13.94700000  | 0.00000000 |
| 289 | 1387.37230000 | 7.70990000   | 0.00000000 |
| 290 | 1402.31170000 | 5.49730000   | 0.00000000 |
| 291 | 1416.82650000 | 9.70940000   | 0.00000000 |
| 292 | 1424.15530000 | 27.35500000  | 0.00000000 |
| 293 | 1425.72110000 | 0.96400000   | 0.00000000 |
| 294 | 1430.16430000 | 10.24980000  | 0.00000000 |
| 295 | 1436.55280000 | 56.53720000  | 0.00000000 |
| 296 | 1442.46260000 | 31.75570000  | 0.00000000 |
| 297 | 1443.67160000 | 157.65190000 | 0.00000000 |
| 298 | 1453.85550000 | 95.74460000  | 0.00000000 |
| 299 | 1458.25820000 | 131.35460000 | 0.00000000 |
| 300 | 1461.61790000 | 35.29220000  | 0.00000000 |
| 301 | 1465.10550000 | 31.30790000  | 0.00000000 |
| 302 | 1473.77430000 | 25.12250000  | 0.00000000 |
| 303 | 1474.58810000 | 14.47570000  | 0.00000000 |
| 304 | 1474.66020000 | 69.61910000  | 0.00000000 |
| 305 | 1475.79990000 | 2.28670000   | 0.00000000 |
| 306 | 1479.16440000 | 91.01500000  | 0.00000000 |
| 307 | 1487.45320000 | 3.05010000   | 0.00000000 |
| 308 | 1489.91440000 | 3.37160000   | 0.00000000 |
| 309 | 1492.55700000 | 6.93340000   | 0.00000000 |
| 310 | 1492.93890000 | 17.07150000  | 0.00000000 |
| 311 | 1500.99620000 | 13.98370000  | 0.00000000 |
| 312 | 1504.06850000 | 7.96880000   | 0.00000000 |
| 313 | 1504.25030000 | 11.10380000  | 0.00000000 |
| 314 | 1506.41900000 | 11.96650000  | 0.00000000 |
| 315 | 1507.89570000 | 10.94270000  | 0.00000000 |
| 316 | 1524.22000000 | 22.99410000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1526.13290000 | 15.32130000   | 0.00000000 |
| 318 | 1526.85820000 | 54.18510000   | 0.00000000 |
| 319 | 1532.27020000 | 136.98700000  | 0.00000000 |
| 320 | 1536.69850000 | 15.94470000   | 0.00000000 |
| 321 | 1537.55060000 | 46.90200000   | 0.00000000 |
| 322 | 1551.89330000 | 9.99080000    | 0.00000000 |
| 323 | 1553.87310000 | 13.10350000   | 0.00000000 |
| 324 | 1557.21530000 | 12.11780000   | 0.00000000 |
| 325 | 1576.99120000 | 4.25000000    | 0.00000000 |
| 326 | 1578.71250000 | 5.26820000    | 0.00000000 |
| 327 | 1581.17870000 | 32.95500000   | 0.00000000 |
| 328 | 1583.22040000 | 7.45260000    | 0.00000000 |
| 329 | 1590.88750000 | 13.40540000   | 0.00000000 |
| 330 | 1592.47660000 | 12.37050000   | 0.00000000 |
| 331 | 1609.66450000 | 1.95100000    | 0.00000000 |
| 332 | 1614.09550000 | 6.16110000    | 0.00000000 |
| 333 | 1623.92610000 | 0.41280000    | 0.00000000 |
| 334 | 1624.89680000 | 6.16680000    | 0.00000000 |
| 335 | 1625.80120000 | 3.27610000    | 0.00000000 |
| 336 | 1630.45260000 | 5.10230000    | 0.00000000 |
| 337 | 1635.93810000 | 0.18010000    | 0.00000000 |
| 338 | 1639.92050000 | 4.35390000    | 0.00000000 |
| 339 | 1658.96200000 | 88.76420000   | 0.00000000 |
| 340 | 1659.55020000 | 128.07850000  | 0.00000000 |
| 341 | 1659.66740000 | 15.51830000   | 0.00000000 |
| 342 | 1661.91690000 | 1.68760000    | 0.00000000 |
| 343 | 1966.41590000 | 2333.94160000 | 0.00000000 |
| 344 | 1970.28800000 | 2418.10640000 | 0.00000000 |
| 345 | 2084.48590000 | 1853.88790000 | 0.00000000 |
| 346 | 3010.03170000 | 34.69020000   | 0.00000000 |
| 347 | 3023.79200000 | 43.14880000   | 0.00000000 |
| 348 | 3028.63820000 | 15.91480000   | 0.00000000 |
| 349 | 3038.24490000 | 24.27750000   | 0.00000000 |
| 350 | 3041.29810000 | 65.63370000   | 0.00000000 |
| 351 | 3043.98710000 | 26.40760000   | 0.00000000 |
| 352 | 3063.85720000 | 60.84800000   | 0.00000000 |
| 353 | 3073.89700000 | 87.32760000   | 0.00000000 |
| 354 | 3080.31990000 | 41.63710000   | 0.00000000 |
| 355 | 3090.59310000 | 71.29540000   | 0.00000000 |
| 356 | 3184.91060000 | 0.86140000    | 0.00000000 |
| 357 | 3186.71140000 | 0.76030000    | 0.00000000 |
| 358 | 3191.79120000 | 1.23460000    | 0.00000000 |
| 359 | 3193.13630000 | 2.11280000    | 0.00000000 |
| 360 | 3194.51140000 | 5.92360000    | 0.00000000 |
| 361 | 3195.36340000 | 0.93190000    | 0.00000000 |
| 362 | 3195.79050000 | 6.54960000    | 0.00000000 |
| 363 | 3196.38460000 | 2.47530000    | 0.00000000 |
| 364 | 3196.56320000 | 2.71410000    | 0.00000000 |
| 365 | 3202.21770000 | 14.34450000   | 0.00000000 |
| 366 | 3204.71070000 | 8.58160000    | 0.00000000 |
| 367 | 3207.93980000 | 36.41610000   | 0.00000000 |
| 368 | 3209.79680000 | 26.62820000   | 0.00000000 |
| 369 | 3211.48420000 | 0.70860000    | 0.00000000 |
| 370 | 3213.78230000 | 0.14230000    | 0.00000000 |
| 371 | 3219.50920000 | 8.25010000    | 0.00000000 |
| 372 | 3220.84220000 | 0.69830000    | 0.00000000 |
| 373 | 3221.68790000 | 2.19190000    | 0.00000000 |
| 374 | 3223.60160000 | 3.82340000    | 0.00000000 |
| 375 | 3224.10600000 | 2.01900000    | 0.00000000 |
| 376 | 3224.79970000 | 6.26700000    | 0.00000000 |
| 377 | 3226.30720000 | 3.91640000    | 0.00000000 |
| 378 | 3231.47980000 | 5.29160000    | 0.00000000 |
| 379 | 3234.72690000 | 6.21740000    | 0.00000000 |
| 380 | 3236.46980000 | 7.33030000    | 0.00000000 |

|     |               |             |            |
|-----|---------------|-------------|------------|
| 381 | 3236.76830000 | 10.82350000 | 0.00000000 |
| 382 | 3240.86020000 | 3.49610000  | 0.00000000 |
| 383 | 3250.27970000 | 8.00820000  | 0.00000000 |
| 384 | 3254.32190000 | 0.49270000  | 0.00000000 |
| 385 | 3258.71930000 | 0.94180000  | 0.00000000 |
| 386 | 3261.12610000 | 0.11030000  | 0.00000000 |
| 387 | 3261.39170000 | 0.93380000  | 0.00000000 |
| 388 | 3269.21180000 | 7.23480000  | 0.00000000 |
| 389 | 3271.38260000 | 6.16470000  | 0.00000000 |
| 390 | 3272.26190000 | 7.03940000  | 0.00000000 |
| 391 | 3284.17400000 | 4.34330000  | 0.00000000 |
| 392 | 3285.41550000 | 4.77740000  | 0.00000000 |
| 393 | 3286.14210000 | 5.27030000  | 0.00000000 |

S8. CALCULATIONS ON ALTERNATIVE CONFORMER OF  $1^{3+}$  ( $^3A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](c6[Re]578(n9ccc[n+](c9C([n+]<br>1n7ccc1)[n+](n8ccc1)[n+](c1ccc(cc1)CCCCCc1cc[n+](cc1)[Re]<br>1([n+](c2cccc3c2c2[n+](c1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -3743.79241160   | a.u. |
| Gibbs Energy                    | : -3742.87309800   | a.u. |
| Number of imaginary frequencies | : 1  |      |

## S8.1. Cartesian Co-ordinates (XYZ format)

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|   |             |            |            |
|---|-------------|------------|------------|
| C | 0.85931200  | 5.11420584 | 3.82540107 |
| H | 0.72639197  | 6.19938612 | 3.84870291 |
| H | 1.37488496  | 4.82056379 | 4.74291277 |
| C | -0.52465999 | 4.43151188 | 3.76373410 |
| H | -0.37385800 | 3.34804296 | 3.73028111 |
| H | -1.01602006 | 4.70518208 | 2.82372403 |
| C | -1.42530596 | 4.81000090 | 4.93837309 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.52076805 | 5.90056276  | 4.97689295  |
| H  | -0.94891500 | 4.50700283  | 5.87800312  |
| C  | -2.85491109 | 2.64977002  | 4.97200298  |
| H  | -3.60281897 | 2.35837007  | 5.71421623  |
| H  | -1.89395702 | 2.28496289  | 5.34005690  |
| C  | -7.45669889 | -0.99464500 | -1.22769797 |
| N  | -7.04477501 | 0.38264599  | -1.39897799 |
| N  | -6.59185505 | -1.88323700 | -1.97960198 |
| N  | -7.44676304 | -1.34517395 | 0.17747800  |
| N  | -5.80880594 | 0.76764899  | -0.98377001 |
| C  | -7.74928999 | 1.43854296  | -1.88060498 |
| N  | -5.26147795 | -1.93059802 | -1.69028199 |
| C  | -6.89466715 | -2.73990893 | -2.98177004 |
| N  | -6.28075790 | -1.27865195 | 0.87368399  |
| C  | -8.47992706 | -1.68842804 | 0.98841202  |
| Ru | -4.54313707 | -0.72376603 | -0.18868101 |
| C  | -5.73437405 | 2.08061504  | -1.21007204 |
| C  | -6.93310308 | 2.54460812  | -1.77363706 |
| H  | -8.75221539 | 1.31900096  | -2.25497103 |
| C  | -4.72480106 | -2.82971597 | -2.52351809 |
| C  | -5.71541214 | -3.36225891 | -3.35341907 |
| H  | -7.90329313 | -2.84067702 | -3.34719801 |
| C  | -6.58459806 | -1.58510303 | 2.13625503  |
| C  | -7.95741987 | -1.85073197 | 2.25402403  |
| H  | -9.48178005 | -1.78962100 | 0.60624897  |
| N  | -2.86285400 | -0.31460300 | -1.32566500 |
| N  | -3.29666591 | -2.25788093 | 0.44646499  |
| H  | -4.84242678 | 2.62780809  | -0.95262599 |
| H  | -7.16838884 | 3.55358005  | -2.06410408 |
| H  | -3.66921902 | -3.04188490 | -2.48278189 |
| H  | -5.59278584 | -4.10324717 | -4.12389278 |
| H  | -5.81988621 | -1.58925796 | 2.89536405  |
| H  | -8.49357128 | -2.12559104 | 3.14548802  |
| C  | -2.71625495 | 0.61953098  | -2.26516008 |
| C  | -1.82503605 | -1.20240295 | -1.08860302 |
| C  | -2.05043101 | -2.21831894 | -0.16033800 |
| C  | -3.56871605 | -3.24153090 | 1.30414796  |
| C  | -1.54088700 | 0.75525898  | -3.00324202 |
| H  | -3.56021190 | 1.26973701  | -2.44242811 |
| C  | -0.58312303 | -1.09169698 | -1.78014898 |
| C  | -1.04399598 | -3.18321800 | 0.14280400  |
| C  | -2.63104391 | -4.21761990 | 1.63978398  |
| H  | -4.56093407 | -3.25510406 | 1.73104203  |
| C  | -0.46896401 | -0.09634100 | -2.74691510 |
| H  | -1.47552001 | 1.52966106  | -3.75261402 |
| C  | 0.49472699  | -2.01164603 | -1.45082295 |
| C  | -1.36275494 | -4.17884016 | 1.06123102  |
| C  | 0.25964999  | -3.07252002 | -0.49972701 |
| H  | -2.90388989 | -4.99018621 | 2.34431195  |
| H  | 0.45905000  | -0.00764100 | -3.29447103 |
| N  | 1.68618500  | -1.82656801 | -2.00374389 |
| H  | -0.61294699 | -4.91850519 | 1.30876100  |
| N  | 1.21809101  | -3.92855310 | -0.17021701 |
| C  | 2.68435907  | -2.68464088 | -1.65553105 |
| C  | 2.44197011  | -3.76095796 | -0.74519402 |
| C  | 3.98519611  | -2.49638295 | -2.17155695 |
| C  | 3.50121307  | -4.63270283 | -0.41266099 |
| C  | 5.00617218  | -3.35370803 | -1.81247199 |
| H  | 4.15358305  | -1.66524398 | -2.84495902 |
| C  | 4.76124001  | -4.43134117 | -0.93686599 |
| H  | 3.29993510  | -5.43725491 | 0.28366899  |
| H  | 6.00543308  | -3.19487810 | -2.19901896 |
| H  | 5.57338810  | -5.09260607 | -0.66102499 |
| N  | 4.85032701  | 1.55834305  | -1.00512803 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 2.38898706  | 0.84681100  | -0.20817199 |
| C  | 6.06192303  | 1.94739997  | -1.41741097 |
| C  | 4.74511290  | 0.42268401  | -0.26598001 |
| C  | 3.42391396  | 0.06880500  | 0.20479800  |
| C  | 1.17923701  | 0.64327800  | 0.32492501  |
| C  | 7.21570587  | 1.21900403  | -1.13080204 |
| H  | 6.10705614  | 2.85839796  | -1.99645495 |
| C  | 5.86110210  | -0.35505101 | 0.07161100  |
| C  | 3.25066304  | -0.99496299 | 1.09859800  |
| C  | 0.94725400  | -0.36168000 | 1.26104701  |
| H  | 0.38605201  | 1.29912698  | -0.00315200 |
| C  | 7.11814404  | 0.05700300  | -0.38850701 |
| H  | 8.16978645  | 1.57610905  | -1.49292898 |
| C  | 5.68029785  | -1.54644096 | 0.89522398  |
| C  | 1.97405005  | -1.20530200 | 1.63405502  |
| C  | 4.38823986  | -1.84134698 | 1.43763304  |
| H  | -0.03871300 | -0.48976099 | 1.67739296  |
| H  | 7.98757410  | -0.53750598 | -0.14427800 |
| N  | 6.72521782  | -2.31931901 | 1.13935995  |
| H  | 1.81862199  | -2.02034092 | 2.32617807  |
| N  | 4.19043112  | -2.88289809 | 2.22808099  |
| C  | 6.53175020  | -3.40772796 | 1.91152894  |
| C  | 5.24110413  | -3.68899894 | 2.47528911  |
| C  | 7.61042213  | -4.29223299 | 2.16971302  |
| C  | 5.07079315  | -4.84313583 | 3.28238106  |
| C  | 7.40992022  | -5.40234423 | 2.94823909  |
| H  | 8.57455730  | -4.06370687 | 1.73356795  |
| C  | 6.13297510  | -5.67911482 | 3.50822496  |
| H  | 4.08900881  | -5.03755379 | 3.69503903  |
| H  | 8.23021507  | -6.08197308 | 3.14331508  |
| H  | 6.00496578  | -6.56466103 | 4.11836720  |
| H  | -8.46763229 | -1.10082197 | -1.60570705 |
| C  | 1.66647899  | 4.72060585  | 2.62341595  |
| C  | 2.57350707  | 3.65992808  | 2.65125299  |
| C  | 1.45235705  | 5.33460188  | 1.38551402  |
| C  | 3.11166501  | 3.18305397  | 1.46776497  |
| H  | 2.82996893  | 3.17090797  | 3.58232188  |
| C  | 2.02107310  | 4.80198288  | 0.24620999  |
| H  | 0.80382103  | 6.19708586  | 1.29777801  |
| N  | 2.79233599  | 3.69275093  | 0.26321799  |
| H  | 3.78625798  | 2.33976293  | 1.47836006  |
| H  | 1.82608998  | 5.23885584  | -0.72257799 |
| C  | -3.20362210 | 1.93653297  | 3.69592190  |
| C  | -2.28818107 | 1.12836599  | 3.01493192  |
| C  | -4.49312115 | 2.02493405  | 3.15333796  |
| C  | -2.68265009 | 0.43388700  | 1.88879895  |
| H  | -1.27330804 | 1.01797605  | 3.37326407  |
| C  | -4.82578897 | 1.30185103  | 2.02722692  |
| H  | -5.25216389 | 2.63590693  | 3.62406707  |
| N  | -3.93676400 | 0.49723101  | 1.39904106  |
| H  | -2.00272989 | -0.21234000 | 1.35894406  |
| H  | -5.82271814 | 1.33606303  | 1.61516500  |
| Re | 2.92239690  | 2.45495105  | -1.62815106 |
| C  | 2.95495605  | 1.30944800  | -3.19280505 |
| O  | 2.98767710  | 0.64601600  | -4.13420486 |
| C  | 1.13599300  | 3.04727507  | -2.09149194 |
| O  | 0.07298600  | 3.40337110  | -2.36274791 |
| C  | 3.66055298  | 3.91383600  | -2.67286801 |
| O  | 4.12593889  | 4.78297806  | -3.27041411 |
| C  | -2.83147192 | 4.20294285  | 4.86727381  |
| H  | -3.31924605 | 4.52039814  | 3.94052291  |
| H  | -3.42823410 | 4.61492682  | 5.68350506  |

## S8.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -6.06260000  | 3.13800000   | 0.00000000      |
| 2    | 9.67350000   | 0.33440000   | 0.00000000      |
| 3    | 19.88140000  | 0.92050000   | 0.00000000      |
| 4    | 21.23540000  | 1.63620000   | 0.00000000      |
| 5    | 24.14020000  | 4.65770000   | 0.00000000      |
| 6    | 26.12610000  | 5.50240000   | 0.00000000      |
| 7    | 32.53020000  | 10.19830000  | 0.00000000      |
| 8    | 38.07330000  | 0.69200000   | 0.00000000      |
| 9    | 42.21030000  | 6.75540000   | 0.00000000      |
| 10   | 45.78230000  | 1.14100000   | 0.00000000      |
| 11   | 49.45840000  | 1.00150000   | 0.00000000      |
| 12   | 50.00070000  | 8.51680000   | 0.00000000      |
| 13   | 56.82050000  | 2.11130000   | 0.00000000      |
| 14   | 61.09300000  | 1.89700000   | 0.00000000      |
| 15   | 63.22630000  | 3.93370000   | 0.00000000      |
| 16   | 66.32290000  | 5.47240000   | 0.00000000      |
| 17   | 68.78850000  | 3.58000000   | 0.00000000      |
| 18   | 71.14430000  | 2.98490000   | 0.00000000      |
| 19   | 73.73490000  | 3.64680000   | 0.00000000      |
| 20   | 77.22680000  | 5.53230000   | 0.00000000      |
| 21   | 83.84330000  | 1.98870000   | 0.00000000      |
| 22   | 84.90980000  | 1.19360000   | 0.00000000      |
| 23   | 90.85330000  | 3.62120000   | 0.00000000      |
| 24   | 94.12380000  | 4.56950000   | 0.00000000      |
| 25   | 95.69190000  | 0.23370000   | 0.00000000      |
| 26   | 98.76560000  | 0.60170000   | 0.00000000      |
| 27   | 103.58830000 | 9.61280000   | 0.00000000      |
| 28   | 111.81650000 | 26.27740000  | 0.00000000      |
| 29   | 112.37340000 | 6.37170000   | 0.00000000      |
| 30   | 117.67380000 | 5.60090000   | 0.00000000      |
| 31   | 124.23250000 | 4.27500000   | 0.00000000      |
| 32   | 134.29940000 | 22.94980000  | 0.00000000      |
| 33   | 135.91140000 | 19.67720000  | 0.00000000      |
| 34   | 138.11280000 | 24.26380000  | 0.00000000      |
| 35   | 140.84060000 | 1.55260000   | 0.00000000      |
| 36   | 144.82450000 | 0.18770000   | 0.00000000      |
| 37   | 152.19780000 | 0.93520000   | 0.00000000      |
| 38   | 163.44270000 | 1.80240000   | 0.00000000      |
| 39   | 166.32650000 | 2.38520000   | 0.00000000      |
| 40   | 167.01450000 | 0.60690000   | 0.00000000      |
| 41   | 173.43700000 | 4.65210000   | 0.00000000      |
| 42   | 175.74940000 | 2.57270000   | 0.00000000      |
| 43   | 181.57690000 | 18.14080000  | 0.00000000      |
| 44   | 184.50550000 | 33.07750000  | 0.00000000      |
| 45   | 186.79380000 | 31.33900000  | 0.00000000      |
| 46   | 190.05360000 | 7.83990000   | 0.00000000      |
| 47   | 191.43750000 | 7.46320000   | 0.00000000      |
| 48   | 196.45790000 | 70.88430000  | 0.00000000      |
| 49   | 198.64810000 | 3.29430000   | 0.00000000      |
| 50   | 207.87640000 | 9.03630000   | 0.00000000      |
| 51   | 211.23790000 | 5.37140000   | 0.00000000      |
| 52   | 214.54370000 | 0.56240000   | 0.00000000      |
| 53   | 223.54370000 | 16.92770000  | 0.00000000      |
| 54   | 229.34120000 | 2.80360000   | 0.00000000      |
| 55   | 237.89140000 | 94.64870000  | 0.00000000      |
| 56   | 245.23830000 | 31.97980000  | 0.00000000      |
| 57   | 253.56620000 | 4.67040000   | 0.00000000      |
| 58   | 270.49740000 | 15.78050000  | 0.00000000      |
| 59   | 276.60820000 | 14.26650000  | 0.00000000      |
| 60   | 277.72900000 | 71.22660000  | 0.00000000      |

|     |              |               |            |
|-----|--------------|---------------|------------|
| 61  | 297.31170000 | 69.24610000   | 0.00000000 |
| 62  | 306.01770000 | 23.53690000   | 0.00000000 |
| 63  | 315.46860000 | 141.05850000  | 0.00000000 |
| 64  | 319.61980000 | 5.90630000    | 0.00000000 |
| 65  | 324.12400000 | 30.98130000   | 0.00000000 |
| 66  | 326.80470000 | 1.82480000    | 0.00000000 |
| 67  | 328.32870000 | 3.34400000    | 0.00000000 |
| 68  | 332.42880000 | 0.87030000    | 0.00000000 |
| 69  | 333.95500000 | 4.02990000    | 0.00000000 |
| 70  | 336.34090000 | 46.17870000   | 0.00000000 |
| 71  | 342.66020000 | 1.97200000    | 0.00000000 |
| 72  | 356.12850000 | 0.06910000    | 0.00000000 |
| 73  | 359.87850000 | 4.25040000    | 0.00000000 |
| 74  | 364.19370000 | 5.22770000    | 0.00000000 |
| 75  | 380.63570000 | 36.38240000   | 0.00000000 |
| 76  | 382.59510000 | 1.66030000    | 0.00000000 |
| 77  | 388.88840000 | 2.12510000    | 0.00000000 |
| 78  | 392.24350000 | 44.81130000   | 0.00000000 |
| 79  | 399.21080000 | 97.09710000   | 0.00000000 |
| 80  | 411.26890000 | 115.89640000  | 0.00000000 |
| 81  | 414.53890000 | 307.88660000  | 0.00000000 |
| 82  | 418.62210000 | 1.08580000    | 0.00000000 |
| 83  | 421.63610000 | 172.34980000  | 0.00000000 |
| 84  | 436.26910000 | 1152.16390000 | 0.00000000 |
| 85  | 438.58250000 | 28.87060000   | 0.00000000 |
| 86  | 442.25900000 | 27.41830000   | 0.00000000 |
| 87  | 445.45070000 | 3.19780000    | 0.00000000 |
| 88  | 450.25450000 | 16.80760000   | 0.00000000 |
| 89  | 455.46750000 | 3.25720000    | 0.00000000 |
| 90  | 476.86610000 | 19.69740000   | 0.00000000 |
| 91  | 479.01840000 | 9.19210000    | 0.00000000 |
| 92  | 480.85240000 | 12.63620000   | 0.00000000 |
| 93  | 487.66390000 | 6.03970000    | 0.00000000 |
| 94  | 491.75090000 | 9.00930000    | 0.00000000 |
| 95  | 494.80240000 | 124.85150000  | 0.00000000 |
| 96  | 495.37070000 | 3.83410000    | 0.00000000 |
| 97  | 496.56860000 | 0.43360000    | 0.00000000 |
| 98  | 498.02190000 | 11.69260000   | 0.00000000 |
| 99  | 514.03500000 | 25.32200000   | 0.00000000 |
| 100 | 529.31290000 | 27.56440000   | 0.00000000 |
| 101 | 532.50480000 | 28.73900000   | 0.00000000 |
| 102 | 535.79290000 | 7.33410000    | 0.00000000 |
| 103 | 537.41410000 | 59.83800000   | 0.00000000 |
| 104 | 562.39690000 | 19.14990000   | 0.00000000 |
| 105 | 562.86340000 | 556.86550000  | 0.00000000 |
| 106 | 565.91680000 | 4649.06980000 | 0.00000000 |
| 107 | 573.59340000 | 9.44630000    | 0.00000000 |
| 108 | 574.65850000 | 1299.13360000 | 0.00000000 |
| 109 | 576.58140000 | 166.30110000  | 0.00000000 |
| 110 | 581.12010000 | 161.68510000  | 0.00000000 |
| 111 | 583.51100000 | 2.57670000    | 0.00000000 |
| 112 | 594.84750000 | 21.27120000   | 0.00000000 |
| 113 | 600.33580000 | 0.13130000    | 0.00000000 |
| 114 | 602.03230000 | 8.23050000    | 0.00000000 |
| 115 | 609.21250000 | 28.24610000   | 0.00000000 |
| 116 | 609.94600000 | 21.64810000   | 0.00000000 |
| 117 | 610.76530000 | 34.15020000   | 0.00000000 |
| 118 | 616.78820000 | 1056.66640000 | 0.00000000 |
| 119 | 618.26110000 | 304.57420000  | 0.00000000 |
| 120 | 625.92010000 | 13.60430000   | 0.00000000 |
| 121 | 633.42580000 | 28.76730000   | 0.00000000 |
| 122 | 639.51470000 | 4.05350000    | 0.00000000 |
| 123 | 646.84190000 | 0.60050000    | 0.00000000 |
| 124 | 647.73160000 | 71.84670000   | 0.00000000 |



|     |              |                |            |
|-----|--------------|----------------|------------|
| 125 | 651.73860000 | 3.54630000     | 0.00000000 |
| 126 | 655.53210000 | 2.93490000     | 0.00000000 |
| 127 | 662.35280000 | 3.16290000     | 0.00000000 |
| 128 | 667.78550000 | 6.25910000     | 0.00000000 |
| 129 | 673.03210000 | 29.83290000    | 0.00000000 |
| 130 | 674.86600000 | 4.56470000     | 0.00000000 |
| 131 | 681.03340000 | 21.54740000    | 0.00000000 |
| 132 | 684.44400000 | 2.54650000     | 0.00000000 |
| 133 | 705.85640000 | 161.15790000   | 0.00000000 |
| 134 | 732.40770000 | 3182.57740000  | 0.00000000 |
| 135 | 735.80000000 | 105.12770000   | 0.00000000 |
| 136 | 740.94980000 | 11.81010000    | 0.00000000 |
| 137 | 741.32090000 | 4.42860000     | 0.00000000 |
| 138 | 742.41410000 | 6.73820000     | 0.00000000 |
| 139 | 745.77870000 | 38.75350000    | 0.00000000 |
| 140 | 748.24670000 | 5.04450000     | 0.00000000 |
| 141 | 751.82370000 | 90.96480000    | 0.00000000 |
| 142 | 757.54680000 | 7.29040000     | 0.00000000 |
| 143 | 760.48780000 | 19.12980000    | 0.00000000 |
| 144 | 763.95270000 | 2358.93380000  | 0.00000000 |
| 145 | 766.77390000 | 59.39870000    | 0.00000000 |
| 146 | 769.26960000 | 91.79800000    | 0.00000000 |
| 147 | 773.83070000 | 117.09260000   | 0.00000000 |
| 148 | 776.64080000 | 148.16410000   | 0.00000000 |
| 149 | 778.62200000 | 30.24140000    | 0.00000000 |
| 150 | 780.29390000 | 110.09690000   | 0.00000000 |
| 151 | 783.37990000 | 13.45420000    | 0.00000000 |
| 152 | 787.13130000 | 3.14140000     | 0.00000000 |
| 153 | 791.14840000 | 5.56980000     | 0.00000000 |
| 154 | 795.80050000 | 95.15220000    | 0.00000000 |
| 155 | 799.37040000 | 104.43650000   | 0.00000000 |
| 156 | 800.35310000 | 99.52780000    | 0.00000000 |
| 157 | 810.52860000 | 8.31000000     | 0.00000000 |
| 158 | 822.40070000 | 8.36020000     | 0.00000000 |
| 159 | 824.51390000 | 42.54390000    | 0.00000000 |
| 160 | 828.59660000 | 193.56430000   | 0.00000000 |
| 161 | 833.80500000 | 117.38240000   | 0.00000000 |
| 162 | 838.31020000 | 17.07520000    | 0.00000000 |
| 163 | 858.91000000 | 32.97760000    | 0.00000000 |
| 164 | 859.76940000 | 34.23520000    | 0.00000000 |
| 165 | 866.17730000 | 113.78830000   | 0.00000000 |
| 166 | 869.10650000 | 43.48410000    | 0.00000000 |
| 167 | 869.26900000 | 2754.48380000  | 0.00000000 |
| 168 | 876.57400000 | 33.21980000    | 0.00000000 |
| 169 | 877.00510000 | 425.73470000   | 0.00000000 |
| 170 | 881.53480000 | 1.98190000     | 0.00000000 |
| 171 | 884.22320000 | 9.70880000     | 0.00000000 |
| 172 | 884.82950000 | 8.84390000     | 0.00000000 |
| 173 | 886.47550000 | 7.41420000     | 0.00000000 |
| 174 | 890.46420000 | 9.03300000     | 0.00000000 |
| 175 | 894.12340000 | 1.44280000     | 0.00000000 |
| 176 | 894.15810000 | 9.83110000     | 0.00000000 |
| 177 | 915.97210000 | 109.08940000   | 0.00000000 |
| 178 | 921.72440000 | 29.94110000    | 0.00000000 |
| 179 | 938.60140000 | 389.26430000   | 0.00000000 |
| 180 | 941.07690000 | 2.47220000     | 0.00000000 |
| 181 | 941.78000000 | 326.56340000   | 0.00000000 |
| 182 | 943.71850000 | 1592.20010000  | 0.00000000 |
| 183 | 944.40990000 | 105.62570000   | 0.00000000 |
| 184 | 947.25000000 | 0.58470000     | 0.00000000 |
| 185 | 949.46280000 | 20061.64380000 | 0.00000000 |
| 186 | 952.31910000 | 1848.60150000  | 0.00000000 |
| 187 | 955.34970000 | 5777.69210000  | 0.00000000 |
| 188 | 963.12560000 | 1447.36700000  | 0.00000000 |

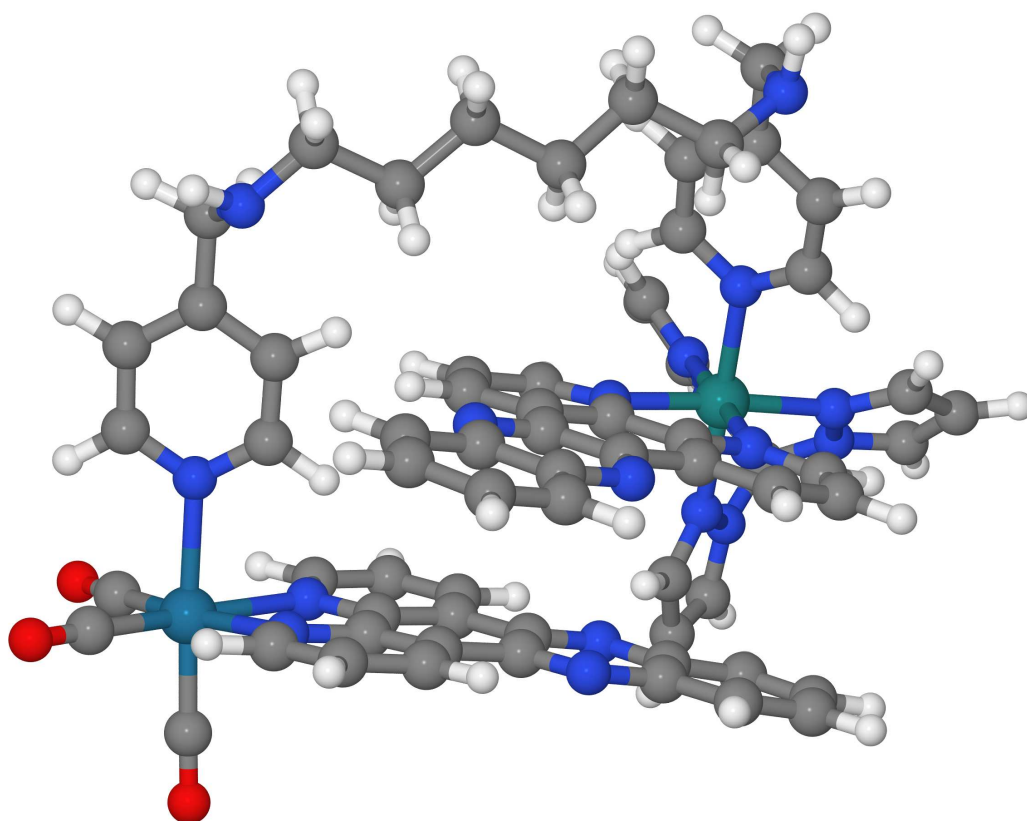
|     |               |               |            |
|-----|---------------|---------------|------------|
| 189 | 969.84370000  | 4.81060000    | 0.00000000 |
| 190 | 971.20560000  | 1.14370000    | 0.00000000 |
| 191 | 972.28960000  | 330.17030000  | 0.00000000 |
| 192 | 983.10160000  | 0.04860000    | 0.00000000 |
| 193 | 991.31920000  | 1.98310000    | 0.00000000 |
| 194 | 995.09640000  | 9.42070000    | 0.00000000 |
| 195 | 998.35190000  | 8.93540000    | 0.00000000 |
| 196 | 1000.10030000 | 38.02090000   | 0.00000000 |
| 197 | 1000.84520000 | 12.32170000   | 0.00000000 |
| 198 | 1004.62640000 | 1.69760000    | 0.00000000 |
| 199 | 1005.75520000 | 5.52440000    | 0.00000000 |
| 200 | 1008.51590000 | 0.33520000    | 0.00000000 |
| 201 | 1010.48240000 | 11.01160000   | 0.00000000 |
| 202 | 1015.14210000 | 15.58300000   | 0.00000000 |
| 203 | 1015.82850000 | 1.29770000    | 0.00000000 |
| 204 | 1017.84200000 | 28.07730000   | 0.00000000 |
| 205 | 1018.53870000 | 36.47740000   | 0.00000000 |
| 206 | 1019.73530000 | 42.58280000   | 0.00000000 |
| 207 | 1020.34170000 | 0.00320000    | 0.00000000 |
| 208 | 1022.92810000 | 235.08100000  | 0.00000000 |
| 209 | 1027.02780000 | 3.56910000    | 0.00000000 |
| 210 | 1030.68350000 | 0.38090000    | 0.00000000 |
| 211 | 1041.01900000 | 173.13530000  | 0.00000000 |
| 212 | 1045.85730000 | 33.67250000   | 0.00000000 |
| 213 | 1053.70710000 | 139.28370000  | 0.00000000 |
| 214 | 1054.85050000 | 19.91700000   | 0.00000000 |
| 215 | 1057.49960000 | 73.16320000   | 0.00000000 |
| 216 | 1070.01420000 | 6.78860000    | 0.00000000 |
| 217 | 1078.13420000 | 14.14560000   | 0.00000000 |
| 218 | 1079.26720000 | 864.87750000  | 0.00000000 |
| 219 | 1081.14290000 | 222.17980000  | 0.00000000 |
| 220 | 1083.31890000 | 10.54930000   | 0.00000000 |
| 221 | 1085.78710000 | 92.09900000   | 0.00000000 |
| 222 | 1090.25910000 | 239.12650000  | 0.00000000 |
| 223 | 1091.13410000 | 31.60300000   | 0.00000000 |
| 224 | 1096.45700000 | 88.13980000   | 0.00000000 |
| 225 | 1098.81950000 | 118.29630000  | 0.00000000 |
| 226 | 1103.49390000 | 402.71040000  | 0.00000000 |
| 227 | 1105.68390000 | 1247.41250000 | 0.00000000 |
| 228 | 1109.54090000 | 44.56390000   | 0.00000000 |
| 229 | 1123.54400000 | 14.90430000   | 0.00000000 |
| 230 | 1123.78240000 | 90.93870000   | 0.00000000 |
| 231 | 1126.82530000 | 17.44420000   | 0.00000000 |
| 232 | 1131.24710000 | 8.10000000    | 0.00000000 |
| 233 | 1133.64070000 | 83.01840000   | 0.00000000 |
| 234 | 1137.16540000 | 33.98350000   | 0.00000000 |
| 235 | 1140.66700000 | 8.04440000    | 0.00000000 |
| 236 | 1146.38020000 | 23.82970000   | 0.00000000 |
| 237 | 1147.16060000 | 11.46340000   | 0.00000000 |
| 238 | 1148.30500000 | 12.80570000   | 0.00000000 |
| 239 | 1151.81260000 | 2.16290000    | 0.00000000 |
| 240 | 1161.39310000 | 26.81400000   | 0.00000000 |
| 241 | 1165.63460000 | 10.85750000   | 0.00000000 |
| 242 | 1170.13330000 | 81.62090000   | 0.00000000 |
| 243 | 1173.53250000 | 0.39440000    | 0.00000000 |
| 244 | 1209.03020000 | 41.20090000   | 0.00000000 |
| 245 | 1210.12220000 | 8.42830000    | 0.00000000 |
| 246 | 1211.64680000 | 26.06740000   | 0.00000000 |
| 247 | 1214.82690000 | 13.07380000   | 0.00000000 |
| 248 | 1219.95170000 | 18.68360000   | 0.00000000 |
| 249 | 1235.69810000 | 18.43500000   | 0.00000000 |
| 250 | 1236.76660000 | 95.86450000   | 0.00000000 |
| 251 | 1239.22170000 | 45.16540000   | 0.00000000 |
| 252 | 1243.22490000 | 993.12970000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1244.87270000 | 2250.27030000 | 0.00000000 |
| 254 | 1248.45180000 | 21.98590000   | 0.00000000 |
| 255 | 1257.57650000 | 19.79590000   | 0.00000000 |
| 256 | 1258.71800000 | 53.72680000   | 0.00000000 |
| 257 | 1264.46640000 | 0.13960000    | 0.00000000 |
| 258 | 1271.15860000 | 65.58300000   | 0.00000000 |
| 259 | 1273.35580000 | 98.10680000   | 0.00000000 |
| 260 | 1274.39340000 | 24.25300000   | 0.00000000 |
| 261 | 1276.41530000 | 91.51470000   | 0.00000000 |
| 262 | 1278.40000000 | 78.14650000   | 0.00000000 |
| 263 | 1280.74340000 | 2.46710000    | 0.00000000 |
| 264 | 1297.55420000 | 2003.45130000 | 0.00000000 |
| 265 | 1305.74930000 | 2.55930000    | 0.00000000 |
| 266 | 1308.87420000 | 41.08490000   | 0.00000000 |
| 267 | 1309.92910000 | 28.12750000   | 0.00000000 |
| 268 | 1310.00390000 | 3.81780000    | 0.00000000 |
| 269 | 1314.98000000 | 20.83960000   | 0.00000000 |
| 270 | 1318.33830000 | 38.17500000   | 0.00000000 |
| 271 | 1319.25800000 | 13.93750000   | 0.00000000 |
| 272 | 1325.75390000 | 164.96380000  | 0.00000000 |
| 273 | 1328.20750000 | 144.53370000  | 0.00000000 |
| 274 | 1335.10510000 | 0.48630000    | 0.00000000 |
| 275 | 1335.88730000 | 3.09070000    | 0.00000000 |
| 276 | 1340.81830000 | 214.10730000  | 0.00000000 |
| 277 | 1344.15780000 | 89.03500000   | 0.00000000 |
| 278 | 1350.59720000 | 13.16290000   | 0.00000000 |
| 279 | 1351.58870000 | 9.50160000    | 0.00000000 |
| 280 | 1359.38820000 | 8.22400000    | 0.00000000 |
| 281 | 1361.50730000 | 14.57390000   | 0.00000000 |
| 282 | 1371.71200000 | 9.46830000    | 0.00000000 |
| 283 | 1373.90710000 | 18.85280000   | 0.00000000 |
| 284 | 1374.92660000 | 8.00000000    | 0.00000000 |
| 285 | 1376.13580000 | 112.54040000  | 0.00000000 |
| 286 | 1382.21930000 | 18.63910000   | 0.00000000 |
| 287 | 1384.66400000 | 32.37180000   | 0.00000000 |
| 288 | 1391.84160000 | 57.38980000   | 0.00000000 |
| 289 | 1394.02770000 | 11.65620000   | 0.00000000 |
| 290 | 1399.29780000 | 159.67330000  | 0.00000000 |
| 291 | 1401.26100000 | 8.56030000    | 0.00000000 |
| 292 | 1407.11090000 | 81.90720000   | 0.00000000 |
| 293 | 1410.88830000 | 117.72670000  | 0.00000000 |
| 294 | 1413.52970000 | 1936.50290000 | 0.00000000 |
| 295 | 1417.59230000 | 127.60240000  | 0.00000000 |
| 296 | 1430.26700000 | 13.74270000   | 0.00000000 |
| 297 | 1440.03210000 | 49.62900000   | 0.00000000 |
| 298 | 1440.99420000 | 227.68990000  | 0.00000000 |
| 299 | 1443.14200000 | 115.97340000  | 0.00000000 |
| 300 | 1456.85440000 | 224.84690000  | 0.00000000 |
| 301 | 1460.08930000 | 44.34750000   | 0.00000000 |
| 302 | 1460.78960000 | 36.70960000   | 0.00000000 |
| 303 | 1473.08320000 | 39.52890000   | 0.00000000 |
| 304 | 1475.31600000 | 7.64290000    | 0.00000000 |
| 305 | 1480.96750000 | 24.87990000   | 0.00000000 |
| 306 | 1484.46250000 | 59.34940000   | 0.00000000 |
| 307 | 1486.73800000 | 639.94960000  | 0.00000000 |
| 308 | 1488.80780000 | 47.34960000   | 0.00000000 |
| 309 | 1489.06200000 | 36.65240000   | 0.00000000 |
| 310 | 1490.19230000 | 3.09690000    | 0.00000000 |
| 311 | 1496.77360000 | 23.82360000   | 0.00000000 |
| 312 | 1500.66280000 | 2.35920000    | 0.00000000 |
| 313 | 1500.93890000 | 63.31760000   | 0.00000000 |
| 314 | 1503.12220000 | 16.99170000   | 0.00000000 |
| 315 | 1505.63130000 | 0.54110000    | 0.00000000 |
| 316 | 1506.05220000 | 11.44430000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1514.82160000 | 538.61380000  | 0.00000000 |
| 318 | 1515.54910000 | 10.14890000   | 0.00000000 |
| 319 | 1525.83270000 | 23.65470000   | 0.00000000 |
| 320 | 1530.05830000 | 181.55180000  | 0.00000000 |
| 321 | 1536.17260000 | 17.80400000   | 0.00000000 |
| 322 | 1541.57160000 | 10.52360000   | 0.00000000 |
| 323 | 1546.77080000 | 71.46100000   | 0.00000000 |
| 324 | 1547.73700000 | 3.65910000    | 0.00000000 |
| 325 | 1553.90970000 | 34.09970000   | 0.00000000 |
| 326 | 1557.38560000 | 15.72770000   | 0.00000000 |
| 327 | 1562.38390000 | 77.15100000   | 0.00000000 |
| 328 | 1573.52190000 | 387.30440000  | 0.00000000 |
| 329 | 1576.53810000 | 21.08770000   | 0.00000000 |
| 330 | 1582.14640000 | 16.52890000   | 0.00000000 |
| 331 | 1586.28230000 | 20.12590000   | 0.00000000 |
| 332 | 1592.49790000 | 12.60750000   | 0.00000000 |
| 333 | 1608.96610000 | 28.39170000   | 0.00000000 |
| 334 | 1610.72770000 | 240.24720000  | 0.00000000 |
| 335 | 1622.31860000 | 343.12270000  | 0.00000000 |
| 336 | 1625.46410000 | 106.18940000  | 0.00000000 |
| 337 | 1628.78860000 | 467.79090000  | 0.00000000 |
| 338 | 1638.02140000 | 4.52310000    | 0.00000000 |
| 339 | 1638.49430000 | 10.54300000   | 0.00000000 |
| 340 | 1657.40200000 | 266.54320000  | 0.00000000 |
| 341 | 1658.98830000 | 240.42200000  | 0.00000000 |
| 342 | 1661.82580000 | 1.76620000    | 0.00000000 |
| 343 | 1963.86560000 | 2356.73110000 | 0.00000000 |
| 344 | 1969.26360000 | 2249.10290000 | 0.00000000 |
| 345 | 2082.71130000 | 1745.57090000 | 0.00000000 |
| 346 | 3012.41410000 | 28.09670000   | 0.00000000 |
| 347 | 3023.64860000 | 48.97240000   | 0.00000000 |
| 348 | 3031.84250000 | 15.57060000   | 0.00000000 |
| 349 | 3042.12930000 | 65.53820000   | 0.00000000 |
| 350 | 3044.62320000 | 31.61680000   | 0.00000000 |
| 351 | 3046.75810000 | 6.60600000    | 0.00000000 |
| 352 | 3063.70500000 | 71.65460000   | 0.00000000 |
| 353 | 3079.81760000 | 75.86120000   | 0.00000000 |
| 354 | 3089.77060000 | 24.08910000   | 0.00000000 |
| 355 | 3091.35590000 | 77.33890000   | 0.00000000 |
| 356 | 3176.29850000 | 0.37270000    | 0.00000000 |
| 357 | 3183.45660000 | 0.71540000    | 0.00000000 |
| 358 | 3185.00030000 | 1.37600000    | 0.00000000 |
| 359 | 3191.81880000 | 2.19790000    | 0.00000000 |
| 360 | 3194.09090000 | 23.44600000   | 0.00000000 |
| 361 | 3195.39010000 | 2.72460000    | 0.00000000 |
| 362 | 3196.90630000 | 2.65490000    | 0.00000000 |
| 363 | 3198.55250000 | 5.35900000    | 0.00000000 |
| 364 | 3200.90970000 | 130.88480000  | 0.00000000 |
| 365 | 3200.95040000 | 8.97380000    | 0.00000000 |
| 366 | 3202.54820000 | 1.53690000    | 0.00000000 |
| 367 | 3204.36180000 | 2.28770000    | 0.00000000 |
| 368 | 3206.64690000 | 1.52500000    | 0.00000000 |
| 369 | 3206.86300000 | 45.82020000   | 0.00000000 |
| 370 | 3212.15730000 | 0.08890000    | 0.00000000 |
| 371 | 3217.95280000 | 36.43420000   | 0.00000000 |
| 372 | 3218.22520000 | 1.78630000    | 0.00000000 |
| 373 | 3218.71570000 | 8.51390000    | 0.00000000 |
| 374 | 3220.83040000 | 3.50190000    | 0.00000000 |
| 375 | 3223.44960000 | 2.27940000    | 0.00000000 |
| 376 | 3226.20940000 | 80.43560000   | 0.00000000 |
| 377 | 3226.49940000 | 1.46340000    | 0.00000000 |
| 378 | 3227.48990000 | 4.34920000    | 0.00000000 |
| 379 | 3230.17600000 | 8.58830000    | 0.00000000 |
| 380 | 3231.38440000 | 15.75080000   | 0.00000000 |

|     |               |             |            |
|-----|---------------|-------------|------------|
| 381 | 3237.61130000 | 4.21660000  | 0.00000000 |
| 382 | 3239.33490000 | 4.07930000  | 0.00000000 |
| 383 | 3253.78440000 | 28.63570000 | 0.00000000 |
| 384 | 3258.69400000 | 16.27140000 | 0.00000000 |
| 385 | 3262.22590000 | 0.64310000  | 0.00000000 |
| 386 | 3263.77440000 | 0.63390000  | 0.00000000 |
| 387 | 3265.68350000 | 13.47690000 | 0.00000000 |
| 388 | 3272.33500000 | 13.85500000 | 0.00000000 |
| 389 | 3275.41750000 | 8.73850000  | 0.00000000 |
| 390 | 3276.22050000 | 31.16650000 | 0.00000000 |
| 391 | 3287.37740000 | 8.45290000  | 0.00000000 |
| 392 | 3289.26300000 | 8.71730000  | 0.00000000 |
| 393 | 3289.48840000 | 7.53250000  | 0.00000000 |

# S9. CALCULATIONS ON ALTERNATIVE CONFORMER OF $2^{3+}$ ( $^1A$ )



|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]<br>1n7ccc1)[n+]1n8ccc1[n+]1ccc(cc1)CNC(CCCCNCc1cc[n+](cc1)[Re]<br>1([n+]2cccc3c2c2[n+]1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 1  |      |
| Energy                          | : -3972.58329708   | a.u. |
| Gibbs Energy                    | : -3971.54548200   | a.u. |
| Number of imaginary frequencies | : 1  |      |

## S9.1. Cartesian Co-ordinates (XYZ format)

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|   |            |            |             |
|---|------------|------------|-------------|
| C | 2.96778893 | 5.70947504 | 0.44015300  |
| H | 2.75522089 | 5.99264812 | 1.47524595  |
| H | 2.92158103 | 4.61584806 | 0.40895900  |
| C | 1.88411403 | 6.28400993 | -0.48079500 |
| H | 2.20479894 | 6.21283102 | -1.52520704 |
| H | 1.75607896 | 7.35197115 | -0.26803699 |
| C | 0.54826999 | 5.55253220 | -0.33800101 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.25259301  | 5.51094723  | 0.71766299  |
| H | 0.68160099  | 4.51100206  | -0.65761000 |
| C | -0.57697600 | 6.19407606  | -1.15321100 |
| H | -0.21853501 | 6.39724922  | -2.16981006 |
| H | -0.82910299 | 7.16808891  | -0.71650398 |
| C | -3.00920200 | 6.00709820  | -1.90935802 |
| H | -2.68993402 | 6.41130304  | -2.88411903 |
| H | -3.32177401 | 6.86018801  | -1.30098999 |
| N | 4.35366917  | 6.10117817  | 0.15062000  |
| C | -4.12616301 | 4.19013023  | -3.17910194 |
| H | -3.12494397 | 4.19881105  | -3.62125301 |
| H | -4.82160521 | 4.48634386  | -3.97036695 |
| N | -4.16277313 | 5.11019802  | -2.03678393 |
| C | 4.85458899  | 5.64530802  | -1.14853597 |
| H | 4.27041101  | 5.99483204  | -2.01043296 |
| H | 5.86873293  | 6.03701687  | -1.27133799 |
| C | 6.09657621  | -3.24359393 | -1.57310200 |
| N | 5.73982191  | -2.51607800 | -2.77129602 |
| N | 6.92981291  | -2.42594695 | -0.71856302 |
| N | 4.91695499  | -3.68630195 | -0.86737800 |
| N | 5.05526876  | -1.34351003 | -2.67220497 |
| C | 6.06532097  | -2.79774499 | -4.06087923 |
| N | 6.46433687  | -1.24019098 | -0.23271000 |
| C | 8.21116066  | -2.65914702 | -0.33071899 |
| N | 4.05020189  | -2.75568891 | -0.39619201 |
| C | 4.50332117  | -4.94705296 | -0.56499201 |
| C | 4.94995022  | -0.88786799 | -3.92114305 |
| C | 5.56607008  | -1.76939702 | -4.82743788 |
| H | 6.61281395  | -3.68897104 | -4.31775904 |
| C | 7.47701979  | -0.72997200 | 0.47047901  |
| C | 8.59250164  | -1.58512604 | 0.43991601  |
| H | 8.73128223  | -3.55311608 | -0.63121402 |
| C | 3.07510996  | -3.43047500 | 0.20892800  |
| C | 3.31933808  | -4.81546783 | 0.12698799  |
| H | 5.07559490  | -5.81008720 | -0.86077899 |
| N | -3.38315201 | -2.22009397 | -0.82062501 |
| N | -4.82437992 | -0.95371199 | 1.05557501  |
| H | 4.44819212  | 0.04081900  | -4.12815523 |
| H | 5.63441181  | -1.66288400 | -5.89609003 |
| H | 7.38618708  | 0.21948300  | 0.96688300  |
| H | 9.54468918  | -1.43130100 | 0.91705298  |
| H | 2.25731111  | -2.90912700 | 0.68037802  |
| H | 2.70950794  | -5.60837603 | 0.52425599  |
| C | -2.68809199 | -2.81011391 | -1.79905200 |
| C | -2.75413895 | -1.93267000 | 0.34950799  |
| C | -3.53022194 | -1.23914099 | 1.35768795  |
| C | -5.55258179 | -0.26174599 | 1.93840599  |
| C | -1.34790599 | -3.16219306 | -1.65091395 |
| H | -3.21966600 | -3.01179194 | -2.71751809 |
| C | -1.40964901 | -2.26344109 | 0.57577902  |
| C | -2.94795203 | -0.85920399 | 2.57299590  |
| C | -5.03426600 | 0.16626200  | 3.16014504  |
| H | -6.57432222 | -0.04694900 | 1.66099799  |
| C | -0.70797497 | -2.90290689 | -0.45497900 |
| H | -0.82984298 | -3.63715005 | -2.47212911 |
| C | -0.80359900 | -1.94758701 | 1.86767399  |
| C | -3.72891307 | -0.14152101 | 3.48871112  |
| C | -1.56574094 | -1.23622501 | 2.85267496  |
| H | -5.66319418 | 0.73292798  | 3.83205509  |
| H | 0.32479900  | -3.17865205 | -0.30688801 |
| N | 0.43584499  | -2.34429598 | 2.11390710  |
| H | -3.29097700 | 0.16541301  | 4.42793417  |
| N | -1.05295396 | -0.92235500 | 4.02999401  |
| C | 0.95490599  | -2.07934809 | 3.33285904  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.20163600  | -1.33210504 | 4.30128622  |
| C | 2.24656701  | -2.55292511 | 3.67824292  |
| C | 0.77900398  | -1.04323399 | 5.56386805  |
| C | 2.76187992  | -2.28204703 | 4.91895199  |
| H | 2.80293107  | -3.12966990 | 2.95246506  |
| C | 2.03047895  | -1.51458597 | 5.86324501  |
| H | 0.19829600  | -0.46322700 | 6.26932716  |
| H | 3.74634695  | -2.64685106 | 5.18365622  |
| H | 2.47208905  | -1.30442202 | 6.82914019  |
| N | 3.76634908  | -0.16309801 | 1.13893294  |
| N | 2.46315193  | -0.35901901 | -1.15322804 |
| C | 4.43495417  | -0.15340200 | 2.29583001  |
| C | 2.51539111  | 0.37197900  | 1.10958600  |
| C | 1.79974198  | 0.25716799  | -0.13736100 |
| C | 1.81027997  | -0.59359902 | -2.29669690 |
| C | 3.91655493  | 0.43515500  | 3.44965911  |
| H | 5.40768623  | -0.62392497 | 2.29338908  |
| C | 1.92147696  | 0.96053803  | 2.23100591  |
| C | 0.48177201  | 0.71474898  | -0.26686800 |
| C | 0.49673200  | -0.17136100 | -2.49854207 |
| H | 2.35821509  | -1.12055600 | -3.06446791 |
| C | 2.65958691  | 1.00931501  | 3.42116308  |
| H | 4.50598192  | 0.42511401  | 4.35559702  |
| C | 0.55874801  | 1.47569394  | 2.11981010  |
| C | -0.16642000 | 0.50562501  | -1.49147701 |
| C | -0.15480199 | 1.36418903  | 0.87786800  |
| H | 0.01458800  | -0.37608200 | -3.44422698 |
| H | 2.22442007  | 1.46932495  | 4.29645777  |
| N | -0.00159500 | 2.01121998  | 3.19061089  |
| H | -1.17799604 | 0.85579097  | -1.62772906 |
| N | -1.39046502 | 1.82431495  | 0.75181502  |
| C | -1.26488495 | 2.46810603  | 3.08159590  |
| C | -1.96847498 | 2.39364290  | 1.83156502  |
| C | -1.91094601 | 3.02577806  | 4.21438217  |
| C | -3.28606391 | 2.91331697  | 1.74741995  |
| C | -3.18966293 | 3.50572896  | 4.10125780  |
| H | -1.36503398 | 3.05754304  | 5.14843607  |
| C | -3.87581801 | 3.45651793  | 2.85881901  |
| H | -3.80680609 | 2.86781192  | 0.80183601  |
| H | -3.68726397 | 3.93092108  | 4.96378279  |
| H | -4.88347387 | 3.84772897  | 2.79599190  |
| H | 6.66879606  | -4.11781311 | -1.86572099 |
| C | 4.89965582  | 4.13717985  | -1.17128003 |
| C | 5.53226423  | 3.43391490  | -0.14522800 |
| C | 4.25449324  | 3.38784099  | -2.15108395 |
| C | 5.46824121  | 2.05576897  | -0.12039200 |
| H | 6.03021622  | 3.96293712  | 0.65573001  |
| C | 4.22880602  | 2.00492311  | -2.05562305 |
| H | 3.73309588  | 3.86946011  | -2.96839595 |
| N | 4.81416607  | 1.32930398  | -1.05047202 |
| H | 5.91322708  | 1.50884402  | 0.69367498  |
| H | 3.68009400  | 1.42305696  | -2.77954698 |
| C | -4.43346977 | 2.77961802  | -2.73171091 |
| C | -3.63419795 | 2.16652393  | -1.76636195 |
| C | -5.52007389 | 2.05014610  | -3.20870900 |
| C | -3.94823503 | 0.90476298  | -1.30977905 |
| H | -2.77777290 | 2.67066097  | -1.34371197 |
| C | -5.78053379 | 0.78667903  | -2.69942498 |
| H | -6.18129015 | 2.46076798  | -3.96124697 |
| N | -5.01650000 | 0.21038599  | -1.75026906 |
| H | -3.33266592 | 0.44605201  | -0.55368900 |
| H | -6.63133097 | 0.21730100  | -3.04594588 |
| H | -5.02154779 | 5.64356422  | -2.06094503 |
| C | -1.82675397 | 5.31892300  | -1.22893000 |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.13487506 | 5.00950003  | -0.22429501 |
| H  | -1.57261205 | 4.40196991  | -1.77298498 |
| H  | 4.45299578  | 7.10897207  | 0.21246099  |
| Ru | 4.45703411  | -0.74780202 | -0.73689902 |
| Re | -5.55342722 | -1.77811801 | -0.86735803 |
| C  | -5.94692993 | -3.49009991 | -0.03298200 |
| O  | -6.17036295 | -4.50272179 | 0.46759099  |
| C  | -5.92914915 | -2.52780008 | -2.61625504 |
| O  | -6.12169409 | -2.97840190 | -3.66004300 |
| C  | -7.41085815 | -1.24966800 | -0.68483800 |
| O  | -8.50755501 | -0.92081499 | -0.54969001 |

## S9.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -5.25870000  | 1.02130000   | 0.00000000      |
| 2    | 10.60340000  | 0.54890000   | 0.00000000      |
| 3    | 11.34060000  | 0.04390000   | 0.00000000      |
| 4    | 17.44030000  | 0.10620000   | 0.00000000      |
| 5    | 21.20100000  | 1.12710000   | 0.00000000      |
| 6    | 27.68370000  | 0.12280000   | 0.00000000      |
| 7    | 33.83720000  | 1.16170000   | 0.00000000      |
| 8    | 35.80860000  | 0.11220000   | 0.00000000      |
| 9    | 38.93840000  | 0.08510000   | 0.00000000      |
| 10   | 41.40250000  | 0.21590000   | 0.00000000      |
| 11   | 45.54560000  | 0.18400000   | 0.00000000      |
| 12   | 51.99740000  | 1.01830000   | 0.00000000      |
| 13   | 55.99100000  | 0.33580000   | 0.00000000      |
| 14   | 56.56350000  | 1.89220000   | 0.00000000      |
| 15   | 63.30760000  | 0.24820000   | 0.00000000      |
| 16   | 63.77230000  | 1.12430000   | 0.00000000      |
| 17   | 64.27860000  | 2.17640000   | 0.00000000      |
| 18   | 69.16580000  | 0.23700000   | 0.00000000      |
| 19   | 71.75240000  | 0.40580000   | 0.00000000      |
| 20   | 72.68230000  | 0.05320000   | 0.00000000      |
| 21   | 77.88040000  | 1.85150000   | 0.00000000      |
| 22   | 81.58450000  | 1.71400000   | 0.00000000      |
| 23   | 84.42540000  | 4.18940000   | 0.00000000      |
| 24   | 87.02360000  | 7.17100000   | 0.00000000      |
| 25   | 90.04020000  | 0.45060000   | 0.00000000      |
| 26   | 92.87910000  | 0.34230000   | 0.00000000      |
| 27   | 93.91840000  | 0.71800000   | 0.00000000      |
| 28   | 95.65020000  | 0.39790000   | 0.00000000      |
| 29   | 97.33990000  | 0.76290000   | 0.00000000      |
| 30   | 102.25630000 | 0.74970000   | 0.00000000      |
| 31   | 103.67290000 | 1.40470000   | 0.00000000      |
| 32   | 107.33370000 | 3.01570000   | 0.00000000      |
| 33   | 113.90880000 | 2.03940000   | 0.00000000      |
| 34   | 121.64070000 | 0.89550000   | 0.00000000      |
| 35   | 128.85280000 | 0.82090000   | 0.00000000      |
| 36   | 135.81030000 | 0.71150000   | 0.00000000      |
| 37   | 136.07280000 | 0.64230000   | 0.00000000      |
| 38   | 140.78190000 | 2.45580000   | 0.00000000      |
| 39   | 141.74670000 | 0.72540000   | 0.00000000      |
| 40   | 150.45920000 | 0.75030000   | 0.00000000      |
| 41   | 153.91730000 | 0.23360000   | 0.00000000      |
| 42   | 156.21690000 | 0.92920000   | 0.00000000      |
| 43   | 161.29840000 | 0.35120000   | 0.00000000      |
| 44   | 166.69420000 | 2.70810000   | 0.00000000      |
| 45   | 172.47350000 | 0.06290000   | 0.00000000      |
| 46   | 175.25650000 | 0.27270000   | 0.00000000      |
| 47   | 180.00700000 | 0.36420000   | 0.00000000      |
| 48   | 183.69040000 | 0.67760000   | 0.00000000      |
| 49   | 185.41850000 | 0.28040000   | 0.00000000      |
| 50   | 188.31950000 | 0.37880000   | 0.00000000      |
| 51   | 191.52570000 | 2.12630000   | 0.00000000      |
| 52   | 194.33930000 | 0.61490000   | 0.00000000      |
| 53   | 200.04030000 | 0.71740000   | 0.00000000      |
| 54   | 204.20880000 | 1.50850000   | 0.00000000      |
| 55   | 207.73520000 | 0.52330000   | 0.00000000      |
| 56   | 213.74020000 | 2.59580000   | 0.00000000      |
| 57   | 217.44930000 | 2.60760000   | 0.00000000      |
| 58   | 218.95410000 | 1.98840000   | 0.00000000      |
| 59   | 228.19940000 | 5.65460000   | 0.00000000      |
| 60   | 229.74160000 | 0.87030000   | 0.00000000      |

|     |              |             |            |
|-----|--------------|-------------|------------|
| 61  | 237.53400000 | 1.54270000  | 0.00000000 |
| 62  | 253.95030000 | 1.09750000  | 0.00000000 |
| 63  | 260.76350000 | 4.49380000  | 0.00000000 |
| 64  | 264.82630000 | 0.67850000  | 0.00000000 |
| 65  | 273.43620000 | 2.73690000  | 0.00000000 |
| 66  | 274.32030000 | 5.68810000  | 0.00000000 |
| 67  | 285.06730000 | 0.48810000  | 0.00000000 |
| 68  | 300.27950000 | 0.10710000  | 0.00000000 |
| 69  | 313.59910000 | 0.79960000  | 0.00000000 |
| 70  | 322.06210000 | 6.35980000  | 0.00000000 |
| 71  | 325.81100000 | 0.41370000  | 0.00000000 |
| 72  | 328.22070000 | 3.82820000  | 0.00000000 |
| 73  | 330.54470000 | 3.50750000  | 0.00000000 |
| 74  | 333.70470000 | 2.50610000  | 0.00000000 |
| 75  | 335.55480000 | 2.65550000  | 0.00000000 |
| 76  | 338.03930000 | 2.29200000  | 0.00000000 |
| 77  | 342.68200000 | 1.65800000  | 0.00000000 |
| 78  | 348.05820000 | 2.69730000  | 0.00000000 |
| 79  | 365.88980000 | 3.57070000  | 0.00000000 |
| 80  | 368.98060000 | 7.33160000  | 0.00000000 |
| 81  | 370.32380000 | 8.76490000  | 0.00000000 |
| 82  | 381.24520000 | 1.12430000  | 0.00000000 |
| 83  | 383.64590000 | 10.16880000 | 0.00000000 |
| 84  | 390.21420000 | 2.25970000  | 0.00000000 |
| 85  | 392.63990000 | 3.80110000  | 0.00000000 |
| 86  | 396.96460000 | 2.22230000  | 0.00000000 |
| 87  | 398.20200000 | 10.65870000 | 0.00000000 |
| 88  | 406.24800000 | 0.24220000  | 0.00000000 |
| 89  | 410.94950000 | 0.52470000  | 0.00000000 |
| 90  | 418.51230000 | 3.06450000  | 0.00000000 |
| 91  | 435.62030000 | 8.39480000  | 0.00000000 |
| 92  | 438.16870000 | 10.15650000 | 0.00000000 |
| 93  | 443.13730000 | 13.12730000 | 0.00000000 |
| 94  | 444.21590000 | 7.80290000  | 0.00000000 |
| 95  | 445.57630000 | 24.11700000 | 0.00000000 |
| 96  | 456.56310000 | 2.01320000  | 0.00000000 |
| 97  | 474.48300000 | 28.02500000 | 0.00000000 |
| 98  | 475.14920000 | 28.32570000 | 0.00000000 |
| 99  | 481.06240000 | 3.94380000  | 0.00000000 |
| 100 | 481.50390000 | 3.45520000  | 0.00000000 |
| 101 | 487.26900000 | 10.87710000 | 0.00000000 |
| 102 | 492.71470000 | 15.77710000 | 0.00000000 |
| 103 | 494.51940000 | 0.21980000  | 0.00000000 |
| 104 | 495.32270000 | 0.77340000  | 0.00000000 |
| 105 | 497.53340000 | 0.71200000  | 0.00000000 |
| 106 | 498.25040000 | 0.29270000  | 0.00000000 |
| 107 | 505.95670000 | 0.30070000  | 0.00000000 |
| 108 | 514.57900000 | 2.56240000  | 0.00000000 |
| 109 | 516.61610000 | 5.54710000  | 0.00000000 |
| 110 | 529.73420000 | 24.08820000 | 0.00000000 |
| 111 | 531.96840000 | 19.75220000 | 0.00000000 |
| 112 | 532.13080000 | 15.54820000 | 0.00000000 |
| 113 | 543.84950000 | 2.42350000  | 0.00000000 |
| 114 | 562.98230000 | 1.22800000  | 0.00000000 |
| 115 | 567.07340000 | 0.05650000  | 0.00000000 |
| 116 | 575.33160000 | 1.99730000  | 0.00000000 |
| 117 | 576.63290000 | 3.23000000  | 0.00000000 |
| 118 | 581.09350000 | 0.71290000  | 0.00000000 |
| 119 | 581.27940000 | 0.74650000  | 0.00000000 |
| 120 | 594.84670000 | 16.72900000 | 0.00000000 |
| 121 | 596.44050000 | 23.49130000 | 0.00000000 |
| 122 | 604.28040000 | 5.76870000  | 0.00000000 |
| 123 | 607.34250000 | 0.06920000  | 0.00000000 |
| 124 | 608.15350000 | 6.97240000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 611.14380000 | 57.06160000  | 0.00000000 |
| 126 | 620.70520000 | 17.89930000  | 0.00000000 |
| 127 | 622.09680000 | 38.70430000  | 0.00000000 |
| 128 | 624.75120000 | 16.65830000  | 0.00000000 |
| 129 | 625.38130000 | 21.59150000  | 0.00000000 |
| 130 | 633.00610000 | 31.35090000  | 0.00000000 |
| 131 | 640.74580000 | 3.12500000   | 0.00000000 |
| 132 | 641.59290000 | 1.57290000   | 0.00000000 |
| 133 | 647.17320000 | 82.88330000  | 0.00000000 |
| 134 | 654.16470000 | 1.96400000   | 0.00000000 |
| 135 | 654.39090000 | 0.71880000   | 0.00000000 |
| 136 | 661.28260000 | 0.79640000   | 0.00000000 |
| 137 | 668.01990000 | 0.45280000   | 0.00000000 |
| 138 | 671.05090000 | 3.84090000   | 0.00000000 |
| 139 | 681.66980000 | 0.91280000   | 0.00000000 |
| 140 | 685.15130000 | 0.18600000   | 0.00000000 |
| 141 | 685.71750000 | 0.13490000   | 0.00000000 |
| 142 | 686.39600000 | 2.93450000   | 0.00000000 |
| 143 | 699.13880000 | 112.28450000 | 0.00000000 |
| 144 | 724.63170000 | 23.93340000  | 0.00000000 |
| 145 | 737.49200000 | 62.10620000  | 0.00000000 |
| 146 | 740.27590000 | 8.27670000   | 0.00000000 |
| 147 | 740.98140000 | 1.33780000   | 0.00000000 |
| 148 | 741.90840000 | 3.15210000   | 0.00000000 |
| 149 | 743.65430000 | 4.60150000   | 0.00000000 |
| 150 | 747.92680000 | 2.00490000   | 0.00000000 |
| 151 | 748.83710000 | 0.03100000   | 0.00000000 |
| 152 | 753.39060000 | 61.20590000  | 0.00000000 |
| 153 | 754.30380000 | 93.60240000  | 0.00000000 |
| 154 | 759.21880000 | 61.12190000  | 0.00000000 |
| 155 | 764.10200000 | 106.75910000 | 0.00000000 |
| 156 | 765.94470000 | 90.92460000  | 0.00000000 |
| 157 | 766.36220000 | 27.81050000  | 0.00000000 |
| 158 | 768.64480000 | 128.00170000 | 0.00000000 |
| 159 | 770.14890000 | 22.62640000  | 0.00000000 |
| 160 | 777.29460000 | 61.61580000  | 0.00000000 |
| 161 | 778.45080000 | 94.97170000  | 0.00000000 |
| 162 | 782.86710000 | 15.11100000  | 0.00000000 |
| 163 | 783.00420000 | 18.56850000  | 0.00000000 |
| 164 | 801.13200000 | 35.95970000  | 0.00000000 |
| 165 | 802.38460000 | 97.28930000  | 0.00000000 |
| 166 | 805.83030000 | 86.33270000  | 0.00000000 |
| 167 | 813.51560000 | 2.45090000   | 0.00000000 |
| 168 | 815.03410000 | 3.54090000   | 0.00000000 |
| 169 | 820.07460000 | 3.17970000   | 0.00000000 |
| 170 | 826.74350000 | 33.65330000  | 0.00000000 |
| 171 | 826.81450000 | 6.80880000   | 0.00000000 |
| 172 | 835.47560000 | 25.96070000  | 0.00000000 |
| 173 | 836.67610000 | 92.38600000  | 0.00000000 |
| 174 | 839.53280000 | 57.30820000  | 0.00000000 |
| 175 | 857.65930000 | 0.62920000   | 0.00000000 |
| 176 | 864.07270000 | 57.39910000  | 0.00000000 |
| 177 | 866.90620000 | 14.64380000  | 0.00000000 |
| 178 | 869.23100000 | 3.54410000   | 0.00000000 |
| 179 | 870.03100000 | 2.18360000   | 0.00000000 |
| 180 | 870.54850000 | 21.55290000  | 0.00000000 |
| 181 | 873.87950000 | 32.87260000  | 0.00000000 |
| 182 | 877.20480000 | 53.34860000  | 0.00000000 |
| 183 | 878.20100000 | 22.20020000  | 0.00000000 |
| 184 | 880.86820000 | 0.26040000   | 0.00000000 |
| 185 | 883.37650000 | 8.51130000   | 0.00000000 |
| 186 | 889.26070000 | 6.32520000   | 0.00000000 |
| 187 | 890.36010000 | 0.04750000   | 0.00000000 |
| 188 | 892.52510000 | 0.18150000   | 0.00000000 |

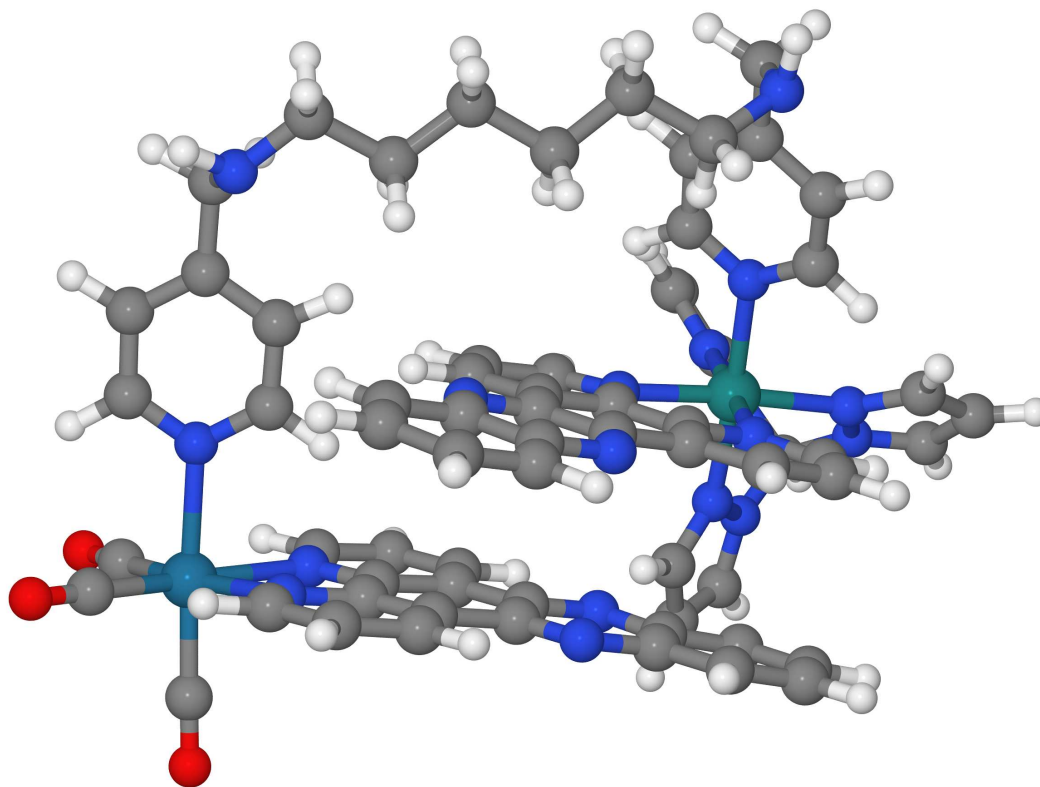
|     |               |             |            |
|-----|---------------|-------------|------------|
| 189 | 900.70560000  | 6.69750000  | 0.00000000 |
| 190 | 916.67300000  | 18.47960000 | 0.00000000 |
| 191 | 919.76130000  | 1.71120000  | 0.00000000 |
| 192 | 920.98640000  | 2.61750000  | 0.00000000 |
| 193 | 921.23170000  | 1.59190000  | 0.00000000 |
| 194 | 922.09790000  | 0.24230000  | 0.00000000 |
| 195 | 946.38910000  | 0.05570000  | 0.00000000 |
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| 197 | 953.09930000  | 2.04430000  | 0.00000000 |
| 198 | 964.65180000  | 4.54640000  | 0.00000000 |
| 199 | 975.63770000  | 11.94940000 | 0.00000000 |
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| 201 | 980.71860000  | 3.57850000  | 0.00000000 |
| 202 | 984.79760000  | 0.88580000  | 0.00000000 |
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| 207 | 993.01510000  | 1.70510000  | 0.00000000 |
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| 212 | 1009.37950000 | 2.58570000  | 0.00000000 |
| 213 | 1009.84250000 | 6.69120000  | 0.00000000 |
| 214 | 1013.26970000 | 20.02660000 | 0.00000000 |
| 215 | 1014.49760000 | 7.97060000  | 0.00000000 |
| 216 | 1018.16990000 | 1.09830000  | 0.00000000 |
| 217 | 1019.56760000 | 1.34460000  | 0.00000000 |
| 218 | 1020.05530000 | 0.28790000  | 0.00000000 |
| 219 | 1021.05830000 | 12.57120000 | 0.00000000 |
| 220 | 1021.96450000 | 14.85290000 | 0.00000000 |
| 221 | 1026.50130000 | 0.46890000  | 0.00000000 |
| 222 | 1027.52890000 | 1.68130000  | 0.00000000 |
| 223 | 1029.80680000 | 2.64430000  | 0.00000000 |
| 224 | 1031.68740000 | 1.66470000  | 0.00000000 |
| 225 | 1033.31720000 | 0.56100000  | 0.00000000 |
| 226 | 1033.52160000 | 3.07220000  | 0.00000000 |
| 227 | 1047.09960000 | 0.15120000  | 0.00000000 |
| 228 | 1051.40600000 | 3.99380000  | 0.00000000 |
| 229 | 1052.78240000 | 10.86610000 | 0.00000000 |
| 230 | 1063.81810000 | 7.67010000  | 0.00000000 |
| 231 | 1070.01100000 | 0.45290000  | 0.00000000 |
| 232 | 1071.12920000 | 0.84790000  | 0.00000000 |
| 233 | 1073.54380000 | 1.89540000  | 0.00000000 |
| 234 | 1074.94280000 | 41.09110000 | 0.00000000 |
| 235 | 1075.44360000 | 54.59560000 | 0.00000000 |
| 236 | 1077.37650000 | 14.54080000 | 0.00000000 |
| 237 | 1080.30230000 | 67.76900000 | 0.00000000 |
| 238 | 1087.39530000 | 8.38540000  | 0.00000000 |
| 239 | 1091.95430000 | 5.10440000  | 0.00000000 |
| 240 | 1092.11430000 | 31.86340000 | 0.00000000 |
| 241 | 1103.58380000 | 4.00610000  | 0.00000000 |
| 242 | 1106.69300000 | 33.17610000 | 0.00000000 |
| 243 | 1111.27490000 | 34.99680000 | 0.00000000 |
| 244 | 1119.78770000 | 0.92430000  | 0.00000000 |
| 245 | 1123.31220000 | 16.26580000 | 0.00000000 |
| 246 | 1125.33570000 | 54.13370000 | 0.00000000 |
| 247 | 1126.20360000 | 47.75000000 | 0.00000000 |
| 248 | 1126.56580000 | 44.31980000 | 0.00000000 |
| 249 | 1131.21000000 | 64.60530000 | 0.00000000 |
| 250 | 1134.36620000 | 80.86200000 | 0.00000000 |
| 251 | 1138.01330000 | 60.98560000 | 0.00000000 |
| 252 | 1145.40850000 | 37.90630000 | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1147.07870000 | 9.26670000   | 0.00000000 |
| 254 | 1150.25660000 | 25.93070000  | 0.00000000 |
| 255 | 1156.08290000 | 1.60160000   | 0.00000000 |
| 256 | 1156.91770000 | 0.69080000   | 0.00000000 |
| 257 | 1162.62220000 | 11.84160000  | 0.00000000 |
| 258 | 1162.90440000 | 21.11040000  | 0.00000000 |
| 259 | 1166.27230000 | 7.27300000   | 0.00000000 |
| 260 | 1176.72720000 | 4.41510000   | 0.00000000 |
| 261 | 1177.42550000 | 0.02460000   | 0.00000000 |
| 262 | 1195.95260000 | 2.37610000   | 0.00000000 |
| 263 | 1212.65090000 | 5.20970000   | 0.00000000 |
| 264 | 1215.58940000 | 4.86370000   | 0.00000000 |
| 265 | 1218.66170000 | 1.68090000   | 0.00000000 |
| 266 | 1220.91940000 | 6.64000000   | 0.00000000 |
| 267 | 1227.02660000 | 10.80980000  | 0.00000000 |
| 268 | 1233.90410000 | 2.36450000   | 0.00000000 |
| 269 | 1238.13200000 | 2.54140000   | 0.00000000 |
| 270 | 1239.13500000 | 0.10700000   | 0.00000000 |
| 271 | 1245.85180000 | 6.81070000   | 0.00000000 |
| 272 | 1245.95810000 | 10.05840000  | 0.00000000 |
| 273 | 1249.81040000 | 9.26870000   | 0.00000000 |
| 274 | 1256.83350000 | 12.94380000  | 0.00000000 |
| 275 | 1262.80480000 | 20.47870000  | 0.00000000 |
| 276 | 1265.33290000 | 7.76790000   | 0.00000000 |
| 277 | 1266.68850000 | 0.35570000   | 0.00000000 |
| 278 | 1268.91220000 | 11.33960000  | 0.00000000 |
| 279 | 1272.13100000 | 63.24840000  | 0.00000000 |
| 280 | 1273.54470000 | 5.80340000   | 0.00000000 |
| 281 | 1275.12730000 | 1.52620000   | 0.00000000 |
| 282 | 1277.26940000 | 9.32800000   | 0.00000000 |
| 283 | 1280.47460000 | 106.07600000 | 0.00000000 |
| 284 | 1294.39750000 | 1.11820000   | 0.00000000 |
| 285 | 1302.18790000 | 0.59180000   | 0.00000000 |
| 286 | 1306.97180000 | 1.78520000   | 0.00000000 |
| 287 | 1307.60840000 | 12.37130000  | 0.00000000 |
| 288 | 1308.95960000 | 2.55020000   | 0.00000000 |
| 289 | 1313.67100000 | 7.33340000   | 0.00000000 |
| 290 | 1317.00020000 | 16.44230000  | 0.00000000 |
| 291 | 1318.45500000 | 21.86670000  | 0.00000000 |
| 292 | 1323.66840000 | 6.29020000   | 0.00000000 |
| 293 | 1327.23480000 | 98.35850000  | 0.00000000 |
| 294 | 1329.03770000 | 128.25620000 | 0.00000000 |
| 295 | 1329.46230000 | 0.78000000   | 0.00000000 |
| 296 | 1330.25190000 | 5.41960000   | 0.00000000 |
| 297 | 1332.65210000 | 6.65640000   | 0.00000000 |
| 298 | 1334.63990000 | 6.24500000   | 0.00000000 |
| 299 | 1339.27110000 | 2.94200000   | 0.00000000 |
| 300 | 1348.10860000 | 9.77150000   | 0.00000000 |
| 301 | 1349.99180000 | 1.12850000   | 0.00000000 |
| 302 | 1360.79550000 | 3.16090000   | 0.00000000 |
| 303 | 1361.83180000 | 2.38690000   | 0.00000000 |
| 304 | 1369.92530000 | 133.54770000 | 0.00000000 |
| 305 | 1370.21590000 | 59.53620000  | 0.00000000 |
| 306 | 1372.18050000 | 60.14280000  | 0.00000000 |
| 307 | 1374.03180000 | 61.88960000  | 0.00000000 |
| 308 | 1374.12640000 | 2.52160000   | 0.00000000 |
| 309 | 1375.44840000 | 76.74880000  | 0.00000000 |
| 310 | 1379.92830000 | 0.50880000   | 0.00000000 |
| 311 | 1380.94040000 | 12.38560000  | 0.00000000 |
| 312 | 1388.62960000 | 20.40130000  | 0.00000000 |
| 313 | 1391.81280000 | 10.44850000  | 0.00000000 |
| 314 | 1399.43650000 | 4.79610000   | 0.00000000 |
| 315 | 1404.27510000 | 10.90730000  | 0.00000000 |
| 316 | 1412.21410000 | 16.79650000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1416.48160000 | 23.22500000   | 0.00000000 |
| 318 | 1418.85170000 | 15.35380000   | 0.00000000 |
| 319 | 1427.14480000 | 2.33570000    | 0.00000000 |
| 320 | 1427.83860000 | 8.52470000    | 0.00000000 |
| 321 | 1440.00820000 | 52.29650000   | 0.00000000 |
| 322 | 1441.84090000 | 37.93110000   | 0.00000000 |
| 323 | 1444.20870000 | 163.33750000  | 0.00000000 |
| 324 | 1453.93370000 | 59.67380000   | 0.00000000 |
| 325 | 1454.93800000 | 138.31790000  | 0.00000000 |
| 326 | 1456.15280000 | 46.85940000   | 0.00000000 |
| 327 | 1463.90760000 | 83.70230000   | 0.00000000 |
| 328 | 1472.77490000 | 14.86960000   | 0.00000000 |
| 329 | 1473.69230000 | 5.91200000    | 0.00000000 |
| 330 | 1474.52100000 | 24.55950000   | 0.00000000 |
| 331 | 1475.41910000 | 2.16740000    | 0.00000000 |
| 332 | 1478.73350000 | 105.63180000  | 0.00000000 |
| 333 | 1479.97480000 | 4.99240000    | 0.00000000 |
| 334 | 1481.23860000 | 70.17660000   | 0.00000000 |
| 335 | 1485.90070000 | 2.34330000    | 0.00000000 |
| 336 | 1491.38380000 | 1.66080000    | 0.00000000 |
| 337 | 1492.93470000 | 19.45860000   | 0.00000000 |
| 338 | 1493.95490000 | 4.73670000    | 0.00000000 |
| 339 | 1494.45230000 | 12.21790000   | 0.00000000 |
| 340 | 1500.70350000 | 8.27640000    | 0.00000000 |
| 341 | 1500.95430000 | 3.16930000    | 0.00000000 |
| 342 | 1502.64110000 | 13.46530000   | 0.00000000 |
| 343 | 1504.97200000 | 4.87150000    | 0.00000000 |
| 344 | 1505.56230000 | 0.67490000    | 0.00000000 |
| 345 | 1505.90020000 | 11.37660000   | 0.00000000 |
| 346 | 1511.14070000 | 17.74570000   | 0.00000000 |
| 347 | 1524.54640000 | 23.13470000   | 0.00000000 |
| 348 | 1525.41900000 | 26.06810000   | 0.00000000 |
| 349 | 1528.28960000 | 44.46160000   | 0.00000000 |
| 350 | 1529.87850000 | 135.71000000  | 0.00000000 |
| 351 | 1536.38130000 | 13.03950000   | 0.00000000 |
| 352 | 1543.72220000 | 19.54690000   | 0.00000000 |
| 353 | 1554.42180000 | 9.17460000    | 0.00000000 |
| 354 | 1555.23420000 | 7.84020000    | 0.00000000 |
| 355 | 1559.45360000 | 12.51520000   | 0.00000000 |
| 356 | 1575.63460000 | 6.18730000    | 0.00000000 |
| 357 | 1576.00150000 | 3.97040000    | 0.00000000 |
| 358 | 1582.32290000 | 34.67260000   | 0.00000000 |
| 359 | 1583.10240000 | 8.65840000    | 0.00000000 |
| 360 | 1601.36890000 | 4.45440000    | 0.00000000 |
| 361 | 1601.77650000 | 9.08770000    | 0.00000000 |
| 362 | 1609.97030000 | 2.00600000    | 0.00000000 |
| 363 | 1613.79160000 | 11.42050000   | 0.00000000 |
| 364 | 1623.03440000 | 0.39170000    | 0.00000000 |
| 365 | 1624.20950000 | 1.79560000    | 0.00000000 |
| 366 | 1625.03420000 | 2.54100000    | 0.00000000 |
| 367 | 1626.01550000 | 4.83880000    | 0.00000000 |
| 368 | 1637.51820000 | 0.23620000    | 0.00000000 |
| 369 | 1639.62150000 | 2.59260000    | 0.00000000 |
| 370 | 1660.76820000 | 3.07110000    | 0.00000000 |
| 371 | 1661.07790000 | 1.24110000    | 0.00000000 |
| 372 | 1663.22130000 | 55.23530000   | 0.00000000 |
| 373 | 1665.19940000 | 110.80250000  | 0.00000000 |
| 374 | 1964.82230000 | 2365.41480000 | 0.00000000 |
| 375 | 1970.90850000 | 2301.50160000 | 0.00000000 |
| 376 | 2084.62310000 | 2076.86660000 | 0.00000000 |
| 377 | 2938.14780000 | 141.55470000  | 0.00000000 |
| 378 | 2983.82020000 | 96.65580000   | 0.00000000 |
| 379 | 2995.40080000 | 8.16950000    | 0.00000000 |
| 380 | 3001.38630000 | 37.28460000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 3011.73070000 | 1.44990000   | 0.00000000 |
| 382 | 3013.82540000 | 192.75010000 | 0.00000000 |
| 383 | 3016.23760000 | 0.16900000   | 0.00000000 |
| 384 | 3023.20660000 | 59.37480000  | 0.00000000 |
| 385 | 3026.46840000 | 80.03540000  | 0.00000000 |
| 386 | 3031.98280000 | 36.22680000  | 0.00000000 |
| 387 | 3045.99250000 | 1.98110000   | 0.00000000 |
| 388 | 3051.12200000 | 57.61280000  | 0.00000000 |
| 389 | 3055.31470000 | 25.90860000  | 0.00000000 |
| 390 | 3064.34640000 | 51.57810000  | 0.00000000 |
| 391 | 3067.19580000 | 34.58580000  | 0.00000000 |
| 392 | 3068.43760000 | 269.38370000 | 0.00000000 |
| 393 | 3187.34150000 | 2.60270000   | 0.00000000 |
| 394 | 3187.59520000 | 2.45710000   | 0.00000000 |
| 395 | 3188.19500000 | 1.33110000   | 0.00000000 |
| 396 | 3194.80160000 | 3.75130000   | 0.00000000 |
| 397 | 3196.36320000 | 3.56100000   | 0.00000000 |
| 398 | 3197.09980000 | 7.94440000   | 0.00000000 |
| 399 | 3197.23970000 | 6.24590000   | 0.00000000 |
| 400 | 3207.43420000 | 21.68840000  | 0.00000000 |
| 401 | 3207.80230000 | 22.25280000  | 0.00000000 |
| 402 | 3213.00270000 | 0.85440000   | 0.00000000 |
| 403 | 3214.44120000 | 0.22970000   | 0.00000000 |
| 404 | 3214.52410000 | 0.05050000   | 0.00000000 |
| 405 | 3215.88130000 | 0.12560000   | 0.00000000 |
| 406 | 3216.37860000 | 13.34510000  | 0.00000000 |
| 407 | 3216.87810000 | 0.10650000   | 0.00000000 |
| 408 | 3217.98330000 | 8.78020000   | 0.00000000 |
| 409 | 3223.75310000 | 9.82970000   | 0.00000000 |
| 410 | 3226.19260000 | 7.13490000   | 0.00000000 |
| 411 | 3226.48060000 | 5.51000000   | 0.00000000 |
| 412 | 3226.57400000 | 2.86590000   | 0.00000000 |
| 413 | 3227.57350000 | 5.25190000   | 0.00000000 |
| 414 | 3231.31920000 | 4.70940000   | 0.00000000 |
| 415 | 3231.79760000 | 2.56310000   | 0.00000000 |
| 416 | 3232.45330000 | 2.72140000   | 0.00000000 |
| 417 | 3237.28580000 | 11.09540000  | 0.00000000 |
| 418 | 3238.50920000 | 86.60270000  | 0.00000000 |
| 419 | 3244.55670000 | 4.72660000   | 0.00000000 |
| 420 | 3245.53630000 | 12.46870000  | 0.00000000 |
| 421 | 3255.47020000 | 0.46450000   | 0.00000000 |
| 422 | 3258.44790000 | 8.59020000   | 0.00000000 |
| 423 | 3268.27830000 | 3.97160000   | 0.00000000 |
| 424 | 3268.75700000 | 13.02870000  | 0.00000000 |
| 425 | 3269.33680000 | 7.08220000   | 0.00000000 |
| 426 | 3279.10410000 | 3.86640000   | 0.00000000 |
| 427 | 3281.11360000 | 4.55980000   | 0.00000000 |
| 428 | 3283.44100000 | 4.40340000   | 0.00000000 |
| 429 | 3289.17870000 | 2.05280000   | 0.00000000 |
| 430 | 3290.86100000 | 1.74270000   | 0.00000000 |
| 431 | 3527.35300000 | 0.91490000   | 0.00000000 |
| 432 | 3564.48160000 | 6.02960000   | 0.00000000 |



S10. CALCULATIONS ON ALTERNATIVE CONFORMER OF  $2^{3+}$  ( $^3A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]<br>1n7ccc1)[n+]1n8ccc1)[n+]1ccc(cc1)CNCCCCCNCCc1cc[n+](cc1)[Re]<br>1([n+]2cccc3c2c2[n+]1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O] |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -3972.51407222   | a.u. |
| Gibbs Energy                    | : -3971.48327600   | a.u. |
| Number of imaginary frequencies | : 0  |      |

## S10.1. Cartesian Co-ordinates (XYZ format)

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|   |            |            |             |
|---|------------|------------|-------------|
| C | 2.63658810 | 5.68639898 | 0.45733401  |
| H | 2.45467496 | 5.91006994 | 1.51244295  |
| H | 2.60113096 | 4.59526014 | 0.36840901  |
| C | 1.52221000 | 6.29957485 | -0.39988101 |
| H | 1.82287097 | 6.30222893 | -1.45269501 |
| H | 1.38178694 | 7.34906816 | -0.11564200 |
| C | 0.20091499 | 5.53790998 | -0.28457400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.09738600 | 5.45211411  | 0.76749998  |
| H | 0.35665700  | 4.51145792  | -0.64023900 |
| C | -0.93219399 | 6.18371201  | -1.08694398 |
| H | -0.56105202 | 6.44911194  | -2.08460808 |
| H | -1.22730994 | 7.12540913  | -0.60862303 |
| C | -3.31616998 | 5.92019176  | -1.96958101 |
| H | -2.96199799 | 6.33886719  | -2.92636800 |
| H | -3.68762994 | 6.75949621  | -1.37499905 |
| N | 4.00817585  | 6.11103916  | 0.14338300  |
| C | -4.29034615 | 4.04411507  | -3.27489400 |
| H | -3.27445197 | 4.10194016  | -3.67679095 |
| H | -4.97146177 | 4.28186178  | -4.09732580 |
| N | -4.43283796 | 4.98728800  | -2.15678811 |
| C | 4.48181200  | 5.69535923  | -1.17793095 |
| H | 3.84392500  | 6.01085377  | -2.01415896 |
| H | 5.46597815  | 6.14446783  | -1.33938599 |
| C | 6.25262499  | -3.10914993 | -1.53289604 |
| N | 5.88362885  | -2.39515090 | -2.73363209 |
| N | 7.03633118  | -2.25697207 | -0.66767699 |
| N | 5.07205296  | -3.58551502 | -0.84153199 |
| N | 5.14185381  | -1.26000595 | -2.63560700 |
| C | 6.23892879  | -2.64140511 | -4.01996613 |
| N | 6.50656080  | -1.10093105 | -0.17665100 |
| C | 8.31488800  | -2.43209410 | -0.25063199 |
| N | 4.15710878  | -2.68168902 | -0.39224699 |
| C | 4.66892195  | -4.84675121 | -0.57389998 |
| C | 5.02983379  | -0.78881001 | -3.87929893 |
| C | 5.70310783  | -1.62590897 | -4.78176785 |
| H | 6.82752085  | -3.50483894 | -4.28155804 |
| C | 7.47602320  | -0.55185503 | 0.56085801  |
| C | 8.62808132  | -1.34976304 | 0.54150802  |
| H | 8.88388634  | -3.29852605 | -0.54368901 |
| C | 3.16327190  | -3.38889790 | 0.16509800  |
| C | 3.44767308  | -4.75310421 | 0.07484800  |
| H | 5.26649094  | -5.69796991 | -0.85574001 |
| N | -3.32331109 | -2.26929402 | -0.78657699 |
| N | -4.71112490 | -0.99108303 | 1.12624204  |
| H | 4.48797894  | 0.11809100  | -4.08265018 |
| H | 5.78290796  | -1.50212395 | -5.84753609 |
| H | 7.32930613  | 0.38103500  | 1.07444096  |
| H | 9.56057358  | -1.15759504 | 1.04249704  |
| H | 2.31373596  | -2.89006996 | 0.61264700  |
| H | 2.84619093  | -5.56858110 | 0.43688801  |
| C | -2.66560102 | -2.88297701 | -1.77266300 |
| C | -2.65059400 | -1.93384600 | 0.35014400  |
| C | -3.39508700 | -1.24939704 | 1.37383604  |
| C | -5.41880798 | -0.32719401 | 2.04316092  |
| C | -1.31473601 | -3.22148108 | -1.66613102 |
| H | -3.23276806 | -3.12228298 | -2.66049004 |
| C | -1.28694499 | -2.24044991 | 0.53305101  |
| C | -2.77304196 | -0.86771500 | 2.57305002  |
| C | -4.86585093 | 0.09280100  | 3.25476098  |
| H | -6.45534611 | -0.13265499 | 1.80772603  |
| C | -0.63117099 | -2.91798401 | -0.50754797 |
| H | -0.82765800 | -3.72663689 | -2.48835897 |
| C | -0.63049603 | -1.89208603 | 1.78408098  |
| C | -3.54227209 | -0.18740900 | 3.52800703  |
| C | -1.37216604 | -1.20367205 | 2.79823709  |
| H | -5.48312616 | 0.63138998  | 3.95956206  |
| H | 0.40444401  | -3.19580293 | -0.39152399 |
| N | 0.64029598  | -2.25318408 | 1.97701299  |
| H | -3.07653904 | 0.11510000  | 4.45487309  |
| N | -0.82622403 | -0.86702102 | 3.95998812  |
| C | 1.19380498  | -1.96392405 | 3.18293405  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.45716399  | -1.23427200 | 4.17565584  |
| C | 2.50798202  | -2.39165902 | 3.48819399  |
| C | 1.07871306  | -0.91174102 | 5.40611410  |
| C | 3.07628202  | -2.08014107 | 4.70132923  |
| H | 3.05603504  | -2.96846390 | 2.75692701  |
| C | 2.36346698  | -1.32767904 | 5.66265297  |
| H | 0.50646001  | -0.34382999 | 6.12880993  |
| H | 4.08359289  | -2.41026902 | 4.92290497  |
| H | 2.83557391  | -1.08254802 | 6.60585594  |
| N | 3.76636600  | -0.08573600 | 1.13954902  |
| N | 2.48271608  | -0.43148899 | -1.15720296 |
| C | 4.44718409  | 0.05772200  | 2.28133392  |
| C | 2.47366905  | 0.38869700  | 1.06625795  |
| C | 1.78575099  | 0.18748300  | -0.14323500 |
| C | 1.85613000  | -0.73533797 | -2.29725909 |
| C | 3.91330791  | 0.71696198  | 3.38362503  |
| H | 5.43882799  | -0.36985001 | 2.31277490  |
| C | 1.86160696  | 1.03814805  | 2.16148710  |
| C | 0.44027600  | 0.59976900  | -0.31630799 |
| C | 0.52630597  | -0.38544500 | -2.51799607 |
| H | 2.43263412  | -1.26175702 | -3.04488492 |
| C | 2.61384201  | 1.21606302  | 3.32009196  |
| H | 4.50953007  | 0.81629097  | 4.27851486  |
| C | 0.47945699  | 1.49183500  | 2.02380395  |
| C | -0.17101599 | 0.30959001  | -1.53401196 |
| C | -0.22656900 | 1.28826404  | 0.78199297  |
| H | 0.05863100  | -0.64837998 | -3.45551896 |
| H | 2.16729593  | 1.72719800  | 4.16097784  |
| N | -0.10421600 | 2.06283903  | 3.06280088  |
| H | -1.19414198 | 0.61274701  | -1.69888794 |
| N | -1.47333002 | 1.71076906  | 0.61965901  |
| C | -1.38960195 | 2.47100210  | 2.92121196  |
| C | -2.07884192 | 2.31422997  | 1.67544305  |
| C | -2.06103396 | 3.05532289  | 4.02006197  |
| C | -3.40876293 | 2.78381705  | 1.56358194  |
| C | -3.36180711 | 3.48175097  | 3.88621497  |
| H | -1.52152598 | 3.14907789  | 4.95418596  |
| C | -4.03409719 | 3.35160089  | 2.64916110  |
| H | -3.92256188 | 2.67916894  | 0.61933100  |
| H | -3.87714911 | 3.92410111  | 4.72976112  |
| H | -5.05598688 | 3.69887900  | 2.55933094  |
| H | 6.85706282  | -3.96518111 | -1.81264901 |
| C | 4.61756420  | 4.19293880  | -1.20630896 |
| C | 5.36010981  | 3.53751493  | -0.22308500 |
| C | 3.95723391  | 3.40182590  | -2.14248896 |
| C | 5.38415813  | 2.16012001  | -0.18860599 |
| H | 5.87987614  | 4.10030508  | 0.53953302  |
| C | 4.01017809  | 2.02202797  | -2.03903699 |
| H | 3.35877705  | 3.84608412  | -2.92684507 |
| N | 4.70286989  | 1.39734697  | -1.06902003 |
| H | 5.92278004  | 1.64903200  | 0.58991897  |
| H | 3.44469905  | 1.40537500  | -2.71965790 |
| C | -4.54187918 | 2.63233399  | -2.79579091 |
| C | -3.66316009 | 2.03086996  | -1.89512396 |
| C | -5.66949987 | 1.89946103  | -3.16220808 |
| C | -3.94706202 | 0.78408998  | -1.37996197 |
| H | -2.77076793 | 2.53346801  | -1.55255699 |
| C | -5.89079285 | 0.64824599  | -2.60705900 |
| H | -6.39114618 | 2.29931903  | -3.86333108 |
| N | -5.05205393 | 0.08908400  | -1.71176398 |
| H | -3.27749109 | 0.34520799  | -0.65871602 |
| H | -6.76865387 | 0.07494600  | -2.86984205 |
| H | -5.30070305 | 5.49688005  | -2.25547099 |
| C | -2.14566398 | 5.26834393  | -1.23536205 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -2.49154711 | 4.92949009  | -0.25319499 |
| H  | -1.82812905 | 4.37210703  | -1.77944005 |
| H  | 4.09288120  | 7.11821604  | 0.22937299  |
| Ru | 4.47652721  | -0.69533098 | -0.70424002 |
| Re | -5.50316906 | -1.87761605 | -0.74338597 |
| C  | -5.81261206 | -3.57171011 | 0.15748601  |
| O  | -5.98507214 | -4.57498598 | 0.69699699  |
| C  | -5.93725920 | -2.68404889 | -2.45244408 |
| O  | -6.16426611 | -3.16761804 | -3.47510004 |
| C  | -7.36147308 | -1.38723505 | -0.48671001 |
| O  | -8.45897198 | -1.08044100 | -0.30700999 |

## S10.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 2.59830000   | 1.51740000   | 0.00000000      |
| 2    | 10.25600000  | 0.72530000   | 0.00000000      |
| 3    | 16.13430000  | 0.95740000   | 0.00000000      |
| 4    | 21.84680000  | 0.61690000   | 0.00000000      |
| 5    | 24.19140000  | 0.41520000   | 0.00000000      |
| 6    | 32.32940000  | 0.32180000   | 0.00000000      |
| 7    | 34.84780000  | 3.71420000   | 0.00000000      |
| 8    | 39.52480000  | 1.26940000   | 0.00000000      |
| 9    | 40.26980000  | 0.05720000   | 0.00000000      |
| 10   | 42.35600000  | 1.82230000   | 0.00000000      |
| 11   | 48.61550000  | 0.80870000   | 0.00000000      |
| 12   | 51.27230000  | 1.04060000   | 0.00000000      |
| 13   | 56.14480000  | 0.80870000   | 0.00000000      |
| 14   | 57.89860000  | 1.52400000   | 0.00000000      |
| 15   | 64.05590000  | 1.60980000   | 0.00000000      |
| 16   | 64.27180000  | 2.27620000   | 0.00000000      |
| 17   | 66.36000000  | 0.87990000   | 0.00000000      |
| 18   | 71.18490000  | 0.57630000   | 0.00000000      |
| 19   | 72.54230000  | 2.78430000   | 0.00000000      |
| 20   | 75.26420000  | 1.15340000   | 0.00000000      |
| 21   | 81.52270000  | 0.69670000   | 0.00000000      |
| 22   | 82.99270000  | 1.20460000   | 0.00000000      |
| 23   | 86.27170000  | 8.58340000   | 0.00000000      |
| 24   | 88.04370000  | 0.90150000   | 0.00000000      |
| 25   | 92.01670000  | 0.68730000   | 0.00000000      |
| 26   | 93.17230000  | 1.26340000   | 0.00000000      |
| 27   | 94.73550000  | 3.76500000   | 0.00000000      |
| 28   | 94.90190000  | 1.18060000   | 0.00000000      |
| 29   | 97.66670000  | 0.94930000   | 0.00000000      |
| 30   | 108.89750000 | 2.59940000   | 0.00000000      |
| 31   | 112.81990000 | 5.38060000   | 0.00000000      |
| 32   | 116.24730000 | 3.20960000   | 0.00000000      |
| 33   | 117.53560000 | 4.80100000   | 0.00000000      |
| 34   | 121.44340000 | 2.18080000   | 0.00000000      |
| 35   | 132.85430000 | 2.97430000   | 0.00000000      |
| 36   | 136.42450000 | 5.97290000   | 0.00000000      |
| 37   | 137.52770000 | 4.36450000   | 0.00000000      |
| 38   | 140.72900000 | 0.14770000   | 0.00000000      |
| 39   | 145.60120000 | 1.69190000   | 0.00000000      |
| 40   | 148.38920000 | 2.06750000   | 0.00000000      |
| 41   | 151.07250000 | 2.39130000   | 0.00000000      |
| 42   | 156.44370000 | 2.93350000   | 0.00000000      |
| 43   | 162.53320000 | 0.24300000   | 0.00000000      |
| 44   | 165.82440000 | 1.59130000   | 0.00000000      |
| 45   | 168.18850000 | 0.30220000   | 0.00000000      |
| 46   | 176.82060000 | 2.19370000   | 0.00000000      |
| 47   | 177.88530000 | 0.48260000   | 0.00000000      |
| 48   | 181.21640000 | 3.76810000   | 0.00000000      |
| 49   | 183.32260000 | 4.63300000   | 0.00000000      |
| 50   | 187.88790000 | 7.06590000   | 0.00000000      |
| 51   | 190.60500000 | 3.77800000   | 0.00000000      |
| 52   | 193.39470000 | 7.07380000   | 0.00000000      |
| 53   | 196.02830000 | 3.51690000   | 0.00000000      |
| 54   | 203.30150000 | 3.97510000   | 0.00000000      |
| 55   | 205.72360000 | 8.43740000   | 0.00000000      |
| 56   | 215.09590000 | 6.69170000   | 0.00000000      |
| 57   | 219.27080000 | 1.56850000   | 0.00000000      |
| 58   | 221.08700000 | 2.22230000   | 0.00000000      |
| 59   | 226.79940000 | 6.08320000   | 0.00000000      |
| 60   | 231.78950000 | 56.41390000  | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 235.75350000 | 2.55260000   | 0.00000000 |
| 62  | 252.97400000 | 2.52450000   | 0.00000000 |
| 63  | 258.47610000 | 1.58720000   | 0.00000000 |
| 64  | 261.43710000 | 4.12970000   | 0.00000000 |
| 65  | 273.89940000 | 16.21640000  | 0.00000000 |
| 66  | 276.84060000 | 11.74780000  | 0.00000000 |
| 67  | 287.82880000 | 20.72110000  | 0.00000000 |
| 68  | 300.57990000 | 26.81870000  | 0.00000000 |
| 69  | 306.05370000 | 7.62640000   | 0.00000000 |
| 70  | 312.28770000 | 20.59610000  | 0.00000000 |
| 71  | 323.10590000 | 15.69790000  | 0.00000000 |
| 72  | 323.57220000 | 4.53970000   | 0.00000000 |
| 73  | 326.89660000 | 5.64910000   | 0.00000000 |
| 74  | 329.85020000 | 10.81440000  | 0.00000000 |
| 75  | 332.38820000 | 3.66390000   | 0.00000000 |
| 76  | 334.21550000 | 9.90170000   | 0.00000000 |
| 77  | 335.59270000 | 12.01270000  | 0.00000000 |
| 78  | 343.70290000 | 7.46480000   | 0.00000000 |
| 79  | 359.13510000 | 1.79330000   | 0.00000000 |
| 80  | 364.53650000 | 2.79010000   | 0.00000000 |
| 81  | 375.44520000 | 2.19600000   | 0.00000000 |
| 82  | 376.42790000 | 136.76580000 | 0.00000000 |
| 83  | 379.38870000 | 7.11970000   | 0.00000000 |
| 84  | 387.91840000 | 1.77730000   | 0.00000000 |
| 85  | 389.69030000 | 1.47770000   | 0.00000000 |
| 86  | 396.98740000 | 42.03700000  | 0.00000000 |
| 87  | 397.21960000 | 8.81740000   | 0.00000000 |
| 88  | 410.03840000 | 106.13630000 | 0.00000000 |
| 89  | 410.39330000 | 0.54710000   | 0.00000000 |
| 90  | 412.88470000 | 5.70950000   | 0.00000000 |
| 91  | 429.55530000 | 16.11400000  | 0.00000000 |
| 92  | 434.15710000 | 44.23240000  | 0.00000000 |
| 93  | 435.76850000 | 20.56470000  | 0.00000000 |
| 94  | 437.57990000 | 35.27640000  | 0.00000000 |
| 95  | 446.06040000 | 24.56070000  | 0.00000000 |
| 96  | 455.91710000 | 5.05520000   | 0.00000000 |
| 97  | 458.92530000 | 7.34360000   | 0.00000000 |
| 98  | 475.06070000 | 27.50440000  | 0.00000000 |
| 99  | 476.09960000 | 26.89670000  | 0.00000000 |
| 100 | 483.32760000 | 6.01810000   | 0.00000000 |
| 101 | 489.14110000 | 13.56700000  | 0.00000000 |
| 102 | 490.29920000 | 16.75500000  | 0.00000000 |
| 103 | 491.53510000 | 11.30540000  | 0.00000000 |
| 104 | 494.09090000 | 2.72360000   | 0.00000000 |
| 105 | 495.55510000 | 1.30860000   | 0.00000000 |
| 106 | 496.46820000 | 2.52420000   | 0.00000000 |
| 107 | 498.20150000 | 10.89360000  | 0.00000000 |
| 108 | 514.80800000 | 7.51700000   | 0.00000000 |
| 109 | 518.27360000 | 2.11270000   | 0.00000000 |
| 110 | 530.94680000 | 15.16470000  | 0.00000000 |
| 111 | 532.89070000 | 18.90860000  | 0.00000000 |
| 112 | 533.22430000 | 51.54950000  | 0.00000000 |
| 113 | 545.63340000 | 3.75540000   | 0.00000000 |
| 114 | 547.15210000 | 8.73250000   | 0.00000000 |
| 115 | 560.57510000 | 27.50020000  | 0.00000000 |
| 116 | 571.85370000 | 5.75880000   | 0.00000000 |
| 117 | 574.52880000 | 0.28090000   | 0.00000000 |
| 118 | 576.69840000 | 15.98690000  | 0.00000000 |
| 119 | 579.01610000 | 7.76200000   | 0.00000000 |
| 120 | 592.10240000 | 8.12910000   | 0.00000000 |
| 121 | 593.59790000 | 146.79050000 | 0.00000000 |
| 122 | 593.82930000 | 204.68360000 | 0.00000000 |
| 123 | 601.54000000 | 5.22750000   | 0.00000000 |
| 124 | 602.29580000 | 0.80580000   | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 610.29400000 | 92.10300000  | 0.00000000 |
| 126 | 611.44030000 | 28.11280000  | 0.00000000 |
| 127 | 616.90810000 | 59.43210000  | 0.00000000 |
| 128 | 619.04990000 | 13.54600000  | 0.00000000 |
| 129 | 625.87020000 | 22.72080000  | 0.00000000 |
| 130 | 630.12520000 | 338.91270000 | 0.00000000 |
| 131 | 630.21430000 | 319.07240000 | 0.00000000 |
| 132 | 633.57940000 | 20.95730000  | 0.00000000 |
| 133 | 647.07380000 | 103.93060000 | 0.00000000 |
| 134 | 647.49260000 | 3.47330000   | 0.00000000 |
| 135 | 653.57890000 | 5.46740000   | 0.00000000 |
| 136 | 654.32350000 | 2.42370000   | 0.00000000 |
| 137 | 668.07770000 | 1.85150000   | 0.00000000 |
| 138 | 669.43260000 | 4.50180000   | 0.00000000 |
| 139 | 670.01440000 | 8.16410000   | 0.00000000 |
| 140 | 674.21000000 | 3.57300000   | 0.00000000 |
| 141 | 683.72140000 | 0.04030000   | 0.00000000 |
| 142 | 686.34850000 | 0.40630000   | 0.00000000 |
| 143 | 700.62840000 | 107.63710000 | 0.00000000 |
| 144 | 720.25730000 | 113.68160000 | 0.00000000 |
| 145 | 725.95610000 | 26.57000000  | 0.00000000 |
| 146 | 736.56190000 | 66.88220000  | 0.00000000 |
| 147 | 737.80040000 | 169.09170000 | 0.00000000 |
| 148 | 738.02080000 | 31.55960000  | 0.00000000 |
| 149 | 739.79310000 | 15.57820000  | 0.00000000 |
| 150 | 742.00470000 | 2.27740000   | 0.00000000 |
| 151 | 744.81910000 | 230.52400000 | 0.00000000 |
| 152 | 748.39790000 | 35.90680000  | 0.00000000 |
| 153 | 750.63110000 | 63.67600000  | 0.00000000 |
| 154 | 753.40820000 | 4.88370000   | 0.00000000 |
| 155 | 765.89220000 | 44.71820000  | 0.00000000 |
| 156 | 769.65490000 | 23.18600000  | 0.00000000 |
| 157 | 771.45610000 | 47.87310000  | 0.00000000 |
| 158 | 772.96300000 | 100.05260000 | 0.00000000 |
| 159 | 774.34810000 | 58.77280000  | 0.00000000 |
| 160 | 774.99550000 | 134.59570000 | 0.00000000 |
| 161 | 776.37180000 | 312.67640000 | 0.00000000 |
| 162 | 780.93530000 | 15.28180000  | 0.00000000 |
| 163 | 784.21640000 | 8.94460000   | 0.00000000 |
| 164 | 793.75850000 | 156.70850000 | 0.00000000 |
| 165 | 794.57050000 | 93.94250000  | 0.00000000 |
| 166 | 799.28240000 | 30.26140000  | 0.00000000 |
| 167 | 799.93130000 | 33.60160000  | 0.00000000 |
| 168 | 801.84300000 | 19.84300000  | 0.00000000 |
| 169 | 804.70660000 | 2.77970000   | 0.00000000 |
| 170 | 808.97780000 | 82.10600000  | 0.00000000 |
| 171 | 814.44130000 | 10.58220000  | 0.00000000 |
| 172 | 825.14070000 | 52.20970000  | 0.00000000 |
| 173 | 831.54640000 | 69.29370000  | 0.00000000 |
| 174 | 834.76050000 | 21.72810000  | 0.00000000 |
| 175 | 841.04300000 | 1.12050000   | 0.00000000 |
| 176 | 856.12380000 | 6.96210000   | 0.00000000 |
| 177 | 865.49830000 | 123.82460000 | 0.00000000 |
| 178 | 866.74390000 | 30.30070000  | 0.00000000 |
| 179 | 873.45960000 | 167.26350000 | 0.00000000 |
| 180 | 875.27290000 | 171.70550000 | 0.00000000 |
| 181 | 876.71360000 | 7.04340000   | 0.00000000 |
| 182 | 879.57300000 | 4.07290000   | 0.00000000 |
| 183 | 880.18110000 | 25.40580000  | 0.00000000 |
| 184 | 881.96490000 | 0.51060000   | 0.00000000 |
| 185 | 883.51060000 | 1.55660000   | 0.00000000 |
| 186 | 884.30730000 | 12.84790000  | 0.00000000 |
| 187 | 888.53410000 | 5.18430000   | 0.00000000 |
| 188 | 900.53830000 | 7.46310000   | 0.00000000 |

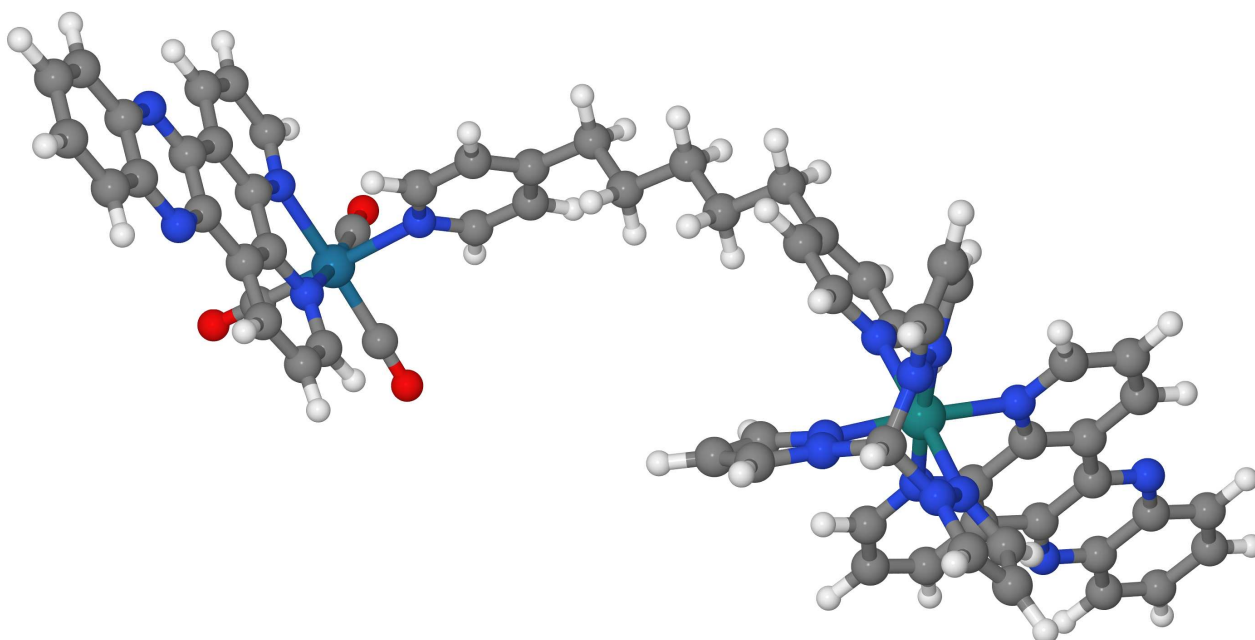
|     |               |               |            |
|-----|---------------|---------------|------------|
| 189 | 912.72970000  | 17.16600000   | 0.00000000 |
| 190 | 916.65120000  | 1.39090000    | 0.00000000 |
| 191 | 918.71330000  | 3.89290000    | 0.00000000 |
| 192 | 919.56910000  | 0.54470000    | 0.00000000 |
| 193 | 930.00300000  | 2.86400000    | 0.00000000 |
| 194 | 935.26230000  | 4.18660000    | 0.00000000 |
| 195 | 940.70380000  | 13.63820000   | 0.00000000 |
| 196 | 945.22770000  | 1.12300000    | 0.00000000 |
| 197 | 950.63120000  | 4.12930000    | 0.00000000 |
| 198 | 963.84980000  | 7.68160000    | 0.00000000 |
| 199 | 972.83200000  | 8.86000000    | 0.00000000 |
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| 205 | 984.04240000  | 5.59190000    | 0.00000000 |
| 206 | 988.40840000  | 38.71960000   | 0.00000000 |
| 207 | 993.22160000  | 0.09350000    | 0.00000000 |
| 208 | 996.62770000  | 58.85530000   | 0.00000000 |
| 209 | 998.51030000  | 4.05540000    | 0.00000000 |
| 210 | 1001.63560000 | 5.24640000    | 0.00000000 |
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| 212 | 1003.90570000 | 30.47770000   | 0.00000000 |
| 213 | 1005.77840000 | 22.09050000   | 0.00000000 |
| 214 | 1005.86560000 | 1.88660000    | 0.00000000 |
| 215 | 1005.92880000 | 8.65480000    | 0.00000000 |
| 216 | 1012.25700000 | 13.74160000   | 0.00000000 |
| 217 | 1013.62710000 | 18.21240000   | 0.00000000 |
| 218 | 1018.54560000 | 39.20320000   | 0.00000000 |
| 219 | 1021.15440000 | 4.27930000    | 0.00000000 |
| 220 | 1024.51930000 | 1.82340000    | 0.00000000 |
| 221 | 1024.70340000 | 3.12530000    | 0.00000000 |
| 222 | 1025.70730000 | 40.46060000   | 0.00000000 |
| 223 | 1030.13070000 | 84.98150000   | 0.00000000 |
| 224 | 1036.01410000 | 117.97310000  | 0.00000000 |
| 225 | 1039.86000000 | 87.23870000   | 0.00000000 |
| 226 | 1043.20860000 | 4.65830000    | 0.00000000 |
| 227 | 1047.45870000 | 0.63620000    | 0.00000000 |
| 228 | 1054.08160000 | 4.44730000    | 0.00000000 |
| 229 | 1057.57750000 | 1376.37440000 | 0.00000000 |
| 230 | 1058.78360000 | 860.19390000  | 0.00000000 |
| 231 | 1062.11020000 | 1151.21980000 | 0.00000000 |
| 232 | 1063.52790000 | 11.02700000   | 0.00000000 |
| 233 | 1067.83110000 | 11.00150000   | 0.00000000 |
| 234 | 1072.94370000 | 5.01280000    | 0.00000000 |
| 235 | 1078.23430000 | 116.15380000  | 0.00000000 |
| 236 | 1081.59470000 | 83.19720000   | 0.00000000 |
| 237 | 1085.05290000 | 113.62630000  | 0.00000000 |
| 238 | 1088.08340000 | 32.38880000   | 0.00000000 |
| 239 | 1092.27540000 | 28.59000000   | 0.00000000 |
| 240 | 1097.86730000 | 617.09220000  | 0.00000000 |
| 241 | 1100.14230000 | 36.52690000   | 0.00000000 |
| 242 | 1103.48880000 | 4.12550000    | 0.00000000 |
| 243 | 1109.48940000 | 30.18430000   | 0.00000000 |
| 244 | 1110.45830000 | 27.49120000   | 0.00000000 |
| 245 | 1119.29460000 | 38.45560000   | 0.00000000 |
| 246 | 1123.96400000 | 20.70560000   | 0.00000000 |
| 247 | 1130.10710000 | 76.62390000   | 0.00000000 |
| 248 | 1131.36400000 | 79.35720000   | 0.00000000 |
| 249 | 1133.80360000 | 772.64240000  | 0.00000000 |
| 250 | 1134.59480000 | 299.83820000  | 0.00000000 |
| 251 | 1143.13810000 | 49.67040000   | 0.00000000 |
| 252 | 1143.86050000 | 463.74810000  | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1147.82330000 | 174.63310000  | 0.00000000 |
| 254 | 1148.76890000 | 0.90200000    | 0.00000000 |
| 255 | 1150.55480000 | 33.28380000   | 0.00000000 |
| 256 | 1153.13460000 | 23.17730000   | 0.00000000 |
| 257 | 1156.04820000 | 507.41550000  | 0.00000000 |
| 258 | 1158.44510000 | 1390.62710000 | 0.00000000 |
| 259 | 1161.70630000 | 1587.92800000 | 0.00000000 |
| 260 | 1167.18580000 | 8.03120000    | 0.00000000 |
| 261 | 1168.45570000 | 579.01840000  | 0.00000000 |
| 262 | 1176.44240000 | 253.17820000  | 0.00000000 |
| 263 | 1195.35530000 | 1.91710000    | 0.00000000 |
| 264 | 1205.54690000 | 53.50660000   | 0.00000000 |
| 265 | 1211.15180000 | 245.75150000  | 0.00000000 |
| 266 | 1216.11410000 | 169.85330000  | 0.00000000 |
| 267 | 1221.74260000 | 4.95530000    | 0.00000000 |
| 268 | 1227.70560000 | 34.06270000   | 0.00000000 |
| 269 | 1233.74590000 | 83.88930000   | 0.00000000 |
| 270 | 1238.22070000 | 37.83650000   | 0.00000000 |
| 271 | 1240.22140000 | 71.76360000   | 0.00000000 |
| 272 | 1246.19950000 | 6.49770000    | 0.00000000 |
| 273 | 1253.10610000 | 248.53970000  | 0.00000000 |
| 274 | 1253.34650000 | 878.88050000  | 0.00000000 |
| 275 | 1258.74520000 | 318.83230000  | 0.00000000 |
| 276 | 1259.95560000 | 58.16260000   | 0.00000000 |
| 277 | 1263.19490000 | 196.14510000  | 0.00000000 |
| 278 | 1265.76680000 | 144.44110000  | 0.00000000 |
| 279 | 1266.96750000 | 349.17790000  | 0.00000000 |
| 280 | 1277.14570000 | 1242.72310000 | 0.00000000 |
| 281 | 1277.39430000 | 141.77490000  | 0.00000000 |
| 282 | 1279.02910000 | 108.66620000  | 0.00000000 |
| 283 | 1283.97110000 | 85.03790000   | 0.00000000 |
| 284 | 1287.18670000 | 830.30300000  | 0.00000000 |
| 285 | 1294.89230000 | 275.55600000  | 0.00000000 |
| 286 | 1295.65950000 | 27.08410000   | 0.00000000 |
| 287 | 1303.94350000 | 2.90760000    | 0.00000000 |
| 288 | 1305.96690000 | 1245.76740000 | 0.00000000 |
| 289 | 1308.79180000 | 23.77340000   | 0.00000000 |
| 290 | 1309.93640000 | 446.49890000  | 0.00000000 |
| 291 | 1315.35700000 | 77.54000000   | 0.00000000 |
| 292 | 1319.05070000 | 224.82480000  | 0.00000000 |
| 293 | 1322.81750000 | 32.77160000   | 0.00000000 |
| 294 | 1323.58300000 | 0.46930000    | 0.00000000 |
| 295 | 1325.16560000 | 165.90890000  | 0.00000000 |
| 296 | 1328.93170000 | 17.40560000   | 0.00000000 |
| 297 | 1330.65000000 | 2.82310000    | 0.00000000 |
| 298 | 1333.94640000 | 6.36110000    | 0.00000000 |
| 299 | 1339.06500000 | 1240.49490000 | 0.00000000 |
| 300 | 1340.20440000 | 5.29840000    | 0.00000000 |
| 301 | 1348.83350000 | 80.80220000   | 0.00000000 |
| 302 | 1350.26110000 | 101.01670000  | 0.00000000 |
| 303 | 1360.88770000 | 2.94600000    | 0.00000000 |
| 304 | 1363.04230000 | 33.34540000   | 0.00000000 |
| 305 | 1364.80010000 | 10.60600000   | 0.00000000 |
| 306 | 1365.51520000 | 2.13630000    | 0.00000000 |
| 307 | 1368.71590000 | 16.47310000   | 0.00000000 |
| 308 | 1370.71730000 | 7.38250000    | 0.00000000 |
| 309 | 1375.47970000 | 221.68390000  | 0.00000000 |
| 310 | 1376.75640000 | 88.40280000   | 0.00000000 |
| 311 | 1386.48020000 | 25.67200000   | 0.00000000 |
| 312 | 1388.60530000 | 469.04490000  | 0.00000000 |
| 313 | 1391.62270000 | 8.67310000    | 0.00000000 |
| 314 | 1398.27030000 | 235.68840000  | 0.00000000 |
| 315 | 1398.52990000 | 170.53800000  | 0.00000000 |
| 316 | 1399.56320000 | 3.05000000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1404.44950000 | 16.11870000   | 0.00000000 |
| 318 | 1405.85470000 | 47.87770000   | 0.00000000 |
| 319 | 1409.07240000 | 14.91450000   | 0.00000000 |
| 320 | 1412.37410000 | 20.22940000   | 0.00000000 |
| 321 | 1427.51430000 | 63.83400000   | 0.00000000 |
| 322 | 1432.13230000 | 360.68080000  | 0.00000000 |
| 323 | 1436.70330000 | 2223.60370000 | 0.00000000 |
| 324 | 1437.63790000 | 251.46250000  | 0.00000000 |
| 325 | 1441.33230000 | 409.03180000  | 0.00000000 |
| 326 | 1442.99730000 | 34.75180000   | 0.00000000 |
| 327 | 1454.20220000 | 1362.97750000 | 0.00000000 |
| 328 | 1459.90360000 | 54.59340000   | 0.00000000 |
| 329 | 1461.87230000 | 73.01220000   | 0.00000000 |
| 330 | 1469.21050000 | 541.79830000  | 0.00000000 |
| 331 | 1474.36600000 | 12.29760000   | 0.00000000 |
| 332 | 1476.21170000 | 2.40050000    | 0.00000000 |
| 333 | 1481.03250000 | 5.63270000    | 0.00000000 |
| 334 | 1486.07010000 | 62.88130000   | 0.00000000 |
| 335 | 1486.61290000 | 9.01350000    | 0.00000000 |
| 336 | 1486.75890000 | 21.54860000   | 0.00000000 |
| 337 | 1489.78370000 | 69.85240000   | 0.00000000 |
| 338 | 1492.38920000 | 5.64840000    | 0.00000000 |
| 339 | 1492.90920000 | 41.67730000   | 0.00000000 |
| 340 | 1493.14330000 | 16.45450000   | 0.00000000 |
| 341 | 1495.13000000 | 1.18480000    | 0.00000000 |
| 342 | 1495.60100000 | 419.87200000  | 0.00000000 |
| 343 | 1499.98210000 | 3.71060000    | 0.00000000 |
| 344 | 1503.26060000 | 1.12140000    | 0.00000000 |
| 345 | 1506.35390000 | 3.33830000    | 0.00000000 |
| 346 | 1509.30080000 | 97.78120000   | 0.00000000 |
| 347 | 1512.19910000 | 38.14170000   | 0.00000000 |
| 348 | 1512.90090000 | 79.59180000   | 0.00000000 |
| 349 | 1514.49760000 | 628.46200000  | 0.00000000 |
| 350 | 1522.92350000 | 4.11790000    | 0.00000000 |
| 351 | 1526.21960000 | 84.21960000   | 0.00000000 |
| 352 | 1529.86030000 | 130.90990000  | 0.00000000 |
| 353 | 1540.65130000 | 7.17650000    | 0.00000000 |
| 354 | 1541.16780000 | 10.78740000   | 0.00000000 |
| 355 | 1547.04360000 | 79.54570000   | 0.00000000 |
| 356 | 1554.12990000 | 44.71780000   | 0.00000000 |
| 357 | 1555.60020000 | 308.62250000  | 0.00000000 |
| 358 | 1559.66460000 | 5.07120000    | 0.00000000 |
| 359 | 1568.47290000 | 79.13360000   | 0.00000000 |
| 360 | 1572.05960000 | 131.80140000  | 0.00000000 |
| 361 | 1577.23490000 | 232.54890000  | 0.00000000 |
| 362 | 1591.88220000 | 625.89160000  | 0.00000000 |
| 363 | 1600.81990000 | 7.68470000    | 0.00000000 |
| 364 | 1601.46840000 | 15.85640000   | 0.00000000 |
| 365 | 1605.96260000 | 144.24960000  | 0.00000000 |
| 366 | 1613.35950000 | 115.98350000  | 0.00000000 |
| 367 | 1618.52740000 | 129.28940000  | 0.00000000 |
| 368 | 1621.58300000 | 52.75290000   | 0.00000000 |
| 369 | 1624.50840000 | 78.03730000   | 0.00000000 |
| 370 | 1647.98170000 | 8.56840000    | 0.00000000 |
| 371 | 1648.67920000 | 1.47310000    | 0.00000000 |
| 372 | 1664.74630000 | 104.45620000  | 0.00000000 |
| 373 | 1664.99220000 | 118.35360000  | 0.00000000 |
| 374 | 1959.20770000 | 2369.34990000 | 0.00000000 |
| 375 | 1965.52990000 | 2318.60840000 | 0.00000000 |
| 376 | 2080.76200000 | 2495.89860000 | 0.00000000 |
| 377 | 2934.28080000 | 153.41050000  | 0.00000000 |
| 378 | 2985.69000000 | 88.64480000   | 0.00000000 |
| 379 | 2997.57920000 | 0.73240000    | 0.00000000 |
| 380 | 3001.71830000 | 54.49020000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 3013.47250000 | 50.34700000  | 0.00000000 |
| 382 | 3016.84180000 | 71.18700000  | 0.00000000 |
| 383 | 3019.41470000 | 65.39080000  | 0.00000000 |
| 384 | 3026.19910000 | 67.67580000  | 0.00000000 |
| 385 | 3026.65570000 | 80.24290000  | 0.00000000 |
| 386 | 3033.53240000 | 38.87260000  | 0.00000000 |
| 387 | 3047.58740000 | 15.51380000  | 0.00000000 |
| 388 | 3052.36070000 | 32.27140000  | 0.00000000 |
| 389 | 3060.30170000 | 23.27290000  | 0.00000000 |
| 390 | 3067.33110000 | 34.88910000  | 0.00000000 |
| 391 | 3068.96740000 | 223.61340000 | 0.00000000 |
| 392 | 3070.98130000 | 97.08960000  | 0.00000000 |
| 393 | 3181.12440000 | 190.72490000 | 0.00000000 |
| 394 | 3181.28690000 | 4.93260000   | 0.00000000 |
| 395 | 3181.83600000 | 36.03200000  | 0.00000000 |
| 396 | 3191.13860000 | 14.22530000  | 0.00000000 |
| 397 | 3191.28160000 | 5.16100000   | 0.00000000 |
| 398 | 3191.70120000 | 4.72750000   | 0.00000000 |
| 399 | 3193.89810000 | 4.45750000   | 0.00000000 |
| 400 | 3201.62650000 | 53.85940000  | 0.00000000 |
| 401 | 3201.93710000 | 57.98030000  | 0.00000000 |
| 402 | 3203.75890000 | 1.22720000   | 0.00000000 |
| 403 | 3213.32970000 | 1.11070000   | 0.00000000 |
| 404 | 3214.03440000 | 4.12210000   | 0.00000000 |
| 405 | 3216.32950000 | 10.00200000  | 0.00000000 |
| 406 | 3216.84060000 | 32.73320000  | 0.00000000 |
| 407 | 3217.10120000 | 11.68400000  | 0.00000000 |
| 408 | 3218.45330000 | 7.11860000   | 0.00000000 |
| 409 | 3219.29350000 | 0.63540000   | 0.00000000 |
| 410 | 3224.54890000 | 5.91620000   | 0.00000000 |
| 411 | 3225.22750000 | 7.55510000   | 0.00000000 |
| 412 | 3226.48440000 | 1.72210000   | 0.00000000 |
| 413 | 3226.84430000 | 7.82940000   | 0.00000000 |
| 414 | 3228.02720000 | 8.45010000   | 0.00000000 |
| 415 | 3228.20220000 | 2.17930000   | 0.00000000 |
| 416 | 3231.54440000 | 2.72450000   | 0.00000000 |
| 417 | 3234.48460000 | 1.85140000   | 0.00000000 |
| 418 | 3238.40730000 | 0.44950000   | 0.00000000 |
| 419 | 3239.60750000 | 7.90880000   | 0.00000000 |
| 420 | 3249.71470000 | 7.80900000   | 0.00000000 |
| 421 | 3250.81040000 | 7.93070000   | 0.00000000 |
| 422 | 3270.14110000 | 2.94410000   | 0.00000000 |
| 423 | 3271.52090000 | 11.86980000  | 0.00000000 |
| 424 | 3271.73570000 | 12.20530000  | 0.00000000 |
| 425 | 3272.76770000 | 11.16130000  | 0.00000000 |
| 426 | 3280.94510000 | 11.60610000  | 0.00000000 |
| 427 | 3284.16780000 | 11.32550000  | 0.00000000 |
| 428 | 3286.20270000 | 7.59100000   | 0.00000000 |
| 429 | 3291.71470000 | 3.65920000   | 0.00000000 |
| 430 | 3294.05020000 | 1.64870000   | 0.00000000 |
| 431 | 3530.30950000 | 1.79540000   | 0.00000000 |
| 432 | 3564.41080000 | 5.66180000   | 0.00000000 |

S11. CALCULATIONS ON EXTENDED CONFORMER OF  $1^{3+}$  ( $^1A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](c6[Ru]578(n9ccc[n+](c9C([n+]<br>1n7ccc1)[n+](c1n8ccc1)[n+](c1ccc(cc1)CCCCCc1cc[n+](c1)[Re]<br>1([n+](c2cccc3c2c2[n+](c1cccc2c1c3nc2cccc2n1)([C][O])([C][O])([C][O]) |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 1  |      |
| Energy                          | : -3743.84161704   | a.u. |
| Gibbs Energy                    | : -3742.92047100   | a.u. |
| Number of imaginary frequencies | : 4  |      |

## S11.1. Cartesian Co-ordinates (XYZ format)

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|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.98803997 | -1.62553406 | -3.51635790 |
| H | -3.24387789 | -0.86145002 | -4.25552416 |
| H | -2.73941398 | -2.54065204 | -4.06041288 |
| C | -1.76151395 | -1.16101599 | -2.70792603 |
| H | -1.50722396 | -1.93000400 | -1.97038400 |
| H | -2.02695489 | -0.26106399 | -2.14258790 |
| C | -0.54868400 | -0.87230802 | -3.59311295 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.81050599 | -0.10290100 | -4.32888412 |
| H  | -0.28856400 | -1.77240205 | -4.16222286 |
| C  | 1.88387597  | -0.09650300 | -3.67398405 |
| H  | 1.61703706  | 0.68916798  | -4.38656378 |
| H  | 2.15233994  | -0.98554802 | -4.25097990 |
| C  | 7.12236595  | 4.71421719  | 1.03920305  |
| N  | 5.82360983  | 4.24827719  | 1.48324299  |
| N  | 8.17878056  | 3.90478611  | 1.60321403  |
| N  | 7.18735695  | 4.71063900  | -0.40858001 |
| N  | 5.41016102  | 2.99816298  | 1.14091396  |
| C  | 4.85079384  | 4.92558289  | 2.15079594  |
| N  | 8.22848415  | 2.57924104  | 1.31150401  |
| C  | 9.19611263  | 4.26727200  | 2.43149209  |
| N  | 7.01584911  | 3.54159403  | -1.08374500 |
| C  | 7.31373787  | 5.76160812  | -1.26312304 |
| Ru | 6.75146198  | 1.80779803  | 0.06132600  |
| C  | 4.16292000  | 2.88917708  | 1.59844196  |
| C  | 3.77098203  | 4.07588816  | 2.24545288  |
| H  | 5.00670385  | 5.93337011  | 2.49696898  |
| C  | 9.28729820  | 2.09922409  | 1.95992398  |
| C  | 9.92762375  | 3.12696004  | 2.67903805  |
| H  | 9.30900097  | 5.28476810  | 2.76550889  |
| C  | 7.03610992  | 3.86273408  | -2.37727308 |
| C  | 7.22587585  | 5.24793291  | -2.53788590 |
| H  | 7.45558596  | 6.76510811  | -0.89873898 |
| N  | 6.62815905  | 0.08008200  | 1.21985900  |
| N  | 8.14698696  | 0.58893597  | -0.89257097 |
| H  | 3.60503006  | 1.98173702  | 1.43593705  |
| H  | 2.82548094  | 4.28037882  | 2.71707606  |
| H  | 9.54185581  | 1.05508494  | 1.88475394  |
| H  | 10.80620861 | 3.04278994  | 3.29493809  |
| H  | 6.90355110  | 3.09915090  | -3.12583089 |
| H  | 7.28939390  | 5.79495907  | -3.46250010 |
| C  | 5.88191986  | -0.11274600 | 2.31151509  |
| C  | 7.43786621  | -0.93083900 | 0.80122298  |
| C  | 8.26641464  | -0.65289801 | -0.34814101 |
| C  | 8.93139744  | 0.90851700  | -1.92611694 |
| C  | 5.88561821  | -1.31883895 | 3.01291704  |
| H  | 5.27241611  | 0.71881998  | 2.63194299  |
| C  | 7.49569416  | -2.16933894 | 1.45233798  |
| C  | 9.15707874  | -1.61194301 | -0.84615803 |
| C  | 9.84332657  | 0.00721400  | -2.47636509 |
| H  | 8.82987499  | 1.91000605  | -2.31645107 |
| C  | 6.68922091  | -2.35858893 | 2.58253193  |
| H  | 5.25721979  | -1.42169797 | 3.88689995  |
| C  | 8.39452839  | -3.19998407 | 0.93738401  |
| C  | 9.95717335  | -1.26316702 | -1.94235694 |
| C  | 9.22086143  | -2.92235398 | -0.20293801 |
| H  | 10.45017624 | 0.31799600  | -3.31567502 |
| H  | 6.71737194  | -3.30791306 | 3.09889507  |
| N  | 8.42947674  | -4.37445498 | 1.54504204  |
| H  | 10.65065479 | -1.98948896 | -2.34273291 |
| N  | 10.05097675 | -3.82945395 | -0.69053799 |
| C  | 9.26914978  | -5.31058598 | 1.05754006  |
| C  | 10.09672356 | -5.03232718 | -0.08243000 |
| C  | 9.34079647  | -6.58660316 | 1.67385304  |
| C  | 10.97017765 | -6.03848314 | -0.57008398 |
| C  | 10.19539261 | -7.53611898 | 1.17716897  |
| H  | 8.70845413  | -6.77613401 | 2.53193498  |
| C  | 11.01470089 | -7.26050997 | 0.04889200  |
| H  | 11.58538723 | -5.80799294 | -1.43059099 |
| H  | 10.25238514 | -8.51103497 | 1.64531696  |
| H  | 11.68018532 | -8.03066826 | -0.32104200 |
| N  | -7.48078012 | -0.70420301 | 1.48207700  |

|    |              |             |             |
|----|--------------|-------------|-------------|
| N  | -9.17023182  | -1.22142601 | -0.53932703 |
| C  | -6.60027981  | -0.48022300 | 2.46327496  |
| C  | -8.16798687  | 0.34904099  | 0.96651399  |
| C  | -9.08292484  | 0.06941700  | -0.12156200 |
| C  | -9.97774792  | -1.51292801 | -1.56464303 |
| C  | -6.36730194  | 0.79415298  | 2.97898197  |
| H  | -6.07229900  | -1.34130299 | 2.84659004  |
| C  | -7.98957682  | 1.65748703  | 1.43506300  |
| C  | -9.81362247  | 1.10031903  | -0.72689998 |
| C  | -10.73647976 | -0.54080898 | -2.21551609 |
| H  | -10.01949310 | -2.54852700 | -1.86934495 |
| C  | -7.06606483  | 1.87063396  | 2.46758199  |
| H  | -5.64369106  | 0.91928601  | 3.77243495  |
| C  | -8.75582695  | 2.74586511  | 0.83416402  |
| C  | -10.65929604 | 0.77305400  | -1.79570901 |
| C  | -9.66407585  | 2.46855998  | -0.23873501 |
| H  | -11.37336922 | -0.83128101 | -3.03941011 |
| H  | -6.91719818  | 2.87466311  | 2.83993793  |
| N  | -8.58790112  | 3.97355700  | 1.29746306  |
| H  | -11.23042583 | 1.55744195  | -2.27257109 |
| N  | -10.37290955 | 3.42856693  | -0.80967999 |
| C  | -9.30414867  | 4.96348286  | 0.72755802  |
| C  | -10.21559620 | 4.68523312  | -0.34742200 |
| C  | -9.16076946  | 6.29713106  | 1.19023502  |
| C  | -10.95481396 | 5.74947500  | -0.92552900 |
| C  | -9.89031696  | 7.30137014  | 0.60943002  |
| H  | -8.46901703  | 6.48530388  | 2.00144100  |
| C  | -10.79225445 | 7.02604198  | -0.45431799 |
| H  | -11.63633823 | 5.51845121  | -1.73429799 |
| H  | -9.78370762  | 8.32032776  | 0.96040499  |
| H  | -11.35503864 | 7.84061289  | -0.89311498 |
| H  | 7.25394392   | 5.73484087  | 1.38346004  |
| C  | -4.16732502  | -1.87303102 | -2.62069392 |
| C  | -5.04780388  | -0.84678400 | -2.27421498 |
| C  | -4.40451479  | -3.12477899 | -2.04657412 |
| C  | -6.08826590  | -1.09296095 | -1.39596701 |
| H  | -4.93014908  | 0.14806500  | -2.68469596 |
| C  | -5.46482992  | -3.29870105 | -1.17683005 |
| H  | -3.76608992  | -3.96918392 | -2.27352500 |
| N  | -6.30784988  | -2.29914308 | -0.83902699 |
| H  | -6.76759291  | -0.29775900 | -1.13257599 |
| H  | -5.65686417  | -4.26340818 | -0.72941899 |
| C  | 3.06013489   | 0.34710801  | -2.85162997 |
| C  | 4.01768398   | -0.55878502 | -2.39087200 |
| C  | 3.21716404   | 1.67886305  | -2.46030498 |
| C  | 5.05367804   | -0.12411800 | -1.58296001 |
| H  | 3.96315503   | -1.60682905 | -2.65735888 |
| C  | 4.27600813   | 2.04482388  | -1.64930904 |
| H  | 2.51638198   | 2.43830395  | -2.78386688 |
| N  | 5.19366503   | 1.16115201  | -1.20242000 |
| H  | 5.79483986   | -0.82310700 | -1.22687197 |
| H  | 4.40677404   | 3.07013297  | -1.33784401 |
| Re | -7.97923517  | -2.67969394 | 0.62231302  |
| C  | -9.43750763  | -2.92022896 | 1.88309300  |
| O  | -10.30486584 | -3.05087399 | 2.62954402  |
| C  | -8.52229881  | -4.27600622 | -0.33797401 |
| O  | -8.85781956  | -5.20738602 | -0.92919898 |
| C  | -6.81563282  | -3.74188304 | 1.75343096  |
| O  | -6.11506414  | -4.34633303 | 2.44195700  |
| C  | 0.66545898   | -0.41156799 | -2.78595996 |
| H  | 0.94208300   | -1.18466198 | -2.06078696 |
| H  | 0.40555000   | 0.48135999  | -2.20684099 |

## S11.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -9.80270000  | 0.81780000   | 0.00000000      |
| 2    | -8.87050000  | 0.34040000   | 0.00000000      |
| 3    | -8.58720000  | 0.27580000   | 0.00000000      |
| 4    | -5.02770000  | 0.18200000   | 0.00000000      |
| 5    | 4.90260000   | 0.14990000   | 0.00000000      |
| 6    | 11.88890000  | 0.24600000   | 0.00000000      |
| 7    | 18.17550000  | 0.54000000   | 0.00000000      |
| 8    | 20.75060000  | 0.88940000   | 0.00000000      |
| 9    | 28.55850000  | 0.30550000   | 0.00000000      |
| 10   | 31.12850000  | 0.14240000   | 0.00000000      |
| 11   | 42.73440000  | 0.53750000   | 0.00000000      |
| 12   | 46.77100000  | 0.15620000   | 0.00000000      |
| 13   | 49.85240000  | 0.38830000   | 0.00000000      |
| 14   | 52.40390000  | 0.55150000   | 0.00000000      |
| 15   | 56.12930000  | 0.44890000   | 0.00000000      |
| 16   | 58.19960000  | 0.14970000   | 0.00000000      |
| 17   | 60.10100000  | 1.27520000   | 0.00000000      |
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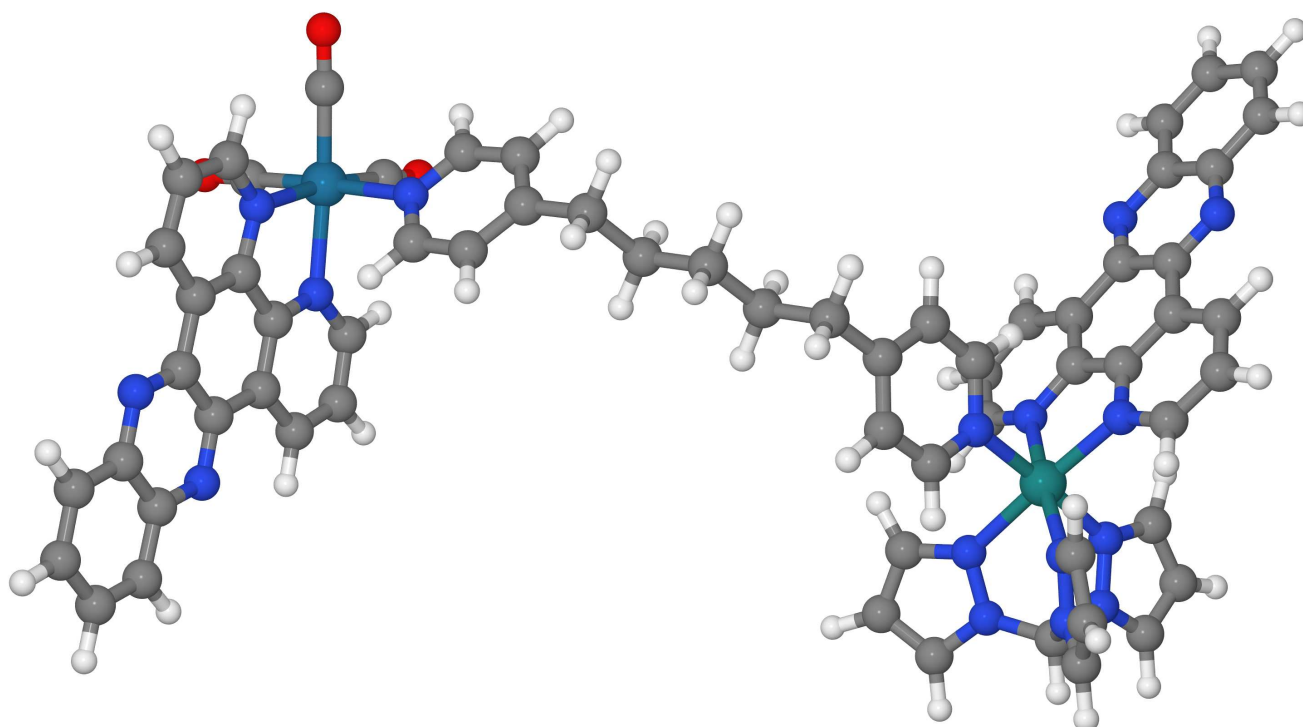
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| 365 | 3200.81670000 | 17.04180000   | 0.00000000 |
| 366 | 3201.44730000 | 16.43900000   | 0.00000000 |
| 367 | 3206.68030000 | 37.90130000   | 0.00000000 |
| 368 | 3207.10020000 | 36.29420000   | 0.00000000 |
| 369 | 3211.00800000 | 1.28350000    | 0.00000000 |
| 370 | 3211.14240000 | 0.48260000    | 0.00000000 |
| 371 | 3213.50700000 | 0.07070000    | 0.00000000 |
| 372 | 3213.56990000 | 0.14570000    | 0.00000000 |
| 373 | 3218.46570000 | 6.68270000    | 0.00000000 |
| 374 | 3224.09460000 | 0.70440000    | 0.00000000 |
| 375 | 3224.14540000 | 3.43240000    | 0.00000000 |
| 376 | 3224.18910000 | 3.36830000    | 0.00000000 |
| 377 | 3224.69250000 | 3.86520000    | 0.00000000 |
| 378 | 3231.07670000 | 6.30670000    | 0.00000000 |
| 379 | 3231.47690000 | 4.78510000    | 0.00000000 |
| 380 | 3232.00760000 | 8.49460000    | 0.00000000 |

|     |               |            |            |
|-----|---------------|------------|------------|
| 381 | 3235.71750000 | 9.64360000 | 0.00000000 |
| 382 | 3236.15640000 | 5.16210000 | 0.00000000 |
| 383 | 3236.74890000 | 2.94060000 | 0.00000000 |
| 384 | 3244.70170000 | 3.18700000 | 0.00000000 |
| 385 | 3259.46360000 | 0.91630000 | 0.00000000 |
| 386 | 3259.55320000 | 1.19690000 | 0.00000000 |
| 387 | 3260.97570000 | 0.28640000 | 0.00000000 |
| 388 | 3269.61370000 | 3.35200000 | 0.00000000 |
| 389 | 3269.85130000 | 9.09310000 | 0.00000000 |
| 390 | 3271.06980000 | 7.30510000 | 0.00000000 |
| 391 | 3284.03530000 | 3.05100000 | 0.00000000 |
| 392 | 3284.47380000 | 4.25160000 | 0.00000000 |
| 393 | 3285.32400000 | 4.92890000 | 0.00000000 |

# **S12. CALCULATIONS ON EXTENDED CONFORMER OF 1<sup>3+</sup> (<sup>3</sup>A)**



|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+]<br>5c4c6c(c3n2)ccc[n+]<br>6[Ru]578(n9ccc[n+]<br>9C([n+]<br>1n7ccc1)[n+]<br>1n8ccc1)[n+]<br>1ccc(cc1)CCCCC1cc[n+]<br>(cc1)[Re]<br>1([n+]<br>2cccc3c2c2[n+]<br>1cccc2c1c3nc2cccc2n1)<br>([C][O])([C][O])[C][O] |      |
| Formula                         | : C <sub>64</sub> H <sub>48</sub> N <sub>16</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -3743.76906278   | a.u. |
| Gibbs Energy                    | : -3742.85199900   | a.u. |
| Number of imaginary frequencies | : 4  |      |

## **S12.1. Cartesian Co-ordinates (XYZ format)**

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|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.92304111 | 1.18279696  | 3.23724103 |
| H | -3.19909310 | 0.37528199  | 3.92034793 |
| H | -2.66981912 | 2.05585694  | 3.84536004 |
| C | -1.68807900 | 0.76036298  | 2.41903806 |
| H | -1.41302896 | 1.57394397  | 1.73915601 |
| H | -1.94986403 | -0.09822100 | 1.79132497 |
| C | -0.49712300 | 0.40582600  | 3.31010008 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -0.77440298 | -0.41922900 | 3.97634912  |
| H  | -0.25745100 | 1.25979102  | 3.95415902  |
| C  | 1.93153501  | -0.35762501 | 3.41601491  |
| H  | 1.65277100  | -1.20833695 | 4.04342604  |
| H  | 2.15842605  | 0.48282000  | 4.07676411  |
| C  | 7.66223001  | -4.65681696 | -1.28482401 |
| N  | 6.36436987  | -4.26010180 | -1.78983295 |
| N  | 8.68353462  | -3.72201204 | -1.71558499 |
| N  | 7.62796593  | -4.74511814 | 0.16007900  |
| N  | 5.83548212  | -3.06418395 | -1.41695702 |
| C  | 5.50253010  | -4.95138216 | -2.57858706 |
| N  | 8.60074902  | -2.41709304 | -1.33536804 |
| C  | 9.77685928  | -3.92830706 | -2.48562789 |
| N  | 7.32155514  | -3.64062595 | 0.89105397  |
| C  | 7.79295015  | -5.83004999 | 0.95968503  |
| Ru | 7.01307821  | -1.83166099 | -0.16142499 |
| C  | 4.62710094  | -3.00375509 | -1.97916198 |
| C  | 4.37588406  | -4.16957283 | -2.71951699 |
| H  | 5.75856876  | -5.92119217 | -2.97085190 |
| C  | 9.65699482  | -1.79810297 | -1.87354600 |
| C  | 10.42369270 | -2.71075201 | -2.60497904 |
| H  | 10.00663280 | -4.90247917 | -2.88408804 |
| C  | 7.29531622  | -4.03543186 | 2.16500592  |
| C  | 7.58676386  | -5.40578890 | 2.25511193  |
| H  | 8.04151058  | -6.79453087 | 0.54981202  |
| N  | 6.85606289  | -0.07509900 | -1.23457301 |
| N  | 8.26922512  | -0.63061398 | 0.95128202  |
| H  | 3.99527192  | -2.14516091 | -1.82231402 |
| H  | 3.48988891  | -4.40541410 | -3.28268194 |
| H  | 9.80572891  | -0.74369800 | -1.70843899 |
| H  | 11.32980824 | -2.51324105 | -3.15063000 |
| H  | 7.06289816  | -3.33181691 | 2.94741011  |
| H  | 7.64044094  | -6.00329590 | 3.14832401  |
| C  | 6.16918278  | 0.14955001  | -2.35960293 |
| C  | 7.61269522  | 0.95573097  | -0.68819499 |
| C  | 8.35112000  | 0.66546702  | 0.45403200  |
| C  | 9.00436783  | -0.96504301 | 2.01744199  |
| C  | 6.15613222  | 1.38652205  | -2.99083900 |
| H  | 5.62041807  | -0.68753302 | -2.76615405 |
| C  | 7.63073683  | 2.25214291  | -1.28570402 |
| C  | 9.16846848  | 1.64769304  | 1.09046698  |
| C  | 9.82476139  | -0.05548300 | 2.67171502  |
| H  | 8.93690205  | -1.99097896 | 2.34873605  |
| C  | 6.88982821  | 2.44690800  | -2.44021106 |
| H  | 5.58146381  | 1.51230097  | -3.89721489 |
| C  | 8.43269253  | 3.29812908  | -0.65705001 |
| C  | 9.89764881  | 1.26476002  | 2.20460892  |
| C  | 9.20139217  | 2.99601889  | 0.53040498  |
| H  | 10.39548111 | -0.37942699 | 3.53013611  |
| H  | 6.89508200  | 3.42276311  | -2.90723705 |
| N  | 8.44281006  | 4.50851297  | -1.19312298 |
| H  | 10.52451038 | 1.99650598  | 2.69673204  |
| N  | 9.94244862  | 3.91912103  | 1.12289000  |
| C  | 9.20002365  | 5.46335697  | -0.59324998 |
| C  | 9.96048641  | 5.16452599  | 0.58080900  |
| C  | 9.24199104  | 6.77063417  | -1.13025701 |
| C  | 10.73787212 | 6.18299913  | 1.17874396  |
| C  | 10.00837994 | 7.74317884  | -0.52649200 |
| H  | 8.65876484  | 6.97558022  | -2.01978707 |
| C  | 10.75989342 | 7.44793177  | 0.63351899  |
| H  | 11.30654621 | 5.93579102  | 2.06694102  |
| H  | 10.03806877 | 8.74361324  | -0.94102502 |
| H  | 11.35691738 | 8.22552013  | 1.09450996  |
| N  | -7.77819395 | 0.56768203  | -1.53362405 |

|    |              |             |             |
|----|--------------|-------------|-------------|
| N  | -9.20826626  | 1.43263900  | 0.56793600  |
| C  | -7.02547693  | 0.16645600  | -2.56349802 |
| C  | -8.56771469  | -0.34371600 | -0.90582299 |
| C  | -9.33827496  | 0.12279100  | 0.22890000  |
| C  | -9.87701893  | 1.89193106  | 1.63094795  |
| C  | -7.02751780  | -1.15134299 | -3.01930189 |
| H  | -6.40971899  | 0.91802198  | -3.03587508 |
| C  | -8.62269115  | -1.68501902 | -1.30721498 |
| C  | -10.15517807 | -0.75712901 | 0.95119399  |
| C  | -10.70771503 | 1.07623100  | 2.39832211  |
| H  | -9.74694633  | 2.93713593  | 1.87113595  |
| C  | -7.83137321  | -2.08413506 | -2.39305496 |
| H  | -6.39962101  | -1.42220998 | -3.85668302 |
| C  | -9.48458481  | -2.61611199 | -0.58413500 |
| C  | -10.85341835 | -0.25467101 | 2.05776095  |
| C  | -10.24599075 | -2.15501094 | 0.53850102  |
| H  | -11.22544289 | 1.49922204  | 3.24798107  |
| H  | -7.86369514  | -3.11577106 | -2.71494794 |
| N  | -9.53715706  | -3.87588501 | -0.98440599 |
| H  | -11.48869610 | -0.92108399 | 2.62448311  |
| N  | -11.03312397 | -2.97008300 | 1.22126806  |
| C  | -10.33628368 | -4.71936083 | -0.30054200 |
| C  | -11.09975624 | -4.25707912 | 0.82512802  |
| C  | -10.42807961 | -6.08021688 | -0.69150400 |
| C  | -11.93080807 | -5.17037296 | 1.52410305  |
| C  | -11.24064827 | -6.93554592 | 0.00575800  |
| H  | -9.84473515  | -6.40809298 | -1.54248703 |
| C  | -11.99618816 | -6.47815084 | 1.11968994  |
| H  | -12.49782276 | -4.80172777 | 2.36941600  |
| H  | -11.31306362 | -7.97480679 | -0.29001400 |
| H  | -12.62952328 | -7.17791414 | 1.65076804  |
| H  | 7.90236282   | -5.63593292 | -1.68535697 |
| C  | -4.08879423  | 1.51115096  | 2.34980392  |
| C  | -5.05401087  | 0.55791801  | 2.02314210  |
| C  | -4.23299789  | 2.77551508  | 1.77121699  |
| C  | -6.09137392  | 0.88648999  | 1.16746104  |
| H  | -5.00820017  | -0.44242200 | 2.43454409  |
| C  | -5.29362917  | 3.03277206  | 0.92375499  |
| H  | -3.52365708  | 3.56608391  | 1.98085296  |
| N  | -6.22658920  | 2.10614800  | 0.61399001  |
| H  | -6.83735609  | 0.14753500  | 0.92063898  |
| H  | -5.41412210  | 4.00741577  | 0.47314700  |
| C  | 3.14671302   | -0.70427901 | 2.60986900  |
| C  | 4.08491898   | 0.26886201  | 2.24981403  |
| C  | 3.36480594   | -2.00430799 | 2.14177990  |
| C  | 5.16945696   | -0.07024100 | 1.46711600  |
| H  | 3.97562599   | 1.29320204  | 2.58157992  |
| C  | 4.46853113   | -2.28091311 | 1.36176705  |
| H  | 2.67892504   | -2.80489707 | 2.38615894  |
| N  | 5.36782789   | -1.33006096 | 1.02188396  |
| H  | 5.90367794   | 0.66845202  | 1.18452704  |
| H  | 4.65682793   | -3.27740097 | 0.99249399  |
| Re | -7.92303324  | 2.63770604  | -0.76852202 |
| C  | -9.41916561  | 3.01119304  | -1.95026302 |
| O  | -10.31019020 | 3.21990991  | -2.64956403 |
| C  | -8.18012524  | 4.34609318  | 0.11404100  |
| O  | -8.35210133  | 5.34740496  | 0.65970403  |
| C  | -6.70040512  | 3.46023989  | -2.03055811 |
| O  | -5.96587706  | 3.92147303  | -2.79055500 |
| C  | 0.74342501   | 0.01531100  | 2.50617099  |
| H  | 1.03766894   | 0.84431702  | 1.85384405  |
| H  | 0.51202798   | -0.83270198 | 1.85283196  |



## S12.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -10.23960000 | 1.58830000   | 0.00000000      |
| 2    | -8.09060000  | 0.97800000   | 0.00000000      |
| 3    | -6.65950000  | 0.43240000   | 0.00000000      |
| 4    | -2.91420000  | 0.14860000   | 0.00000000      |
| 5    | 4.60930000   | 0.77330000   | 0.00000000      |
| 6    | 13.71730000  | 0.06920000   | 0.00000000      |
| 7    | 18.55450000  | 1.36110000   | 0.00000000      |
| 8    | 19.53450000  | 0.73830000   | 0.00000000      |
| 9    | 30.67860000  | 0.13210000   | 0.00000000      |
| 10   | 34.79710000  | 0.37160000   | 0.00000000      |
| 11   | 42.53600000  | 0.60510000   | 0.00000000      |
| 12   | 48.14110000  | 0.83130000   | 0.00000000      |
| 13   | 49.74260000  | 0.63010000   | 0.00000000      |
| 14   | 54.93210000  | 0.79460000   | 0.00000000      |
| 15   | 56.78640000  | 0.41100000   | 0.00000000      |
| 16   | 58.20680000  | 0.77440000   | 0.00000000      |
| 17   | 59.43470000  | 2.62650000   | 0.00000000      |
| 18   | 61.88930000  | 1.61610000   | 0.00000000      |
| 19   | 63.74840000  | 2.12070000   | 0.00000000      |
| 20   | 66.08420000  | 1.68560000   | 0.00000000      |
| 21   | 67.75920000  | 0.01310000   | 0.00000000      |
| 22   | 69.21710000  | 0.49340000   | 0.00000000      |
| 23   | 71.20800000  | 4.50380000   | 0.00000000      |
| 24   | 73.67000000  | 0.47900000   | 0.00000000      |
| 25   | 82.56150000  | 2.98500000   | 0.00000000      |
| 26   | 84.53310000  | 9.70690000   | 0.00000000      |
| 27   | 89.64810000  | 3.16090000   | 0.00000000      |
| 28   | 91.88100000  | 0.76520000   | 0.00000000      |
| 29   | 95.16600000  | 1.28350000   | 0.00000000      |
| 30   | 100.49620000 | 0.03590000   | 0.00000000      |
| 31   | 106.45900000 | 1.16870000   | 0.00000000      |
| 32   | 113.91930000 | 3.39240000   | 0.00000000      |
| 33   | 129.60910000 | 0.91010000   | 0.00000000      |
| 34   | 132.47670000 | 0.02830000   | 0.00000000      |
| 35   | 136.20080000 | 0.47970000   | 0.00000000      |
| 36   | 142.04460000 | 0.17850000   | 0.00000000      |
| 37   | 146.82250000 | 10.75020000  | 0.00000000      |
| 38   | 152.32000000 | 0.57170000   | 0.00000000      |
| 39   | 154.88710000 | 1.10880000   | 0.00000000      |
| 40   | 169.27100000 | 0.42410000   | 0.00000000      |
| 41   | 169.42040000 | 0.86080000   | 0.00000000      |
| 42   | 171.47350000 | 0.80370000   | 0.00000000      |
| 43   | 173.94570000 | 0.38460000   | 0.00000000      |
| 44   | 175.81720000 | 0.36540000   | 0.00000000      |
| 45   | 177.51180000 | 0.37660000   | 0.00000000      |
| 46   | 181.66510000 | 13.99660000  | 0.00000000      |
| 47   | 187.08670000 | 0.41130000   | 0.00000000      |
| 48   | 189.09690000 | 11.69870000  | 0.00000000      |
| 49   | 189.64960000 | 13.44670000  | 0.00000000      |
| 50   | 196.99500000 | 20.91830000  | 0.00000000      |
| 51   | 205.75500000 | 1.09080000   | 0.00000000      |
| 52   | 209.92890000 | 1.09670000   | 0.00000000      |
| 53   | 217.38420000 | 1.32400000   | 0.00000000      |
| 54   | 221.86100000 | 1.44340000   | 0.00000000      |
| 55   | 237.25510000 | 53.27540000  | 0.00000000      |
| 56   | 241.73310000 | 0.12180000   | 0.00000000      |
| 57   | 245.72320000 | 0.27400000   | 0.00000000      |
| 58   | 258.65140000 | 2.63140000   | 0.00000000      |
| 59   | 273.11650000 | 3.32450000   | 0.00000000      |
| 60   | 280.76440000 | 1.26670000   | 0.00000000      |

|     |              |               |            |
|-----|--------------|---------------|------------|
| 61  | 293.82040000 | 82.85880000   | 0.00000000 |
| 62  | 297.67080000 | 1.90590000    | 0.00000000 |
| 63  | 309.56500000 | 2.43870000    | 0.00000000 |
| 64  | 314.65450000 | 1.32070000    | 0.00000000 |
| 65  | 318.84460000 | 130.58900000  | 0.00000000 |
| 66  | 325.13350000 | 21.34720000   | 0.00000000 |
| 67  | 327.08800000 | 0.04100000    | 0.00000000 |
| 68  | 328.04090000 | 0.31830000    | 0.00000000 |
| 69  | 330.48440000 | 2.07950000    | 0.00000000 |
| 70  | 332.05050000 | 2.87040000    | 0.00000000 |
| 71  | 359.48530000 | 6.04670000    | 0.00000000 |
| 72  | 360.19220000 | 6.35650000    | 0.00000000 |
| 73  | 361.32490000 | 0.59450000    | 0.00000000 |
| 74  | 380.17800000 | 0.81830000    | 0.00000000 |
| 75  | 382.21960000 | 16.66580000   | 0.00000000 |
| 76  | 382.74980000 | 8.34100000    | 0.00000000 |
| 77  | 386.16210000 | 4.76100000    | 0.00000000 |
| 78  | 390.99140000 | 46.50680000   | 0.00000000 |
| 79  | 397.37780000 | 67.94700000   | 0.00000000 |
| 80  | 402.87030000 | 0.20730000    | 0.00000000 |
| 81  | 406.14910000 | 0.55650000    | 0.00000000 |
| 82  | 406.48770000 | 0.86350000    | 0.00000000 |
| 83  | 413.71740000 | 55.64920000   | 0.00000000 |
| 84  | 421.63620000 | 14.49470000   | 0.00000000 |
| 85  | 435.74900000 | 10.42430000   | 0.00000000 |
| 86  | 439.01420000 | 260.64330000  | 0.00000000 |
| 87  | 440.09980000 | 171.75920000  | 0.00000000 |
| 88  | 441.88890000 | 20.52530000   | 0.00000000 |
| 89  | 454.85130000 | 1.86920000    | 0.00000000 |
| 90  | 474.82010000 | 31.83900000   | 0.00000000 |
| 91  | 475.88270000 | 25.59280000   | 0.00000000 |
| 92  | 481.56340000 | 10.96940000   | 0.00000000 |
| 93  | 486.83260000 | 6.06310000    | 0.00000000 |
| 94  | 488.46290000 | 0.11950000    | 0.00000000 |
| 95  | 489.33380000 | 3.23950000    | 0.00000000 |
| 96  | 489.86490000 | 0.00940000    | 0.00000000 |
| 97  | 494.62590000 | 3.00390000    | 0.00000000 |
| 98  | 497.37720000 | 0.09760000    | 0.00000000 |
| 99  | 516.29160000 | 2.40800000    | 0.00000000 |
| 100 | 531.91450000 | 24.79840000   | 0.00000000 |
| 101 | 532.38480000 | 4.70100000    | 0.00000000 |
| 102 | 532.50140000 | 23.45390000   | 0.00000000 |
| 103 | 544.26030000 | 24.81020000   | 0.00000000 |
| 104 | 561.71180000 | 16.58430000   | 0.00000000 |
| 105 | 562.03740000 | 0.82930000    | 0.00000000 |
| 106 | 571.46930000 | 0.93460000    | 0.00000000 |
| 107 | 572.50090000 | 1.30100000    | 0.00000000 |
| 108 | 575.60450000 | 1.39740000    | 0.00000000 |
| 109 | 581.89830000 | 1.09790000    | 0.00000000 |
| 110 | 583.44460000 | 417.45070000  | 0.00000000 |
| 111 | 585.97290000 | 1293.43040000 | 0.00000000 |
| 112 | 594.13060000 | 28.14930000   | 0.00000000 |
| 113 | 602.80990000 | 0.19340000    | 0.00000000 |
| 114 | 605.14140000 | 4.75080000    | 0.00000000 |
| 115 | 612.47290000 | 41.99250000   | 0.00000000 |
| 116 | 613.51940000 | 31.10840000   | 0.00000000 |
| 117 | 619.16870000 | 442.69550000  | 0.00000000 |
| 118 | 620.46140000 | 680.85780000  | 0.00000000 |
| 119 | 625.14760000 | 8.82050000    | 0.00000000 |
| 120 | 633.87840000 | 36.81970000   | 0.00000000 |
| 121 | 638.50470000 | 12.15830000   | 0.00000000 |
| 122 | 638.73020000 | 2.77450000    | 0.00000000 |
| 123 | 646.77950000 | 74.44490000   | 0.00000000 |
| 124 | 648.76730000 | 0.77770000    | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 650.36270000 | 3.44110000   | 0.00000000 |
| 126 | 653.92800000 | 0.31500000   | 0.00000000 |
| 127 | 659.91550000 | 0.00770000   | 0.00000000 |
| 128 | 668.68730000 | 5.42470000   | 0.00000000 |
| 129 | 670.95920000 | 5.76970000   | 0.00000000 |
| 130 | 676.12030000 | 5.04280000   | 0.00000000 |
| 131 | 680.87870000 | 4.23400000   | 0.00000000 |
| 132 | 686.13120000 | 0.56780000   | 0.00000000 |
| 133 | 701.45520000 | 128.30190000 | 0.00000000 |
| 134 | 735.11420000 | 0.01330000   | 0.00000000 |
| 135 | 736.82550000 | 7.62700000   | 0.00000000 |
| 136 | 738.80930000 | 510.17970000 | 0.00000000 |
| 137 | 739.83530000 | 8.98550000   | 0.00000000 |
| 138 | 740.50230000 | 0.59260000   | 0.00000000 |
| 139 | 746.75470000 | 0.58790000   | 0.00000000 |
| 140 | 752.38100000 | 0.05890000   | 0.00000000 |
| 141 | 757.83400000 | 97.94110000  | 0.00000000 |
| 142 | 761.15820000 | 0.40930000   | 0.00000000 |
| 143 | 761.53450000 | 0.36080000   | 0.00000000 |
| 144 | 763.79380000 | 0.38730000   | 0.00000000 |
| 145 | 767.10750000 | 0.43820000   | 0.00000000 |
| 146 | 770.40070000 | 789.98220000 | 0.00000000 |
| 147 | 771.58290000 | 47.45400000  | 0.00000000 |
| 148 | 771.81360000 | 127.28940000 | 0.00000000 |
| 149 | 773.66340000 | 197.14390000 | 0.00000000 |
| 150 | 779.22010000 | 70.77390000  | 0.00000000 |
| 151 | 781.49320000 | 11.00250000  | 0.00000000 |
| 152 | 781.85090000 | 114.74510000 | 0.00000000 |
| 153 | 786.04730000 | 85.18530000  | 0.00000000 |
| 154 | 788.84890000 | 0.36510000   | 0.00000000 |
| 155 | 795.73270000 | 71.47450000  | 0.00000000 |
| 156 | 797.86580000 | 122.78290000 | 0.00000000 |
| 157 | 815.51360000 | 0.07300000   | 0.00000000 |
| 158 | 826.77630000 | 0.31670000   | 0.00000000 |
| 159 | 835.34930000 | 33.32180000  | 0.00000000 |
| 160 | 836.30430000 | 0.84830000   | 0.00000000 |
| 161 | 840.74070000 | 2.44340000   | 0.00000000 |
| 162 | 841.51410000 | 79.12670000  | 0.00000000 |
| 163 | 842.51770000 | 23.94390000  | 0.00000000 |
| 164 | 862.66660000 | 39.73690000  | 0.00000000 |
| 165 | 866.54970000 | 15.61060000  | 0.00000000 |
| 166 | 872.91320000 | 202.46030000 | 0.00000000 |
| 167 | 874.76480000 | 0.04790000   | 0.00000000 |
| 168 | 875.47420000 | 314.34280000 | 0.00000000 |
| 169 | 876.68990000 | 2.47250000   | 0.00000000 |
| 170 | 878.65820000 | 5.61920000   | 0.00000000 |
| 171 | 880.62360000 | 0.34320000   | 0.00000000 |
| 172 | 884.58320000 | 0.02300000   | 0.00000000 |
| 173 | 887.67350000 | 6.46880000   | 0.00000000 |
| 174 | 888.05790000 | 17.28710000  | 0.00000000 |
| 175 | 897.26150000 | 0.00260000   | 0.00000000 |
| 176 | 899.03890000 | 0.32410000   | 0.00000000 |
| 177 | 915.72770000 | 6.29130000   | 0.00000000 |
| 178 | 920.85310000 | 1.36620000   | 0.00000000 |
| 179 | 938.61840000 | 10.62820000  | 0.00000000 |
| 180 | 939.14060000 | 23.64370000  | 0.00000000 |
| 181 | 942.12340000 | 0.67590000   | 0.00000000 |
| 182 | 944.72470000 | 7.49600000   | 0.00000000 |
| 183 | 946.43580000 | 0.24580000   | 0.00000000 |
| 184 | 952.16210000 | 7.59660000   | 0.00000000 |
| 185 | 957.66650000 | 1.31410000   | 0.00000000 |
| 186 | 968.01820000 | 12.78260000  | 0.00000000 |
| 187 | 968.77520000 | 3.83260000   | 0.00000000 |
| 188 | 971.56940000 | 3.68840000   | 0.00000000 |

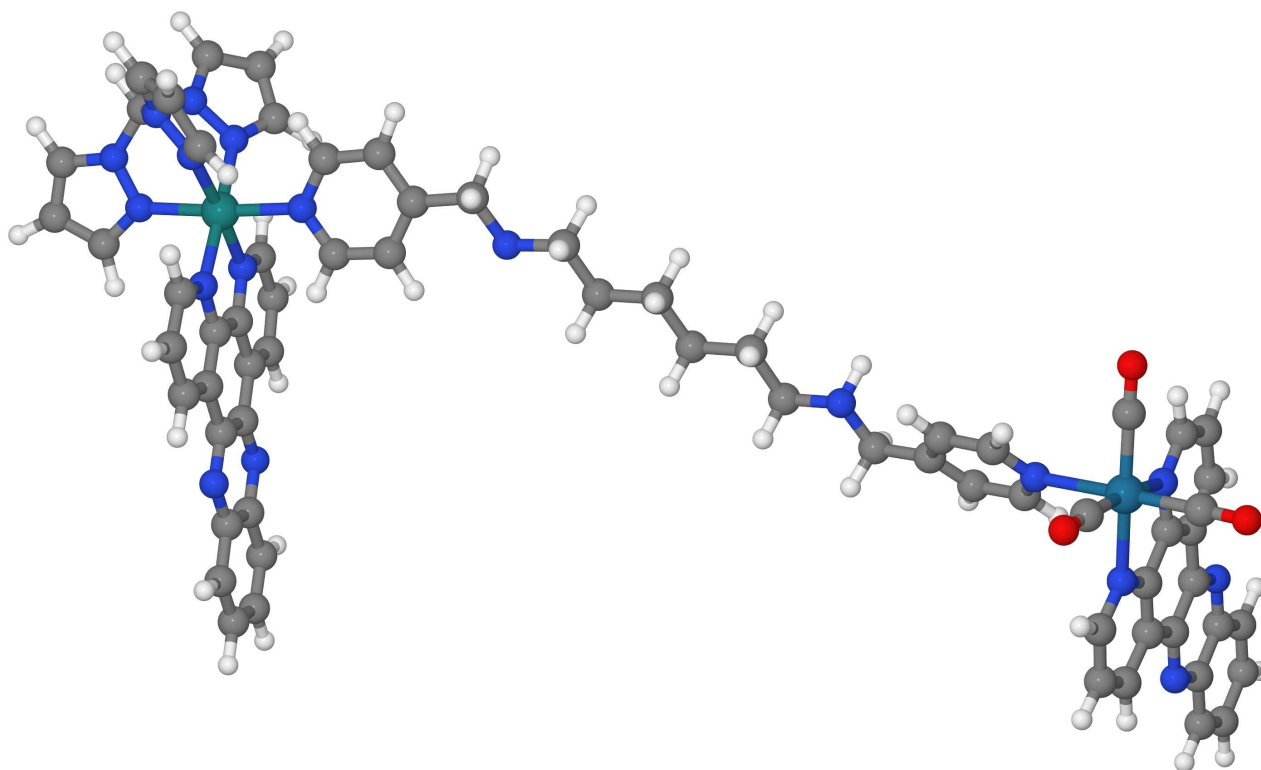
|     |               |                |            |
|-----|---------------|----------------|------------|
| 189 | 984.14910000  | 0.05870000     | 0.00000000 |
| 190 | 985.34200000  | 78.85020000    | 0.00000000 |
| 191 | 985.62810000  | 2.37590000     | 0.00000000 |
| 192 | 986.14650000  | 71.04410000    | 0.00000000 |
| 193 | 986.81650000  | 2.18090000     | 0.00000000 |
| 194 | 992.57690000  | 1.38970000     | 0.00000000 |
| 195 | 994.56180000  | 257.54420000   | 0.00000000 |
| 196 | 997.25760000  | 119.14520000   | 0.00000000 |
| 197 | 1001.56640000 | 16844.87010000 | 0.00000000 |
| 198 | 1002.34420000 | 13.33320000    | 0.00000000 |
| 199 | 1003.77760000 | 1138.74850000  | 0.00000000 |
| 200 | 1006.10450000 | 37.28400000    | 0.00000000 |
| 201 | 1008.14240000 | 3.58180000     | 0.00000000 |
| 202 | 1012.30400000 | 0.12650000     | 0.00000000 |
| 203 | 1019.79350000 | 104.00560000   | 0.00000000 |
| 204 | 1020.43110000 | 203.42670000   | 0.00000000 |
| 205 | 1021.39400000 | 0.00010000     | 0.00000000 |
| 206 | 1023.23780000 | 413.47000000   | 0.00000000 |
| 207 | 1026.93200000 | 4.03540000     | 0.00000000 |
| 208 | 1028.71220000 | 3.48560000     | 0.00000000 |
| 209 | 1032.81330000 | 0.33630000     | 0.00000000 |
| 210 | 1033.49270000 | 0.02500000     | 0.00000000 |
| 211 | 1035.20410000 | 200.54160000   | 0.00000000 |
| 212 | 1048.96030000 | 18.22550000    | 0.00000000 |
| 213 | 1051.92840000 | 12.40010000    | 0.00000000 |
| 214 | 1055.17190000 | 167.68100000   | 0.00000000 |
| 215 | 1063.42370000 | 1.17810000     | 0.00000000 |
| 216 | 1068.12120000 | 0.18540000     | 0.00000000 |
| 217 | 1072.73160000 | 1.64110000     | 0.00000000 |
| 218 | 1078.89720000 | 84.92000000    | 0.00000000 |
| 219 | 1079.82360000 | 96.41110000    | 0.00000000 |
| 220 | 1081.05400000 | 1.04690000     | 0.00000000 |
| 221 | 1085.29790000 | 220.03790000   | 0.00000000 |
| 222 | 1086.66400000 | 445.56240000   | 0.00000000 |
| 223 | 1090.05360000 | 759.39000000   | 0.00000000 |
| 224 | 1091.59660000 | 20.20050000    | 0.00000000 |
| 225 | 1094.36030000 | 57.64830000    | 0.00000000 |
| 226 | 1101.56520000 | 315.80680000   | 0.00000000 |
| 227 | 1107.91880000 | 4092.45320000  | 0.00000000 |
| 228 | 1108.09860000 | 137.04430000   | 0.00000000 |
| 229 | 1115.34970000 | 24.20230000    | 0.00000000 |
| 230 | 1121.59140000 | 18.18170000    | 0.00000000 |
| 231 | 1126.77540000 | 136.13210000   | 0.00000000 |
| 232 | 1129.40930000 | 110.78520000   | 0.00000000 |
| 233 | 1134.22160000 | 128.53580000   | 0.00000000 |
| 234 | 1134.86810000 | 2.78200000     | 0.00000000 |
| 235 | 1141.81470000 | 2.03020000     | 0.00000000 |
| 236 | 1145.31100000 | 19.50620000    | 0.00000000 |
| 237 | 1147.36230000 | 37.15920000    | 0.00000000 |
| 238 | 1150.42100000 | 5.46370000     | 0.00000000 |
| 239 | 1151.93100000 | 1.52920000     | 0.00000000 |
| 240 | 1160.08580000 | 24.77800000    | 0.00000000 |
| 241 | 1160.92700000 | 0.97280000     | 0.00000000 |
| 242 | 1169.49680000 | 115.30680000   | 0.00000000 |
| 243 | 1172.99670000 | 0.52590000     | 0.00000000 |
| 244 | 1206.27280000 | 48.38050000    | 0.00000000 |
| 245 | 1211.41960000 | 39.18380000    | 0.00000000 |
| 246 | 1215.35840000 | 5.51600000     | 0.00000000 |
| 247 | 1217.85780000 | 0.79920000     | 0.00000000 |
| 248 | 1236.12610000 | 269.63690000   | 0.00000000 |
| 249 | 1237.89980000 | 22.62810000    | 0.00000000 |
| 250 | 1240.59030000 | 2600.98500000  | 0.00000000 |
| 251 | 1241.45040000 | 13.84850000    | 0.00000000 |
| 252 | 1243.02770000 | 34.35790000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1244.80180000 | 0.55890000    | 0.00000000 |
| 254 | 1247.46460000 | 25.75570000   | 0.00000000 |
| 255 | 1261.38300000 | 48.64210000   | 0.00000000 |
| 256 | 1262.43380000 | 3.78140000    | 0.00000000 |
| 257 | 1263.38010000 | 0.44950000    | 0.00000000 |
| 258 | 1265.25200000 | 9.38790000    | 0.00000000 |
| 259 | 1273.44780000 | 6.20800000    | 0.00000000 |
| 260 | 1273.66180000 | 30.38740000   | 0.00000000 |
| 261 | 1274.48910000 | 107.96890000  | 0.00000000 |
| 262 | 1278.45610000 | 127.47780000  | 0.00000000 |
| 263 | 1286.27990000 | 0.62910000    | 0.00000000 |
| 264 | 1298.87420000 | 1709.91030000 | 0.00000000 |
| 265 | 1306.39980000 | 35.51440000   | 0.00000000 |
| 266 | 1307.05070000 | 1.23940000    | 0.00000000 |
| 267 | 1308.17700000 | 123.58240000  | 0.00000000 |
| 268 | 1311.28350000 | 2.11360000    | 0.00000000 |
| 269 | 1314.12720000 | 4.38250000    | 0.00000000 |
| 270 | 1317.36730000 | 18.82590000   | 0.00000000 |
| 271 | 1318.70370000 | 34.22530000   | 0.00000000 |
| 272 | 1321.42490000 | 125.50830000  | 0.00000000 |
| 273 | 1323.29200000 | 134.80700000  | 0.00000000 |
| 274 | 1331.84020000 | 0.33970000    | 0.00000000 |
| 275 | 1333.30190000 | 0.27880000    | 0.00000000 |
| 276 | 1335.66600000 | 0.10030000    | 0.00000000 |
| 277 | 1336.55660000 | 7.93820000    | 0.00000000 |
| 278 | 1349.35720000 | 0.08590000    | 0.00000000 |
| 279 | 1349.92780000 | 18.16660000   | 0.00000000 |
| 280 | 1351.93250000 | 67.85310000   | 0.00000000 |
| 281 | 1359.39220000 | 4.85930000    | 0.00000000 |
| 282 | 1372.77320000 | 15.86170000   | 0.00000000 |
| 283 | 1374.62150000 | 118.01590000  | 0.00000000 |
| 284 | 1376.44550000 | 4.20320000    | 0.00000000 |
| 285 | 1378.53820000 | 1.62240000    | 0.00000000 |
| 286 | 1379.54540000 | 8.82820000    | 0.00000000 |
| 287 | 1380.34940000 | 24.90120000   | 0.00000000 |
| 288 | 1381.38660000 | 17.51830000   | 0.00000000 |
| 289 | 1392.69070000 | 214.34880000  | 0.00000000 |
| 290 | 1399.67250000 | 2.54390000    | 0.00000000 |
| 291 | 1405.14490000 | 37.57370000   | 0.00000000 |
| 292 | 1406.10320000 | 540.86240000  | 0.00000000 |
| 293 | 1408.47050000 | 82.24270000   | 0.00000000 |
| 294 | 1416.96130000 | 1462.79750000 | 0.00000000 |
| 295 | 1424.38940000 | 314.99940000  | 0.00000000 |
| 296 | 1429.35900000 | 7.44750000    | 0.00000000 |
| 297 | 1431.53630000 | 55.09280000   | 0.00000000 |
| 298 | 1434.09580000 | 66.07750000   | 0.00000000 |
| 299 | 1442.54300000 | 313.18280000  | 0.00000000 |
| 300 | 1453.89800000 | 121.22350000  | 0.00000000 |
| 301 | 1462.97320000 | 31.95420000   | 0.00000000 |
| 302 | 1469.31220000 | 1.51580000    | 0.00000000 |
| 303 | 1471.79790000 | 27.21810000   | 0.00000000 |
| 304 | 1472.61290000 | 47.93210000   | 0.00000000 |
| 305 | 1475.20090000 | 1.42260000    | 0.00000000 |
| 306 | 1480.22160000 | 6.29200000    | 0.00000000 |
| 307 | 1482.01490000 | 52.68960000   | 0.00000000 |
| 308 | 1486.56460000 | 56.47730000   | 0.00000000 |
| 309 | 1491.84170000 | 0.32180000    | 0.00000000 |
| 310 | 1499.97480000 | 12.77130000   | 0.00000000 |
| 311 | 1501.38140000 | 12.05960000   | 0.00000000 |
| 312 | 1503.57930000 | 17.66430000   | 0.00000000 |
| 313 | 1503.82450000 | 284.99890000  | 0.00000000 |
| 314 | 1504.71250000 | 0.94400000    | 0.00000000 |
| 315 | 1505.63030000 | 97.25020000   | 0.00000000 |
| 316 | 1509.86330000 | 15.93540000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1512.31520000 | 12.41580000   | 0.00000000 |
| 318 | 1516.79540000 | 555.08810000  | 0.00000000 |
| 319 | 1524.23610000 | 24.04300000   | 0.00000000 |
| 320 | 1529.48610000 | 135.17500000  | 0.00000000 |
| 321 | 1537.44300000 | 13.51840000   | 0.00000000 |
| 322 | 1539.78120000 | 26.76620000   | 0.00000000 |
| 323 | 1547.74800000 | 66.26070000   | 0.00000000 |
| 324 | 1550.74580000 | 3.64390000    | 0.00000000 |
| 325 | 1553.17200000 | 36.25130000   | 0.00000000 |
| 326 | 1557.16290000 | 52.63400000   | 0.00000000 |
| 327 | 1559.96850000 | 99.93450000   | 0.00000000 |
| 328 | 1576.87250000 | 291.58610000  | 0.00000000 |
| 329 | 1577.98210000 | 3.51760000    | 0.00000000 |
| 330 | 1582.36980000 | 10.34570000   | 0.00000000 |
| 331 | 1587.96660000 | 14.76210000   | 0.00000000 |
| 332 | 1595.43720000 | 12.16040000   | 0.00000000 |
| 333 | 1610.70700000 | 264.76500000  | 0.00000000 |
| 334 | 1613.68160000 | 5.71960000    | 0.00000000 |
| 335 | 1625.81720000 | 2.02190000    | 0.00000000 |
| 336 | 1626.39280000 | 5.28000000    | 0.00000000 |
| 337 | 1639.49000000 | 5.78030000    | 0.00000000 |
| 338 | 1641.00620000 | 426.75540000  | 0.00000000 |
| 339 | 1644.69690000 | 0.02770000    | 0.00000000 |
| 340 | 1657.44180000 | 370.29000000  | 0.00000000 |
| 341 | 1661.61230000 | 0.01990000    | 0.00000000 |
| 342 | 1661.89780000 | 127.74360000  | 0.00000000 |
| 343 | 1963.00670000 | 2393.94640000 | 0.00000000 |
| 344 | 1969.05510000 | 2324.95350000 | 0.00000000 |
| 345 | 2083.43390000 | 1957.96850000 | 0.00000000 |
| 346 | 3008.68830000 | 18.72520000   | 0.00000000 |
| 347 | 3016.45610000 | 2.74870000    | 0.00000000 |
| 348 | 3022.03500000 | 72.18460000   | 0.00000000 |
| 349 | 3032.77620000 | 1.47520000    | 0.00000000 |
| 350 | 3040.27580000 | 58.06810000   | 0.00000000 |
| 351 | 3043.73790000 | 57.76220000   | 0.00000000 |
| 352 | 3050.16480000 | 1.53030000    | 0.00000000 |
| 353 | 3063.18920000 | 69.46510000   | 0.00000000 |
| 354 | 3086.23550000 | 60.18010000   | 0.00000000 |
| 355 | 3090.95110000 | 70.99270000   | 0.00000000 |
| 356 | 3174.74960000 | 0.00530000    | 0.00000000 |
| 357 | 3182.62040000 | 1.04920000    | 0.00000000 |
| 358 | 3183.70400000 | 0.87650000    | 0.00000000 |
| 359 | 3184.61690000 | 3.81970000    | 0.00000000 |
| 360 | 3191.31330000 | 32.48930000   | 0.00000000 |
| 361 | 3192.06400000 | 2.24560000    | 0.00000000 |
| 362 | 3194.77960000 | 3.16090000    | 0.00000000 |
| 363 | 3196.41010000 | 3.31880000    | 0.00000000 |
| 364 | 3199.04070000 | 147.93590000  | 0.00000000 |
| 365 | 3200.98260000 | 1.68070000    | 0.00000000 |
| 366 | 3201.25910000 | 16.45990000   | 0.00000000 |
| 367 | 3202.95840000 | 2.10120000    | 0.00000000 |
| 368 | 3206.09870000 | 9.75400000    | 0.00000000 |
| 369 | 3206.90720000 | 36.36880000   | 0.00000000 |
| 370 | 3206.93470000 | 8.64630000    | 0.00000000 |
| 371 | 3212.90050000 | 0.06680000    | 0.00000000 |
| 372 | 3213.00720000 | 0.12500000    | 0.00000000 |
| 373 | 3217.31550000 | 14.38730000   | 0.00000000 |
| 374 | 3217.44260000 | 9.07860000    | 0.00000000 |
| 375 | 3218.61070000 | 7.19910000    | 0.00000000 |
| 376 | 3223.44810000 | 1.26190000    | 0.00000000 |
| 377 | 3223.54890000 | 2.90010000    | 0.00000000 |
| 378 | 3230.34300000 | 15.83730000   | 0.00000000 |
| 379 | 3230.52740000 | 8.11320000    | 0.00000000 |
| 380 | 3230.66140000 | 2.94420000    | 0.00000000 |

|     |               |             |            |
|-----|---------------|-------------|------------|
| 381 | 3231.76390000 | 15.20870000 | 0.00000000 |
| 382 | 3235.63320000 | 22.70950000 | 0.00000000 |
| 383 | 3240.82620000 | 13.06250000 | 0.00000000 |
| 384 | 3244.35260000 | 3.21490000  | 0.00000000 |
| 385 | 3262.64910000 | 0.53050000  | 0.00000000 |
| 386 | 3263.61460000 | 0.21080000  | 0.00000000 |
| 387 | 3264.26570000 | 7.18020000  | 0.00000000 |
| 388 | 3270.85510000 | 10.17210000 | 0.00000000 |
| 389 | 3271.86560000 | 15.72110000 | 0.00000000 |
| 390 | 3274.28010000 | 22.03550000 | 0.00000000 |
| 391 | 3287.25390000 | 6.41910000  | 0.00000000 |
| 392 | 3287.34020000 | 7.33110000  | 0.00000000 |
| 393 | 3288.20150000 | 6.32080000  | 0.00000000 |

### S13. CALCULATIONS ON EXTENDED CONFORMER OF $2^{3+}$ ( $^1A$ )



|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4)c6c(c3n2)ccc[n+](c6)[Ru]578(n9ccc[n+](c9)C([n+]<br>1n7ccc1)[n+](c1)n8ccc1)[n+](c1)ccc(cc1)CNC(CCCCNCc1cc[n+](c1)[Re]<br>1([n+](c1)2cccc3c2c2[n+](c1)cccc2c1c3nc2cccc2n1)([C]([O]))([C]([O]))([C]([O]) |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 1  |      |
| Energy                          | : -3972.55012320   | a.u. |
| Gibbs Energy                    | : -3971.51989400   | a.u. |
| Number of imaginary frequencies | : 4  |      |

#### S13.1. Cartesian Co-ordinates (XYZ format)

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|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.14897203 | -0.48144001 | 0.61128300  |
| H | 2.96508598 | 0.31297299  | -0.12061400 |
| H | 3.04525805 | -0.02174300 | 1.60898602  |
| C | 2.10592508 | -1.58160305 | 0.44553101  |
| H | 2.31059694 | -2.38312101 | 1.16647601  |
| H | 2.21484208 | -2.02171803 | -0.55161202 |
| C | 0.67421103 | -1.07957304 | 0.64003497  |



|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | 0.47209701   | -0.27392599 | -0.07639000 |
| H  | 0.57469398   | -0.63631701 | 1.63831902  |
| C  | -0.37563300  | -2.17958498 | 0.46981201  |
| H  | -0.17723900  | -2.98302388 | 1.18957102  |
| H  | -0.27212101  | -2.62611294 | -0.52670401 |
| C  | -2.85177994  | -2.77376604 | 0.48088899  |
| H  | -2.64938307  | -3.58880901 | 1.19671595  |
| H  | -2.76802993  | -3.20898795 | -0.52126402 |
| N  | 4.49991179   | -0.99793398 | 0.37947199  |
| C  | -5.23920918  | -3.25869608 | 0.50165302  |
| H  | -5.18339396  | -4.03559589 | 1.28111100  |
| H  | -5.08720398  | -3.77868390 | -0.45239300 |
| N  | -4.20741415  | -2.23835993 | 0.62397403  |
| C  | 5.53280783   | 0.01416700  | 0.54320800  |
| H  | 5.27234888   | 0.86847401  | -0.09377500 |
| H  | 5.60126877   | 0.41256899  | 1.56835401  |
| C  | -13.71871376 | -2.49343991 | 1.15921295  |
| N  | -12.83309078 | -2.47473407 | 2.30615091  |
| N  | -14.13130379 | -1.15371299 | 0.80620003  |
| N  | -13.07026386 | -3.14466190 | 0.03838700  |
| N  | -11.63214970 | -1.84214497 | 2.21365190  |
| C  | -12.97107697 | -3.10170698 | 3.50531197  |
| N  | -13.19198799 | -0.24359301 | 0.43952700  |
| C  | -15.38046360 | -0.61451697 | 0.77426398  |
| N  | -11.91268158 | -2.62863398 | -0.45689800 |
| C  | -13.39928722 | -4.30871820 | -0.58387297 |
| Ru | -11.20302486 | -0.86161798 | 0.41462499  |
| C  | -11.00984383 | -2.07260489 | 3.36966896  |
| C  | -11.81648827 | -2.85693502 | 4.21510696  |
| H  | -13.86244869 | -3.65566111 | 3.74662900  |
| C  | -13.85285378 | 0.88090801  | 0.17383400  |
| C  | -15.23463154 | 0.69420099  | 0.37107700  |
| H  | -16.24810982 | -1.19595098 | 1.03644896  |
| C  | -11.51151276 | -3.47782898 | -1.40278101 |
| C  | -12.41845131 | -4.54755402 | -1.52077305 |
| H  | -14.28761101 | -4.85482311 | -0.31414300 |
| N  | -10.58806229 | 0.96651697  | 1.20252097  |
| N  | -10.85029984 | 0.22346801  | -1.32902896 |
| H  | -10.02055836 | -1.68044198 | 3.53813601  |
| H  | -11.58308697 | -3.19666505 | 5.20924807  |
| H  | -13.31916237 | 1.76168895  | -0.14250199 |
| H  | -16.01712418 | 1.42067695  | 0.23598900  |
| H  | -10.59768200 | -3.29215693 | -1.94263196 |
| H  | -12.36065483 | -5.38014078 | -2.20023799 |
| C  | -10.51737309 | 1.31192303  | 2.49142504  |
| C  | -10.25934982 | 1.89553702  | 0.26351899  |
| C  | -10.40189457 | 1.49074602  | -1.11512196 |
| C  | -11.04298496 | -0.17943101 | -2.58838391 |
| C  | -10.09565639 | 2.57697010  | 2.90191889  |
| H  | -10.80964756 | 0.55993301  | 3.20884991  |
| C  | -9.82586384  | 3.18444991  | 0.59785402  |
| C  | -10.11102676 | 2.37415004  | -2.16203308 |
| C  | -10.77635002 | 0.64357001  | -3.68308306 |
| H  | -11.42359924 | -1.18106198 | -2.72071099 |
| C  | -9.74055481  | 3.52050090  | 1.95554602  |
| H  | -10.05322838 | 2.80081391  | 3.95901299  |
| C  | -9.49082947  | 4.11994314  | -0.47338700 |
| C  | -10.30195904 | 1.92579699  | -3.47584009 |
| C  | -9.63252735  | 3.71767497  | -1.84386802 |
| H  | -10.94584179 | 0.26387399  | -4.68129110 |
| H  | -9.40663528  | 4.51001501  | 2.23503995  |
| N  | -9.06467438  | 5.32975101  | -0.15006299 |
| H  | -10.08193588 | 2.59165311  | -4.29859781 |
| N  | -9.34247303  | 4.54085398  | -2.83786607 |

|    |              |             |             |
|----|--------------|-------------|-------------|
| C  | -8.76320076  | 6.17973423  | -1.15279806 |
| C  | -8.90493107  | 5.77733898  | -2.52380991 |
| C  | -8.30058098  | 7.48784494  | -0.85616601 |
| C  | -8.57964802  | 6.69575119  | -3.55523801 |
| C  | -7.99493885  | 8.35015392  | -1.87671697 |
| H  | -8.20088482  | 7.77102613  | 0.18400200  |
| C  | -8.13535309  | 7.95189285  | -3.23388290 |
| H  | -8.69361496  | 6.37242699  | -4.58214808 |
| H  | -7.64151096  | 9.34926128  | -1.65366900 |
| H  | -7.88638020  | 8.65523434  | -4.01885080 |
| N  | 12.09516621  | 0.15191901  | -1.57208598 |
| N  | 12.31498623  | -1.42968595 | 0.61764699  |
| C  | 11.94522953  | 0.91346997  | -2.66017389 |
| C  | 12.63082409  | 0.70213300  | -0.45075899 |
| C  | 12.74969387  | -0.14612000 | 0.72304899  |
| C  | 12.38505459  | -2.22789192 | 1.68734205  |
| C  | 12.32353210  | 2.25525594  | -2.68933201 |
| H  | 11.51359081  | 0.43702301  | -3.52884197 |
| C  | 13.03490257  | 2.04402900  | -0.40566999 |
| C  | 13.27130318  | 0.36216101  | 1.92119503  |
| C  | 12.89189053  | -1.79232895 | 2.91121602  |
| H  | 12.02814579  | -3.23995304 | 1.56015897  |
| C  | 12.87425041  | 2.82519197  | -1.55846703 |
| H  | 12.18015671  | 2.82713199  | -3.59556794 |
| C  | 13.59825516  | 2.58764911  | 0.82692200  |
| C  | 13.34003735  | -0.49164701 | 3.03085208  |
| C  | 13.71575069  | 1.75171602  | 1.98344100  |
| H  | 12.92580509  | -2.47851610 | 3.74594593  |
| H  | 13.18300438  | 3.86110711  | -1.53589296 |
| N  | 13.98628998  | 3.85232997  | 0.84579402  |
| H  | 13.74079037  | -0.11082100 | 3.96003199  |
| N  | 14.21711254  | 2.20929503  | 3.11902404  |
| C  | 14.50128078  | 4.33430481  | 1.99476099  |
| C  | 14.61895847  | 3.49568796  | 3.15509796  |
| C  | 14.93313599  | 5.68406296  | 2.06547499  |
| C  | 15.16451645  | 4.03336382  | 4.34949493  |
| C  | 15.45561790  | 6.17130089  | 3.23498011  |
| H  | 14.83591843  | 6.29908895  | 1.17988801  |
| C  | 15.57189369  | 5.34140205  | 4.38330984  |
| H  | 15.24437141  | 3.38453603  | 5.21241522  |
| H  | 15.78634071  | 7.20091820  | 3.29243994  |
| H  | 15.98880768  | 5.75500107  | 5.29323006  |
| H  | -14.60254097 | -3.06551909 | 1.42168403  |
| C  | 6.89564180   | -0.47223899 | 0.11859000  |
| C  | 8.05351543   | 0.18223301  | 0.54259199  |
| C  | 7.05655718   | -1.56869304 | -0.72885799 |
| C  | 9.29099560   | -0.26099899 | 0.11157600  |
| H  | 8.00065136   | 1.03431499  | 1.20867205  |
| C  | 8.32766914   | -1.95747697 | -1.11395800 |
| H  | 6.19095087   | -2.11204600 | -1.08029103 |
| N  | 9.44234562   | -1.31789696 | -0.70798397 |
| H  | 10.18890381  | 0.24227300  | 0.43612301  |
| H  | 8.46933079   | -2.80600309 | -1.76882994 |
| C  | -6.62958097  | -2.67450404 | 0.49362299  |
| C  | -6.87058020  | -1.35030901 | 0.12798300  |
| C  | -7.73939180  | -3.45159888 | 0.83037698  |
| C  | -8.16650581  | -0.86514002 | 0.11024000  |
| H  | -6.04633617  | -0.70264298 | -0.13529600 |
| C  | -9.00741673  | -2.90163898 | 0.78680599  |
| H  | -7.62482023  | -4.48523998 | 1.13248098  |
| N  | -9.23601055  | -1.61863995 | 0.43281701  |
| H  | -8.35750771  | 0.15922700  | -0.17052899 |
| H  | -9.87488174  | -3.48964310 | 1.04566300  |
| Re | 11.55755806  | -2.06345391 | -1.44301605 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 13.33457947 | -2.59428000 | -1.99213398 |
| O | 14.39948082 | -2.89884496 | -2.31070399 |
| C | 11.10871124 | -3.90155411 | -1.03434896 |
| O | 10.84360218 | -4.98973322 | -0.75871497 |
| C | 10.90806293 | -2.29952002 | -3.25045490 |
| O | 10.52424145 | -2.40597606 | -4.33305788 |
| H | -4.29005289 | -1.79577506 | 1.53592098  |
| H | 4.67639399  | -1.75803399 | 1.03169703  |
| C | -1.80809605 | -1.67488503 | 0.65132397  |
| H | -2.01680803 | -0.87668198 | -0.06930400 |
| H | -1.91280997 | -1.23164701 | 1.64971697  |

## S13.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -15.08320000 | 0.12120000   | 0.00000000      |
| 2    | -13.39520000 | 0.72490000   | 0.00000000      |
| 3    | -9.23940000  | 0.98430000   | 0.00000000      |
| 4    | -5.43420000  | 0.37260000   | 0.00000000      |
| 5    | 2.09740000   | 0.11410000   | 0.00000000      |
| 6    | 10.55530000  | 0.32890000   | 0.00000000      |
| 7    | 12.22780000  | 0.69800000   | 0.00000000      |
| 8    | 18.33510000  | 0.63560000   | 0.00000000      |
| 9    | 19.67000000  | 0.32340000   | 0.00000000      |
| 10   | 24.39110000  | 0.24800000   | 0.00000000      |
| 11   | 28.48540000  | 0.05970000   | 0.00000000      |
| 12   | 31.80190000  | 0.52450000   | 0.00000000      |
| 13   | 38.73870000  | 1.31840000   | 0.00000000      |
| 14   | 38.93730000  | 0.81060000   | 0.00000000      |
| 15   | 42.86810000  | 1.45690000   | 0.00000000      |
| 16   | 46.71460000  | 0.06350000   | 0.00000000      |
| 17   | 49.98460000  | 0.37090000   | 0.00000000      |
| 18   | 53.94440000  | 1.89610000   | 0.00000000      |
| 19   | 56.77700000  | 1.05380000   | 0.00000000      |
| 20   | 62.02990000  | 0.78810000   | 0.00000000      |
| 21   | 62.63650000  | 0.65530000   | 0.00000000      |
| 22   | 63.53360000  | 0.11550000   | 0.00000000      |
| 23   | 66.83210000  | 0.09820000   | 0.00000000      |
| 24   | 67.30010000  | 3.10450000   | 0.00000000      |
| 25   | 70.25040000  | 0.94560000   | 0.00000000      |
| 26   | 71.92510000  | 0.52180000   | 0.00000000      |
| 27   | 78.66310000  | 0.14930000   | 0.00000000      |
| 28   | 83.79810000  | 18.10240000  | 0.00000000      |
| 29   | 85.73420000  | 0.14320000   | 0.00000000      |
| 30   | 87.59320000  | 0.35740000   | 0.00000000      |
| 31   | 90.85230000  | 0.69630000   | 0.00000000      |
| 32   | 93.02640000  | 1.02450000   | 0.00000000      |
| 33   | 95.98330000  | 0.71050000   | 0.00000000      |
| 34   | 99.53830000  | 0.36990000   | 0.00000000      |
| 35   | 104.32010000 | 0.80600000   | 0.00000000      |
| 36   | 110.74040000 | 0.81470000   | 0.00000000      |
| 37   | 119.84150000 | 1.18970000   | 0.00000000      |
| 38   | 124.90430000 | 0.19940000   | 0.00000000      |
| 39   | 129.60550000 | 1.66330000   | 0.00000000      |
| 40   | 137.31470000 | 1.08010000   | 0.00000000      |
| 41   | 139.73310000 | 0.79020000   | 0.00000000      |
| 42   | 140.49970000 | 3.04030000   | 0.00000000      |
| 43   | 147.45780000 | 0.27290000   | 0.00000000      |
| 44   | 151.81430000 | 0.64690000   | 0.00000000      |
| 45   | 154.98670000 | 2.14810000   | 0.00000000      |
| 46   | 165.39270000 | 0.89990000   | 0.00000000      |
| 47   | 168.11020000 | 0.26560000   | 0.00000000      |
| 48   | 170.66590000 | 1.05790000   | 0.00000000      |
| 49   | 172.83740000 | 0.53570000   | 0.00000000      |
| 50   | 174.72890000 | 0.47450000   | 0.00000000      |
| 51   | 175.66630000 | 0.50630000   | 0.00000000      |
| 52   | 180.02940000 | 1.62170000   | 0.00000000      |
| 53   | 181.98630000 | 0.45090000   | 0.00000000      |
| 54   | 188.92920000 | 1.55230000   | 0.00000000      |
| 55   | 190.23960000 | 0.63890000   | 0.00000000      |
| 56   | 191.80390000 | 0.41510000   | 0.00000000      |
| 57   | 198.03290000 | 0.01980000   | 0.00000000      |
| 58   | 198.78390000 | 0.25760000   | 0.00000000      |
| 59   | 208.52470000 | 1.26890000   | 0.00000000      |
| 60   | 220.38100000 | 0.32840000   | 0.00000000      |

|     |              |             |            |
|-----|--------------|-------------|------------|
| 61  | 237.67810000 | 0.54190000  | 0.00000000 |
| 62  | 238.41090000 | 1.32480000  | 0.00000000 |
| 63  | 243.03730000 | 0.03550000  | 0.00000000 |
| 64  | 253.37030000 | 0.09140000  | 0.00000000 |
| 65  | 258.29980000 | 1.02200000  | 0.00000000 |
| 66  | 272.69420000 | 0.83050000  | 0.00000000 |
| 67  | 275.36900000 | 6.64000000  | 0.00000000 |
| 68  | 283.45790000 | 0.33270000  | 0.00000000 |
| 69  | 298.27340000 | 1.62690000  | 0.00000000 |
| 70  | 313.70240000 | 1.82940000  | 0.00000000 |
| 71  | 323.74130000 | 3.58070000  | 0.00000000 |
| 72  | 326.98190000 | 0.26950000  | 0.00000000 |
| 73  | 327.69980000 | 0.30980000  | 0.00000000 |
| 74  | 328.83630000 | 0.08740000  | 0.00000000 |
| 75  | 331.70840000 | 5.17080000  | 0.00000000 |
| 76  | 332.63410000 | 4.64280000  | 0.00000000 |
| 77  | 336.48420000 | 3.43640000  | 0.00000000 |
| 78  | 342.52080000 | 3.64290000  | 0.00000000 |
| 79  | 349.82530000 | 1.29450000  | 0.00000000 |
| 80  | 358.67250000 | 2.56530000  | 0.00000000 |
| 81  | 366.68640000 | 8.84870000  | 0.00000000 |
| 82  | 372.39040000 | 7.14440000  | 0.00000000 |
| 83  | 379.98690000 | 0.08250000  | 0.00000000 |
| 84  | 389.75500000 | 1.25340000  | 0.00000000 |
| 85  | 391.19270000 | 0.20330000  | 0.00000000 |
| 86  | 401.84750000 | 4.41930000  | 0.00000000 |
| 87  | 402.77410000 | 0.18490000  | 0.00000000 |
| 88  | 407.37220000 | 0.53520000  | 0.00000000 |
| 89  | 412.79260000 | 0.49470000  | 0.00000000 |
| 90  | 417.30530000 | 2.05550000  | 0.00000000 |
| 91  | 440.92670000 | 20.10760000 | 0.00000000 |
| 92  | 442.52270000 | 2.04780000  | 0.00000000 |
| 93  | 443.53500000 | 15.30140000 | 0.00000000 |
| 94  | 446.14810000 | 10.98560000 | 0.00000000 |
| 95  | 453.07230000 | 0.46830000  | 0.00000000 |
| 96  | 473.73690000 | 23.99670000 | 0.00000000 |
| 97  | 477.35210000 | 2.27650000  | 0.00000000 |
| 98  | 477.80480000 | 7.50770000  | 0.00000000 |
| 99  | 479.78780000 | 20.76650000 | 0.00000000 |
| 100 | 487.70580000 | 14.61550000 | 0.00000000 |
| 101 | 489.63520000 | 7.58350000  | 0.00000000 |
| 102 | 494.28770000 | 1.05580000  | 0.00000000 |
| 103 | 497.05960000 | 0.12410000  | 0.00000000 |
| 104 | 497.61830000 | 0.10480000  | 0.00000000 |
| 105 | 498.46190000 | 23.13200000 | 0.00000000 |
| 106 | 499.30740000 | 1.01640000  | 0.00000000 |
| 107 | 504.19440000 | 0.87850000  | 0.00000000 |
| 108 | 511.49620000 | 14.36970000 | 0.00000000 |
| 109 | 513.96650000 | 4.55460000  | 0.00000000 |
| 110 | 524.81570000 | 12.44590000 | 0.00000000 |
| 111 | 527.79180000 | 10.42130000 | 0.00000000 |
| 112 | 537.02250000 | 1.15480000  | 0.00000000 |
| 113 | 548.13090000 | 13.62710000 | 0.00000000 |
| 114 | 561.45920000 | 0.12960000  | 0.00000000 |
| 115 | 564.06560000 | 0.39510000  | 0.00000000 |
| 116 | 575.05880000 | 0.61200000  | 0.00000000 |
| 117 | 575.30460000 | 1.10270000  | 0.00000000 |
| 118 | 579.82090000 | 0.67770000  | 0.00000000 |
| 119 | 580.22170000 | 0.00460000  | 0.00000000 |
| 120 | 594.79150000 | 29.73810000 | 0.00000000 |
| 121 | 596.11830000 | 20.06210000 | 0.00000000 |
| 122 | 602.10520000 | 5.38970000  | 0.00000000 |
| 123 | 605.62540000 | 0.35140000  | 0.00000000 |
| 124 | 609.35690000 | 6.48690000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 617.88180000 | 23.10780000  | 0.00000000 |
| 126 | 622.81420000 | 32.59110000  | 0.00000000 |
| 127 | 628.04940000 | 18.30950000  | 0.00000000 |
| 128 | 632.29950000 | 13.07140000  | 0.00000000 |
| 129 | 636.56700000 | 14.93980000  | 0.00000000 |
| 130 | 636.75830000 | 10.70350000  | 0.00000000 |
| 131 | 638.53280000 | 0.86710000   | 0.00000000 |
| 132 | 649.31460000 | 70.63890000  | 0.00000000 |
| 133 | 651.33640000 | 2.33850000   | 0.00000000 |
| 134 | 653.18290000 | 1.39760000   | 0.00000000 |
| 135 | 655.65880000 | 12.31650000  | 0.00000000 |
| 136 | 659.25850000 | 0.01790000   | 0.00000000 |
| 137 | 667.41750000 | 1.30610000   | 0.00000000 |
| 138 | 668.82030000 | 3.45710000   | 0.00000000 |
| 139 | 678.52260000 | 2.62020000   | 0.00000000 |
| 140 | 684.61090000 | 0.42390000   | 0.00000000 |
| 141 | 684.69890000 | 0.26630000   | 0.00000000 |
| 142 | 686.54440000 | 0.31280000   | 0.00000000 |
| 143 | 732.72140000 | 9.06830000   | 0.00000000 |
| 144 | 736.46150000 | 9.66220000   | 0.00000000 |
| 145 | 739.19020000 | 10.05110000  | 0.00000000 |
| 146 | 740.80470000 | 7.27410000   | 0.00000000 |
| 147 | 741.13510000 | 4.95750000   | 0.00000000 |
| 148 | 741.40420000 | 1.35870000   | 0.00000000 |
| 149 | 750.90470000 | 5.73890000   | 0.00000000 |
| 150 | 751.34240000 | 0.00490000   | 0.00000000 |
| 151 | 752.09940000 | 103.49470000 | 0.00000000 |
| 152 | 757.95300000 | 101.55310000 | 0.00000000 |
| 153 | 758.42240000 | 91.58670000  | 0.00000000 |
| 154 | 759.79850000 | 0.51990000   | 0.00000000 |
| 155 | 761.21040000 | 99.60150000  | 0.00000000 |
| 156 | 763.87580000 | 120.21400000 | 0.00000000 |
| 157 | 778.76750000 | 76.78770000  | 0.00000000 |
| 158 | 779.15170000 | 61.75710000  | 0.00000000 |
| 159 | 779.36910000 | 19.70170000  | 0.00000000 |
| 160 | 781.54650000 | 15.17210000  | 0.00000000 |
| 161 | 796.09690000 | 94.60370000  | 0.00000000 |
| 162 | 799.52750000 | 117.42010000 | 0.00000000 |
| 163 | 801.38800000 | 24.10510000  | 0.00000000 |
| 164 | 804.97730000 | 150.93100000 | 0.00000000 |
| 165 | 811.54800000 | 0.08960000   | 0.00000000 |
| 166 | 811.77600000 | 34.15980000  | 0.00000000 |
| 167 | 815.48950000 | 0.06550000   | 0.00000000 |
| 168 | 818.12810000 | 14.92880000  | 0.00000000 |
| 169 | 820.20440000 | 0.16410000   | 0.00000000 |
| 170 | 826.68350000 | 0.15910000   | 0.00000000 |
| 171 | 833.88000000 | 22.55710000  | 0.00000000 |
| 172 | 835.80780000 | 63.75820000  | 0.00000000 |
| 173 | 838.80020000 | 123.42030000 | 0.00000000 |
| 174 | 840.82420000 | 65.03440000  | 0.00000000 |
| 175 | 854.02650000 | 10.47810000  | 0.00000000 |
| 176 | 858.02120000 | 10.93330000  | 0.00000000 |
| 177 | 859.93760000 | 0.01390000   | 0.00000000 |
| 178 | 863.50530000 | 10.29190000  | 0.00000000 |
| 179 | 868.96150000 | 19.88720000  | 0.00000000 |
| 180 | 873.38690000 | 0.02940000   | 0.00000000 |
| 181 | 873.78080000 | 9.63550000   | 0.00000000 |
| 182 | 875.37580000 | 11.40220000  | 0.00000000 |
| 183 | 879.91180000 | 54.82930000  | 0.00000000 |
| 184 | 884.08650000 | 0.13610000   | 0.00000000 |
| 185 | 892.00370000 | 2.08290000   | 0.00000000 |
| 186 | 895.99840000 | 0.00010000   | 0.00000000 |
| 187 | 896.95720000 | 0.00210000   | 0.00000000 |
| 188 | 900.08680000 | 5.69040000   | 0.00000000 |

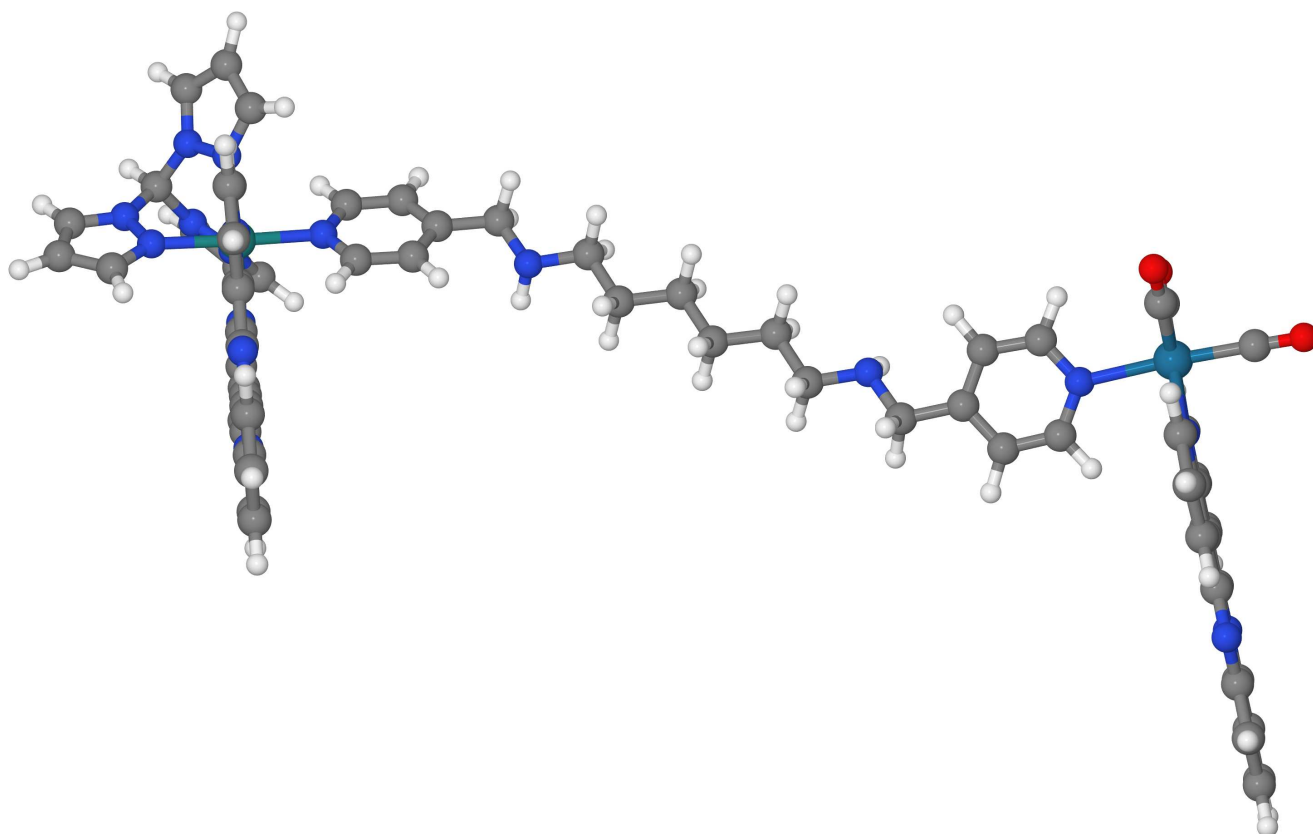
|     |               |              |            |
|-----|---------------|--------------|------------|
| 189 | 915.26540000  | 1.33160000   | 0.00000000 |
| 190 | 917.26880000  | 1.24390000   | 0.00000000 |
| 191 | 920.91750000  | 0.24230000   | 0.00000000 |
| 192 | 924.45250000  | 3.92860000   | 0.00000000 |
| 193 | 926.73190000  | 5.05090000   | 0.00000000 |
| 194 | 932.58010000  | 18.41370000  | 0.00000000 |
| 195 | 947.93800000  | 0.04950000   | 0.00000000 |
| 196 | 948.54080000  | 0.05110000   | 0.00000000 |
| 197 | 953.69470000  | 0.67460000   | 0.00000000 |
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| 199 | 977.25370000  | 0.10630000   | 0.00000000 |
| 200 | 977.41920000  | 0.18900000   | 0.00000000 |
| 201 | 981.68190000  | 41.84050000  | 0.00000000 |
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| 204 | 991.66500000  | 1.39860000   | 0.00000000 |
| 205 | 992.40440000  | 1.35140000   | 0.00000000 |
| 206 | 995.39250000  | 5.62190000   | 0.00000000 |
| 207 | 999.54160000  | 7.05190000   | 0.00000000 |
| 208 | 1000.72930000 | 17.94880000  | 0.00000000 |
| 209 | 1001.78600000 | 2.22090000   | 0.00000000 |
| 210 | 1006.65980000 | 2.76790000   | 0.00000000 |
| 211 | 1008.99470000 | 1.15460000   | 0.00000000 |
| 212 | 1009.07850000 | 10.85420000  | 0.00000000 |
| 213 | 1009.28410000 | 12.93620000  | 0.00000000 |
| 214 | 1011.91230000 | 5.20640000   | 0.00000000 |
| 215 | 1013.85940000 | 13.14260000  | 0.00000000 |
| 216 | 1018.92210000 | 6.54150000   | 0.00000000 |
| 217 | 1020.58380000 | 0.00250000   | 0.00000000 |
| 218 | 1021.36700000 | 0.00090000   | 0.00000000 |
| 219 | 1025.05340000 | 0.10090000   | 0.00000000 |
| 220 | 1026.00720000 | 0.02910000   | 0.00000000 |
| 221 | 1027.08830000 | 2.92420000   | 0.00000000 |
| 222 | 1027.17780000 | 5.45720000   | 0.00000000 |
| 223 | 1031.13570000 | 0.64710000   | 0.00000000 |
| 224 | 1033.24710000 | 0.40340000   | 0.00000000 |
| 225 | 1033.97940000 | 0.05770000   | 0.00000000 |
| 226 | 1051.41090000 | 0.20810000   | 0.00000000 |
| 227 | 1057.50300000 | 65.34090000  | 0.00000000 |
| 228 | 1060.02100000 | 23.46270000  | 0.00000000 |
| 229 | 1066.75710000 | 2.07100000   | 0.00000000 |
| 230 | 1067.02570000 | 0.11850000   | 0.00000000 |
| 231 | 1068.11520000 | 0.11420000   | 0.00000000 |
| 232 | 1071.46520000 | 0.07840000   | 0.00000000 |
| 233 | 1074.18130000 | 42.29410000  | 0.00000000 |
| 234 | 1075.53120000 | 49.46430000  | 0.00000000 |
| 235 | 1077.28840000 | 24.17320000  | 0.00000000 |
| 236 | 1083.03300000 | 7.92140000   | 0.00000000 |
| 237 | 1083.88880000 | 39.85190000  | 0.00000000 |
| 238 | 1087.15640000 | 5.12590000   | 0.00000000 |
| 239 | 1093.17180000 | 6.11400000   | 0.00000000 |
| 240 | 1105.03750000 | 41.81680000  | 0.00000000 |
| 241 | 1105.55380000 | 11.94930000  | 0.00000000 |
| 242 | 1117.30010000 | 15.63080000  | 0.00000000 |
| 243 | 1120.40540000 | 82.62380000  | 0.00000000 |
| 244 | 1121.20730000 | 14.34650000  | 0.00000000 |
| 245 | 1121.69710000 | 100.46020000 | 0.00000000 |
| 246 | 1123.22430000 | 24.40370000  | 0.00000000 |
| 247 | 1130.40340000 | 2.98250000   | 0.00000000 |
| 248 | 1130.82930000 | 43.53130000  | 0.00000000 |
| 249 | 1135.22340000 | 1.74160000   | 0.00000000 |
| 250 | 1136.05420000 | 41.18350000  | 0.00000000 |
| 251 | 1143.45520000 | 34.79360000  | 0.00000000 |
| 252 | 1148.02550000 | 150.26820000 | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1150.63140000 | 0.51910000   | 0.00000000 |
| 254 | 1150.91890000 | 4.74060000   | 0.00000000 |
| 255 | 1151.09100000 | 3.34690000   | 0.00000000 |
| 256 | 1157.85990000 | 30.70410000  | 0.00000000 |
| 257 | 1159.44480000 | 18.36630000  | 0.00000000 |
| 258 | 1170.49860000 | 8.55490000   | 0.00000000 |
| 259 | 1172.16440000 | 0.89110000   | 0.00000000 |
| 260 | 1173.18250000 | 0.44840000   | 0.00000000 |
| 261 | 1186.42720000 | 1.41350000   | 0.00000000 |
| 262 | 1211.91380000 | 3.48720000   | 0.00000000 |
| 263 | 1212.83040000 | 1.12290000   | 0.00000000 |
| 264 | 1214.03000000 | 1.82580000   | 0.00000000 |
| 265 | 1215.05760000 | 0.81750000   | 0.00000000 |
| 266 | 1221.95670000 | 11.14730000  | 0.00000000 |
| 267 | 1223.06830000 | 10.98660000  | 0.00000000 |
| 268 | 1235.33480000 | 4.79990000   | 0.00000000 |
| 269 | 1239.07460000 | 0.19180000   | 0.00000000 |
| 270 | 1243.52190000 | 0.48470000   | 0.00000000 |
| 271 | 1247.37530000 | 6.69600000   | 0.00000000 |
| 272 | 1255.83890000 | 1.50570000   | 0.00000000 |
| 273 | 1256.82230000 | 28.82410000  | 0.00000000 |
| 274 | 1257.14550000 | 19.50560000  | 0.00000000 |
| 275 | 1262.79000000 | 0.39870000   | 0.00000000 |
| 276 | 1263.49140000 | 0.63670000   | 0.00000000 |
| 277 | 1268.88060000 | 94.49030000  | 0.00000000 |
| 278 | 1269.62850000 | 7.43680000   | 0.00000000 |
| 279 | 1272.68560000 | 7.75090000   | 0.00000000 |
| 280 | 1272.74440000 | 10.02680000  | 0.00000000 |
| 281 | 1273.93290000 | 112.72930000 | 0.00000000 |
| 282 | 1282.99600000 | 8.29990000   | 0.00000000 |
| 283 | 1284.71990000 | 7.04620000   | 0.00000000 |
| 284 | 1301.00150000 | 0.64300000   | 0.00000000 |
| 285 | 1302.08010000 | 0.63200000   | 0.00000000 |
| 286 | 1305.32230000 | 0.32660000   | 0.00000000 |
| 287 | 1306.99020000 | 0.05370000   | 0.00000000 |
| 288 | 1310.81270000 | 8.68050000   | 0.00000000 |
| 289 | 1316.90640000 | 20.20220000  | 0.00000000 |
| 290 | 1317.89340000 | 58.04560000  | 0.00000000 |
| 291 | 1320.68090000 | 10.58850000  | 0.00000000 |
| 292 | 1320.98430000 | 41.73950000  | 0.00000000 |
| 293 | 1323.49190000 | 3.36230000   | 0.00000000 |
| 294 | 1323.62050000 | 103.13750000 | 0.00000000 |
| 295 | 1329.13190000 | 0.18780000   | 0.00000000 |
| 296 | 1331.12110000 | 0.15670000   | 0.00000000 |
| 297 | 1332.54470000 | 0.15450000   | 0.00000000 |
| 298 | 1336.08770000 | 0.20430000   | 0.00000000 |
| 299 | 1342.72660000 | 62.24610000  | 0.00000000 |
| 300 | 1346.41400000 | 0.83570000   | 0.00000000 |
| 301 | 1346.92100000 | 8.84980000   | 0.00000000 |
| 302 | 1351.20390000 | 1.54330000   | 0.00000000 |
| 303 | 1365.09050000 | 3.61400000   | 0.00000000 |
| 304 | 1371.91390000 | 11.27460000  | 0.00000000 |
| 305 | 1372.29820000 | 187.24820000 | 0.00000000 |
| 306 | 1372.76680000 | 17.86840000  | 0.00000000 |
| 307 | 1374.70440000 | 100.65560000 | 0.00000000 |
| 308 | 1376.66950000 | 1.16800000   | 0.00000000 |
| 309 | 1378.24230000 | 49.85230000  | 0.00000000 |
| 310 | 1378.27320000 | 2.94780000   | 0.00000000 |
| 311 | 1384.66000000 | 1.20310000   | 0.00000000 |
| 312 | 1393.85850000 | 64.52080000  | 0.00000000 |
| 313 | 1404.43450000 | 0.40260000   | 0.00000000 |
| 314 | 1415.71790000 | 6.83630000   | 0.00000000 |
| 315 | 1420.35290000 | 9.07970000   | 0.00000000 |
| 316 | 1424.34160000 | 0.97130000   | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1425.75220000 | 1.44880000    | 0.00000000 |
| 318 | 1427.95190000 | 1.46270000    | 0.00000000 |
| 319 | 1428.80580000 | 8.95430000    | 0.00000000 |
| 320 | 1435.60910000 | 60.56190000   | 0.00000000 |
| 321 | 1437.35780000 | 53.55810000   | 0.00000000 |
| 322 | 1443.51590000 | 157.95430000  | 0.00000000 |
| 323 | 1453.17440000 | 88.22010000   | 0.00000000 |
| 324 | 1453.77420000 | 124.33660000  | 0.00000000 |
| 325 | 1460.91230000 | 42.03380000   | 0.00000000 |
| 326 | 1461.30540000 | 33.39260000   | 0.00000000 |
| 327 | 1468.49760000 | 22.84230000   | 0.00000000 |
| 328 | 1473.37870000 | 32.51450000   | 0.00000000 |
| 329 | 1473.78230000 | 59.96090000   | 0.00000000 |
| 330 | 1475.04470000 | 0.02140000    | 0.00000000 |
| 331 | 1475.41790000 | 88.55370000   | 0.00000000 |
| 332 | 1479.20690000 | 12.17760000   | 0.00000000 |
| 333 | 1481.47830000 | 6.23980000    | 0.00000000 |
| 334 | 1484.72850000 | 16.77890000   | 0.00000000 |
| 335 | 1491.16540000 | 0.13990000    | 0.00000000 |
| 336 | 1492.42640000 | 6.26110000    | 0.00000000 |
| 337 | 1499.25400000 | 27.83120000   | 0.00000000 |
| 338 | 1500.02720000 | 9.56520000    | 0.00000000 |
| 339 | 1500.28890000 | 94.43110000   | 0.00000000 |
| 340 | 1500.90410000 | 15.63210000   | 0.00000000 |
| 341 | 1501.13730000 | 11.13800000   | 0.00000000 |
| 342 | 1503.48940000 | 8.10440000    | 0.00000000 |
| 343 | 1503.84440000 | 13.35950000   | 0.00000000 |
| 344 | 1516.84520000 | 5.61720000    | 0.00000000 |
| 345 | 1517.55610000 | 24.59890000   | 0.00000000 |
| 346 | 1518.27850000 | 24.57820000   | 0.00000000 |
| 347 | 1523.85590000 | 21.76260000   | 0.00000000 |
| 348 | 1524.42890000 | 26.03360000   | 0.00000000 |
| 349 | 1526.70510000 | 56.02550000   | 0.00000000 |
| 350 | 1530.17440000 | 116.92350000  | 0.00000000 |
| 351 | 1536.91180000 | 41.21790000   | 0.00000000 |
| 352 | 1551.98470000 | 10.22990000   | 0.00000000 |
| 353 | 1553.54000000 | 13.45640000   | 0.00000000 |
| 354 | 1557.07360000 | 12.33290000   | 0.00000000 |
| 355 | 1577.94790000 | 2.30760000    | 0.00000000 |
| 356 | 1578.09860000 | 3.67160000    | 0.00000000 |
| 357 | 1581.87190000 | 7.00000000    | 0.00000000 |
| 358 | 1582.00200000 | 36.91830000   | 0.00000000 |
| 359 | 1594.02540000 | 8.24230000    | 0.00000000 |
| 360 | 1597.32170000 | 6.63290000    | 0.00000000 |
| 361 | 1610.81710000 | 0.84690000    | 0.00000000 |
| 362 | 1611.95430000 | 15.34440000   | 0.00000000 |
| 363 | 1619.30070000 | 2.77560000    | 0.00000000 |
| 364 | 1624.63360000 | 0.84080000    | 0.00000000 |
| 365 | 1626.39300000 | 5.05920000    | 0.00000000 |
| 366 | 1626.75050000 | 11.08470000   | 0.00000000 |
| 367 | 1637.28160000 | 0.67610000    | 0.00000000 |
| 368 | 1638.51440000 | 5.77770000    | 0.00000000 |
| 369 | 1652.00520000 | 130.86000000  | 0.00000000 |
| 370 | 1660.97080000 | 0.40870000    | 0.00000000 |
| 371 | 1661.38330000 | 0.04060000    | 0.00000000 |
| 372 | 1662.19040000 | 54.71530000   | 0.00000000 |
| 373 | 1846.14610000 | 44.68760000   | 0.00000000 |
| 374 | 1960.77290000 | 2363.79490000 | 0.00000000 |
| 375 | 1964.74730000 | 2302.22340000 | 0.00000000 |
| 376 | 2084.01650000 | 1703.86230000 | 0.00000000 |
| 377 | 2927.69860000 | 156.33010000  | 0.00000000 |
| 378 | 2928.57200000 | 137.97880000  | 0.00000000 |
| 379 | 2948.24910000 | 109.95400000  | 0.00000000 |
| 380 | 2949.30940000 | 98.30910000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 2999.22110000 | 0.63800000   | 0.00000000 |
| 382 | 2999.63580000 | 0.11030000   | 0.00000000 |
| 383 | 3003.80290000 | 2.67140000   | 0.00000000 |
| 384 | 3008.44300000 | 181.92460000 | 0.00000000 |
| 385 | 3018.97250000 | 14.96910000  | 0.00000000 |
| 386 | 3019.53530000 | 19.94930000  | 0.00000000 |
| 387 | 3022.86720000 | 19.75430000  | 0.00000000 |
| 388 | 3025.84080000 | 38.30980000  | 0.00000000 |
| 389 | 3027.47010000 | 90.18630000  | 0.00000000 |
| 390 | 3035.35950000 | 3.30480000   | 0.00000000 |
| 391 | 3051.32590000 | 0.66630000   | 0.00000000 |
| 392 | 3058.12720000 | 333.76700000 | 0.00000000 |
| 393 | 3183.27080000 | 0.71420000   | 0.00000000 |
| 394 | 3183.81020000 | 0.87190000   | 0.00000000 |
| 395 | 3188.73120000 | 1.65340000   | 0.00000000 |
| 396 | 3191.49170000 | 1.80820000   | 0.00000000 |
| 397 | 3191.75420000 | 6.48890000   | 0.00000000 |
| 398 | 3192.16010000 | 2.38120000   | 0.00000000 |
| 399 | 3193.70000000 | 3.47720000   | 0.00000000 |
| 400 | 3200.51800000 | 17.37950000  | 0.00000000 |
| 401 | 3201.37600000 | 16.45560000  | 0.00000000 |
| 402 | 3206.46440000 | 38.54480000  | 0.00000000 |
| 403 | 3207.01560000 | 36.62190000  | 0.00000000 |
| 404 | 3207.50180000 | 4.68350000   | 0.00000000 |
| 405 | 3210.87570000 | 1.22660000   | 0.00000000 |
| 406 | 3211.07650000 | 0.65100000   | 0.00000000 |
| 407 | 3211.86680000 | 0.05220000   | 0.00000000 |
| 408 | 3212.57140000 | 0.07390000   | 0.00000000 |
| 409 | 3216.75050000 | 0.91790000   | 0.00000000 |
| 410 | 3221.81920000 | 1.95860000   | 0.00000000 |
| 411 | 3222.22310000 | 2.29120000   | 0.00000000 |
| 412 | 3222.78850000 | 4.16960000   | 0.00000000 |
| 413 | 3224.19090000 | 1.96010000   | 0.00000000 |
| 414 | 3224.27090000 | 5.23900000   | 0.00000000 |
| 415 | 3228.48290000 | 7.07740000   | 0.00000000 |
| 416 | 3229.32410000 | 5.52420000   | 0.00000000 |
| 417 | 3232.20710000 | 8.21370000   | 0.00000000 |
| 418 | 3236.14540000 | 3.82830000   | 0.00000000 |
| 419 | 3237.41000000 | 11.32180000  | 0.00000000 |
| 420 | 3237.60660000 | 2.92840000   | 0.00000000 |
| 421 | 3238.17920000 | 1.79700000   | 0.00000000 |
| 422 | 3261.15250000 | 0.80630000   | 0.00000000 |
| 423 | 3261.32740000 | 1.03520000   | 0.00000000 |
| 424 | 3263.49130000 | 0.41140000   | 0.00000000 |
| 425 | 3271.14200000 | 6.06470000   | 0.00000000 |
| 426 | 3272.05760000 | 4.92450000   | 0.00000000 |
| 427 | 3272.48760000 | 7.31360000   | 0.00000000 |
| 428 | 3285.33550000 | 4.43570000   | 0.00000000 |
| 429 | 3285.84790000 | 2.99090000   | 0.00000000 |
| 430 | 3285.98130000 | 6.54010000   | 0.00000000 |
| 431 | 3489.79350000 | 0.90480000   | 0.00000000 |
| 432 | 3492.07630000 | 0.61540000   | 0.00000000 |

S14. CALCULATIONS ON EXTENDED CONFORMER OF  $2^{3+}$  ( $^3A$ )

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity<br>empiricaldispersion=gd3bj int=ultrafine pop=regular  |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](6[Ru]578(n9ccc[n+](9C([n+]<br>1n7ccc1)[n+](1n8ccc1)[n+](1ccc(cc1)CNC(CCCCCNCc1cc[n+](cc1)[Re]<br>1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O]) |      |
| Formula                         | : C <sub>67</sub> H <sub>56</sub> N <sub>18</sub> O <sub>3</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -3972.47541013   | a.u. |
| Gibbs Energy                    | : -3971.45045600   | a.u. |
| Number of imaginary frequencies | : 4  |      |

## S14.1. Cartesian Co-ordinates (XYZ format)

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|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.14410591 | -0.35284799 | 0.34162599  |
| H | 2.95674992 | 0.40934700  | -0.42292801 |
| H | 3.03712797 | 0.14759301  | 1.31919897  |
| C | 2.10718989 | -1.46472895 | 0.22280601  |
| H | 2.32233500 | -2.23766303 | 0.97140801  |
| H | 2.21134400 | -1.94095004 | -0.75809300 |
| C | 0.67394698 | -0.96474802 | 0.41134200  |

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | 0.45786801   | -0.19066501 | -0.33509699 |
| H  | 0.58245200   | -0.48160201 | 1.39172399  |
| C  | -0.36940101  | -2.07833695 | 0.29991201  |
| H  | -0.14950299  | -2.85427403 | 1.04319704  |
| H  | -0.28231701  | -2.55874801 | -0.68225700 |
| C  | -2.83762193  | -2.69389606 | 0.39315501  |
| H  | -2.60178590  | -3.48399806 | 1.12589002  |
| H  | -2.78492999  | -3.15800309 | -0.59787101 |
| N  | 4.49839783   | -0.87125498 | 0.13416301  |
| C  | -5.21635008  | -3.20021510 | 0.52050298  |
| H  | -5.14124203  | -3.93856812 | 1.33488202  |
| H  | -5.08477402  | -3.76744604 | -0.40971899 |
| N  | -4.19383812  | -2.16757488 | 0.56983298  |
| C  | 5.52470016   | 0.15197501  | 0.27063501  |
| H  | 5.27380514   | 0.97519398  | -0.40982801 |
| H  | 5.57195091   | 0.59673703  | 1.27769804  |
| C  | -13.72085190 | -2.48665595 | 1.20967698  |
| N  | -12.83609295 | -2.47969604 | 2.35578799  |
| N  | -14.09465885 | -1.13402998 | 0.84607601  |
| N  | -13.08515644 | -3.15715504 | 0.09473300  |
| N  | -11.62740612 | -1.86397505 | 2.26569390  |
| C  | -12.99213123 | -3.07672095 | 3.56477809  |
| N  | -13.12988758 | -0.24780600 | 0.47435501  |
| C  | -15.31720161 | -0.55560100 | 0.80971497  |
| N  | -11.92197704 | -2.66517997 | -0.40836000 |
| C  | -13.44006062 | -4.30887985 | -0.53042001 |
| Ru | -11.17004585 | -0.88210601 | 0.44761100  |
| C  | -11.01767921 | -2.07475805 | 3.43358207  |
| C  | -11.83989239 | -2.83328009 | 4.28158617  |
| H  | -13.89349747 | -3.61251712 | 3.81021810  |
| C  | -13.75706863 | 0.90120202  | 0.20056400  |
| C  | -15.13367367 | 0.75286698  | 0.39808601  |
| H  | -16.20540428 | -1.10508001 | 1.07442498  |
| C  | -11.54248333 | -3.51668501 | -1.36270297 |
| C  | -12.46864414 | -4.56589985 | -1.47436595 |
| H  | -14.33882904 | -4.83692598 | -0.25928199 |
| N  | -10.56218910 | 0.92487901  | 1.23806500  |
| N  | -10.84252644 | 0.16805500  | -1.29832494 |
| H  | -10.02658844 | -1.68935299 | 3.60766006  |
| H  | -11.61991787 | -3.15762305 | 5.28367186  |
| H  | -13.19194126 | 1.76109695  | -0.11933500 |
| H  | -15.89728546 | 1.49829900  | 0.26031101  |
| H  | -10.63105965 | -3.34652305 | -1.91195405 |
| H  | -12.43146801 | -5.39800882 | -2.15552998 |
| C  | -10.48298645 | 1.28133500  | 2.52434301  |
| C  | -10.24508381 | 1.85854995  | 0.25770700  |
| C  | -10.39146042 | 1.46307099  | -1.06761503 |
| C  | -11.04635143 | -0.23437600 | -2.55715489 |
| C  | -10.06291676 | 2.54366589  | 2.92345500  |
| H  | -10.77062130 | 0.53607899  | 3.25149107  |
| C  | -9.79681015  | 3.16831493  | 0.60602099  |
| C  | -10.10216331 | 2.34576988  | -2.15163898 |
| C  | -10.79240417 | 0.58286703  | -3.65106893 |
| H  | -11.42923355 | -1.23600698 | -2.68810892 |
| C  | -9.70988941  | 3.48991489  | 1.95110798  |
| H  | -10.01591587 | 2.77718306  | 3.97742605  |
| C  | -9.46403313  | 4.09984112  | -0.46806300 |
| C  | -10.30815411 | 1.88178504  | -3.44101501 |
| C  | -9.61665726  | 3.68877912  | -1.84651506 |
| H  | -10.97292614 | 0.20517500  | -4.64722776 |
| H  | -9.37461185  | 4.47946882  | 2.23202205  |
| N  | -9.03057861  | 5.31110382  | -0.15568399 |
| H  | -10.09710217 | 2.53932905  | -4.27382803 |
| N  | -9.32826614  | 4.50929880  | -2.84460402 |

|    |              |             |             |
|----|--------------|-------------|-------------|
| C  | -8.73164558  | 6.16119289  | -1.17222095 |
| C  | -8.88263512  | 5.75477219  | -2.53529406 |
| C  | -8.26469040  | 7.46490002  | -0.88717002 |
| C  | -8.56181717  | 6.66565418  | -3.56789303 |
| C  | -7.95926619  | 8.33135796  | -1.91381001 |
| H  | -8.15756798  | 7.75250721  | 0.15169699  |
| C  | -8.10867500  | 7.92989683  | -3.26056910 |
| H  | -8.68350506  | 6.33781624  | -4.59314919 |
| H  | -7.60157013  | 9.32941341  | -1.69119501 |
| H  | -7.86387110  | 8.62487030  | -4.05472279 |
| N  | 12.10207558  | 0.14809300  | -1.54883003 |
| N  | 12.15706539  | -1.46741402 | 0.59487599  |
| C  | 12.02402496  | 0.93428397  | -2.62765193 |
| C  | 12.62979889  | 0.65754497  | -0.40435800 |
| C  | 12.65905952  | -0.21410100 | 0.75248200  |
| C  | 12.13483047  | -2.28935099 | 1.64934003  |
| C  | 12.47137070  | 2.25497103  | -2.62118912 |
| H  | 11.59584045  | 0.49520200  | -3.51707911 |
| C  | 13.10042000  | 1.97466803  | -0.32188100 |
| C  | 13.15991592  | 0.23980100  | 1.97979200  |
| C  | 12.61522388  | -1.90827501 | 2.90169311  |
| H  | 11.72561264  | -3.27570391 | 1.48599195  |
| C  | 13.01643753  | 2.78048706  | -1.46561098 |
| H  | 12.38452816  | 2.84716606  | -3.52153492 |
| C  | 13.64778996  | 2.46363211  | 0.94064599  |
| C  | 13.13465023  | -0.63935500 | 3.07110906  |
| C  | 13.67759895  | 1.60135400  | 2.08446002  |
| H  | 12.57382011  | -2.61272812 | 3.72079992  |
| H  | 13.37630844  | 3.79887509  | -1.41793001 |
| N  | 14.10219669  | 3.70465994  | 0.99876797  |
| H  | 13.51887894  | -0.30377299 | 4.02437878  |
| N  | 14.16104889  | 2.01044512  | 3.24589205  |
| C  | 14.59994602  | 4.13686705  | 2.17485595  |
| C  | 14.63018894  | 3.27216411  | 3.32162094  |
| C  | 15.10059834  | 5.45968580  | 2.28784108  |
| C  | 15.16030598  | 3.75765395  | 4.54495192  |
| C  | 15.60571003  | 5.89657688  | 3.48455405  |
| H  | 15.06858444  | 6.09494591  | 1.41183996  |
| C  | 15.63574791  | 5.04082489  | 4.61929083  |
| H  | 15.17395973  | 3.09000397  | 5.39701796  |
| H  | 15.98876476  | 6.90554190  | 3.57422400  |
| H  | 16.04113960  | 5.41456985  | 5.55139208  |
| H  | -14.62099171 | -3.03186989 | 1.47265899  |
| C  | 6.89591408   | -0.34955099 | -0.10466600 |
| C  | 8.04596233   | 0.30331901  | 0.34008601  |
| C  | 7.07513523   | -1.46275699 | -0.92680299 |
| C  | 9.29216862   | -0.15743800 | -0.04412300 |
| H  | 7.98175907   | 1.16834795  | 0.98809099  |
| C  | 8.35287666   | -1.86796701 | -1.26625800 |
| H  | 6.21714020   | -2.00813293 | -1.29347301 |
| N  | 9.46414661   | -1.23164296 | -0.83870202 |
| H  | 10.18040371  | 0.34852201  | 0.29970601  |
| H  | 8.50538540   | -2.72872710 | -1.90163398 |
| C  | -6.61169815  | -2.63467693 | 0.50716299  |
| C  | -6.86584806  | -1.31409001 | 0.13026500  |
| C  | -7.70866585  | -3.42916799 | 0.85467601  |
| C  | -8.16278458  | -0.84181798 | 0.11336700  |
| H  | -6.04745722  | -0.66354603 | -0.14253099 |
| C  | -8.98043346  | -2.89811611 | 0.81498402  |
| H  | -7.57686710  | -4.45833921 | 1.16270602  |
| N  | -9.21590614  | -1.61623597 | 0.45158499  |
| H  | -8.37871838  | 0.17577000  | -0.17393599 |
| H  | -9.84197521  | -3.49068093 | 1.08184600  |
| Re | 11.49813938  | -1.97713196 | -1.45352805 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 13.29033279 | -2.55245209 | -1.93447602 |
| O | 14.35786057 | -2.88363290 | -2.21254110 |
| C | 10.98826027 | -3.81565690 | -1.10232496 |
| O | 10.69232655 | -4.90426493 | -0.86281502 |
| C | 10.93044853 | -2.15833712 | -3.29983902 |
| O | 10.59901142 | -2.23513103 | -4.40170383 |
| H | -4.24577188 | -1.69495702 | 1.46884799  |
| H | 4.67457724  | -1.60623300 | 0.81477201  |
| C | -1.80205905 | -1.57919502 | 0.49493301  |
| H | -2.03572106 | -0.81109202 | -0.25021100 |
| H | -1.88733399 | -1.09915805 | 1.47803295  |

## S14.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -13.14090000 | 0.74410000   | 0.00000000      |
| 2    | -12.07650000 | 0.28240000   | 0.00000000      |
| 3    | -9.31520000  | 2.57920000   | 0.00000000      |
| 4    | -5.12640000  | 1.52320000   | 0.00000000      |
| 5    | 2.73780000   | 0.09210000   | 0.00000000      |
| 6    | 10.98570000  | 0.26160000   | 0.00000000      |
| 7    | 12.67330000  | 0.75960000   | 0.00000000      |
| 8    | 19.18010000  | 0.48490000   | 0.00000000      |
| 9    | 21.04510000  | 0.50260000   | 0.00000000      |
| 10   | 26.66270000  | 0.32630000   | 0.00000000      |
| 11   | 31.73590000  | 0.23970000   | 0.00000000      |
| 12   | 33.77890000  | 0.66570000   | 0.00000000      |
| 13   | 38.64020000  | 1.82380000   | 0.00000000      |
| 14   | 40.78460000  | 3.03210000   | 0.00000000      |
| 15   | 43.68190000  | 1.57130000   | 0.00000000      |
| 16   | 49.28040000  | 0.66780000   | 0.00000000      |
| 17   | 52.06830000  | 1.48250000   | 0.00000000      |
| 18   | 56.58230000  | 0.49770000   | 0.00000000      |
| 19   | 57.59470000  | 0.39300000   | 0.00000000      |
| 20   | 60.45390000  | 1.58320000   | 0.00000000      |
| 21   | 64.05050000  | 1.44200000   | 0.00000000      |
| 22   | 65.58800000  | 0.50870000   | 0.00000000      |
| 23   | 67.01540000  | 0.54560000   | 0.00000000      |
| 24   | 68.77880000  | 0.14160000   | 0.00000000      |
| 25   | 70.17240000  | 3.84960000   | 0.00000000      |
| 26   | 71.67450000  | 1.33040000   | 0.00000000      |
| 27   | 81.28690000  | 0.30110000   | 0.00000000      |
| 28   | 84.14200000  | 18.65750000  | 0.00000000      |
| 29   | 86.48070000  | 0.53810000   | 0.00000000      |
| 30   | 88.22600000  | 1.31240000   | 0.00000000      |
| 31   | 91.11640000  | 1.06260000   | 0.00000000      |
| 32   | 92.28930000  | 0.99680000   | 0.00000000      |
| 33   | 94.67140000  | 1.03850000   | 0.00000000      |
| 34   | 99.47230000  | 1.04430000   | 0.00000000      |
| 35   | 105.27970000 | 1.23580000   | 0.00000000      |
| 36   | 111.41820000 | 0.66520000   | 0.00000000      |
| 37   | 127.16560000 | 2.02360000   | 0.00000000      |
| 38   | 134.02260000 | 1.87730000   | 0.00000000      |
| 39   | 135.75870000 | 3.78730000   | 0.00000000      |
| 40   | 139.37120000 | 0.13060000   | 0.00000000      |
| 41   | 141.33330000 | 1.76040000   | 0.00000000      |
| 42   | 143.29920000 | 10.60840000  | 0.00000000      |
| 43   | 147.32040000 | 2.55700000   | 0.00000000      |
| 44   | 153.91630000 | 3.14960000   | 0.00000000      |
| 45   | 156.72360000 | 0.99170000   | 0.00000000      |
| 46   | 161.46230000 | 2.75780000   | 0.00000000      |
| 47   | 165.70470000 | 1.64320000   | 0.00000000      |
| 48   | 169.41810000 | 0.40320000   | 0.00000000      |
| 49   | 170.21140000 | 1.57890000   | 0.00000000      |
| 50   | 171.78070000 | 0.40450000   | 0.00000000      |
| 51   | 174.81110000 | 0.40400000   | 0.00000000      |
| 52   | 175.74220000 | 0.70050000   | 0.00000000      |
| 53   | 182.24330000 | 10.70500000  | 0.00000000      |
| 54   | 188.61920000 | 5.72270000   | 0.00000000      |
| 55   | 189.11830000 | 8.68740000   | 0.00000000      |
| 56   | 194.46600000 | 1.25730000   | 0.00000000      |
| 57   | 200.59620000 | 21.56560000  | 0.00000000      |
| 58   | 211.07020000 | 1.35740000   | 0.00000000      |
| 59   | 211.45640000 | 4.66460000   | 0.00000000      |
| 60   | 218.87860000 | 4.34580000   | 0.00000000      |

|     |              |               |            |
|-----|--------------|---------------|------------|
| 61  | 224.52190000 | 29.27630000   | 0.00000000 |
| 62  | 239.32380000 | 32.99330000   | 0.00000000 |
| 63  | 241.14800000 | 2.98660000    | 0.00000000 |
| 64  | 245.67280000 | 1.52070000    | 0.00000000 |
| 65  | 258.59580000 | 1.99020000    | 0.00000000 |
| 66  | 270.11090000 | 3.95880000    | 0.00000000 |
| 67  | 272.66970000 | 3.04100000    | 0.00000000 |
| 68  | 280.45590000 | 3.70470000    | 0.00000000 |
| 69  | 281.47880000 | 19.56870000   | 0.00000000 |
| 70  | 291.28590000 | 49.96820000   | 0.00000000 |
| 71  | 308.35330000 | 3.15950000    | 0.00000000 |
| 72  | 313.52030000 | 1.41040000    | 0.00000000 |
| 73  | 321.53960000 | 58.88400000   | 0.00000000 |
| 74  | 323.48690000 | 19.61130000   | 0.00000000 |
| 75  | 326.63550000 | 0.03650000    | 0.00000000 |
| 76  | 328.56540000 | 2.40390000    | 0.00000000 |
| 77  | 329.90860000 | 80.93460000   | 0.00000000 |
| 78  | 330.43730000 | 11.26340000   | 0.00000000 |
| 79  | 332.06610000 | 1.49320000    | 0.00000000 |
| 80  | 356.58480000 | 10.27920000   | 0.00000000 |
| 81  | 359.77490000 | 2.57740000    | 0.00000000 |
| 82  | 375.61950000 | 14.63250000   | 0.00000000 |
| 83  | 380.00980000 | 1.04290000    | 0.00000000 |
| 84  | 387.80470000 | 3.12530000    | 0.00000000 |
| 85  | 389.65860000 | 53.51830000   | 0.00000000 |
| 86  | 397.69000000 | 76.72000000   | 0.00000000 |
| 87  | 404.34630000 | 0.10560000    | 0.00000000 |
| 88  | 406.92890000 | 1.28300000    | 0.00000000 |
| 89  | 412.14610000 | 37.93070000   | 0.00000000 |
| 90  | 420.99390000 | 20.42010000   | 0.00000000 |
| 91  | 422.50500000 | 4.29760000    | 0.00000000 |
| 92  | 435.75820000 | 8.42590000    | 0.00000000 |
| 93  | 438.25140000 | 397.94350000  | 0.00000000 |
| 94  | 440.18340000 | 74.87500000   | 0.00000000 |
| 95  | 441.89100000 | 19.67840000   | 0.00000000 |
| 96  | 446.44760000 | 7.40580000    | 0.00000000 |
| 97  | 455.22070000 | 1.40160000    | 0.00000000 |
| 98  | 474.75140000 | 33.96290000   | 0.00000000 |
| 99  | 476.25910000 | 26.46140000   | 0.00000000 |
| 100 | 478.74820000 | 13.89480000   | 0.00000000 |
| 101 | 485.89900000 | 5.38320000    | 0.00000000 |
| 102 | 488.13080000 | 0.08210000    | 0.00000000 |
| 103 | 489.57250000 | 1.97060000    | 0.00000000 |
| 104 | 489.75790000 | 0.02060000    | 0.00000000 |
| 105 | 494.50290000 | 1.63850000    | 0.00000000 |
| 106 | 497.21660000 | 0.09340000    | 0.00000000 |
| 107 | 500.64900000 | 15.18040000   | 0.00000000 |
| 108 | 501.10330000 | 22.57660000   | 0.00000000 |
| 109 | 517.93960000 | 2.64260000    | 0.00000000 |
| 110 | 524.63130000 | 3.08190000    | 0.00000000 |
| 111 | 532.50130000 | 3.91130000    | 0.00000000 |
| 112 | 532.67320000 | 13.67920000   | 0.00000000 |
| 113 | 536.72250000 | 16.43670000   | 0.00000000 |
| 114 | 545.93430000 | 7.94540000    | 0.00000000 |
| 115 | 562.39330000 | 0.18030000    | 0.00000000 |
| 116 | 571.41840000 | 0.51150000    | 0.00000000 |
| 117 | 572.33370000 | 0.93550000    | 0.00000000 |
| 118 | 575.71610000 | 1.49620000    | 0.00000000 |
| 119 | 581.89590000 | 1.21280000    | 0.00000000 |
| 120 | 583.11920000 | 494.38120000  | 0.00000000 |
| 121 | 585.61140000 | 1311.19420000 | 0.00000000 |
| 122 | 594.09260000 | 28.14000000   | 0.00000000 |
| 123 | 602.68500000 | 0.27290000    | 0.00000000 |
| 124 | 605.14590000 | 5.20470000    | 0.00000000 |



|     |              |               |            |
|-----|--------------|---------------|------------|
| 125 | 612.15090000 | 31.40110000   | 0.00000000 |
| 126 | 619.39380000 | 1018.37070000 | 0.00000000 |
| 127 | 621.00440000 | 118.68190000  | 0.00000000 |
| 128 | 624.65110000 | 22.88350000   | 0.00000000 |
| 129 | 633.14980000 | 3.97290000    | 0.00000000 |
| 130 | 633.65570000 | 33.32630000   | 0.00000000 |
| 131 | 638.61240000 | 2.75250000    | 0.00000000 |
| 132 | 643.28800000 | 11.49090000   | 0.00000000 |
| 133 | 646.84470000 | 76.70710000   | 0.00000000 |
| 134 | 648.66530000 | 1.07690000    | 0.00000000 |
| 135 | 650.41360000 | 3.06010000    | 0.00000000 |
| 136 | 653.77520000 | 0.32410000    | 0.00000000 |
| 137 | 660.16010000 | 0.00190000    | 0.00000000 |
| 138 | 668.85320000 | 5.72910000    | 0.00000000 |
| 139 | 671.19630000 | 5.66160000    | 0.00000000 |
| 140 | 675.88680000 | 5.38540000    | 0.00000000 |
| 141 | 679.67900000 | 6.32640000    | 0.00000000 |
| 142 | 684.88850000 | 0.29150000    | 0.00000000 |
| 143 | 701.52040000 | 129.47730000  | 0.00000000 |
| 144 | 733.89480000 | 9.15240000    | 0.00000000 |
| 145 | 735.49130000 | 2.25980000    | 0.00000000 |
| 146 | 737.02520000 | 4.85650000    | 0.00000000 |
| 147 | 739.19930000 | 535.75590000  | 0.00000000 |
| 148 | 739.78580000 | 9.75400000    | 0.00000000 |
| 149 | 740.52210000 | 0.55790000    | 0.00000000 |
| 150 | 741.47750000 | 6.06810000    | 0.00000000 |
| 151 | 746.89550000 | 0.28640000    | 0.00000000 |
| 152 | 752.69950000 | 0.02670000    | 0.00000000 |
| 153 | 757.72850000 | 98.12640000   | 0.00000000 |
| 154 | 759.87900000 | 0.52340000    | 0.00000000 |
| 155 | 761.74870000 | 0.34310000    | 0.00000000 |
| 156 | 770.04560000 | 862.20120000  | 0.00000000 |
| 157 | 771.64270000 | 59.84710000   | 0.00000000 |
| 158 | 773.69180000 | 77.48600000   | 0.00000000 |
| 159 | 774.34540000 | 214.59150000  | 0.00000000 |
| 160 | 779.19390000 | 70.93540000   | 0.00000000 |
| 161 | 779.90260000 | 104.51030000  | 0.00000000 |
| 162 | 781.56430000 | 10.78400000   | 0.00000000 |
| 163 | 786.27780000 | 80.15790000   | 0.00000000 |
| 164 | 788.79880000 | 0.47410000    | 0.00000000 |
| 165 | 796.95400000 | 95.66670000   | 0.00000000 |
| 166 | 797.19670000 | 103.01160000  | 0.00000000 |
| 167 | 801.34300000 | 21.83370000   | 0.00000000 |
| 168 | 805.90050000 | 165.84730000  | 0.00000000 |
| 169 | 813.31480000 | 4.52030000    | 0.00000000 |
| 170 | 815.12150000 | 0.06660000    | 0.00000000 |
| 171 | 827.07160000 | 0.45500000    | 0.00000000 |
| 172 | 835.40380000 | 26.23350000   | 0.00000000 |
| 173 | 836.20230000 | 1.92420000    | 0.00000000 |
| 174 | 840.57520000 | 119.62790000  | 0.00000000 |
| 175 | 840.95360000 | 67.99370000   | 0.00000000 |
| 176 | 855.64800000 | 13.92830000   | 0.00000000 |
| 177 | 857.08280000 | 23.23970000   | 0.00000000 |
| 178 | 866.51090000 | 14.74010000   | 0.00000000 |
| 179 | 873.13780000 | 115.43780000  | 0.00000000 |
| 180 | 874.91670000 | 0.03900000    | 0.00000000 |
| 181 | 878.39080000 | 401.18840000  | 0.00000000 |
| 182 | 884.33950000 | 0.01160000    | 0.00000000 |
| 183 | 885.30820000 | 1.01690000    | 0.00000000 |
| 184 | 889.97370000 | 26.86490000   | 0.00000000 |
| 185 | 890.06530000 | 1.66340000    | 0.00000000 |
| 186 | 891.10030000 | 19.16200000   | 0.00000000 |
| 187 | 892.93950000 | 3.74180000    | 0.00000000 |
| 188 | 897.24570000 | 0.00600000    | 0.00000000 |

|     |               |                |            |
|-----|---------------|----------------|------------|
| 189 | 900.55540000  | 4.39380000     | 0.00000000 |
| 190 | 915.80900000  | 5.59500000     | 0.00000000 |
| 191 | 920.88660000  | 1.35620000     | 0.00000000 |
| 192 | 937.15980000  | 18.44400000    | 0.00000000 |
| 193 | 940.03870000  | 0.52650000     | 0.00000000 |
| 194 | 941.80960000  | 16.14510000    | 0.00000000 |
| 195 | 944.72090000  | 6.63010000     | 0.00000000 |
| 196 | 947.66610000  | 0.91770000     | 0.00000000 |
| 197 | 952.78440000  | 11.97580000    | 0.00000000 |
| 198 | 969.14350000  | 13.37840000    | 0.00000000 |
| 199 | 969.44230000  | 1.08350000     | 0.00000000 |
| 200 | 971.12370000  | 3.12860000     | 0.00000000 |
| 201 | 974.09760000  | 3.69070000     | 0.00000000 |
| 202 | 983.28470000  | 67.37050000    | 0.00000000 |
| 203 | 984.42450000  | 0.07030000     | 0.00000000 |
| 204 | 985.48700000  | 0.29730000     | 0.00000000 |
| 205 | 985.72950000  | 123.69830000   | 0.00000000 |
| 206 | 987.48290000  | 2.96430000     | 0.00000000 |
| 207 | 992.54360000  | 1.34220000     | 0.00000000 |
| 208 | 997.02550000  | 40.79330000    | 0.00000000 |
| 209 | 997.57120000  | 122.19250000   | 0.00000000 |
| 210 | 999.12690000  | 2928.63480000  | 0.00000000 |
| 211 | 999.99970000  | 15871.60260000 | 0.00000000 |
| 212 | 1002.09540000 | 16.36270000    | 0.00000000 |
| 213 | 1006.75050000 | 32.93010000    | 0.00000000 |
| 214 | 1008.01450000 | 2.49650000     | 0.00000000 |
| 215 | 1010.97680000 | 29.11010000    | 0.00000000 |
| 216 | 1018.00020000 | 1.17150000     | 0.00000000 |
| 217 | 1018.98590000 | 36.56550000    | 0.00000000 |
| 218 | 1019.40880000 | 191.63250000   | 0.00000000 |
| 219 | 1020.87020000 | 5.87430000     | 0.00000000 |
| 220 | 1021.40720000 | 0.00250000     | 0.00000000 |
| 221 | 1022.66430000 | 463.33730000   | 0.00000000 |
| 222 | 1027.27200000 | 3.89910000     | 0.00000000 |
| 223 | 1031.50880000 | 1.66220000     | 0.00000000 |
| 224 | 1032.39970000 | 0.38940000     | 0.00000000 |
| 225 | 1033.00170000 | 0.00420000     | 0.00000000 |
| 226 | 1035.18960000 | 188.07290000   | 0.00000000 |
| 227 | 1047.87620000 | 8.33250000     | 0.00000000 |
| 228 | 1051.74930000 | 12.38440000    | 0.00000000 |
| 229 | 1053.29530000 | 161.25540000   | 0.00000000 |
| 230 | 1060.81810000 | 11.97540000    | 0.00000000 |
| 231 | 1067.26780000 | 2.84670000     | 0.00000000 |
| 232 | 1067.88760000 | 0.14090000     | 0.00000000 |
| 233 | 1071.89110000 | 0.03380000     | 0.00000000 |
| 234 | 1078.95220000 | 86.01010000    | 0.00000000 |
| 235 | 1081.19770000 | 140.73180000   | 0.00000000 |
| 236 | 1083.26880000 | 87.81310000    | 0.00000000 |
| 237 | 1086.53320000 | 38.30260000    | 0.00000000 |
| 238 | 1086.66350000 | 467.37150000   | 0.00000000 |
| 239 | 1087.19800000 | 5.06380000     | 0.00000000 |
| 240 | 1090.13580000 | 930.79960000   | 0.00000000 |
| 241 | 1094.71870000 | 64.46660000    | 0.00000000 |
| 242 | 1101.77810000 | 423.09080000   | 0.00000000 |
| 243 | 1107.69010000 | 3952.35770000  | 0.00000000 |
| 244 | 1107.87340000 | 39.43020000    | 0.00000000 |
| 245 | 1121.39010000 | 17.56280000    | 0.00000000 |
| 246 | 1126.08460000 | 117.08010000   | 0.00000000 |
| 247 | 1129.73390000 | 53.56100000    | 0.00000000 |
| 248 | 1132.10110000 | 19.28920000    | 0.00000000 |
| 249 | 1133.60480000 | 162.48880000   | 0.00000000 |
| 250 | 1134.03310000 | 50.81970000    | 0.00000000 |
| 251 | 1134.75880000 | 6.89870000     | 0.00000000 |
| 252 | 1135.43310000 | 14.51960000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1141.57390000 | 1.78560000    | 0.00000000 |
| 254 | 1144.86790000 | 15.52180000   | 0.00000000 |
| 255 | 1147.20240000 | 38.68080000   | 0.00000000 |
| 256 | 1148.51340000 | 134.13880000  | 0.00000000 |
| 257 | 1151.55160000 | 6.89590000    | 0.00000000 |
| 258 | 1152.23090000 | 0.88580000    | 0.00000000 |
| 259 | 1159.67600000 | 25.58390000   | 0.00000000 |
| 260 | 1169.15350000 | 127.65810000  | 0.00000000 |
| 261 | 1170.33430000 | 5.40480000    | 0.00000000 |
| 262 | 1173.68800000 | 0.69220000    | 0.00000000 |
| 263 | 1186.17650000 | 1.31680000    | 0.00000000 |
| 264 | 1206.59760000 | 48.71160000   | 0.00000000 |
| 265 | 1211.19420000 | 43.41380000   | 0.00000000 |
| 266 | 1213.43030000 | 1.17290000    | 0.00000000 |
| 267 | 1217.88100000 | 1.27490000    | 0.00000000 |
| 268 | 1219.24840000 | 41.54130000   | 0.00000000 |
| 269 | 1224.51930000 | 10.05640000   | 0.00000000 |
| 270 | 1235.59320000 | 6.50190000    | 0.00000000 |
| 271 | 1240.44230000 | 2800.21020000 | 0.00000000 |
| 272 | 1242.63480000 | 9.16160000    | 0.00000000 |
| 273 | 1244.90520000 | 0.31440000    | 0.00000000 |
| 274 | 1248.14000000 | 5.85910000    | 0.00000000 |
| 275 | 1257.25240000 | 23.95780000   | 0.00000000 |
| 276 | 1259.52040000 | 9.78960000    | 0.00000000 |
| 277 | 1260.98910000 | 27.94110000   | 0.00000000 |
| 278 | 1263.55990000 | 0.56120000    | 0.00000000 |
| 279 | 1269.70890000 | 4.21880000    | 0.00000000 |
| 280 | 1273.73740000 | 8.44600000    | 0.00000000 |
| 281 | 1273.74680000 | 11.40790000   | 0.00000000 |
| 282 | 1274.30510000 | 138.02970000  | 0.00000000 |
| 283 | 1277.65490000 | 121.99030000  | 0.00000000 |
| 284 | 1283.17380000 | 14.17980000   | 0.00000000 |
| 285 | 1291.55900000 | 0.87270000    | 0.00000000 |
| 286 | 1298.94710000 | 1744.82010000 | 0.00000000 |
| 287 | 1302.33010000 | 18.68540000   | 0.00000000 |
| 288 | 1307.05300000 | 5.97740000    | 0.00000000 |
| 289 | 1307.16280000 | 0.79510000    | 0.00000000 |
| 290 | 1309.59870000 | 101.53870000  | 0.00000000 |
| 291 | 1314.25780000 | 5.18750000    | 0.00000000 |
| 292 | 1317.34540000 | 19.24330000   | 0.00000000 |
| 293 | 1320.73950000 | 78.09540000   | 0.00000000 |
| 294 | 1321.36760000 | 118.77840000  | 0.00000000 |
| 295 | 1321.83630000 | 113.12050000  | 0.00000000 |
| 296 | 1323.98930000 | 4.15650000    | 0.00000000 |
| 297 | 1331.71420000 | 0.24590000    | 0.00000000 |
| 298 | 1331.96910000 | 0.28590000    | 0.00000000 |
| 299 | 1336.04050000 | 0.39270000    | 0.00000000 |
| 300 | 1336.70510000 | 3.54570000    | 0.00000000 |
| 301 | 1344.34620000 | 61.66080000   | 0.00000000 |
| 302 | 1349.51540000 | 0.51430000    | 0.00000000 |
| 303 | 1351.59380000 | 68.79670000   | 0.00000000 |
| 304 | 1352.57900000 | 1.85520000    | 0.00000000 |
| 305 | 1359.26910000 | 4.64370000    | 0.00000000 |
| 306 | 1365.74480000 | 6.10790000    | 0.00000000 |
| 307 | 1373.06280000 | 15.14780000   | 0.00000000 |
| 308 | 1374.74450000 | 125.74040000  | 0.00000000 |
| 309 | 1380.40810000 | 26.34330000   | 0.00000000 |
| 310 | 1382.61170000 | 16.27110000   | 0.00000000 |
| 311 | 1385.02000000 | 1.89420000    | 0.00000000 |
| 312 | 1392.70590000 | 196.13140000  | 0.00000000 |
| 313 | 1394.14890000 | 58.43500000   | 0.00000000 |
| 314 | 1404.65720000 | 0.70570000    | 0.00000000 |
| 315 | 1405.92070000 | 467.49160000  | 0.00000000 |
| 316 | 1407.65170000 | 132.85150000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1410.41410000 | 18.25740000   | 0.00000000 |
| 318 | 1417.23490000 | 1515.82680000 | 0.00000000 |
| 319 | 1424.33120000 | 0.63110000    | 0.00000000 |
| 320 | 1424.88210000 | 300.92080000  | 0.00000000 |
| 321 | 1425.93870000 | 0.98230000    | 0.00000000 |
| 322 | 1429.27600000 | 7.37510000    | 0.00000000 |
| 323 | 1431.24010000 | 95.56520000   | 0.00000000 |
| 324 | 1433.11790000 | 36.95120000   | 0.00000000 |
| 325 | 1441.62450000 | 324.51250000  | 0.00000000 |
| 326 | 1454.24780000 | 118.51700000  | 0.00000000 |
| 327 | 1462.30300000 | 38.18990000   | 0.00000000 |
| 328 | 1469.07060000 | 1.16260000    | 0.00000000 |
| 329 | 1469.54250000 | 51.75600000   | 0.00000000 |
| 330 | 1471.72960000 | 27.54490000   | 0.00000000 |
| 331 | 1475.00170000 | 7.80500000    | 0.00000000 |
| 332 | 1475.87510000 | 37.16640000   | 0.00000000 |
| 333 | 1479.79690000 | 1.60200000    | 0.00000000 |
| 334 | 1480.78140000 | 52.99230000   | 0.00000000 |
| 335 | 1482.49640000 | 15.79620000   | 0.00000000 |
| 336 | 1486.40220000 | 56.06740000   | 0.00000000 |
| 337 | 1490.90990000 | 0.10060000    | 0.00000000 |
| 338 | 1500.18760000 | 93.39100000   | 0.00000000 |
| 339 | 1500.24390000 | 13.22360000   | 0.00000000 |
| 340 | 1501.43090000 | 29.32310000   | 0.00000000 |
| 341 | 1501.43550000 | 11.97100000   | 0.00000000 |
| 342 | 1503.34120000 | 299.37270000  | 0.00000000 |
| 343 | 1503.90010000 | 20.97590000   | 0.00000000 |
| 344 | 1504.88730000 | 0.66560000    | 0.00000000 |
| 345 | 1505.59300000 | 93.20910000   | 0.00000000 |
| 346 | 1512.26640000 | 14.11300000   | 0.00000000 |
| 347 | 1516.76810000 | 552.09430000  | 0.00000000 |
| 348 | 1517.15380000 | 0.06240000    | 0.00000000 |
| 349 | 1518.40630000 | 13.44860000   | 0.00000000 |
| 350 | 1524.25210000 | 24.03930000   | 0.00000000 |
| 351 | 1529.66930000 | 132.30660000  | 0.00000000 |
| 352 | 1534.97640000 | 8.19440000    | 0.00000000 |
| 353 | 1539.35160000 | 23.39490000   | 0.00000000 |
| 354 | 1547.53200000 | 63.39280000   | 0.00000000 |
| 355 | 1550.52140000 | 4.47000000    | 0.00000000 |
| 356 | 1553.83680000 | 36.38480000   | 0.00000000 |
| 357 | 1557.49110000 | 55.75310000   | 0.00000000 |
| 358 | 1560.12030000 | 98.13690000   | 0.00000000 |
| 359 | 1576.75240000 | 290.31980000  | 0.00000000 |
| 360 | 1578.16070000 | 3.43320000    | 0.00000000 |
| 361 | 1582.47620000 | 10.63290000   | 0.00000000 |
| 362 | 1588.13430000 | 13.51830000   | 0.00000000 |
| 363 | 1596.02400000 | 5.77250000    | 0.00000000 |
| 364 | 1610.80880000 | 265.97290000  | 0.00000000 |
| 365 | 1613.70090000 | 5.77310000    | 0.00000000 |
| 366 | 1625.81410000 | 1.48310000    | 0.00000000 |
| 367 | 1626.38890000 | 5.64430000    | 0.00000000 |
| 368 | 1639.58500000 | 5.84650000    | 0.00000000 |
| 369 | 1640.84340000 | 432.67870000  | 0.00000000 |
| 370 | 1644.47070000 | 0.02350000    | 0.00000000 |
| 371 | 1658.61890000 | 322.45280000  | 0.00000000 |
| 372 | 1661.62670000 | 0.02820000    | 0.00000000 |
| 373 | 1663.19370000 | 132.85890000  | 0.00000000 |
| 374 | 1962.97370000 | 2392.69050000 | 0.00000000 |
| 375 | 1968.95550000 | 2318.39370000 | 0.00000000 |
| 376 | 2083.28750000 | 1950.44370000 | 0.00000000 |
| 377 | 2928.33070000 | 144.24950000  | 0.00000000 |
| 378 | 2932.47490000 | 151.39660000  | 0.00000000 |
| 379 | 2948.84280000 | 98.81270000   | 0.00000000 |
| 380 | 2951.57630000 | 91.42340000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 381 | 2999.52450000 | 0.74380000   | 0.00000000 |
| 382 | 2999.80460000 | 0.16350000   | 0.00000000 |
| 383 | 3003.80300000 | 3.14450000   | 0.00000000 |
| 384 | 3008.64030000 | 181.70860000 | 0.00000000 |
| 385 | 3019.43620000 | 16.86080000  | 0.00000000 |
| 386 | 3020.41650000 | 21.85280000  | 0.00000000 |
| 387 | 3021.51100000 | 20.55980000  | 0.00000000 |
| 388 | 3026.88060000 | 37.39090000  | 0.00000000 |
| 389 | 3028.89490000 | 81.75370000  | 0.00000000 |
| 390 | 3036.16590000 | 3.39940000   | 0.00000000 |
| 391 | 3052.01340000 | 0.57000000   | 0.00000000 |
| 392 | 3058.63360000 | 332.23940000 | 0.00000000 |
| 393 | 3174.57930000 | 0.02150000   | 0.00000000 |
| 394 | 3182.28720000 | 1.55380000   | 0.00000000 |
| 395 | 3183.66030000 | 0.88630000   | 0.00000000 |
| 396 | 3190.92880000 | 32.91720000  | 0.00000000 |
| 397 | 3192.13910000 | 2.34820000   | 0.00000000 |
| 398 | 3194.13420000 | 5.27270000   | 0.00000000 |
| 399 | 3195.36420000 | 3.54920000   | 0.00000000 |
| 400 | 3198.83720000 | 149.43780000 | 0.00000000 |
| 401 | 3200.69830000 | 2.19080000   | 0.00000000 |
| 402 | 3201.36090000 | 16.50380000  | 0.00000000 |
| 403 | 3206.35500000 | 0.65900000   | 0.00000000 |
| 404 | 3206.40600000 | 16.74840000  | 0.00000000 |
| 405 | 3206.97760000 | 36.42890000  | 0.00000000 |
| 406 | 3210.53960000 | 2.44560000   | 0.00000000 |
| 407 | 3212.48890000 | 0.11890000   | 0.00000000 |
| 408 | 3212.91620000 | 0.07440000   | 0.00000000 |
| 409 | 3217.25460000 | 13.11250000  | 0.00000000 |
| 410 | 3217.64670000 | 10.88870000  | 0.00000000 |
| 411 | 3222.08220000 | 10.95660000  | 0.00000000 |
| 412 | 3223.03100000 | 2.23630000   | 0.00000000 |
| 413 | 3223.21960000 | 3.62170000   | 0.00000000 |
| 414 | 3223.82160000 | 2.17570000   | 0.00000000 |
| 415 | 3230.30660000 | 8.53110000   | 0.00000000 |
| 416 | 3230.40570000 | 1.98890000   | 0.00000000 |
| 417 | 3231.11890000 | 17.63170000  | 0.00000000 |
| 418 | 3232.14080000 | 14.51380000  | 0.00000000 |
| 419 | 3236.51530000 | 14.66100000  | 0.00000000 |
| 420 | 3241.11010000 | 13.07080000  | 0.00000000 |
| 421 | 3245.51510000 | 3.20080000   | 0.00000000 |
| 422 | 3263.03630000 | 0.48860000   | 0.00000000 |
| 423 | 3264.39570000 | 0.47970000   | 0.00000000 |
| 424 | 3264.58890000 | 6.56160000   | 0.00000000 |
| 425 | 3273.09210000 | 21.50100000  | 0.00000000 |
| 426 | 3274.91450000 | 10.45000000  | 0.00000000 |
| 427 | 3275.84950000 | 13.04240000  | 0.00000000 |
| 428 | 3287.89650000 | 5.92700000   | 0.00000000 |
| 429 | 3288.64070000 | 8.13840000   | 0.00000000 |
| 430 | 3289.43070000 | 9.21760000   | 0.00000000 |
| 431 | 3489.39490000 | 0.83960000   | 0.00000000 |
| 432 | 3492.29310000 | 1.15140000   | 0.00000000 |

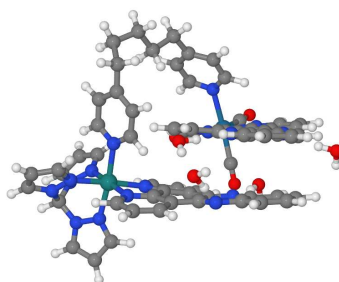
S15. CALCULATIONS ON  $1\mathbf{w}^{3+}$  ( $^1\mathbf{A}$ )

FIG. S25. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](6[Ru]578(n9ccc[n+](9C([n+]
            : 1n7ccc1)[n+](1n8ccc1)[n+](1ccc(cc1)CCCCC1cc[n+](cc1)[Re]
            : 1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O].O.O.O.O
Formula    : C64H56N16O7ReRu3+
Charge     : 3
Multiplicity : 1
Energy     : -4049.76457201
Gibbs Energy : -4048.75098700
Number of imaginary frequencies : 0

```

a.u.

a.u.

## S15.1. Cartesian Co-ordinates (XYZ format)

145

```

C   1.19130099  3.07712889  5.12920189
H   1.01775801  3.98428893  5.71727991
H   1.88878500  2.45445800  5.69474983
C  -0.15179300  2.33216310  4.97011518
H  -0.00589000  1.44430697  4.34636784
H  -0.86304200  2.97404695  4.43976688
C  -0.71857601  1.94830894  6.33964682
H  -0.69305801  2.83481312  6.98340607
H  -0.05420500  1.21254599  6.80822611
C  -2.35163689  0.04170900  5.66273022
H  -3.18292904 -0.47353101  6.15860510
H  -1.47258794 -0.58792901  5.82602596
C  -6.84223890  0.96267998 -1.46937704
N  -5.96305323  2.04381108 -1.06882799
N  -6.26639223  0.22263700 -2.57062292
N  -7.11126184  0.09027000 -0.34463999
N  -4.72242212  1.75202703 -0.59426999
C  -6.18371201  3.38526106 -1.08540297
N  -5.06670094 -0.39328900 -2.40445495
C  -6.74784994  0.03266600 -3.82923102
N  -6.07948685 -0.56045598  0.25762400
C  -8.28420544 -0.13556901  0.30674100
Ru -4.17001677 -0.26614201 -0.53490698
C  -4.15686083  2.92542100 -0.30675501
C  -5.03918886  3.98069811 -0.60108298
H  -7.11704016  3.79520702 -1.43306804

```

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.78793192 | -0.97833103 | -3.56719708 |
| C | -5.81930399 | -0.73642099 | -4.49493885 |
| H | -7.69074678 | 0.45256600  | -4.13663578 |
| C | -6.60917091 | -1.20498204 | 1.29624295  |
| C | -7.99536180 | -0.97010303 | 1.36380398  |
| H | -9.20663166 | 0.30566999  | -0.03157500 |
| N | -2.30839992 | -0.04491600 | -1.42834306 |
| N | -3.52841806 | -2.24228907 | -0.62639302 |
| H | -3.16056991 | 2.95802689  | 0.10315900  |
| H | -4.86197805 | 5.03447390  | -0.47347900 |
| H | -3.87587094 | -1.53911102 | -3.68664098 |
| H | -5.87415886 | -1.07947695 | -5.51355410 |
| H | -5.98048019 | -1.79399395 | 1.94342995  |
| H | -8.68870926 | -1.36042905 | 2.08847094  |
| C | -1.82221401 | 1.04607701  | -2.03081608 |
| C | -1.55671299 | -1.17772901 | -1.43289602 |
| C | -2.22051597 | -2.37669110 | -0.98155099 |
| C | -4.22922897 | -3.34390497 | -0.34260699 |
| C | -0.55435002 | 1.06823397  | -2.60728192 |
| H | -2.46096802 | 1.91628695  | -2.04500103 |
| C | -0.24686401 | -1.21394503 | -1.93310297 |
| C | -1.56058204 | -3.60932803 | -0.97849500 |
| C | -3.65473700 | -4.61419392 | -0.37559199 |
| H | -5.26851797 | -3.20006204 | -0.08457400 |
| C | 0.25362501  | -0.05283200 | -2.53698707 |
| H | -0.20861700 | 1.97321999  | -3.08695412 |
| C | 0.51548100  | -2.45417404 | -1.79377997 |
| C | -2.31312394 | -4.75400686 | -0.68189198 |
| C | -0.13099501 | -3.63241100 | -1.28190100 |
| H | -4.26633978 | -5.47652197 | -0.14907500 |
| H | 1.25726795  | -0.02785400 | -2.93261003 |
| N | 1.80460095  | -2.46418095 | -2.10096002 |
| H | -1.84754598 | -5.72711515 | -0.68618000 |
| N | 0.55301398  | -4.74414921 | -1.06243896 |
| C | 2.50641704  | -3.60423493 | -1.91346204 |
| C | 1.86872005  | -4.76466322 | -1.36268306 |
| C | 3.88925409  | -3.65256095 | -2.22487497 |
| C | 2.63304090  | -5.93243408 | -1.11972201 |
| C | 4.59744787  | -4.80128908 | -1.98546004 |
| H | 4.36343002  | -2.76671290 | -2.62736797 |
| C | 3.96822095  | -5.94450903 | -1.42724204 |
| H | 2.14008689  | -6.79604483 | -0.69360900 |
| H | 5.65888405  | -4.83334398 | -2.19202900 |
| H | 4.55809498  | -6.83156109 | -1.23724604 |
| N | 4.39919186  | 1.98898900  | -0.67430103 |
| N | 1.78021204  | 1.81450903  | -0.17595001 |
| C | 5.69922018  | 2.11216497  | -0.96299201 |
| C | 3.94113207  | 0.79610997  | -0.21876200 |
| C | 2.53281903  | 0.72054499  | 0.10370800  |
| C | 0.51294601  | 1.85418403  | 0.24438700  |
| C | 6.59890079  | 1.06222498  | -0.79632801 |
| H | 6.02607298  | 3.07585502  | -1.32565105 |
| C | 4.78756905  | -0.29746601 | -0.00168900 |
| C | 2.00048089  | -0.40522400 | 0.74862897  |
| C | -0.06092300 | 0.81127900  | 0.96168602  |
| H | -0.04939000 | 2.74661398  | 0.01435600  |
| C | 6.14813805  | -0.14772800 | -0.30458099 |
| H | 7.64103889  | 1.21337104  | -1.04085195 |
| C | 4.22917891  | -1.52831495 | 0.54999697  |
| C | 0.67505699  | -0.33315000 | 1.20052803  |
| C | 2.85110092  | -1.57674396 | 0.94863802  |
| H | -1.07726395 | 0.91265702  | 1.30706501  |
| H | 6.83390379  | -0.96904701 | -0.15371500 |
| N | 5.01410007  | -2.58600211 | 0.68340498  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.24093300  | -1.16122699 | 1.73769796  |
| N  | 2.33303809  | -2.67461109 | 1.48080206  |
| C  | 4.50883818  | -3.70132399 | 1.24792802  |
| C  | 3.13826990  | -3.74431491 | 1.66494703  |
| C  | 5.33222008  | -4.84168911 | 1.42622805  |
| C  | 2.63576007  | -4.92389488 | 2.27057004  |
| C  | 4.81460619  | -5.96485186 | 2.01597095  |
| H  | 6.35820103  | -4.79653120 | 1.08524895  |
| C  | 3.46169806  | -6.00382900 | 2.44309306  |
| H  | 1.60563099  | -4.94241619 | 2.59471607  |
| H  | 5.43978500  | -6.83724022 | 2.15754294  |
| H  | 3.07950997  | -6.90340614 | 2.90876102  |
| H  | -7.78143311 | 1.39180100  | -1.80199206 |
| C  | 1.80854595  | 3.45449591  | 3.81375694  |
| C  | 2.98646402  | 2.86608791  | 3.34994507  |
| C  | 1.20801103  | 4.39900017  | 2.97496510  |
| C  | 3.44169593  | 3.14195395  | 2.07184410  |
| H  | 3.53678703  | 2.16567993  | 3.96478009  |
| C  | 1.71322703  | 4.61681509  | 1.70796502  |
| H  | 0.32484800  | 4.94100285  | 3.28788900  |
| N  | 2.78456593  | 3.95312595  | 1.22013295  |
| H  | 4.33516693  | 2.66692710  | 1.69563603  |
| H  | 1.23044097  | 5.31531191  | 1.04086196  |
| C  | -2.68800712 | 0.03996100  | 4.19225216  |
| C  | -2.18333793 | -0.94460100 | 3.33991694  |
| C  | -3.59809089 | 0.93685901  | 3.62456298  |
| C  | -2.58244491 | -0.99979800 | 2.01552701  |
| H  | -1.48290801 | -1.69448602 | 3.68376398  |
| C  | -3.95643592 | 0.82201499  | 2.29299212  |
| H  | -4.05661488 | 1.72120297  | 4.21144581  |
| N  | -3.45391011 | -0.12503999 | 1.47084498  |
| H  | -2.17540693 | -1.77433801 | 1.38650000  |
| H  | -4.67820787 | 1.49815202  | 1.86257398  |
| Re | 2.85994697  | 3.54261303  | -1.01927495 |
| C  | 2.79066992  | 2.97413301  | -2.87153792 |
| O  | 2.73438501  | 2.63820004  | -3.97191405 |
| C  | 1.33865297  | 4.69067001  | -1.36683702 |
| O  | 0.41433400  | 5.33774281  | -1.61095297 |
| C  | 4.05122519  | 5.01001692  | -1.46829498 |
| O  | 4.77932787  | 5.87131023  | -1.70294905 |
| C  | -2.15219688 | 1.40618002  | 6.35047102  |
| H  | -2.82913208 | 2.15213990  | 5.92343903  |
| H  | -2.45421410 | 1.29649103  | 7.39541912  |
| H  | 2.98159695  | -1.02981400 | -2.74045110 |
| O  | 3.57760096  | -0.28246599 | -2.93242311 |
| H  | 3.53184891  | -0.16506800 | -3.88743091 |
| H  | 0.00587900  | -5.85874319 | 0.45160499  |
| O  | -0.41672900 | -6.06298494 | 1.30723298  |
| H  | 0.11103900  | -6.76353979 | 1.70438194  |
| H  | 0.44588301  | -3.15152597 | 1.88200402  |
| O  | -0.47243199 | -3.35885000 | 2.12488103  |
| H  | -0.56276101 | -4.31081486 | 1.93950999  |
| H  | 6.61227179  | -2.99632692 | -0.34120399 |
| O  | 7.45458603  | -3.23283195 | -0.77002001 |
| H  | 7.34940910  | -2.95550203 | -1.68614101 |



## S15.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 12.87030000  | 2.08000000   | 0.00000000      |
| 2    | 19.89080000  | 0.30180000   | 0.00000000      |
| 3    | 20.42210000  | 2.40020000   | 0.00000000      |
| 4    | 24.05100000  | 0.55850000   | 0.00000000      |
| 5    | 25.04480000  | 0.20120000   | 0.00000000      |
| 6    | 29.90450000  | 0.91130000   | 0.00000000      |
| 7    | 35.48270000  | 0.75850000   | 0.00000000      |
| 8    | 38.45880000  | 0.25470000   | 0.00000000      |
| 9    | 45.87180000  | 1.76770000   | 0.00000000      |
| 10   | 47.57790000  | 2.03400000   | 0.00000000      |
| 11   | 49.33760000  | 2.60160000   | 0.00000000      |
| 12   | 53.27970000  | 1.63880000   | 0.00000000      |
| 13   | 55.52760000  | 0.23060000   | 0.00000000      |
| 14   | 55.69620000  | 10.25940000  | 0.00000000      |
| 15   | 60.53500000  | 4.44610000   | 0.00000000      |
| 16   | 65.01600000  | 1.74490000   | 0.00000000      |
| 17   | 69.15530000  | 3.13910000   | 0.00000000      |
| 18   | 70.33090000  | 4.10800000   | 0.00000000      |
| 19   | 72.18780000  | 4.52140000   | 0.00000000      |
| 20   | 78.13260000  | 0.88900000   | 0.00000000      |
| 21   | 79.18390000  | 9.06750000   | 0.00000000      |
| 22   | 81.16550000  | 8.96870000   | 0.00000000      |
| 23   | 83.95000000  | 6.50190000   | 0.00000000      |
| 24   | 87.70450000  | 7.97350000   | 0.00000000      |
| 25   | 88.78570000  | 3.01310000   | 0.00000000      |
| 26   | 91.31980000  | 2.02620000   | 0.00000000      |
| 27   | 91.87250000  | 4.57160000   | 0.00000000      |
| 28   | 94.88190000  | 7.01490000   | 0.00000000      |
| 29   | 98.24470000  | 7.28940000   | 0.00000000      |
| 30   | 100.14340000 | 5.84390000   | 0.00000000      |
| 31   | 104.55510000 | 0.95310000   | 0.00000000      |
| 32   | 107.93850000 | 4.20380000   | 0.00000000      |
| 33   | 110.45590000 | 2.86860000   | 0.00000000      |
| 34   | 111.44140000 | 5.41650000   | 0.00000000      |
| 35   | 114.17810000 | 1.78650000   | 0.00000000      |
| 36   | 116.53800000 | 3.76490000   | 0.00000000      |
| 37   | 120.95380000 | 2.91100000   | 0.00000000      |
| 38   | 129.37600000 | 5.08800000   | 0.00000000      |
| 39   | 135.51670000 | 0.22180000   | 0.00000000      |
| 40   | 139.22610000 | 2.15820000   | 0.00000000      |
| 41   | 140.31890000 | 5.49660000   | 0.00000000      |
| 42   | 140.96800000 | 2.88710000   | 0.00000000      |
| 43   | 145.10370000 | 1.50420000   | 0.00000000      |
| 44   | 146.64340000 | 1.29180000   | 0.00000000      |
| 45   | 150.04410000 | 7.46110000   | 0.00000000      |
| 46   | 155.04990000 | 1.05850000   | 0.00000000      |
| 47   | 157.09190000 | 1.80160000   | 0.00000000      |
| 48   | 162.15170000 | 0.42440000   | 0.00000000      |
| 49   | 163.70220000 | 3.14180000   | 0.00000000      |
| 50   | 172.28580000 | 0.68800000   | 0.00000000      |
| 51   | 175.35360000 | 1.10690000   | 0.00000000      |
| 52   | 177.11210000 | 2.82240000   | 0.00000000      |
| 53   | 180.12470000 | 3.80750000   | 0.00000000      |
| 54   | 180.68060000 | 0.04960000   | 0.00000000      |
| 55   | 185.60810000 | 4.92710000   | 0.00000000      |
| 56   | 188.62420000 | 1.58080000   | 0.00000000      |
| 57   | 193.84270000 | 4.11060000   | 0.00000000      |
| 58   | 197.74310000 | 2.23780000   | 0.00000000      |
| 59   | 201.19870000 | 3.39350000   | 0.00000000      |
| 60   | 205.80830000 | 5.31670000   | 0.00000000      |

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| 61  | 209.48830000 | 3.53210000   | 0.00000000 |
| 62  | 219.29330000 | 2.38520000   | 0.00000000 |
| 63  | 230.42200000 | 3.48240000   | 0.00000000 |
| 64  | 233.15870000 | 3.42520000   | 0.00000000 |
| 65  | 235.05200000 | 8.83650000   | 0.00000000 |
| 66  | 239.08330000 | 2.00240000   | 0.00000000 |
| 67  | 253.81010000 | 8.82510000   | 0.00000000 |
| 68  | 256.30750000 | 19.14220000  | 0.00000000 |
| 69  | 261.94650000 | 80.99800000  | 0.00000000 |
| 70  | 271.12530000 | 128.20000000 | 0.00000000 |
| 71  | 275.39390000 | 1.03480000   | 0.00000000 |
| 72  | 280.83170000 | 61.66400000  | 0.00000000 |
| 73  | 282.19160000 | 23.91130000  | 0.00000000 |
| 74  | 287.65970000 | 189.10640000 | 0.00000000 |
| 75  | 297.95770000 | 2.78680000   | 0.00000000 |
| 76  | 312.33280000 | 23.59770000  | 0.00000000 |
| 77  | 317.06900000 | 110.71050000 | 0.00000000 |
| 78  | 322.66530000 | 10.32590000  | 0.00000000 |
| 79  | 327.13750000 | 11.19970000  | 0.00000000 |
| 80  | 328.51640000 | 2.34060000   | 0.00000000 |
| 81  | 334.33070000 | 23.96120000  | 0.00000000 |
| 82  | 338.99920000 | 3.30450000   | 0.00000000 |
| 83  | 339.95510000 | 21.71610000  | 0.00000000 |
| 84  | 341.74940000 | 0.03500000   | 0.00000000 |
| 85  | 342.45640000 | 11.89490000  | 0.00000000 |
| 86  | 346.23770000 | 7.03390000   | 0.00000000 |
| 87  | 357.42590000 | 0.57940000   | 0.00000000 |
| 88  | 368.07170000 | 8.91690000   | 0.00000000 |
| 89  | 372.02260000 | 5.92320000   | 0.00000000 |
| 90  | 381.97560000 | 30.15090000  | 0.00000000 |
| 91  | 389.42090000 | 1.62420000   | 0.00000000 |
| 92  | 390.77810000 | 81.15300000  | 0.00000000 |
| 93  | 393.36030000 | 27.29020000  | 0.00000000 |
| 94  | 397.65650000 | 1.07950000   | 0.00000000 |
| 95  | 397.97580000 | 1.66340000   | 0.00000000 |
| 96  | 409.95560000 | 0.77300000   | 0.00000000 |
| 97  | 417.28170000 | 1.36010000   | 0.00000000 |
| 98  | 421.15280000 | 2.98880000   | 0.00000000 |
| 99  | 426.26470000 | 33.46080000  | 0.00000000 |
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| 102 | 445.55780000 | 3.48660000   | 0.00000000 |
| 103 | 446.29040000 | 42.82090000  | 0.00000000 |
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| 105 | 462.39060000 | 53.10290000  | 0.00000000 |
| 106 | 468.26510000 | 1.15800000   | 0.00000000 |
| 107 | 476.53810000 | 37.38360000  | 0.00000000 |
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| 111 | 487.89540000 | 2.22020000   | 0.00000000 |
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| 113 | 497.64260000 | 6.79370000   | 0.00000000 |
| 114 | 498.23570000 | 3.09640000   | 0.00000000 |
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| 116 | 508.32560000 | 12.73470000  | 0.00000000 |
| 117 | 513.58630000 | 1.07510000   | 0.00000000 |
| 118 | 517.07270000 | 9.55280000   | 0.00000000 |
| 119 | 524.35520000 | 33.75260000  | 0.00000000 |
| 120 | 535.48260000 | 10.83490000  | 0.00000000 |
| 121 | 544.81680000 | 47.24580000  | 0.00000000 |
| 122 | 554.25860000 | 34.48170000  | 0.00000000 |
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| 124 | 560.08890000 | 4.76870000   | 0.00000000 |

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| 128 | 583.47010000 | 2.54900000   | 0.00000000 |
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| 131 | 595.18870000 | 12.08470000  | 0.00000000 |
| 132 | 603.76140000 | 14.88090000  | 0.00000000 |
| 133 | 605.55200000 | 0.39890000   | 0.00000000 |
| 134 | 609.47470000 | 10.96060000  | 0.00000000 |
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| 141 | 647.53530000 | 83.18130000  | 0.00000000 |
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| 148 | 670.48090000 | 67.79670000  | 0.00000000 |
| 149 | 676.62010000 | 50.45850000  | 0.00000000 |
| 150 | 677.68490000 | 4.96380000   | 0.00000000 |
| 151 | 684.43610000 | 1.82740000   | 0.00000000 |
| 152 | 684.60260000 | 0.05140000   | 0.00000000 |
| 153 | 686.11190000 | 0.57620000   | 0.00000000 |
| 154 | 726.31490000 | 152.10960000 | 0.00000000 |
| 155 | 738.92540000 | 21.05250000  | 0.00000000 |
| 156 | 743.21050000 | 8.83990000   | 0.00000000 |
| 157 | 743.79580000 | 35.15570000  | 0.00000000 |
| 158 | 744.65660000 | 12.81760000  | 0.00000000 |
| 159 | 745.24130000 | 68.69530000  | 0.00000000 |
| 160 | 745.71930000 | 12.72230000  | 0.00000000 |
| 161 | 746.30600000 | 16.41100000  | 0.00000000 |
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| 163 | 748.92830000 | 23.88360000  | 0.00000000 |
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| 165 | 756.83500000 | 17.11260000  | 0.00000000 |
| 166 | 758.72820000 | 98.40790000  | 0.00000000 |
| 167 | 761.47090000 | 73.55910000  | 0.00000000 |
| 168 | 762.40180000 | 116.23890000 | 0.00000000 |
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| 170 | 767.84580000 | 89.15240000  | 0.00000000 |
| 171 | 774.23940000 | 144.47630000 | 0.00000000 |
| 172 | 780.74670000 | 21.72120000  | 0.00000000 |
| 173 | 783.71340000 | 2.58100000   | 0.00000000 |
| 174 | 792.76080000 | 32.17120000  | 0.00000000 |
| 175 | 793.40880000 | 52.50690000  | 0.00000000 |
| 176 | 796.16290000 | 91.76170000  | 0.00000000 |
| 177 | 799.59820000 | 112.93720000 | 0.00000000 |
| 178 | 813.98870000 | 4.35470000   | 0.00000000 |
| 179 | 814.31690000 | 9.68850000   | 0.00000000 |
| 180 | 818.41770000 | 8.21330000   | 0.00000000 |
| 181 | 822.04660000 | 42.56410000  | 0.00000000 |
| 182 | 827.32290000 | 2.41270000   | 0.00000000 |
| 183 | 836.81070000 | 26.78950000  | 0.00000000 |
| 184 | 837.10710000 | 46.95480000  | 0.00000000 |
| 185 | 839.06960000 | 97.73360000  | 0.00000000 |
| 186 | 844.21090000 | 24.52110000  | 0.00000000 |
| 187 | 857.77660000 | 6.66960000   | 0.00000000 |
| 188 | 862.71510000 | 26.80500000  | 0.00000000 |

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| 190 | 865.82580000  | 2.71070000  | 0.00000000 |
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| 192 | 871.09730000  | 19.83820000 | 0.00000000 |
| 193 | 873.90460000  | 35.78720000 | 0.00000000 |
| 194 | 878.49340000  | 47.85960000 | 0.00000000 |
| 195 | 880.71690000  | 14.12010000 | 0.00000000 |
| 196 | 881.26280000  | 2.51000000  | 0.00000000 |
| 197 | 883.98860000  | 1.96930000  | 0.00000000 |
| 198 | 890.02490000  | 6.89580000  | 0.00000000 |
| 199 | 890.69420000  | 7.06870000  | 0.00000000 |
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| 201 | 916.18130000  | 1.25210000  | 0.00000000 |
| 202 | 921.52600000  | 2.90440000  | 0.00000000 |
| 203 | 922.75660000  | 0.61390000  | 0.00000000 |
| 204 | 922.92240000  | 1.84880000  | 0.00000000 |
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| 206 | 936.37750000  | 19.74870000 | 0.00000000 |
| 207 | 947.53310000  | 0.16410000  | 0.00000000 |
| 208 | 948.64730000  | 0.02390000  | 0.00000000 |
| 209 | 953.63800000  | 0.37560000  | 0.00000000 |
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| 212 | 980.35270000  | 0.35250000  | 0.00000000 |
| 213 | 983.48900000  | 2.36010000  | 0.00000000 |
| 214 | 985.14350000  | 0.42380000  | 0.00000000 |
| 215 | 986.88200000  | 1.03180000  | 0.00000000 |
| 216 | 990.84900000  | 3.24080000  | 0.00000000 |
| 217 | 998.81820000  | 2.63100000  | 0.00000000 |
| 218 | 1000.47720000 | 1.64190000  | 0.00000000 |
| 219 | 1008.10090000 | 0.34850000  | 0.00000000 |
| 220 | 1009.10250000 | 3.88790000  | 0.00000000 |
| 221 | 1011.00750000 | 1.65070000  | 0.00000000 |
| 222 | 1011.28870000 | 17.53820000 | 0.00000000 |
| 223 | 1012.15440000 | 32.13720000 | 0.00000000 |
| 224 | 1012.90190000 | 1.63540000  | 0.00000000 |
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| 226 | 1014.94760000 | 0.64490000  | 0.00000000 |
| 227 | 1016.16350000 | 0.41880000  | 0.00000000 |
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| 229 | 1019.30370000 | 1.31700000  | 0.00000000 |
| 230 | 1029.19930000 | 1.02380000  | 0.00000000 |
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| 232 | 1039.29920000 | 0.12420000  | 0.00000000 |
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| 234 | 1042.14050000 | 0.99070000  | 0.00000000 |
| 235 | 1042.21350000 | 22.75030000 | 0.00000000 |
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| 237 | 1054.93490000 | 6.46110000  | 0.00000000 |
| 238 | 1071.93290000 | 4.60200000  | 0.00000000 |
| 239 | 1074.94660000 | 4.64950000  | 0.00000000 |
| 240 | 1075.28100000 | 48.10380000 | 0.00000000 |
| 241 | 1076.35690000 | 48.54240000 | 0.00000000 |
| 242 | 1080.03340000 | 14.95070000 | 0.00000000 |
| 243 | 1082.88660000 | 5.11540000  | 0.00000000 |
| 244 | 1085.47050000 | 13.05190000 | 0.00000000 |
| 245 | 1086.40740000 | 82.90560000 | 0.00000000 |
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| 248 | 1097.39660000 | 0.22410000  | 0.00000000 |
| 249 | 1116.33240000 | 81.08890000 | 0.00000000 |
| 250 | 1117.49690000 | 80.08320000 | 0.00000000 |
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| 252 | 1123.86590000 | 25.65250000 | 0.00000000 |

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| 253 | 1125.76760000 | 47.84210000  | 0.00000000 |
| 254 | 1125.87600000 | 0.58360000   | 0.00000000 |
| 255 | 1134.01830000 | 16.09980000  | 0.00000000 |
| 256 | 1138.71130000 | 4.84000000   | 0.00000000 |
| 257 | 1146.03330000 | 19.70930000  | 0.00000000 |
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| 259 | 1154.81410000 | 15.41100000  | 0.00000000 |
| 260 | 1165.83130000 | 2.01970000   | 0.00000000 |
| 261 | 1166.67220000 | 0.63540000   | 0.00000000 |
| 262 | 1167.44210000 | 5.50080000   | 0.00000000 |
| 263 | 1171.30710000 | 17.93870000  | 0.00000000 |
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| 268 | 1214.02670000 | 0.73310000   | 0.00000000 |
| 269 | 1224.00080000 | 16.96250000  | 0.00000000 |
| 270 | 1225.78680000 | 17.28990000  | 0.00000000 |
| 271 | 1230.94660000 | 6.23910000   | 0.00000000 |
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| 273 | 1237.19670000 | 22.18510000  | 0.00000000 |
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| 277 | 1254.95470000 | 36.13550000  | 0.00000000 |
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| 283 | 1279.08380000 | 0.94680000   | 0.00000000 |
| 284 | 1280.90180000 | 0.55400000   | 0.00000000 |
| 285 | 1281.71930000 | 19.59310000  | 0.00000000 |
| 286 | 1282.05670000 | 0.37290000   | 0.00000000 |
| 287 | 1287.78550000 | 10.04780000  | 0.00000000 |
| 288 | 1307.99220000 | 3.77690000   | 0.00000000 |
| 289 | 1308.95200000 | 1.36320000   | 0.00000000 |
| 290 | 1309.72910000 | 4.81270000   | 0.00000000 |
| 291 | 1310.68170000 | 5.48250000   | 0.00000000 |
| 292 | 1316.47890000 | 1.18370000   | 0.00000000 |
| 293 | 1319.21010000 | 67.15140000  | 0.00000000 |
| 294 | 1321.45210000 | 51.34450000  | 0.00000000 |
| 295 | 1322.54890000 | 54.30820000  | 0.00000000 |
| 296 | 1323.18470000 | 54.65800000  | 0.00000000 |
| 297 | 1334.07780000 | 2.60150000   | 0.00000000 |
| 298 | 1337.08510000 | 0.50270000   | 0.00000000 |
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| 300 | 1350.38160000 | 13.76560000  | 0.00000000 |
| 301 | 1351.51320000 | 2.21620000   | 0.00000000 |
| 302 | 1356.30620000 | 0.28360000   | 0.00000000 |
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| 307 | 1377.29590000 | 5.71290000   | 0.00000000 |
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| 315 | 1416.86000000 | 10.89330000  | 0.00000000 |
| 316 | 1419.65440000 | 10.16840000  | 0.00000000 |

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| 317 | 1429.49900000 | 5.09180000    | 0.00000000 |
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| 320 | 1436.63250000 | 51.31010000   | 0.00000000 |
| 321 | 1442.86080000 | 177.90120000  | 0.00000000 |
| 322 | 1454.05540000 | 41.54340000   | 0.00000000 |
| 323 | 1456.97500000 | 93.71630000   | 0.00000000 |
| 324 | 1458.52640000 | 130.16020000  | 0.00000000 |
| 325 | 1459.05010000 | 17.24690000   | 0.00000000 |
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| 327 | 1474.42750000 | 71.34060000   | 0.00000000 |
| 328 | 1475.34700000 | 71.31990000   | 0.00000000 |
| 329 | 1476.86230000 | 9.86230000    | 0.00000000 |
| 330 | 1479.67670000 | 24.34210000   | 0.00000000 |
| 331 | 1480.35870000 | 12.81530000   | 0.00000000 |
| 332 | 1485.22910000 | 1.10830000    | 0.00000000 |
| 333 | 1489.38280000 | 12.83020000   | 0.00000000 |
| 334 | 1492.40740000 | 6.86160000    | 0.00000000 |
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| 356 | 1616.49710000 | 15.77500000   | 0.00000000 |
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| 358 | 1625.38540000 | 1.47840000    | 0.00000000 |
| 359 | 1627.86370000 | 4.38570000    | 0.00000000 |
| 360 | 1628.05100000 | 5.03220000    | 0.00000000 |
| 361 | 1637.47610000 | 3.41470000    | 0.00000000 |
| 362 | 1642.84230000 | 0.42940000    | 0.00000000 |
| 363 | 1644.06640000 | 135.67310000  | 0.00000000 |
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| 367 | 1661.12610000 | 13.52160000   | 0.00000000 |
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| 369 | 1666.59770000 | 87.25950000   | 0.00000000 |
| 370 | 1707.99780000 | 61.80010000   | 0.00000000 |
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| 374 | 3007.65730000 | 33.46610000   | 0.00000000 |
| 375 | 3015.67500000 | 17.57650000   | 0.00000000 |
| 376 | 3022.27560000 | 31.96080000   | 0.00000000 |
| 377 | 3030.44410000 | 13.74740000   | 0.00000000 |
| 378 | 3033.60440000 | 68.67920000   | 0.00000000 |
| 379 | 3042.08870000 | 37.84070000   | 0.00000000 |
| 380 | 3060.31920000 | 58.26850000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 3063.68440000 | 33.92690000   | 0.00000000 |
| 382 | 3071.31340000 | 90.15280000   | 0.00000000 |
| 383 | 3084.68260000 | 77.24840000   | 0.00000000 |
| 384 | 3190.01890000 | 4.82280000    | 0.00000000 |
| 385 | 3190.31820000 | 1.04500000    | 0.00000000 |
| 386 | 3194.24180000 | 2.44770000    | 0.00000000 |
| 387 | 3196.59440000 | 3.58920000    | 0.00000000 |
| 388 | 3198.79980000 | 0.17210000    | 0.00000000 |
| 389 | 3198.93350000 | 2.95690000    | 0.00000000 |
| 390 | 3200.27430000 | 8.77660000    | 0.00000000 |
| 391 | 3202.21110000 | 7.50910000    | 0.00000000 |
| 392 | 3202.98920000 | 0.78660000    | 0.00000000 |
| 393 | 3209.43270000 | 6.08360000    | 0.00000000 |
| 394 | 3210.30570000 | 14.04740000   | 0.00000000 |
| 395 | 3213.62480000 | 2.28080000    | 0.00000000 |
| 396 | 3213.88300000 | 0.70630000    | 0.00000000 |
| 397 | 3216.46690000 | 18.58300000   | 0.00000000 |
| 398 | 3217.75420000 | 1.42510000    | 0.00000000 |
| 399 | 3224.38460000 | 16.14390000   | 0.00000000 |
| 400 | 3227.64460000 | 6.17280000    | 0.00000000 |
| 401 | 3228.25760000 | 5.94850000    | 0.00000000 |
| 402 | 3228.29860000 | 4.90890000    | 0.00000000 |
| 403 | 3228.75530000 | 8.54290000    | 0.00000000 |
| 404 | 3230.34980000 | 6.52220000    | 0.00000000 |
| 405 | 3232.75470000 | 5.81680000    | 0.00000000 |
| 406 | 3238.23890000 | 12.41470000   | 0.00000000 |
| 407 | 3242.43140000 | 25.54450000   | 0.00000000 |
| 408 | 3244.01760000 | 5.43970000    | 0.00000000 |
| 409 | 3246.66330000 | 3.95460000    | 0.00000000 |
| 410 | 3253.02860000 | 4.77870000    | 0.00000000 |
| 411 | 3256.68310000 | 8.85890000    | 0.00000000 |
| 412 | 3259.98380000 | 20.02100000   | 0.00000000 |
| 413 | 3260.85240000 | 0.50630000    | 0.00000000 |
| 414 | 3261.00440000 | 0.18180000    | 0.00000000 |
| 415 | 3264.50220000 | 3.44560000    | 0.00000000 |
| 416 | 3270.43450000 | 5.22170000    | 0.00000000 |
| 417 | 3271.08260000 | 6.17150000    | 0.00000000 |
| 418 | 3271.43620000 | 9.48360000    | 0.00000000 |
| 419 | 3284.95620000 | 4.31960000    | 0.00000000 |
| 420 | 3285.09220000 | 4.30500000    | 0.00000000 |
| 421 | 3285.47120000 | 5.33140000    | 0.00000000 |
| 422 | 3565.24810000 | 727.60130000  | 0.00000000 |
| 423 | 3578.39140000 | 656.80220000  | 0.00000000 |
| 424 | 3585.73780000 | 983.41770000  | 0.00000000 |
| 425 | 3608.89990000 | 332.93240000  | 0.00000000 |
| 426 | 3652.93920000 | 1007.13550000 | 0.00000000 |
| 427 | 3854.21540000 | 143.60130000  | 0.00000000 |
| 428 | 3858.65780000 | 106.78780000  | 0.00000000 |
| 429 | 3862.70710000 | 131.98890000  | 0.00000000 |

# S16. CALCULATIONS ON $1\mathbf{w}^{3+}$ ( $^3\mathbf{A}$ )

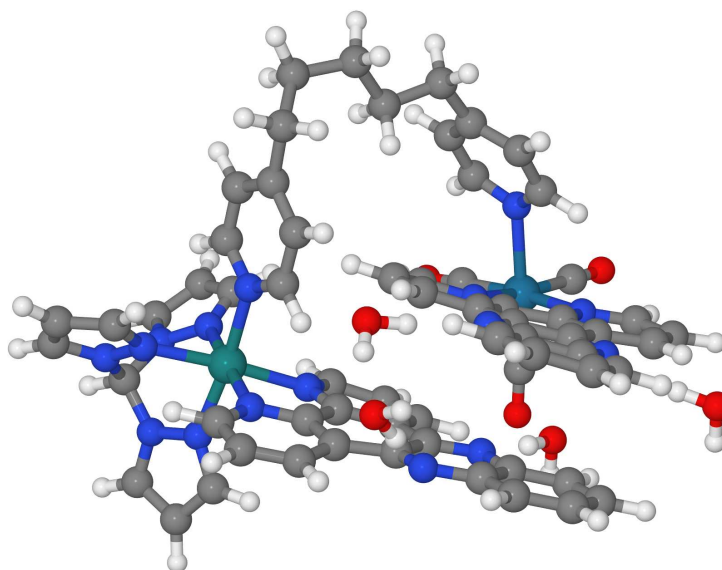


FIG. S26. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]
            : 1n7ccc1)[n+](n8ccc1)[n+](1ccc(cc1)CCCCc1cc[n+](cc1)[Re]
            : 1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1))([C][O])([C][O])([C][O]).O.O.O.O
            : C64H56N16O7ReRu3+,3
Formula    :
Charge     : 3
Multiplicity : 3
Energy     : -4049.70092806
Gibbs Energy : -4048.69118500
Number of imaginary frequencies : 0

```

a.u.

a.u.

## S16.1. Cartesian Co-ordinates (XYZ format)

145

```

C -1.26485395 -2.89891291 5.16933918
H -1.12051201 -3.78496695 5.79620790
H -1.94665301 -2.23290491 5.70354223
C 0.10093200 -2.20144606 4.98712587
H -0.02133000 -1.32262003 4.34548712
H 0.78740102 -2.87746692 4.46650696
C 0.69056797 -1.80954397 6.34459305
H 0.64552897 -2.68359303 7.00380993
H 0.05403600 -1.04605603 6.80698919
C 2.36844492 0.04708400 5.64283180
H 3.21350503 0.54449600 6.13455200
H 1.50517094 0.69772100 5.80313587
C 6.83941507 -0.96614701 -1.50329804
N 5.98398304 -2.05164194 -1.07316899
N 6.21847916 -0.23296399 -2.59003901

```



|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 7.11989403  | -0.08067100 | -0.39294699 |
| N  | 4.75322485  | -1.77031100 | -0.57062298 |
| C  | 6.21459103  | -3.38878798 | -1.08073997 |
| N  | 5.02303123  | 0.38766599  | -2.38321710 |
| C  | 6.65725279  | -0.01669300 | -3.85045195 |
| N  | 6.09619284  | 0.57948202  | 0.21247999  |
| C  | 8.30224228  | 0.19720000  | 0.21149801  |
| Ru | 4.15893698  | 0.25193101  | -0.52895099 |
| C  | 4.20190382  | -2.94617200 | -0.25804999 |
| C  | 5.08797884  | -3.99097395 | -0.56073898 |
| H  | 7.14180899  | -3.79396701 | -1.45009601 |
| C  | 4.71010113  | 1.00008500  | -3.53232098 |
| C  | 5.70807791  | 0.76930702  | -4.48204613 |
| H  | 7.59060717  | -0.42775699 | -4.19819307 |
| C  | 6.64193392  | 1.28079295  | 1.20841503  |
| C  | 8.02801895  | 1.06914794  | 1.24468803  |
| H  | 9.22420406  | -0.23680100 | -0.13774000 |
| N  | 2.30663610  | -0.02049700 | -1.40902305 |
| N  | 3.50502896  | 2.22020793  | -0.64926600 |
| H  | 3.21449208  | -2.98858809 | 0.17309500  |
| H  | 4.92478085  | -5.04479122 | -0.41766700 |
| H  | 3.79589295  | 1.56402302  | -3.61435390 |
| H  | 5.73847294  | 1.12604403  | -5.49666691 |
| H  | 6.02623892  | 1.88812399  | 1.85086501  |
| H  | 8.73404694  | 1.49868703  | 1.93365598  |
| C  | 1.83446097  | -1.13073301 | -1.97180700 |
| C  | 1.54656398  | 1.12003899  | -1.41927195 |
| C  | 2.18191695  | 2.30880904  | -1.00793505 |
| C  | 4.18571615  | 3.33130789  | -0.38556099 |
| C  | 0.55320799  | -1.17296195 | -2.53085399 |
| H  | 2.48069310  | -1.99498606 | -1.97962201 |
| C  | 0.20787200  | 1.13098001  | -1.88756895 |
| C  | 1.48149502  | 3.53497291  | -1.00921905 |
| C  | 3.57837605  | 4.59146500  | -0.44542900 |
| H  | 5.22923279  | 3.21893907  | -0.12957300 |
| C  | -0.26452601 | -0.05979400 | -2.46653605 |
| H  | 0.21297500  | -2.08898807 | -2.99206710 |
| C  | -0.57714897 | 2.34338689  | -1.76195002 |
| C  | 2.23214507  | 4.69249105  | -0.74147701 |
| C  | 0.05589100  | 3.53684711  | -1.28103602 |
| H  | 4.17426395  | 5.47079515  | -0.24565899 |
| H  | -1.27221406 | -0.10891000 | -2.85359693 |
| N  | -1.88234603 | 2.32273602  | -2.07716894 |
| H  | 1.74941802  | 5.65769005  | -0.75827003 |
| N  | -0.63343602 | 4.66598511  | -1.07973003 |
| C  | -2.58334994 | 3.49525309  | -1.94751501 |
| C  | -1.96026397 | 4.66733313  | -1.41856694 |
| C  | -3.94258308 | 3.55033493  | -2.31441593 |
| C  | -2.72458792 | 5.83412695  | -1.24074697 |
| C  | -4.66648197 | 4.71855402  | -2.14878988 |
| H  | -4.40713692 | 2.65657997  | -2.71209002 |
| C  | -4.06087208 | 5.85839796  | -1.59919000 |
| H  | -2.24153590 | 6.70790720  | -0.82129300 |
| H  | -5.71130705 | 4.75185680  | -2.42937493 |
| H  | -4.64239311 | 6.75987720  | -1.45239401 |
| N  | -4.35418510 | -1.95394695 | -0.72396803 |
| N  | -1.74906695 | -1.83631694 | -0.14495200 |
| C  | -5.64214277 | -2.04582906 | -1.06985795 |
| C  | -3.88154888 | -0.76539302 | -0.27121401 |
| C  | -2.48400211 | -0.72112101 | 0.09573400  |
| C  | -0.49228701 | -1.89471304 | 0.30448601  |
| C  | -6.51638699 | -0.96754998 | -0.96063298 |
| H  | -5.97976923 | -3.00596189 | -1.43232906 |
| C  | -4.70490599 | 0.35519400  | -0.10218000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.94680095 | 0.40209901  | 0.73928201  |
| C  | 0.08672600  | -0.84889603 | 1.01415098  |
| H  | 0.05644500  | -2.80310106 | 0.10688500  |
| C  | -6.05454683 | 0.23650201  | -0.46479100 |
| H  | -7.55040598 | -1.09236896 | -1.25076795 |
| C  | -4.13921881 | 1.57347500  | 0.47127500  |
| C  | -0.63159901 | 0.31312999  | 1.21659601  |
| C  | -2.77767301 | 1.58684695  | 0.91981697  |
| H  | 1.09158099  | -0.96836799 | 1.38662100  |
| H  | -6.72718000 | 1.07509995  | -0.35357699 |
| N  | -4.90440798 | 2.64811492  | 0.58927602  |
| H  | -0.19910701 | 1.14465201  | 1.74893105  |
| N  | -2.25827789 | 2.65801191  | 1.50452006  |
| C  | -4.39601088 | 3.74347210  | 1.19371498  |
| C  | -3.04914689 | 3.74025011  | 1.68175399  |
| C  | -5.19809580 | 4.90007687  | 1.36095202  |
| C  | -2.55747294 | 4.87957621  | 2.36529303  |
| C  | -4.68815804 | 5.99053907  | 2.01776505  |
| H  | -6.20499516 | 4.89148903  | 0.96471798  |
| C  | -3.36553192 | 5.97661781  | 2.52780890  |
| H  | -1.55316603 | 4.84838200  | 2.76192093  |
| H  | -5.29911184 | 6.87424898  | 2.15200210  |
| H  | -2.99320102 | 6.84523821  | 3.05696607  |
| H  | 7.77489185  | -1.38255095 | -1.86088896 |
| C  | -1.88470995 | -3.31572104 | 3.86680198  |
| C  | -3.03882504 | -2.71237612 | 3.36390805  |
| C  | -1.30794704 | -4.31761694 | 3.07945895  |
| C  | -3.48886609 | -3.03095007 | 2.09359598  |
| H  | -3.57244897 | -1.96742201 | 3.93996692  |
| C  | -1.80612600 | -4.57550287 | 1.81736600  |
| H  | -0.44704899 | -4.87375116 | 3.42776394  |
| N  | -2.84773707 | -3.89815402 | 1.28621805  |
| H  | -4.36168289 | -2.54425406 | 1.68488300  |
| H  | -1.33946705 | -5.31855011 | 1.18792701  |
| C  | 2.71110010  | 0.03923800  | 4.17807817  |
| C  | 2.19536304  | 1.00985396  | 3.31358004  |
| C  | 3.63826299  | -0.85609800 | 3.62886596  |
| C  | 2.59300804  | 1.05510902  | 1.99246299  |
| H  | 1.48857796  | 1.75809300  | 3.64677811  |
| C  | 4.00524616  | -0.75305498 | 2.30335212  |
| H  | 4.10336304  | -1.62479305 | 4.23020077  |
| N  | 3.48211288  | 0.17912200  | 1.47014999  |
| H  | 2.18049192  | 1.81538606  | 1.35019898  |
| H  | 4.74230003  | -1.41905904 | 1.88416302  |
| Re | -2.85092306 | -3.55872989 | -0.96970099 |
| C  | -2.70901108 | -3.05874991 | -2.83712101 |
| O  | -2.60517907 | -2.76967001 | -3.94723392 |
| C  | -1.35380399 | -4.75901318 | -1.23422396 |
| O  | -0.44116899 | -5.43864107 | -1.43095303 |
| C  | -4.07193995 | -5.00596619 | -1.40338004 |
| O  | -4.81897116 | -5.85375786 | -1.62855697 |
| C  | 2.14072990  | -1.31318796 | 6.33324003  |
| H  | 2.78726697  | -2.07887506 | 5.89443016  |
| H  | 2.46353889  | -1.21178699 | 7.37227678  |
| H  | -2.95673394 | 0.95538700  | -2.71959591 |
| O  | -3.52009606 | 0.20528300  | -3.01825809 |
| H  | -3.40897989 | 0.17972399  | -3.97440100 |
| H  | -0.11311000 | 5.70087194  | 0.31885499  |
| O  | 0.30868301  | 6.04197216  | 1.14518499  |
| H  | -0.34501600 | 6.61873007  | 1.55294299  |
| H  | -0.38408899 | 3.14775610  | 1.89907503  |
| O  | 0.51449603  | 3.41216803  | 2.16448498  |
| H  | 0.57462299  | 4.34451580  | 1.88202798  |
| H  | -6.58757401 | 3.06381989  | -0.23366900 |

|   |             |            |             |
|---|-------------|------------|-------------|
| O | -7.48707724 | 3.25736594 | -0.56042302 |
| H | -7.40170622 | 3.24541402 | -1.51933801 |

## S16.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 11.44520000  | 3.64020000   | 0.00000000      |
| 2    | 17.84320000  | 4.03450000   | 0.00000000      |
| 3    | 18.47740000  | 0.62390000   | 0.00000000      |
| 4    | 22.88260000  | 0.01700000   | 0.00000000      |
| 5    | 26.59910000  | 0.60400000   | 0.00000000      |
| 6    | 31.49920000  | 0.60070000   | 0.00000000      |
| 7    | 33.87470000  | 0.47260000   | 0.00000000      |
| 8    | 37.22870000  | 1.75470000   | 0.00000000      |
| 9    | 42.35220000  | 5.45630000   | 0.00000000      |
| 10   | 46.42230000  | 3.37270000   | 0.00000000      |
| 11   | 48.75690000  | 3.76290000   | 0.00000000      |
| 12   | 52.64390000  | 3.06770000   | 0.00000000      |
| 13   | 55.88490000  | 1.92820000   | 0.00000000      |
| 14   | 57.32820000  | 5.48290000   | 0.00000000      |
| 15   | 63.65010000  | 3.25180000   | 0.00000000      |
| 16   | 64.92140000  | 5.53780000   | 0.00000000      |
| 17   | 69.46330000  | 9.97240000   | 0.00000000      |
| 18   | 72.27790000  | 1.08840000   | 0.00000000      |
| 19   | 72.75390000  | 3.63840000   | 0.00000000      |
| 20   | 80.10580000  | 1.29980000   | 0.00000000      |
| 21   | 83.26840000  | 3.08060000   | 0.00000000      |
| 22   | 84.75940000  | 1.05580000   | 0.00000000      |
| 23   | 88.17180000  | 6.85730000   | 0.00000000      |
| 24   | 90.86520000  | 6.11810000   | 0.00000000      |
| 25   | 91.40300000  | 1.48180000   | 0.00000000      |
| 26   | 92.41650000  | 8.56930000   | 0.00000000      |
| 27   | 93.96330000  | 0.01840000   | 0.00000000      |
| 28   | 97.25550000  | 9.89890000   | 0.00000000      |
| 29   | 100.48790000 | 17.92470000  | 0.00000000      |
| 30   | 102.31530000 | 5.23210000   | 0.00000000      |
| 31   | 103.75770000 | 0.49810000   | 0.00000000      |
| 32   | 107.84520000 | 4.89890000   | 0.00000000      |
| 33   | 110.15060000 | 6.20690000   | 0.00000000      |
| 34   | 111.58570000 | 11.25780000  | 0.00000000      |
| 35   | 113.77960000 | 6.25960000   | 0.00000000      |
| 36   | 117.47340000 | 0.69340000   | 0.00000000      |
| 37   | 124.52100000 | 0.35670000   | 0.00000000      |
| 38   | 132.17860000 | 1.52570000   | 0.00000000      |
| 39   | 136.00210000 | 2.74840000   | 0.00000000      |
| 40   | 138.01770000 | 0.36760000   | 0.00000000      |
| 41   | 140.65210000 | 2.46770000   | 0.00000000      |
| 42   | 142.66270000 | 1.11980000   | 0.00000000      |
| 43   | 144.81060000 | 0.11210000   | 0.00000000      |
| 44   | 151.99690000 | 4.85470000   | 0.00000000      |
| 45   | 154.25640000 | 3.22170000   | 0.00000000      |
| 46   | 160.11810000 | 1.14910000   | 0.00000000      |
| 47   | 161.78710000 | 4.09670000   | 0.00000000      |
| 48   | 164.41490000 | 12.94700000  | 0.00000000      |
| 49   | 168.41930000 | 0.64570000   | 0.00000000      |
| 50   | 170.40410000 | 5.09910000   | 0.00000000      |
| 51   | 173.27350000 | 6.54600000   | 0.00000000      |
| 52   | 175.68610000 | 3.45590000   | 0.00000000      |
| 53   | 179.11960000 | 4.72750000   | 0.00000000      |
| 54   | 181.79090000 | 2.31060000   | 0.00000000      |
| 55   | 184.28590000 | 5.39580000   | 0.00000000      |
| 56   | 190.17980000 | 2.66620000   | 0.00000000      |
| 57   | 193.57120000 | 4.31340000   | 0.00000000      |
| 58   | 194.06570000 | 2.39420000   | 0.00000000      |
| 59   | 200.84060000 | 0.70110000   | 0.00000000      |
| 60   | 204.55790000 | 31.48480000  | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 207.96480000 | 17.04140000  | 0.00000000 |
| 62  | 219.44860000 | 0.82360000   | 0.00000000 |
| 63  | 224.49780000 | 6.96060000   | 0.00000000 |
| 64  | 230.32860000 | 10.87660000  | 0.00000000 |
| 65  | 235.75190000 | 18.11540000  | 0.00000000 |
| 66  | 237.57640000 | 5.28720000   | 0.00000000 |
| 67  | 244.15150000 | 42.76530000  | 0.00000000 |
| 68  | 246.96330000 | 67.35650000  | 0.00000000 |
| 69  | 253.31800000 | 4.81040000   | 0.00000000 |
| 70  | 262.16850000 | 66.68410000  | 0.00000000 |
| 71  | 273.58200000 | 3.65420000   | 0.00000000 |
| 72  | 282.22240000 | 24.17080000  | 0.00000000 |
| 73  | 284.61840000 | 1.47850000   | 0.00000000 |
| 74  | 294.87690000 | 38.80360000  | 0.00000000 |
| 75  | 295.97990000 | 144.13970000 | 0.00000000 |
| 76  | 302.15110000 | 28.93480000  | 0.00000000 |
| 77  | 313.95560000 | 24.98360000  | 0.00000000 |
| 78  | 321.37910000 | 10.35910000  | 0.00000000 |
| 79  | 323.73250000 | 11.28920000  | 0.00000000 |
| 80  | 326.86520000 | 22.89090000  | 0.00000000 |
| 81  | 332.44780000 | 20.27770000  | 0.00000000 |
| 82  | 334.29970000 | 75.82610000  | 0.00000000 |
| 83  | 334.71000000 | 81.75190000  | 0.00000000 |
| 84  | 338.50840000 | 47.55470000  | 0.00000000 |
| 85  | 342.93940000 | 69.76370000  | 0.00000000 |
| 86  | 346.62110000 | 65.69340000  | 0.00000000 |
| 87  | 357.81810000 | 0.32820000   | 0.00000000 |
| 88  | 361.80710000 | 120.17000000 | 0.00000000 |
| 89  | 363.85730000 | 6.00480000   | 0.00000000 |
| 90  | 376.90770000 | 2.02660000   | 0.00000000 |
| 91  | 383.11880000 | 6.75720000   | 0.00000000 |
| 92  | 389.66600000 | 1.33290000   | 0.00000000 |
| 93  | 393.09960000 | 15.54550000  | 0.00000000 |
| 94  | 394.15310000 | 8.81150000   | 0.00000000 |
| 95  | 396.37560000 | 1.05390000   | 0.00000000 |
| 96  | 408.92960000 | 73.90570000  | 0.00000000 |
| 97  | 413.73330000 | 3.02810000   | 0.00000000 |
| 98  | 420.61300000 | 5.75180000   | 0.00000000 |
| 99  | 421.71330000 | 24.58560000  | 0.00000000 |
| 100 | 440.41020000 | 21.09600000  | 0.00000000 |
| 101 | 446.34020000 | 30.06660000  | 0.00000000 |
| 102 | 446.75920000 | 96.23470000  | 0.00000000 |
| 103 | 449.33900000 | 39.80290000  | 0.00000000 |
| 104 | 454.29170000 | 39.51130000  | 0.00000000 |
| 105 | 463.71470000 | 2.85550000   | 0.00000000 |
| 106 | 467.84540000 | 59.27500000  | 0.00000000 |
| 107 | 476.56180000 | 39.91550000  | 0.00000000 |
| 108 | 479.25430000 | 32.69580000  | 0.00000000 |
| 109 | 482.57300000 | 25.52510000  | 0.00000000 |
| 110 | 483.59090000 | 41.09340000  | 0.00000000 |
| 111 | 488.34360000 | 3.00320000   | 0.00000000 |
| 112 | 494.08030000 | 17.13580000  | 0.00000000 |
| 113 | 497.99420000 | 24.77520000  | 0.00000000 |
| 114 | 498.76200000 | 0.61160000   | 0.00000000 |
| 115 | 504.93890000 | 9.67140000   | 0.00000000 |
| 116 | 513.68260000 | 27.18880000  | 0.00000000 |
| 117 | 514.06320000 | 28.23190000  | 0.00000000 |
| 118 | 516.46200000 | 36.33850000  | 0.00000000 |
| 119 | 524.25620000 | 39.81630000  | 0.00000000 |
| 120 | 536.06280000 | 12.18130000  | 0.00000000 |
| 121 | 551.54580000 | 22.04540000  | 0.00000000 |
| 122 | 554.39350000 | 37.70990000  | 0.00000000 |
| 123 | 555.57790000 | 28.69990000  | 0.00000000 |
| 124 | 560.85110000 | 4.67120000   | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 571.22690000 | 2.96190000   | 0.00000000 |
| 126 | 578.42440000 | 2.87130000   | 0.00000000 |
| 127 | 578.89440000 | 3.38130000   | 0.00000000 |
| 128 | 582.95960000 | 5.92040000   | 0.00000000 |
| 129 | 589.43800000 | 103.56290000 | 0.00000000 |
| 130 | 592.95940000 | 8.04300000   | 0.00000000 |
| 131 | 594.34890000 | 21.78510000  | 0.00000000 |
| 132 | 597.01700000 | 170.09590000 | 0.00000000 |
| 133 | 599.26410000 | 2.08890000   | 0.00000000 |
| 134 | 602.40410000 | 11.29970000  | 0.00000000 |
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| 138 | 625.44220000 | 31.15180000  | 0.00000000 |
| 139 | 635.48070000 | 58.74140000  | 0.00000000 |
| 140 | 636.97750000 | 188.08520000 | 0.00000000 |
| 141 | 645.13790000 | 2.04230000   | 0.00000000 |
| 142 | 646.94680000 | 78.69160000  | 0.00000000 |
| 143 | 650.67590000 | 53.05380000  | 0.00000000 |
| 144 | 656.06910000 | 10.86120000  | 0.00000000 |
| 145 | 658.32010000 | 12.23050000  | 0.00000000 |
| 146 | 666.92650000 | 12.22490000  | 0.00000000 |
| 147 | 670.39250000 | 12.21850000  | 0.00000000 |
| 148 | 670.93110000 | 9.48720000   | 0.00000000 |
| 149 | 673.52760000 | 6.05530000   | 0.00000000 |
| 150 | 680.25810000 | 3.67070000   | 0.00000000 |
| 151 | 684.07140000 | 3.50590000   | 0.00000000 |
| 152 | 684.98020000 | 46.20640000  | 0.00000000 |
| 153 | 706.56510000 | 343.32340000 | 0.00000000 |
| 154 | 723.82330000 | 89.56030000  | 0.00000000 |
| 155 | 731.63820000 | 4.76640000   | 0.00000000 |
| 156 | 738.91190000 | 6.93370000   | 0.00000000 |
| 157 | 740.05380000 | 24.06730000  | 0.00000000 |
| 158 | 743.94200000 | 12.30340000  | 0.00000000 |
| 159 | 746.22440000 | 26.49820000  | 0.00000000 |
| 160 | 746.46160000 | 34.13480000  | 0.00000000 |
| 161 | 747.43710000 | 3.41420000   | 0.00000000 |
| 162 | 747.98910000 | 221.02390000 | 0.00000000 |
| 163 | 753.50530000 | 71.07220000  | 0.00000000 |
| 164 | 758.97520000 | 75.11950000  | 0.00000000 |
| 165 | 760.59900000 | 56.87150000  | 0.00000000 |
| 166 | 773.23570000 | 79.95620000  | 0.00000000 |
| 167 | 775.53040000 | 87.80310000  | 0.00000000 |
| 168 | 775.89320000 | 136.12710000 | 0.00000000 |
| 169 | 776.90770000 | 375.78470000 | 0.00000000 |
| 170 | 779.17760000 | 100.71540000 | 0.00000000 |
| 171 | 782.40260000 | 1.76500000   | 0.00000000 |
| 172 | 784.32820000 | 27.18260000  | 0.00000000 |
| 173 | 785.00290000 | 7.27160000   | 0.00000000 |
| 174 | 794.78960000 | 13.30600000  | 0.00000000 |
| 175 | 796.55570000 | 100.57310000 | 0.00000000 |
| 176 | 798.14260000 | 93.01340000  | 0.00000000 |
| 177 | 800.10440000 | 64.54000000  | 0.00000000 |
| 178 | 813.27010000 | 28.15290000  | 0.00000000 |
| 179 | 819.21770000 | 83.93370000  | 0.00000000 |
| 180 | 822.19540000 | 42.87320000  | 0.00000000 |
| 181 | 824.12020000 | 5.41160000   | 0.00000000 |
| 182 | 832.09790000 | 148.36830000 | 0.00000000 |
| 183 | 835.07420000 | 45.40200000  | 0.00000000 |
| 184 | 837.29520000 | 21.11560000  | 0.00000000 |
| 185 | 843.18120000 | 16.72250000  | 0.00000000 |
| 186 | 845.20940000 | 380.67260000 | 0.00000000 |
| 187 | 861.56140000 | 5.54860000   | 0.00000000 |
| 188 | 862.45860000 | 32.16520000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 189 | 864.56460000  | 303.35750000  | 0.00000000 |
| 190 | 870.46480000  | 8.57700000    | 0.00000000 |
| 191 | 872.86470000  | 63.72270000   | 0.00000000 |
| 192 | 877.08520000  | 183.85970000  | 0.00000000 |
| 193 | 880.49180000  | 3.99480000    | 0.00000000 |
| 194 | 886.01340000  | 30.91390000   | 0.00000000 |
| 195 | 887.34870000  | 54.75020000   | 0.00000000 |
| 196 | 889.80490000  | 7.64710000    | 0.00000000 |
| 197 | 889.94180000  | 1.67560000    | 0.00000000 |
| 198 | 892.50210000  | 2.86670000    | 0.00000000 |
| 199 | 895.51480000  | 2.15560000    | 0.00000000 |
| 200 | 901.70310000  | 1.48180000    | 0.00000000 |
| 201 | 917.74750000  | 8.73320000    | 0.00000000 |
| 202 | 923.01950000  | 5.05950000    | 0.00000000 |
| 203 | 935.48250000  | 2.90280000    | 0.00000000 |
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| 205 | 940.63900000  | 1.06650000    | 0.00000000 |
| 206 | 943.61950000  | 1.54890000    | 0.00000000 |
| 207 | 947.18490000  | 0.43240000    | 0.00000000 |
| 208 | 948.44040000  | 3.02990000    | 0.00000000 |
| 209 | 952.39080000  | 0.08490000    | 0.00000000 |
| 210 | 953.97920000  | 8.04780000    | 0.00000000 |
| 211 | 966.20310000  | 2.61780000    | 0.00000000 |
| 212 | 970.47470000  | 2.62810000    | 0.00000000 |
| 213 | 974.33800000  | 2.79770000    | 0.00000000 |
| 214 | 975.14540000  | 3.28960000    | 0.00000000 |
| 215 | 975.53590000  | 5.99680000    | 0.00000000 |
| 216 | 984.73220000  | 0.31260000    | 0.00000000 |
| 217 | 988.33170000  | 0.37390000    | 0.00000000 |
| 218 | 996.36420000  | 2.30910000    | 0.00000000 |
| 219 | 1004.27740000 | 18.93620000   | 0.00000000 |
| 220 | 1004.46090000 | 0.71300000    | 0.00000000 |
| 221 | 1007.11130000 | 7.42560000    | 0.00000000 |
| 222 | 1011.93900000 | 2.81680000    | 0.00000000 |
| 223 | 1013.56930000 | 3.35490000    | 0.00000000 |
| 224 | 1015.62180000 | 3.69150000    | 0.00000000 |
| 225 | 1015.74920000 | 0.45630000    | 0.00000000 |
| 226 | 1017.90380000 | 59.24870000   | 0.00000000 |
| 227 | 1018.22780000 | 1.09810000    | 0.00000000 |
| 228 | 1023.53660000 | 75.35050000   | 0.00000000 |
| 229 | 1025.25490000 | 82.28670000   | 0.00000000 |
| 230 | 1037.68210000 | 19.35070000   | 0.00000000 |
| 231 | 1038.75220000 | 0.44410000    | 0.00000000 |
| 232 | 1041.47410000 | 29.55170000   | 0.00000000 |
| 233 | 1042.82820000 | 7.53940000    | 0.00000000 |
| 234 | 1045.22810000 | 64.53920000   | 0.00000000 |
| 235 | 1046.38030000 | 78.63240000   | 0.00000000 |
| 236 | 1052.62650000 | 407.60610000  | 0.00000000 |
| 237 | 1055.19540000 | 6.24450000    | 0.00000000 |
| 238 | 1059.54770000 | 189.43480000  | 0.00000000 |
| 239 | 1071.38210000 | 1580.68910000 | 0.00000000 |
| 240 | 1074.92660000 | 5.44170000    | 0.00000000 |
| 241 | 1079.94330000 | 166.69630000  | 0.00000000 |
| 242 | 1084.81500000 | 20.75420000   | 0.00000000 |
| 243 | 1085.53760000 | 89.30690000   | 0.00000000 |
| 244 | 1087.47350000 | 85.75960000   | 0.00000000 |
| 245 | 1089.43090000 | 103.16520000  | 0.00000000 |
| 246 | 1090.43300000 | 21.40980000   | 0.00000000 |
| 247 | 1095.79420000 | 0.29020000    | 0.00000000 |
| 248 | 1102.90910000 | 349.19890000  | 0.00000000 |
| 249 | 1105.28970000 | 727.54770000  | 0.00000000 |
| 250 | 1124.25590000 | 45.65110000   | 0.00000000 |
| 251 | 1126.82440000 | 86.91970000   | 0.00000000 |
| 252 | 1127.41060000 | 21.77110000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1127.67130000 | 139.60780000  | 0.00000000 |
| 254 | 1133.09250000 | 99.12130000   | 0.00000000 |
| 255 | 1136.17170000 | 132.50060000  | 0.00000000 |
| 256 | 1138.67960000 | 4.21980000    | 0.00000000 |
| 257 | 1141.07150000 | 724.39260000  | 0.00000000 |
| 258 | 1147.63120000 | 59.02450000   | 0.00000000 |
| 259 | 1148.18130000 | 21.52020000   | 0.00000000 |
| 260 | 1157.22210000 | 7.61490000    | 0.00000000 |
| 261 | 1165.69930000 | 11.40990000   | 0.00000000 |
| 262 | 1167.60640000 | 95.75890000   | 0.00000000 |
| 263 | 1169.45430000 | 6.11830000    | 0.00000000 |
| 264 | 1175.86380000 | 60.91850000   | 0.00000000 |
| 265 | 1177.52560000 | 36.01850000   | 0.00000000 |
| 266 | 1181.85250000 | 146.48310000  | 0.00000000 |
| 267 | 1198.15460000 | 1993.35340000 | 0.00000000 |
| 268 | 1206.40590000 | 57.85100000   | 0.00000000 |
| 269 | 1213.01260000 | 42.37620000   | 0.00000000 |
| 270 | 1215.88660000 | 116.54100000  | 0.00000000 |
| 271 | 1226.02400000 | 53.49990000   | 0.00000000 |
| 272 | 1232.12070000 | 27.84690000   | 0.00000000 |
| 273 | 1235.23460000 | 12.45790000   | 0.00000000 |
| 274 | 1237.01320000 | 28.88540000   | 0.00000000 |
| 275 | 1246.16230000 | 6.98630000    | 0.00000000 |
| 276 | 1250.25040000 | 2.37330000    | 0.00000000 |
| 277 | 1255.62380000 | 37.14850000   | 0.00000000 |
| 278 | 1257.33490000 | 10.85610000   | 0.00000000 |
| 279 | 1259.22160000 | 13.59990000   | 0.00000000 |
| 280 | 1261.77280000 | 243.19120000  | 0.00000000 |
| 281 | 1271.85750000 | 1005.75510000 | 0.00000000 |
| 282 | 1273.56130000 | 1222.30170000 | 0.00000000 |
| 283 | 1277.19350000 | 690.15640000  | 0.00000000 |
| 284 | 1280.71810000 | 146.20410000  | 0.00000000 |
| 285 | 1281.12700000 | 16.02430000   | 0.00000000 |
| 286 | 1282.20470000 | 1.43260000    | 0.00000000 |
| 287 | 1288.34590000 | 685.75530000  | 0.00000000 |
| 288 | 1294.24050000 | 694.95130000  | 0.00000000 |
| 289 | 1296.94630000 | 29.94110000   | 0.00000000 |
| 290 | 1306.89510000 | 31.49190000   | 0.00000000 |
| 291 | 1308.36200000 | 80.71980000   | 0.00000000 |
| 292 | 1309.76240000 | 1.23540000    | 0.00000000 |
| 293 | 1317.36450000 | 2.23100000    | 0.00000000 |
| 294 | 1320.30330000 | 164.18340000  | 0.00000000 |
| 295 | 1321.98360000 | 25.33550000   | 0.00000000 |
| 296 | 1323.77420000 | 69.43210000   | 0.00000000 |
| 297 | 1323.93070000 | 115.16400000  | 0.00000000 |
| 298 | 1327.11330000 | 2.49390000    | 0.00000000 |
| 299 | 1334.55900000 | 4.20830000    | 0.00000000 |
| 300 | 1339.96690000 | 5.78850000    | 0.00000000 |
| 301 | 1352.14680000 | 1.66550000    | 0.00000000 |
| 302 | 1353.90110000 | 115.24420000  | 0.00000000 |
| 303 | 1358.88710000 | 34.93600000   | 0.00000000 |
| 304 | 1360.94640000 | 2.17480000    | 0.00000000 |
| 305 | 1368.18920000 | 3.81880000    | 0.00000000 |
| 306 | 1377.08500000 | 252.19170000  | 0.00000000 |
| 307 | 1377.29340000 | 13.24510000   | 0.00000000 |
| 308 | 1378.08650000 | 7.39550000    | 0.00000000 |
| 309 | 1379.00250000 | 3.52820000    | 0.00000000 |
| 310 | 1380.07680000 | 89.38860000   | 0.00000000 |
| 311 | 1380.78650000 | 70.58470000   | 0.00000000 |
| 312 | 1382.23700000 | 54.22050000   | 0.00000000 |
| 313 | 1386.26370000 | 225.32360000  | 0.00000000 |
| 314 | 1394.33080000 | 126.17310000  | 0.00000000 |
| 315 | 1399.18450000 | 5.34110000    | 0.00000000 |
| 316 | 1403.38320000 | 15.40780000   | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1404.58680000 | 7.45880000    | 0.00000000 |
| 318 | 1410.87490000 | 30.06120000   | 0.00000000 |
| 319 | 1426.07690000 | 37.47840000   | 0.00000000 |
| 320 | 1430.05500000 | 42.45120000   | 0.00000000 |
| 321 | 1435.99200000 | 124.42770000  | 0.00000000 |
| 322 | 1441.63990000 | 445.67720000  | 0.00000000 |
| 323 | 1454.68290000 | 486.52810000  | 0.00000000 |
| 324 | 1457.21660000 | 451.69080000  | 0.00000000 |
| 325 | 1458.27580000 | 24.53930000   | 0.00000000 |
| 326 | 1459.45270000 | 530.31920000  | 0.00000000 |
| 327 | 1459.82000000 | 123.72080000  | 0.00000000 |
| 328 | 1468.88290000 | 44.09390000   | 0.00000000 |
| 329 | 1474.55920000 | 171.11490000  | 0.00000000 |
| 330 | 1477.19560000 | 9.90120000    | 0.00000000 |
| 331 | 1480.86210000 | 19.12280000   | 0.00000000 |
| 332 | 1483.49800000 | 58.72910000   | 0.00000000 |
| 333 | 1485.38090000 | 1.12620000    | 0.00000000 |
| 334 | 1486.93100000 | 62.06890000   | 0.00000000 |
| 335 | 1488.48380000 | 12.89640000   | 0.00000000 |
| 336 | 1490.29020000 | 41.11820000   | 0.00000000 |
| 337 | 1501.31290000 | 4.89990000    | 0.00000000 |
| 338 | 1503.56740000 | 30.33670000   | 0.00000000 |
| 339 | 1504.73620000 | 17.43730000   | 0.00000000 |
| 340 | 1506.23280000 | 328.57730000  | 0.00000000 |
| 341 | 1515.95630000 | 26.04950000   | 0.00000000 |
| 342 | 1521.38330000 | 475.60950000  | 0.00000000 |
| 343 | 1527.26700000 | 72.69720000   | 0.00000000 |
| 344 | 1531.15270000 | 12.53870000   | 0.00000000 |
| 345 | 1534.67220000 | 50.83510000   | 0.00000000 |
| 346 | 1535.19480000 | 103.68560000  | 0.00000000 |
| 347 | 1545.45920000 | 68.68370000   | 0.00000000 |
| 348 | 1552.23050000 | 35.96950000   | 0.00000000 |
| 349 | 1556.56720000 | 8.56640000    | 0.00000000 |
| 350 | 1565.18210000 | 77.72850000   | 0.00000000 |
| 351 | 1575.65700000 | 323.14980000  | 0.00000000 |
| 352 | 1578.21890000 | 76.40530000   | 0.00000000 |
| 353 | 1579.45260000 | 18.80840000   | 0.00000000 |
| 354 | 1581.48290000 | 198.43980000  | 0.00000000 |
| 355 | 1584.53910000 | 87.53430000   | 0.00000000 |
| 356 | 1589.80080000 | 9.66300000    | 0.00000000 |
| 357 | 1606.85110000 | 251.81510000  | 0.00000000 |
| 358 | 1611.33760000 | 80.64310000   | 0.00000000 |
| 359 | 1616.92860000 | 39.35350000   | 0.00000000 |
| 360 | 1626.40470000 | 7.90230000    | 0.00000000 |
| 361 | 1627.55580000 | 5.75360000    | 0.00000000 |
| 362 | 1629.10670000 | 19.52720000   | 0.00000000 |
| 363 | 1640.52970000 | 5.71210000    | 0.00000000 |
| 364 | 1649.74900000 | 356.11820000  | 0.00000000 |
| 365 | 1652.90190000 | 66.84810000   | 0.00000000 |
| 366 | 1656.20500000 | 137.62560000  | 0.00000000 |
| 367 | 1656.77050000 | 111.88390000  | 0.00000000 |
| 368 | 1660.87490000 | 47.20040000   | 0.00000000 |
| 369 | 1669.45240000 | 120.01830000  | 0.00000000 |
| 370 | 1709.51470000 | 62.96740000   | 0.00000000 |
| 371 | 1958.35070000 | 2248.12560000 | 0.00000000 |
| 372 | 1972.48810000 | 2376.54620000 | 0.00000000 |
| 373 | 2082.78330000 | 2122.30180000 | 0.00000000 |
| 374 | 3010.14210000 | 27.38130000   | 0.00000000 |
| 375 | 3015.20590000 | 19.89780000   | 0.00000000 |
| 376 | 3021.72610000 | 37.71360000   | 0.00000000 |
| 377 | 3032.81300000 | 22.46050000   | 0.00000000 |
| 378 | 3034.10140000 | 55.83990000   | 0.00000000 |
| 379 | 3045.03600000 | 32.13930000   | 0.00000000 |
| 380 | 3060.99460000 | 71.34780000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 3071.14580000 | 20.60840000   | 0.00000000 |
| 382 | 3076.99590000 | 78.52670000   | 0.00000000 |
| 383 | 3085.63140000 | 76.04870000   | 0.00000000 |
| 384 | 3178.24980000 | 0.12160000    | 0.00000000 |
| 385 | 3184.47230000 | 4.51080000    | 0.00000000 |
| 386 | 3184.55880000 | 9.70250000    | 0.00000000 |
| 387 | 3192.91470000 | 25.74620000   | 0.00000000 |
| 388 | 3193.40070000 | 5.88190000    | 0.00000000 |
| 389 | 3195.79340000 | 18.49420000   | 0.00000000 |
| 390 | 3196.18360000 | 3.55920000    | 0.00000000 |
| 391 | 3198.42030000 | 2.54280000    | 0.00000000 |
| 392 | 3203.12360000 | 64.83310000   | 0.00000000 |
| 393 | 3207.47930000 | 20.38620000   | 0.00000000 |
| 394 | 3208.96000000 | 7.60380000    | 0.00000000 |
| 395 | 3210.40160000 | 13.73950000   | 0.00000000 |
| 396 | 3211.77940000 | 0.62410000    | 0.00000000 |
| 397 | 3215.28710000 | 52.26180000   | 0.00000000 |
| 398 | 3215.53470000 | 1.80930000    | 0.00000000 |
| 399 | 3219.12390000 | 24.62650000   | 0.00000000 |
| 400 | 3223.48580000 | 7.65440000    | 0.00000000 |
| 401 | 3224.14450000 | 1.70570000    | 0.00000000 |
| 402 | 3226.21430000 | 6.12760000    | 0.00000000 |
| 403 | 3228.27400000 | 8.65140000    | 0.00000000 |
| 404 | 3228.92960000 | 3.33590000    | 0.00000000 |
| 405 | 3229.71920000 | 6.03730000    | 0.00000000 |
| 406 | 3230.22080000 | 2.27690000    | 0.00000000 |
| 407 | 3241.63820000 | 7.35620000    | 0.00000000 |
| 408 | 3242.33790000 | 0.90380000    | 0.00000000 |
| 409 | 3250.59700000 | 3.91960000    | 0.00000000 |
| 410 | 3253.37260000 | 0.69970000    | 0.00000000 |
| 411 | 3260.04310000 | 12.72740000   | 0.00000000 |
| 412 | 3262.11520000 | 34.55800000   | 0.00000000 |
| 413 | 3263.90360000 | 1.03610000    | 0.00000000 |
| 414 | 3266.00210000 | 0.71750000    | 0.00000000 |
| 415 | 3268.14050000 | 0.84060000    | 0.00000000 |
| 416 | 3271.57250000 | 12.96560000   | 0.00000000 |
| 417 | 3272.46570000 | 36.25240000   | 0.00000000 |
| 418 | 3276.37410000 | 13.69410000   | 0.00000000 |
| 419 | 3288.17060000 | 9.59740000    | 0.00000000 |
| 420 | 3288.76410000 | 6.33210000    | 0.00000000 |
| 421 | 3289.80720000 | 8.81590000    | 0.00000000 |
| 422 | 3301.51450000 | 1191.50200000 | 0.00000000 |
| 423 | 3377.49750000 | 1509.68830000 | 0.00000000 |
| 424 | 3544.86670000 | 1592.35840000 | 0.00000000 |
| 425 | 3576.36710000 | 438.88510000  | 0.00000000 |
| 426 | 3617.44360000 | 647.09920000  | 0.00000000 |
| 427 | 3853.01970000 | 113.00670000  | 0.00000000 |
| 428 | 3857.44970000 | 96.94030000   | 0.00000000 |
| 429 | 3861.15480000 | 75.58180000   | 0.00000000 |

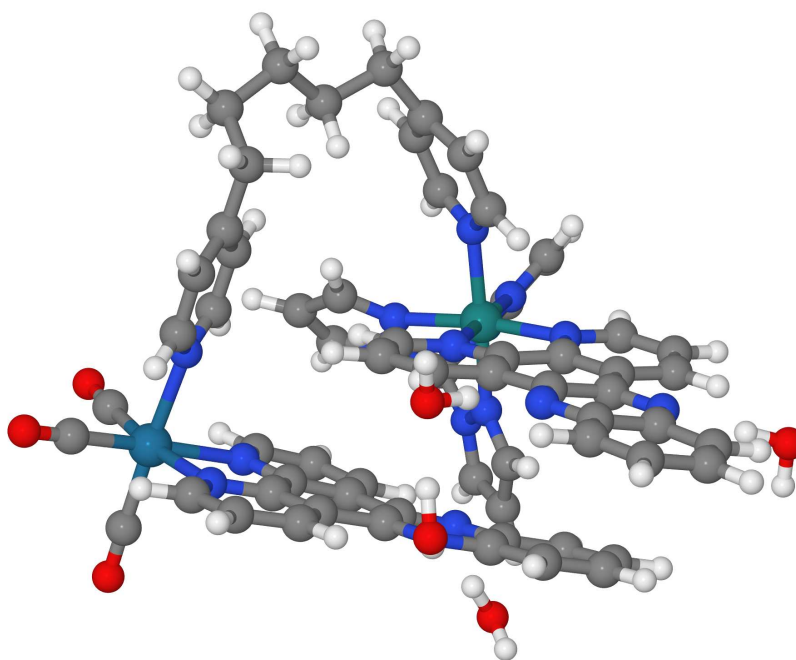
**S17. CALCULATIONS ON ALTERNATIVE CONFORMER OF  $1w^{3+}$  ( $^1A$ )**


FIG. S27. Molecule

Route : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric  
 : aldispersion=gd3bj int=ultrafine pop=regular  
 SMILES : c1ccc2c(c1)nc3c4ccc[n+](c3n2)ccc[n+](c4)[Ru]578(n9ccc[n+](c9C([n+]  
 1n7ccc1)[n+](c1n8ccc1)[n+](c1ccc(cc1)CCCCC1cc[n+](c1)[Re]  
 1([n+](c2ccc3c2c2[n+](c1ccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O].O.O.O.O  
 Formula :  $C_{64}H_{56}N_{16}O_7ReRu^{3+}$   
 Charge : 3  
 Multiplicity : 1  
 Energy : -4049.75809674 a.u.

**S17.1. Cartesian Co-ordinates (XYZ format)**

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|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.05469100 | 3.90782189  | 5.55381584  |
| H | -0.23334500 | 4.92780876  | 5.90118980  |
| H | 0.40503499  | 3.34420991  | 6.36946821  |
| C | -1.38131201 | 3.23558688  | 5.13259888  |
| H | -1.12005699 | 2.34073091  | 4.55936289  |
| H | -1.90312004 | 3.90002394  | 4.43500519  |
| C | -2.32449198 | 2.84091592  | 6.26558113  |
| H | -2.69322109 | 3.73549104  | 6.77692509  |
| H | -1.78050494 | 2.25123191  | 7.01249790  |
| C | -3.10242891 | 0.63605797  | 5.17371511  |
| H | -3.45978904 | -0.15524100 | 5.83394384  |
| H | -2.01002502 | 0.55041301  | 5.17396593  |
| C | 1.38764203  | 4.60314512  | -2.66757989 |
| N | 2.41736007  | 5.26957321  | -1.89750695 |
| N | 1.85698700  | 3.32490897  | -3.14917302 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.18734300  | 4.44140720  | -1.87147701 |
| N | 2.89000201  | 4.68032503  | -0.76614797 |
| C | 2.98029804  | 6.49336195  | -2.08881593 |
| N | 2.21200800  | 2.36902595  | -2.25167203 |
| C | 2.06896806  | 2.90616012  | -4.42741585 |
| N | 0.24650501  | 3.75894904  | -0.69524097 |
| C | -1.04861498 | 4.97085285  | -2.07780409 |
| C | 3.75986600  | 5.54195309  | -0.24041800 |
| C | 3.85179305  | 6.69559383  | -1.04169798 |
| H | 2.72151709  | 7.10171223  | -2.93901205 |
| C | 2.65644908  | 1.33950305  | -2.96923804 |
| C | 2.58134890  | 1.63026404  | -4.34508419 |
| H | 1.83536994  | 3.53755999  | -5.26820803 |
| C | -0.96853799 | 3.86769390  | -0.15553300 |
| C | -1.81845701 | 4.61187220  | -0.99314201 |
| H | -1.27090895 | 5.54574680  | -2.96112704 |
| N | -3.21283388 | -0.18866000 | -1.68467700 |
| N | -3.96055198 | -2.55292702 | -0.66491097 |
| H | 4.26760483  | 5.30146122  | 0.67914999  |
| H | 4.47371197  | 7.55785084  | -0.87457901 |
| H | 2.99281502  | 0.44519600  | -2.47473407 |
| H | 2.82651901  | 0.96102500  | -5.15055513 |
| H | -1.17605603 | 3.43701601  | 0.80875599  |
| H | -2.85266304 | 4.85508108  | -0.82211900 |
| C | -2.90064502 | 0.97866899  | -2.25968909 |
| C | -2.26663089 | -1.16198504 | -1.62142003 |
| C | -2.65637994 | -2.42179608 | -1.02253401 |
| C | -4.37056684 | -3.71244502 | -0.13980800 |
| C | -1.64078605 | 1.22940505  | -2.79940510 |
| H | -3.67936397 | 1.72690904  | -2.29513407 |
| C | -0.97081202 | -0.97450298 | -2.12083793 |
| C | -1.72129095 | -3.45071912 | -0.83433598 |
| C | -3.49867702 | -4.77316093 | 0.09185400  |
| H | -5.42088985 | -3.79137397 | 0.10207700  |
| C | -0.66874301 | 0.25068000  | -2.73080206 |
| H | -1.44605100 | 2.18554807  | -3.26390696 |
| C | 0.02059800  | -2.03160906 | -1.94412601 |
| C | -2.16459894 | -4.64374924 | -0.24275300 |
| C | -0.33843499 | -3.24240899 | -1.26236701 |
| H | -3.87815690 | -5.68403482 | 0.53349102  |
| H | 0.32045701  | 0.41889599  | -3.12741590 |
| N | 1.25367796  | -1.83270395 | -2.38503194 |
| H | -1.47234905 | -5.45116282 | -0.04934900 |
| N | 0.56433702  | -4.18265104 | -1.02585995 |
| C | 2.18815207  | -2.77251410 | -2.12576509 |
| C | 1.83669198  | -3.97112298 | -1.42167199 |
| C | 3.53197503  | -2.57014298 | -2.53150392 |
| C | 2.84033394  | -4.93392801 | -1.14189196 |
| C | 4.48149014  | -3.50944400 | -2.22519302 |
| H | 3.77632403  | -1.67556500 | -3.08635402 |
| C | 4.13261986  | -4.69843578 | -1.53103602 |
| H | 2.56560397  | -5.82931805 | -0.60022599 |
| H | 5.51305914  | -3.34758592 | -2.51060796 |
| H | 4.90407324  | -5.42237711 | -1.30241501 |
| N | 3.84126401  | 1.76091397  | 0.03415000  |
| N | 1.34419000  | 0.96750998  | 0.36480200  |
| C | 5.07750988  | 2.18924689  | -0.23700400 |
| C | 3.66685796  | 0.45590901  | 0.38339001  |
| C | 2.30586004  | 0.03875700  | 0.62156999  |
| C | 0.07252000  | 0.65258998  | 0.62566900  |
| C | 6.18451691  | 1.34521496  | -0.16664501 |
| H | 5.17586184  | 3.22518706  | -0.52601200 |
| C | 4.73311806  | -0.44460601 | 0.50570703  |
| C | 2.01073289  | -1.24208903 | 1.11325896  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.29538199 | -0.57852900 | 1.16095495  |
| H  | -0.66645902 | 1.40393400  | 0.40105900  |
| C  | 6.02256489  | 0.02408100  | 0.20865400  |
| H  | 7.16324186  | 1.73884904  | -0.40400600 |
| C  | 4.45100594  | -1.80755401 | 0.95559400  |
| C  | 0.66919500  | -1.54029799 | 1.39849699  |
| C  | 3.10969591  | -2.18799400 | 1.30733705  |
| H  | -1.33515596 | -0.77008301 | 1.38332200  |
| H  | 6.87694407  | -0.63575602 | 0.26434201  |
| N  | 5.44911718  | -2.67149711 | 1.05923402  |
| H  | 0.38658601  | -2.50274611 | 1.79959297  |
| N  | 2.85015512  | -3.39697790 | 1.78583705  |
| C  | 5.19211006  | -3.91393805 | 1.51617205  |
| C  | 3.86251593  | -4.28201723 | 1.90432703  |
| C  | 6.23614597  | -4.87111282 | 1.59719002  |
| C  | 3.61296105  | -5.59843016 | 2.36940503  |
| C  | 5.95945597  | -6.13594103 | 2.04547405  |
| H  | 7.23135185  | -4.57846403 | 1.28808105  |
| C  | 4.64256001  | -6.50025320 | 2.43336105  |
| H  | 2.60423708  | -5.87334681 | 2.64401603  |
| H  | 6.75068712  | -6.87265396 | 2.10382009  |
| H  | 4.45312214  | -7.50896692 | 2.77806711  |
| H  | 1.14536595  | 5.22393322  | -3.52321196 |
| C  | 0.82669502  | 3.88280392  | 4.33918905  |
| C  | 1.63319194  | 2.77387309  | 4.06979990  |
| C  | 0.71742201  | 4.84252977  | 3.33073807  |
| C  | 2.14438009  | 2.58773494  | 2.80022907  |
| H  | 1.80776799  | 2.01778007  | 4.82478523  |
| C  | 1.25522196  | 4.58956718  | 2.08127904  |
| H  | 0.15382101  | 5.75362206  | 3.48738003  |
| N  | 1.89413404  | 3.43888903  | 1.78518796  |
| H  | 2.72848392  | 1.70985794  | 2.56969309  |
| H  | 1.12502897  | 5.28789520  | 1.26801002  |
| C  | -3.56581998 | 0.33723199  | 3.77195692  |
| C  | -4.18689299 | -0.87386000 | 3.46129489  |
| C  | -3.37637997 | 1.23090005  | 2.71025705  |
| C  | -4.59120512 | -1.13800704 | 2.16510892  |
| H  | -4.36705112 | -1.61604500 | 4.22806311  |
| C  | -3.80765295 | 0.90130401  | 1.43735099  |
| H  | -2.90080094 | 2.18983507  | 2.86346197  |
| N  | -4.41539621 | -0.26841700 | 1.15149295  |
| H  | -5.08163118 | -2.07065606 | 1.92870402  |
| H  | -3.67277694 | 1.58881497  | 0.61408901  |
| C  | -3.51326704 | 2.02447605  | 5.73592710  |
| H  | -4.02506781 | 2.60581303  | 4.96317482  |
| H  | -4.24283409 | 1.87763500  | 6.53504801  |
| Re | -5.20559502 | -0.74256802 | -0.90069002 |
| Ru | 2.08083200  | 2.83445597  | -0.22616000 |
| C  | -5.80249214 | -1.22304797 | -2.68714309 |
| O  | -6.14678621 | -1.51270103 | -3.74674702 |
| C  | -6.04008722 | 1.00215697  | -1.06290102 |
| O  | -6.50446415 | 2.05297804  | -1.15717196 |
| C  | -6.85530806 | -1.43970299 | -0.15328200 |
| O  | -7.82581186 | -1.87510204 | 0.29086399  |
| H  | 7.24464893  | -2.58705306 | 0.38550699  |
| O  | 8.16383457  | -2.54762006 | 0.06178900  |
| H  | 8.08525944  | -2.71925497 | -0.88304800 |
| H  | 1.24728799  | -4.15329790 | 2.43913507  |
| O  | 0.39762801  | -4.59247017 | 2.65228105  |
| H  | 0.34928399  | -4.61932707 | 3.61401796  |
| H  | 0.45998999  | -5.91449308 | 0.00031300  |
| O  | 0.36714700  | -6.58627415 | 0.69453502  |
| H  | 0.32910401  | -6.03481817 | 1.49785197  |
| H  | 1.71291006  | -1.32423604 | -4.34975910 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 2.16801095 | -1.27621400 | -5.20380116 |
| H | 2.39042497 | -2.19255900 | -5.40029192 |

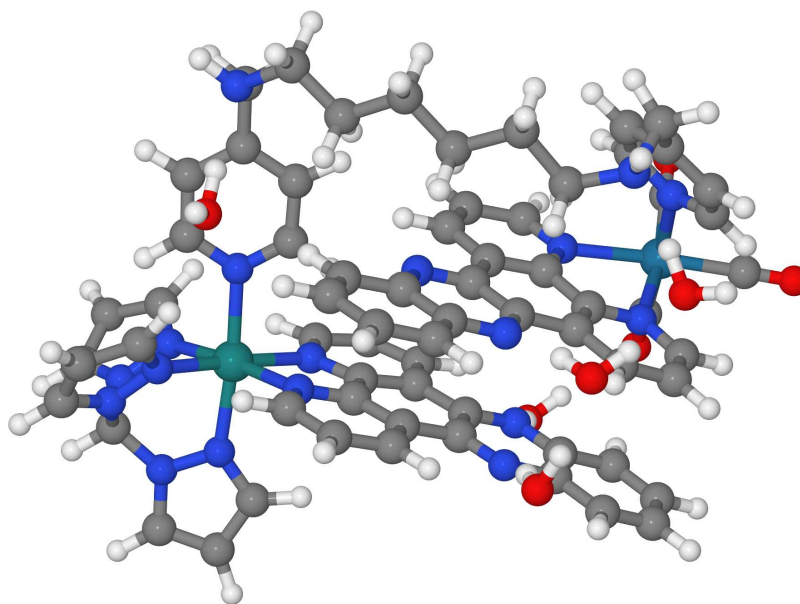
S18. CALCULATIONS ON  $2\mathbf{w}^{3+}$  ( $^1\mathbf{A}$ )

FIG. S28. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](6[Ru]578(n9ccc[n+](9C([n+](n7ccc1)[n+](1n8ccc1)[n+](1ccc(cc1)CNCCCCCNCCc1cc[n+](cc1)[Re]1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C]([O])([C]([O])([C]([O].O.O.O.O.O
Formula    : C67H66N18O8ReRu3+
Charge     : 3
Multiplicity : 1
Energy     : -4354.97649559
Gibbs Energy : -4353.82290300
Number of imaginary frequencies : 1

```

a.u.  
a.u.

## S18.1. Cartesian Co-ordinates (XYZ format)

161

```

C  2.71265697  4.64000416  0.86645699
H  2.25364709  4.51161814  1.85025704
H  2.68817592  3.65936208  0.38195100
C  1.89155805  5.64126396  0.04685300
H  2.35361099  5.79844618 -0.93294299
H  1.88957405  6.61187315  0.55602902
C  0.46053499  5.14248800 -0.15413500
H -0.02170100  5.01412296  0.82115602
H  0.50298899  4.14616394 -0.60855597
C -0.41800100  6.03347588 -1.03798401
H  0.10537500  6.23600388 -1.98028004
H -0.57858801  7.00374317 -0.55405003
C -2.65602803  6.09860277 -2.31610703
H -2.08300805  6.38396502 -3.21098709
H -3.02187490  7.02148914 -1.85851097

```

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 4.12852478  | 4.98306894  | 1.09359002  |
| C  | -3.57118511 | 4.22579813  | -3.68306899 |
| H  | -2.54775000 | 4.30569983  | -4.05987310 |
| H  | -4.24344778 | 4.34910679  | -4.53405285 |
| N  | -3.83829188 | 5.29110718  | -2.68363690 |
| C  | 4.96078300  | 5.00824022  | -0.12555300 |
| H  | 4.52666807  | 5.62260580  | -0.92116898 |
| H  | 5.92020082  | 5.45300722  | 0.14469200  |
| C  | -7.48584318 | -2.21979594 | 0.15574200  |
| N  | -7.14918423 | -2.34745598 | -1.24955595 |
| N  | -6.55925083 | -2.96901608 | 0.97401798  |
| N  | -7.50666094 | -0.82251197 | 0.54098499  |
| N  | -5.95335579 | -1.87866604 | -1.70203400 |
| C  | -7.92213488 | -2.79839993 | -2.27431607 |
| N  | -5.23858309 | -2.65125489 | 0.95250797  |
| C  | -6.80262613 | -4.01698399 | 1.80712795  |
| N  | -6.37759495 | -0.08051100 | 0.38703501  |
| C  | -8.55901241 | -0.04396800 | 0.91368598  |
| Ru | -4.66019487 | -1.05899096 | -0.27413300 |
| C  | -5.97714186 | -2.03973007 | -3.02468109 |
| C  | -7.19375086 | -2.61963797 | -3.42910600 |
| H  | -8.90447426 | -3.20296788 | -2.09800506 |
| C  | -4.64272881 | -3.50529790 | 1.78234303  |
| C  | -5.58865499 | -4.38394785 | 2.34382296  |
| H  | -7.79847097 | -4.40453005 | 1.94266605  |
| C  | -6.71782017 | 1.17850006  | 0.66823399  |
| C  | -8.08187485 | 1.24430299  | 1.01268697  |
| H  | -9.53706455 | -0.46435499 | 1.07615602  |
| N  | -2.86670399 | -2.01168489 | -0.79802501 |
| N  | -3.39194012 | -0.45551300 | 1.27500904  |
| H  | -5.14027977 | -1.72280300 | -3.62469697 |
| H  | -7.49513388 | -2.87180901 | -4.43098879 |
| H  | -3.57844806 | -3.45906210 | 1.94203496  |
| H  | -5.40455198 | -5.17870522 | 3.04576397  |
| H  | -5.99471188 | 1.97684801  | 0.57757503  |
| H  | -8.64056873 | 2.12035894  | 1.29338002  |
| C  | -2.62382007 | -2.73550701 | -1.89408505 |
| C  | -1.87091899 | -1.88080096 | 0.12410900  |
| C  | -2.17209005 | -1.06020701 | 1.27313900  |
| C  | -3.73211503 | 0.28296101  | 2.33590293  |
| C  | -1.39237404 | -3.34659600 | -2.12583089 |
| H  | -3.43729591 | -2.83559895 | -2.59642506 |
| C  | -0.62866598 | -2.52003598 | -0.00675800 |
| C  | -1.26526403 | -0.93620700 | 2.33510494  |
| C  | -2.88613796 | 0.44845501  | 3.43158603  |
| H  | -4.70845509 | 0.74246597  | 2.31128001  |
| C  | -0.38891801 | -3.25210810 | -1.17969203 |
| H  | -1.24413705 | -3.90653396 | -3.03881001 |
| C  | 0.32473901  | -2.43734407 | 1.10104096  |
| C  | -1.64588499 | -0.16070101 | 3.44096208  |
| C  | 0.00204400  | -1.66071498 | 2.26723790  |
| H  | -3.21174693 | 1.05940902  | 4.26129007  |
| H  | 0.55378598  | -3.75898004 | -1.32875705 |
| N  | 1.46059406  | -3.11940908 | 1.03439903  |
| H  | -0.97697699 | -0.04189800 | 4.28187799  |
| N  | 0.82194698  | -1.61402500 | 3.30756688  |
| C  | 2.28746295  | -3.10821295 | 2.10214996  |
| C  | 1.95065999  | -2.35231304 | 3.27373695  |
| C  | 3.49176502  | -3.85787606 | 2.08334994  |
| C  | 2.80951190  | -2.38775802 | 4.40244389  |
| C  | 4.29546595  | -3.87864709 | 3.19374108  |
| H  | 3.74311209  | -4.42008114 | 1.19442999  |
| C  | 3.94961691  | -3.14637995 | 4.36021280  |
| H  | 2.54069304  | -1.79785895 | 5.26943302  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 5.20982981  | -4.45810509 | 3.18397593  |
| H  | 4.60602188  | -3.18171096 | 5.22033119  |
| N  | 4.46607304  | -0.93973899 | 0.36805701  |
| N  | 3.12377000  | -0.90110201 | -1.96867096 |
| C  | 5.15775204  | -0.99094099 | 1.51086700  |
| C  | 3.28299499  | -0.27406001 | 0.34128299  |
| C  | 2.53585291  | -0.30060500 | -0.90193498 |
| C  | 2.43365788  | -1.02772701 | -3.10691404 |
| C  | 4.73986101  | -0.32464099 | 2.65812612  |
| H  | 6.07625389  | -1.55977595 | 1.49507999  |
| C  | 2.79345608  | 0.41540900  | 1.45869505  |
| C  | 1.25827599  | 0.26789200  | -0.98256803 |
| C  | 1.14034498  | -0.52810502 | -3.24834299 |
| H  | 2.93542099  | -1.52617705 | -3.92399502 |
| C  | 3.56478095  | 0.39839000  | 2.62972689  |
| H  | 5.34036922  | -0.37665501 | 3.55426598  |
| C  | 1.51018798  | 1.10657203  | 1.36142504  |
| C  | 0.56080401  | 0.14566401  | -2.19186306 |
| C  | 0.72312403  | 0.98849499  | 0.16966300  |
| H  | 0.61964703  | -0.65422702 | -4.18694210 |
| H  | 3.23875809  | 0.93836099  | 3.50358200  |
| N  | 1.07672298  | 1.82344902  | 2.38620591  |
| H  | -0.42197600 | 0.57754600  | -2.28610802 |
| N  | -0.47487399 | 1.54305696  | 0.07741200  |
| C  | -0.12884100 | 2.42341590  | 2.29915905  |
| C  | -0.93636900 | 2.25853395  | 1.12434399  |
| C  | -0.60137802 | 3.21710396  | 3.37444210  |
| C  | -2.21024609 | 2.87658000  | 1.07254505  |
| C  | -1.83273101 | 3.81245995  | 3.28209901  |
| H  | 0.02533800  | 3.33621812  | 4.24828291  |
| C  | -2.63858700 | 3.63752699  | 2.12856507  |
| H  | -2.83268595 | 2.76515388  | 0.19841400  |
| H  | -2.19998288 | 4.42073202  | 4.09901714  |
| H  | -3.60824490 | 4.11292505  | 2.07328105  |
| H  | -8.47840214 | -2.63124204 | 0.30521500  |
| C  | 5.19481993  | 3.60854411  | -0.64114398 |
| C  | 4.55112410  | 3.12191391  | -1.77761900 |
| C  | 6.05889893  | 2.74014091  | 0.02898500  |
| C  | 4.73360014  | 1.80003595  | -2.16000795 |
| H  | 3.88793206  | 3.75214601  | -2.35579491 |
| C  | 6.20570898  | 1.44238698  | -0.42065099 |
| H  | 6.59696198  | 3.06001711  | 0.91066599  |
| N  | 5.52550316  | 0.95524198  | -1.47843599 |
| H  | 4.21647882  | 1.39709699  | -3.01982498 |
| H  | 6.86535215  | 0.75661302  | 0.09152600  |
| C  | -3.79029298 | 2.86419606  | -3.06515503 |
| C  | -2.75023293 | 2.14509201  | -2.48099589 |
| C  | -5.07224798 | 2.32663989  | -2.95097303 |
| C  | -3.02747107 | 1.01424205  | -1.73635101 |
| H  | -1.72656703 | 2.48617411  | -2.55075407 |
| C  | -5.27611780 | 1.17668700  | -2.21107101 |
| H  | -5.92381191 | 2.81930208  | -3.40259504 |
| N  | -4.27355814 | 0.54292202  | -1.56604898 |
| H  | -2.24163294 | 0.50170797  | -1.20903301 |
| H  | -6.26410103 | 0.75924802  | -2.09441090 |
| Re | 5.31471682  | -1.42319202 | -1.68071604 |
| C  | 4.98476791  | -3.31317806 | -1.66208899 |
| O  | 4.77571678  | -4.45076895 | -1.63831699 |
| C  | 5.82999897  | -1.49766600 | -3.55002189 |
| O  | 6.10742998  | -1.51520395 | -4.66719818 |
| C  | 7.16345501  | -1.72858906 | -1.17779100 |
| O  | 8.25383282  | -1.90740097 | -0.85282099 |
| H  | -4.55145597 | 5.90743780  | -3.05382800 |
| C  | -1.75532603 | 5.35422087  | -1.33642697 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.31001997 | 5.18479681  | -0.41108200 |
| H | -1.53661895 | 4.36467218  | -1.74272501 |
| H | 4.18125296  | 5.89924288  | 1.53048098  |
| H | 4.63485289  | 3.89043999  | 2.46329999  |
| O | 4.82047081  | 3.28788209  | 3.23011398  |
| H | 5.61089516  | 3.64631701  | 3.64723802  |
| H | -4.58730221 | 4.49008989  | -1.08904195 |
| O | -4.93964100 | 4.06434822  | -0.27340800 |
| H | -5.17856121 | 4.80405283  | 0.29440200  |
| H | 2.02910900  | 2.52314997  | 3.84959888  |
| O | 2.52221704  | 2.73534989  | 4.66394186  |
| H | 3.40060902  | 3.00262403  | 4.31791782  |
| H | 1.08045197  | -0.15457299 | 4.75651598  |
| O | 1.16547406  | 0.35267299  | 5.57754278  |
| H | 1.71586704  | 1.12418997  | 5.35896301  |
| H | 1.90449798  | -4.65143108 | -0.14063400 |
| O | 2.04467607  | -5.39966488 | -0.74574202 |
| H | 2.90311694  | -5.22518396 | -1.14728403 |

## S18.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -10.95680000 | 0.60670000   | 0.00000000      |
| 2    | 7.03280000   | 0.77970000   | 0.00000000      |
| 3    | 19.63410000  | 1.60680000   | 0.00000000      |
| 4    | 21.98410000  | 1.02870000   | 0.00000000      |
| 5    | 25.93560000  | 0.20340000   | 0.00000000      |
| 6    | 28.32580000  | 1.31150000   | 0.00000000      |
| 7    | 32.84560000  | 2.07250000   | 0.00000000      |
| 8    | 37.99330000  | 0.67160000   | 0.00000000      |
| 9    | 40.36650000  | 5.24000000   | 0.00000000      |
| 10   | 43.23140000  | 0.56510000   | 0.00000000      |
| 11   | 45.34460000  | 2.91500000   | 0.00000000      |
| 12   | 48.19330000  | 0.09110000   | 0.00000000      |
| 13   | 51.75340000  | 1.49990000   | 0.00000000      |
| 14   | 53.96830000  | 4.92270000   | 0.00000000      |
| 15   | 56.03260000  | 0.59430000   | 0.00000000      |
| 16   | 58.15400000  | 12.15070000  | 0.00000000      |
| 17   | 60.51510000  | 7.89150000   | 0.00000000      |
| 18   | 63.98530000  | 0.89490000   | 0.00000000      |
| 19   | 65.36380000  | 0.33980000   | 0.00000000      |
| 20   | 66.17680000  | 9.29500000   | 0.00000000      |
| 21   | 67.92560000  | 2.91120000   | 0.00000000      |
| 22   | 71.95840000  | 0.67850000   | 0.00000000      |
| 23   | 72.81340000  | 1.22970000   | 0.00000000      |
| 24   | 77.59160000  | 1.93370000   | 0.00000000      |
| 25   | 78.36050000  | 1.15610000   | 0.00000000      |
| 26   | 82.02010000  | 2.74080000   | 0.00000000      |
| 27   | 83.45310000  | 0.47300000   | 0.00000000      |
| 28   | 87.22130000  | 2.84540000   | 0.00000000      |
| 29   | 88.87430000  | 1.11860000   | 0.00000000      |
| 30   | 89.83880000  | 7.65100000   | 0.00000000      |
| 31   | 91.28850000  | 2.24550000   | 0.00000000      |
| 32   | 92.51870000  | 4.74340000   | 0.00000000      |
| 33   | 96.09220000  | 8.44000000   | 0.00000000      |
| 34   | 97.81860000  | 3.96350000   | 0.00000000      |
| 35   | 103.99090000 | 5.04350000   | 0.00000000      |
| 36   | 104.29530000 | 44.03290000  | 0.00000000      |
| 37   | 110.89790000 | 4.91600000   | 0.00000000      |
| 38   | 116.59150000 | 0.95720000   | 0.00000000      |
| 39   | 118.12100000 | 3.63180000   | 0.00000000      |
| 40   | 121.10420000 | 2.67870000   | 0.00000000      |
| 41   | 122.13190000 | 1.55850000   | 0.00000000      |
| 42   | 126.10980000 | 3.74570000   | 0.00000000      |
| 43   | 130.62120000 | 2.41530000   | 0.00000000      |
| 44   | 132.35560000 | 0.95990000   | 0.00000000      |
| 45   | 135.21220000 | 18.56830000  | 0.00000000      |
| 46   | 137.37620000 | 3.61790000   | 0.00000000      |
| 47   | 140.27620000 | 1.83180000   | 0.00000000      |
| 48   | 144.05280000 | 0.50390000   | 0.00000000      |
| 49   | 144.92280000 | 3.03980000   | 0.00000000      |
| 50   | 147.97220000 | 4.48700000   | 0.00000000      |
| 51   | 151.72670000 | 0.81880000   | 0.00000000      |
| 52   | 155.04240000 | 3.13830000   | 0.00000000      |
| 53   | 157.46450000 | 6.07400000   | 0.00000000      |
| 54   | 158.48750000 | 18.99530000  | 0.00000000      |
| 55   | 165.70750000 | 0.97240000   | 0.00000000      |
| 56   | 167.34450000 | 1.64430000   | 0.00000000      |
| 57   | 169.38070000 | 16.36600000  | 0.00000000      |
| 58   | 179.06780000 | 2.25840000   | 0.00000000      |
| 59   | 180.71110000 | 0.94860000   | 0.00000000      |
| 60   | 180.98300000 | 8.77650000   | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 182.56810000 | 0.34550000   | 0.00000000 |
| 62  | 183.74360000 | 3.77630000   | 0.00000000 |
| 63  | 188.26930000 | 4.35480000   | 0.00000000 |
| 64  | 191.05660000 | 24.57720000  | 0.00000000 |
| 65  | 191.69830000 | 9.38580000   | 0.00000000 |
| 66  | 195.39960000 | 0.61150000   | 0.00000000 |
| 67  | 197.66690000 | 25.98740000  | 0.00000000 |
| 68  | 198.06490000 | 9.72790000   | 0.00000000 |
| 69  | 202.79160000 | 4.03430000   | 0.00000000 |
| 70  | 209.46320000 | 45.69360000  | 0.00000000 |
| 71  | 211.56310000 | 50.69570000  | 0.00000000 |
| 72  | 215.15610000 | 11.77640000  | 0.00000000 |
| 73  | 226.74920000 | 24.93290000  | 0.00000000 |
| 74  | 235.00510000 | 5.34750000   | 0.00000000 |
| 75  | 242.88580000 | 21.31460000  | 0.00000000 |
| 76  | 243.25650000 | 25.55310000  | 0.00000000 |
| 77  | 252.37190000 | 51.11950000  | 0.00000000 |
| 78  | 256.53610000 | 9.76550000   | 0.00000000 |
| 79  | 260.11880000 | 2.65980000   | 0.00000000 |
| 80  | 262.96770000 | 1.56840000   | 0.00000000 |
| 81  | 277.09680000 | 6.89090000   | 0.00000000 |
| 82  | 278.98190000 | 11.39770000  | 0.00000000 |
| 83  | 296.86890000 | 1.54580000   | 0.00000000 |
| 84  | 303.60750000 | 97.70360000  | 0.00000000 |
| 85  | 304.85450000 | 40.19200000  | 0.00000000 |
| 86  | 317.69770000 | 6.95540000   | 0.00000000 |
| 87  | 320.02970000 | 3.39800000   | 0.00000000 |
| 88  | 329.78520000 | 3.53590000   | 0.00000000 |
| 89  | 331.36690000 | 2.29690000   | 0.00000000 |
| 90  | 334.34750000 | 5.08710000   | 0.00000000 |
| 91  | 335.28160000 | 4.89990000   | 0.00000000 |
| 92  | 340.33000000 | 2.04290000   | 0.00000000 |
| 93  | 340.46370000 | 2.55980000   | 0.00000000 |
| 94  | 343.68800000 | 6.07400000   | 0.00000000 |
| 95  | 347.00280000 | 9.55150000   | 0.00000000 |
| 96  | 358.71180000 | 3.95960000   | 0.00000000 |
| 97  | 364.55600000 | 6.56630000   | 0.00000000 |
| 98  | 370.26880000 | 8.59550000   | 0.00000000 |
| 99  | 378.28790000 | 6.74290000   | 0.00000000 |
| 100 | 381.30190000 | 0.91370000   | 0.00000000 |
| 101 | 386.84790000 | 1.31100000   | 0.00000000 |
| 102 | 390.97980000 | 0.88960000   | 0.00000000 |
| 103 | 394.16300000 | 12.02600000  | 0.00000000 |
| 104 | 394.85220000 | 105.86300000 | 0.00000000 |
| 105 | 403.33940000 | 5.35370000   | 0.00000000 |
| 106 | 404.42380000 | 2.32540000   | 0.00000000 |
| 107 | 405.82230000 | 1.32510000   | 0.00000000 |
| 108 | 408.60510000 | 2.93090000   | 0.00000000 |
| 109 | 417.22980000 | 7.75770000   | 0.00000000 |
| 110 | 419.56170000 | 1.22570000   | 0.00000000 |
| 111 | 439.57230000 | 8.02670000   | 0.00000000 |
| 112 | 441.33450000 | 16.38030000  | 0.00000000 |
| 113 | 446.46390000 | 21.94110000  | 0.00000000 |
| 114 | 450.71170000 | 0.46950000   | 0.00000000 |
| 115 | 471.88650000 | 52.23940000  | 0.00000000 |
| 116 | 472.87550000 | 28.02420000  | 0.00000000 |
| 117 | 475.18940000 | 8.96610000   | 0.00000000 |
| 118 | 476.51280000 | 32.17780000  | 0.00000000 |
| 119 | 481.16120000 | 13.95900000  | 0.00000000 |
| 120 | 484.27040000 | 6.95620000   | 0.00000000 |
| 121 | 485.53730000 | 45.50730000  | 0.00000000 |
| 122 | 488.42880000 | 27.96300000  | 0.00000000 |
| 123 | 496.09680000 | 0.70750000   | 0.00000000 |
| 124 | 501.42900000 | 26.53470000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 504.25520000 | 8.99470000   | 0.00000000 |
| 126 | 506.26240000 | 29.28740000  | 0.00000000 |
| 127 | 506.95370000 | 3.81460000   | 0.00000000 |
| 128 | 508.77110000 | 7.59640000   | 0.00000000 |
| 129 | 512.39410000 | 27.18720000  | 0.00000000 |
| 130 | 515.17420000 | 37.44400000  | 0.00000000 |
| 131 | 525.05940000 | 16.69420000  | 0.00000000 |
| 132 | 527.72210000 | 30.03730000  | 0.00000000 |
| 133 | 531.12790000 | 37.04150000  | 0.00000000 |
| 134 | 551.46980000 | 25.13350000  | 0.00000000 |
| 135 | 554.88160000 | 89.63540000  | 0.00000000 |
| 136 | 559.11180000 | 11.41450000  | 0.00000000 |
| 137 | 560.11220000 | 5.15120000   | 0.00000000 |
| 138 | 565.29920000 | 35.73690000  | 0.00000000 |
| 139 | 574.75670000 | 0.38880000   | 0.00000000 |
| 140 | 576.03130000 | 1.47210000   | 0.00000000 |
| 141 | 577.63770000 | 5.61940000   | 0.00000000 |
| 142 | 579.19410000 | 4.42240000   | 0.00000000 |
| 143 | 594.52560000 | 11.71560000  | 0.00000000 |
| 144 | 597.05720000 | 6.90090000   | 0.00000000 |
| 145 | 598.76000000 | 24.19800000  | 0.00000000 |
| 146 | 605.20700000 | 0.85640000   | 0.00000000 |
| 147 | 607.27000000 | 12.67140000  | 0.00000000 |
| 148 | 615.66790000 | 5.89740000   | 0.00000000 |
| 149 | 617.54040000 | 17.90180000  | 0.00000000 |
| 150 | 622.99370000 | 33.40010000  | 0.00000000 |
| 151 | 630.55060000 | 31.65470000  | 0.00000000 |
| 152 | 631.57330000 | 26.07680000  | 0.00000000 |
| 153 | 636.22260000 | 15.60490000  | 0.00000000 |
| 154 | 646.12560000 | 94.16450000  | 0.00000000 |
| 155 | 647.31920000 | 5.38540000   | 0.00000000 |
| 156 | 651.29830000 | 75.64700000  | 0.00000000 |
| 157 | 653.10250000 | 15.40310000  | 0.00000000 |
| 158 | 657.94640000 | 17.76490000  | 0.00000000 |
| 159 | 658.59670000 | 11.77890000  | 0.00000000 |
| 160 | 660.74900000 | 13.01140000  | 0.00000000 |
| 161 | 667.24920000 | 177.19010000 | 0.00000000 |
| 162 | 677.16770000 | 8.03400000   | 0.00000000 |
| 163 | 677.93050000 | 33.29160000  | 0.00000000 |
| 164 | 682.86890000 | 69.00660000  | 0.00000000 |
| 165 | 684.40920000 | 1.01670000   | 0.00000000 |
| 166 | 685.95730000 | 0.29770000   | 0.00000000 |
| 167 | 686.80360000 | 2.47130000   | 0.00000000 |
| 168 | 689.66530000 | 113.20980000 | 0.00000000 |
| 169 | 724.64290000 | 60.78060000  | 0.00000000 |
| 170 | 735.01300000 | 10.51130000  | 0.00000000 |
| 171 | 735.34910000 | 72.44210000  | 0.00000000 |
| 172 | 740.62430000 | 16.38480000  | 0.00000000 |
| 173 | 742.56170000 | 9.79700000   | 0.00000000 |
| 174 | 746.28320000 | 32.73420000  | 0.00000000 |
| 175 | 747.98370000 | 6.01880000   | 0.00000000 |
| 176 | 749.74410000 | 16.75810000  | 0.00000000 |
| 177 | 752.08360000 | 199.47750000 | 0.00000000 |
| 178 | 753.25500000 | 17.30560000  | 0.00000000 |
| 179 | 755.73130000 | 18.50880000  | 0.00000000 |
| 180 | 758.29800000 | 17.23690000  | 0.00000000 |
| 181 | 759.52750000 | 78.22820000  | 0.00000000 |
| 182 | 761.03130000 | 122.63350000 | 0.00000000 |
| 183 | 763.81880000 | 109.23160000 | 0.00000000 |
| 184 | 765.92860000 | 37.30960000  | 0.00000000 |
| 185 | 771.73790000 | 34.49780000  | 0.00000000 |
| 186 | 784.81070000 | 89.22920000  | 0.00000000 |
| 187 | 785.43370000 | 41.52990000  | 0.00000000 |
| 188 | 787.61630000 | 33.50420000  | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 189 | 788.23260000  | 91.84110000  | 0.00000000 |
| 190 | 794.41450000  | 102.44230000 | 0.00000000 |
| 191 | 795.47380000  | 143.00760000 | 0.00000000 |
| 192 | 797.73660000  | 112.61590000 | 0.00000000 |
| 193 | 804.01640000  | 26.19270000  | 0.00000000 |
| 194 | 815.18970000  | 4.74060000   | 0.00000000 |
| 195 | 815.80240000  | 2.39280000   | 0.00000000 |
| 196 | 818.61820000  | 37.99290000  | 0.00000000 |
| 197 | 819.07030000  | 186.35650000 | 0.00000000 |
| 198 | 819.21640000  | 25.66940000  | 0.00000000 |
| 199 | 823.73520000  | 55.08290000  | 0.00000000 |
| 200 | 829.73370000  | 121.88810000 | 0.00000000 |
| 201 | 835.50560000  | 69.36190000  | 0.00000000 |
| 202 | 836.62760000  | 9.59480000   | 0.00000000 |
| 203 | 841.32420000  | 51.41640000  | 0.00000000 |
| 204 | 853.25800000  | 2.20680000   | 0.00000000 |
| 205 | 858.58370000  | 4.43270000   | 0.00000000 |
| 206 | 865.18070000  | 8.16080000   | 0.00000000 |
| 207 | 869.90220000  | 29.69030000  | 0.00000000 |
| 208 | 871.43690000  | 42.84930000  | 0.00000000 |
| 209 | 874.55300000  | 35.08510000  | 0.00000000 |
| 210 | 876.14060000  | 1.86690000   | 0.00000000 |
| 211 | 877.40040000  | 30.71750000  | 0.00000000 |
| 212 | 882.10250000  | 24.00090000  | 0.00000000 |
| 213 | 882.59950000  | 15.35340000  | 0.00000000 |
| 214 | 887.76650000  | 40.00930000  | 0.00000000 |
| 215 | 895.64680000  | 23.58840000  | 0.00000000 |
| 216 | 899.23570000  | 0.47990000   | 0.00000000 |
| 217 | 899.68840000  | 6.24140000   | 0.00000000 |
| 218 | 902.97840000  | 39.97290000  | 0.00000000 |
| 219 | 915.86150000  | 145.04190000 | 0.00000000 |
| 220 | 916.68870000  | 3.80040000   | 0.00000000 |
| 221 | 918.79030000  | 3.46130000   | 0.00000000 |
| 222 | 921.69830000  | 0.39370000   | 0.00000000 |
| 223 | 930.80030000  | 6.14400000   | 0.00000000 |
| 224 | 936.21760000  | 37.53570000  | 0.00000000 |
| 225 | 939.53770000  | 7.02680000   | 0.00000000 |
| 226 | 947.48840000  | 0.05230000   | 0.00000000 |
| 227 | 948.95360000  | 2.32580000   | 0.00000000 |
| 228 | 953.57500000  | 1.02270000   | 0.00000000 |
| 229 | 966.31920000  | 11.16270000  | 0.00000000 |
| 230 | 978.52030000  | 3.63860000   | 0.00000000 |
| 231 | 979.10580000  | 1.11810000   | 0.00000000 |
| 232 | 985.36930000  | 1.01900000   | 0.00000000 |
| 233 | 985.62370000  | 12.15790000  | 0.00000000 |
| 234 | 987.77620000  | 7.90800000   | 0.00000000 |
| 235 | 988.82030000  | 5.90550000   | 0.00000000 |
| 236 | 990.49670000  | 1.11330000   | 0.00000000 |
| 237 | 991.82340000  | 1.92850000   | 0.00000000 |
| 238 | 1001.87950000 | 7.80160000   | 0.00000000 |
| 239 | 1002.34280000 | 0.94810000   | 0.00000000 |
| 240 | 1003.93750000 | 0.60960000   | 0.00000000 |
| 241 | 1004.51060000 | 1.31090000   | 0.00000000 |
| 242 | 1006.67710000 | 3.18290000   | 0.00000000 |
| 243 | 1007.95030000 | 0.53560000   | 0.00000000 |
| 244 | 1009.94820000 | 16.41760000  | 0.00000000 |
| 245 | 1012.07190000 | 20.19220000  | 0.00000000 |
| 246 | 1015.09390000 | 11.04180000  | 0.00000000 |
| 247 | 1016.62420000 | 9.02560000   | 0.00000000 |
| 248 | 1019.65530000 | 1.53530000   | 0.00000000 |
| 249 | 1026.01200000 | 0.87100000   | 0.00000000 |
| 250 | 1026.43810000 | 1.44780000   | 0.00000000 |
| 251 | 1027.23110000 | 14.29660000  | 0.00000000 |
| 252 | 1028.47830000 | 0.26690000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1031.68590000 | 0.80010000   | 0.00000000 |
| 254 | 1033.28650000 | 0.67930000   | 0.00000000 |
| 255 | 1037.58820000 | 0.46080000   | 0.00000000 |
| 256 | 1038.01890000 | 0.21160000   | 0.00000000 |
| 257 | 1047.29460000 | 8.55810000   | 0.00000000 |
| 258 | 1059.00430000 | 0.03350000   | 0.00000000 |
| 259 | 1064.14090000 | 47.81840000  | 0.00000000 |
| 260 | 1065.23430000 | 34.16490000  | 0.00000000 |
| 261 | 1072.14790000 | 1.01770000   | 0.00000000 |
| 262 | 1072.56230000 | 4.62970000   | 0.00000000 |
| 263 | 1072.83440000 | 57.56760000  | 0.00000000 |
| 264 | 1074.06580000 | 3.34470000   | 0.00000000 |
| 265 | 1074.65380000 | 51.54610000  | 0.00000000 |
| 266 | 1077.83650000 | 18.87180000  | 0.00000000 |
| 267 | 1089.77820000 | 6.92810000   | 0.00000000 |
| 268 | 1092.32990000 | 3.75490000   | 0.00000000 |
| 269 | 1096.32900000 | 6.87660000   | 0.00000000 |
| 270 | 1104.40560000 | 50.15590000  | 0.00000000 |
| 271 | 1107.34140000 | 44.62570000  | 0.00000000 |
| 272 | 1115.82660000 | 26.01050000  | 0.00000000 |
| 273 | 1118.53120000 | 109.35940000 | 0.00000000 |
| 274 | 1120.52090000 | 66.45650000  | 0.00000000 |
| 275 | 1122.68360000 | 70.40270000  | 0.00000000 |
| 276 | 1123.57040000 | 24.69520000  | 0.00000000 |
| 277 | 1123.79310000 | 8.94100000   | 0.00000000 |
| 278 | 1132.98250000 | 5.59990000   | 0.00000000 |
| 279 | 1133.69310000 | 23.55560000  | 0.00000000 |
| 280 | 1138.83180000 | 2.75650000   | 0.00000000 |
| 281 | 1141.51930000 | 36.43510000  | 0.00000000 |
| 282 | 1144.91040000 | 5.70010000   | 0.00000000 |
| 283 | 1147.27800000 | 25.40750000  | 0.00000000 |
| 284 | 1159.10040000 | 7.64330000   | 0.00000000 |
| 285 | 1163.36370000 | 1.77420000   | 0.00000000 |
| 286 | 1167.05960000 | 18.02610000  | 0.00000000 |
| 287 | 1169.90980000 | 19.90430000  | 0.00000000 |
| 288 | 1173.90650000 | 12.83960000  | 0.00000000 |
| 289 | 1177.37120000 | 2.61570000   | 0.00000000 |
| 290 | 1180.14090000 | 5.70000000   | 0.00000000 |
| 291 | 1198.43200000 | 1.35100000   | 0.00000000 |
| 292 | 1213.28030000 | 1.50640000   | 0.00000000 |
| 293 | 1216.39000000 | 2.13230000   | 0.00000000 |
| 294 | 1223.09900000 | 16.11820000  | 0.00000000 |
| 295 | 1224.22210000 | 3.23610000   | 0.00000000 |
| 296 | 1236.98520000 | 9.50140000   | 0.00000000 |
| 297 | 1238.81940000 | 3.35020000   | 0.00000000 |
| 298 | 1240.71320000 | 0.66900000   | 0.00000000 |
| 299 | 1245.52610000 | 2.54990000   | 0.00000000 |
| 300 | 1246.08320000 | 4.66040000   | 0.00000000 |
| 301 | 1251.12800000 | 0.25620000   | 0.00000000 |
| 302 | 1253.74540000 | 13.73250000  | 0.00000000 |
| 303 | 1259.11110000 | 65.10590000  | 0.00000000 |
| 304 | 1260.12870000 | 8.03630000   | 0.00000000 |
| 305 | 1263.52330000 | 2.20620000   | 0.00000000 |
| 306 | 1269.61980000 | 89.72670000  | 0.00000000 |
| 307 | 1270.50930000 | 2.25650000   | 0.00000000 |
| 308 | 1275.25110000 | 52.22460000  | 0.00000000 |
| 309 | 1275.60320000 | 50.18480000  | 0.00000000 |
| 310 | 1276.70120000 | 9.22370000   | 0.00000000 |
| 311 | 1280.39290000 | 4.47660000   | 0.00000000 |
| 312 | 1281.45590000 | 10.15160000  | 0.00000000 |
| 313 | 1303.39950000 | 0.80170000   | 0.00000000 |
| 314 | 1303.60400000 | 1.06530000   | 0.00000000 |
| 315 | 1305.58840000 | 5.57380000   | 0.00000000 |
| 316 | 1307.16370000 | 3.24870000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 317 | 1309.10910000 | 11.97490000  | 0.00000000 |
| 318 | 1310.43920000 | 16.63800000  | 0.00000000 |
| 319 | 1317.28240000 | 60.25660000  | 0.00000000 |
| 320 | 1319.44340000 | 49.98080000  | 0.00000000 |
| 321 | 1321.61950000 | 7.72180000   | 0.00000000 |
| 322 | 1322.22540000 | 96.09180000  | 0.00000000 |
| 323 | 1326.24160000 | 0.91270000   | 0.00000000 |
| 324 | 1336.11860000 | 1.50340000   | 0.00000000 |
| 325 | 1337.42560000 | 1.18560000   | 0.00000000 |
| 326 | 1337.85680000 | 1.23520000   | 0.00000000 |
| 327 | 1339.34830000 | 2.77710000   | 0.00000000 |
| 328 | 1350.12390000 | 10.02770000  | 0.00000000 |
| 329 | 1350.49590000 | 7.57690000   | 0.00000000 |
| 330 | 1350.61190000 | 0.40020000   | 0.00000000 |
| 331 | 1357.45850000 | 12.95120000  | 0.00000000 |
| 332 | 1370.54090000 | 203.18380000 | 0.00000000 |
| 333 | 1370.75600000 | 51.00440000  | 0.00000000 |
| 334 | 1374.06690000 | 3.78320000   | 0.00000000 |
| 335 | 1375.02460000 | 8.34670000   | 0.00000000 |
| 336 | 1375.22200000 | 5.27280000   | 0.00000000 |
| 337 | 1376.52080000 | 161.28100000 | 0.00000000 |
| 338 | 1378.48330000 | 13.90520000  | 0.00000000 |
| 339 | 1379.15690000 | 12.16810000  | 0.00000000 |
| 340 | 1381.46830000 | 1.81170000   | 0.00000000 |
| 341 | 1383.95250000 | 23.85370000  | 0.00000000 |
| 342 | 1391.21160000 | 12.79370000  | 0.00000000 |
| 343 | 1402.45720000 | 3.84310000   | 0.00000000 |
| 344 | 1410.21070000 | 3.07740000   | 0.00000000 |
| 345 | 1410.46390000 | 13.38590000  | 0.00000000 |
| 346 | 1415.97440000 | 5.59790000   | 0.00000000 |
| 347 | 1417.75140000 | 14.32210000  | 0.00000000 |
| 348 | 1428.67830000 | 7.60890000   | 0.00000000 |
| 349 | 1430.30890000 | 15.53190000  | 0.00000000 |
| 350 | 1436.14700000 | 73.07370000  | 0.00000000 |
| 351 | 1436.63610000 | 63.43310000  | 0.00000000 |
| 352 | 1444.09730000 | 163.48320000 | 0.00000000 |
| 353 | 1453.00530000 | 86.35830000  | 0.00000000 |
| 354 | 1456.29100000 | 83.91250000  | 0.00000000 |
| 355 | 1457.88100000 | 53.18920000  | 0.00000000 |
| 356 | 1465.47160000 | 85.77370000  | 0.00000000 |
| 357 | 1472.45800000 | 13.69310000  | 0.00000000 |
| 358 | 1473.08570000 | 54.43380000  | 0.00000000 |
| 359 | 1474.07940000 | 68.36830000  | 0.00000000 |
| 360 | 1476.36030000 | 9.17940000   | 0.00000000 |
| 361 | 1477.11940000 | 16.56620000  | 0.00000000 |
| 362 | 1482.64500000 | 6.43460000   | 0.00000000 |
| 363 | 1483.94130000 | 1.36310000   | 0.00000000 |
| 364 | 1490.91810000 | 0.97820000   | 0.00000000 |
| 365 | 1491.03890000 | 5.77800000   | 0.00000000 |
| 366 | 1493.38500000 | 23.86000000  | 0.00000000 |
| 367 | 1495.64660000 | 3.98350000   | 0.00000000 |
| 368 | 1499.47470000 | 11.88830000  | 0.00000000 |
| 369 | 1500.78590000 | 11.08740000  | 0.00000000 |
| 370 | 1502.02910000 | 16.72720000  | 0.00000000 |
| 371 | 1503.42700000 | 4.96080000   | 0.00000000 |
| 372 | 1504.63090000 | 4.29430000   | 0.00000000 |
| 373 | 1509.53700000 | 4.41420000   | 0.00000000 |
| 374 | 1510.36220000 | 4.00140000   | 0.00000000 |
| 375 | 1518.11690000 | 5.49850000   | 0.00000000 |
| 376 | 1520.06850000 | 35.41790000  | 0.00000000 |
| 377 | 1524.24900000 | 24.22900000  | 0.00000000 |
| 378 | 1525.16400000 | 33.73510000  | 0.00000000 |
| 379 | 1527.79010000 | 63.16620000  | 0.00000000 |
| 380 | 1533.10760000 | 139.07880000 | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 1540.44030000 | 21.75760000   | 0.00000000 |
| 382 | 1551.60190000 | 10.79740000   | 0.00000000 |
| 383 | 1553.32950000 | 13.28650000   | 0.00000000 |
| 384 | 1556.82190000 | 10.70250000   | 0.00000000 |
| 385 | 1570.95750000 | 6.59260000    | 0.00000000 |
| 386 | 1575.80040000 | 4.96330000    | 0.00000000 |
| 387 | 1583.30480000 | 30.44440000   | 0.00000000 |
| 388 | 1586.46710000 | 5.81100000    | 0.00000000 |
| 389 | 1599.64790000 | 4.25670000    | 0.00000000 |
| 390 | 1601.50870000 | 11.70480000   | 0.00000000 |
| 391 | 1609.88260000 | 12.45250000   | 0.00000000 |
| 392 | 1612.10300000 | 18.90160000   | 0.00000000 |
| 393 | 1621.28190000 | 8.41780000    | 0.00000000 |
| 394 | 1621.56240000 | 16.36190000   | 0.00000000 |
| 395 | 1623.04210000 | 1.19280000    | 0.00000000 |
| 396 | 1626.60490000 | 17.93010000   | 0.00000000 |
| 397 | 1634.31340000 | 1.07430000    | 0.00000000 |
| 398 | 1640.75390000 | 7.11440000    | 0.00000000 |
| 399 | 1649.92430000 | 55.55510000   | 0.00000000 |
| 400 | 1651.59660000 | 171.40220000  | 0.00000000 |
| 401 | 1654.96200000 | 147.75230000  | 0.00000000 |
| 402 | 1659.56770000 | 14.19170000   | 0.00000000 |
| 403 | 1660.02580000 | 29.32920000   | 0.00000000 |
| 404 | 1666.20910000 | 27.77640000   | 0.00000000 |
| 405 | 1672.50500000 | 118.36490000  | 0.00000000 |
| 406 | 1675.42660000 | 50.70710000   | 0.00000000 |
| 407 | 1718.91120000 | 76.10830000   | 0.00000000 |
| 408 | 1843.06380000 | 63.86830000   | 0.00000000 |
| 409 | 1947.97250000 | 2479.88290000 | 0.00000000 |
| 410 | 1974.95290000 | 2224.57030000 | 0.00000000 |
| 411 | 2085.19210000 | 1995.44090000 | 0.00000000 |
| 412 | 2965.20160000 | 136.85000000  | 0.00000000 |
| 413 | 3005.01580000 | 42.61200000   | 0.00000000 |
| 414 | 3012.33470000 | 7.31250000    | 0.00000000 |
| 415 | 3018.12950000 | 56.82150000   | 0.00000000 |
| 416 | 3026.39910000 | 148.26890000  | 0.00000000 |
| 417 | 3030.70880000 | 21.47000000   | 0.00000000 |
| 418 | 3035.61310000 | 62.15980000   | 0.00000000 |
| 419 | 3038.81540000 | 74.55120000   | 0.00000000 |
| 420 | 3044.91470000 | 19.10840000   | 0.00000000 |
| 421 | 3060.52480000 | 63.02690000   | 0.00000000 |
| 422 | 3062.13780000 | 16.40290000   | 0.00000000 |
| 423 | 3064.19040000 | 58.62020000   | 0.00000000 |
| 424 | 3079.71130000 | 115.05920000  | 0.00000000 |
| 425 | 3090.29450000 | 21.02360000   | 0.00000000 |
| 426 | 3091.57250000 | 29.65480000   | 0.00000000 |
| 427 | 3104.63460000 | 89.20380000   | 0.00000000 |
| 428 | 3180.51590000 | 0.65890000    | 0.00000000 |
| 429 | 3189.59250000 | 5.50030000    | 0.00000000 |
| 430 | 3192.24940000 | 6.82430000    | 0.00000000 |
| 431 | 3196.73300000 | 5.88700000    | 0.00000000 |
| 432 | 3197.76130000 | 1.09110000    | 0.00000000 |
| 433 | 3197.78720000 | 1.65280000    | 0.00000000 |
| 434 | 3204.99820000 | 6.26790000    | 0.00000000 |
| 435 | 3206.20040000 | 14.56660000   | 0.00000000 |
| 436 | 3208.14780000 | 6.54370000    | 0.00000000 |
| 437 | 3208.46270000 | 0.88850000    | 0.00000000 |
| 438 | 3212.54190000 | 15.75620000   | 0.00000000 |
| 439 | 3213.21460000 | 20.95180000   | 0.00000000 |
| 440 | 3214.18320000 | 22.81950000   | 0.00000000 |
| 441 | 3216.08820000 | 15.64870000   | 0.00000000 |
| 442 | 3216.21360000 | 9.60260000    | 0.00000000 |
| 443 | 3216.88530000 | 21.42540000   | 0.00000000 |
| 444 | 3217.94940000 | 44.67380000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 445 | 3218.42370000 | 0.34510000    | 0.00000000 |
| 446 | 3222.12000000 | 27.59900000   | 0.00000000 |
| 447 | 3223.12070000 | 40.70110000   | 0.00000000 |
| 448 | 3223.29330000 | 8.68920000    | 0.00000000 |
| 449 | 3226.86090000 | 1484.66910000 | 0.00000000 |
| 450 | 3230.13050000 | 2.56810000    | 0.00000000 |
| 451 | 3231.73290000 | 9.03140000    | 0.00000000 |
| 452 | 3237.96540000 | 6.88010000    | 0.00000000 |
| 453 | 3239.89160000 | 5.24350000    | 0.00000000 |
| 454 | 3241.81470000 | 5.42390000    | 0.00000000 |
| 455 | 3244.26010000 | 16.22020000   | 0.00000000 |
| 456 | 3251.77730000 | 49.09980000   | 0.00000000 |
| 457 | 3261.05120000 | 1.17330000    | 0.00000000 |
| 458 | 3261.63780000 | 0.43000000    | 0.00000000 |
| 459 | 3263.06180000 | 1.88990000    | 0.00000000 |
| 460 | 3266.44760000 | 9.39330000    | 0.00000000 |
| 461 | 3267.53300000 | 6.90650000    | 0.00000000 |
| 462 | 3269.36170000 | 8.87270000    | 0.00000000 |
| 463 | 3270.85370000 | 6.90530000    | 0.00000000 |
| 464 | 3282.47260000 | 3.09910000    | 0.00000000 |
| 465 | 3284.29940000 | 3.35650000    | 0.00000000 |
| 466 | 3285.01770000 | 4.99820000    | 0.00000000 |
| 467 | 3386.80830000 | 874.49040000  | 0.00000000 |
| 468 | 3497.16230000 | 806.41860000  | 0.00000000 |
| 469 | 3510.14530000 | 5.99670000    | 0.00000000 |
| 470 | 3549.29780000 | 8.71980000    | 0.00000000 |
| 471 | 3562.22420000 | 1075.64120000 | 0.00000000 |
| 472 | 3627.47130000 | 728.05500000  | 0.00000000 |
| 473 | 3638.82090000 | 218.20130000  | 0.00000000 |
| 474 | 3724.17740000 | 738.06390000  | 0.00000000 |
| 475 | 3841.73610000 | 288.63310000  | 0.00000000 |
| 476 | 3854.31770000 | 81.64790000   | 0.00000000 |
| 477 | 3855.92810000 | 62.46800000   | 0.00000000 |

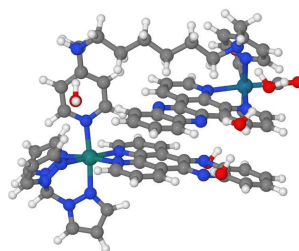
S19. CALCULATIONS ON  $2w^{3+}$  ( $^3A$ )

FIG. S29. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](6[Ru]578(n9ccc[n+](9C([n+](n7ccc1)[n+](n8ccc1)[n+](1ccc(cc1)CNCCCCCNCCc1cc[n+](cc1)[Re]1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2ccccc2n1)([C][O])([C][O])([C][O].O.O.O.O.O
Formula    : C67H66N18O8ReRu3+,3
Charge     : 3
Multiplicity : 3
Energy     : -4354.91691833 a.u.
Gibbs Energy : -4353.76604000 a.u.
Number of imaginary frequencies : 0

```

## S19.1. Cartesian Co-ordinates (XYZ format)

161

```

C   2.77753901  4.61535120  0.64060998
H   2.39843106  4.53012514  1.66227603
H   2.71773791  3.61382294  0.20466000
C   1.90034997  5.58469915 -0.15741199
H   2.31724596  5.73049021 -1.15908301
H   1.90754497  6.56538391  0.33246899
C   0.46825901  5.06808281 -0.29270300
H   0.01791400  4.95923901  0.69961202
H   0.50297701  4.06039381 -0.72264802
C  -0.43505901  5.93756390 -1.17356801
H   0.07652200  6.13934517 -2.12265205
H  -0.60437799  6.91020584 -0.69746500
C  -2.66141009  5.95145321 -2.46784401
H  -2.07113099  6.26156902 -3.34256196
H  -3.08213711  6.85682011 -2.02331591
N   4.20628595  4.97154713  0.73513401
C  -3.43711305  4.03479910 -3.85212588
H  -2.39152002  4.12732506 -4.15496778
H  -4.05085611  4.12983608 -4.74922991
N  -3.79491210  5.09559011 -2.87809706
C   4.94070578  4.90914679 -0.54322797
H   4.43150520  5.44580221 -1.35049498
H   5.90660477  5.39342690 -0.38779199
C  -7.56209612 -2.21022892  0.07694800
N  -7.14786911 -2.41754198 -1.29740798
N  -6.65208578 -2.88649201  0.98050302
N  -7.62285423 -0.79504299  0.37025899

```

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -5.92979813 | -1.97143304 | -1.71300495 |
| C  | -7.83582115 | -2.97791910 | -2.32268095 |
| N  | -5.33156490 | -2.54963899 | 0.98302799  |
| C  | -6.89165878 | -3.89674592 | 1.84703398  |
| N  | -6.50172901 | -0.04383800 | 0.22016700  |
| C  | -8.69415188 | -0.01231200 | 0.66113400  |
| Ru | -4.71787024 | -1.02961397 | -0.27225500 |
| C  | -5.85776711 | -2.25471210 | -3.01638794 |
| C  | -7.03348112 | -2.88814998 | -3.44134498 |
| H  | -8.81968498 | -3.39154410 | -2.17689896 |
| C  | -4.73874378 | -3.36037707 | 1.86887300  |
| C  | -5.68179321 | -4.22056103 | 2.43668795  |
| H  | -7.88231993 | -4.30051279 | 1.97695100  |
| C  | -6.86245823 | 1.22637498  | 0.42040700  |
| C  | -8.23705482 | 1.28749597  | 0.70623398  |
| H  | -9.67221737 | -0.43703800 | 0.81114203  |
| N  | -2.88669491 | -1.97561300 | -0.63564599 |
| N  | -3.58527493 | -0.31831700 | 1.31810498  |
| H  | -4.98840714 | -1.97953606 | -3.59024000 |
| H  | -7.26427603 | -3.23443103 | -4.43355083 |
| H  | -3.68030596 | -3.28433609 | 2.05379796  |
| H  | -5.50879622 | -4.97999716 | 3.17897797  |
| H  | -6.14389610 | 2.02933002  | 0.31438100  |
| H  | -8.81740856 | 2.16917896  | 0.91538203  |
| C  | -2.57476306 | -2.77012992 | -1.65532005 |
| C  | -1.94669998 | -1.73050296 | 0.33503500  |
| C  | -2.33275199 | -0.87294400 | 1.39432895  |
| C  | -4.02755022 | 0.43443099  | 2.32623291  |
| C  | -1.30719995 | -3.34908009 | -1.77678502 |
| H  | -3.34612203 | -2.95806098 | -2.38617110 |
| C  | -0.66968203 | -2.33912706 | 0.31884399  |
| C  | -1.48636794 | -0.65262401 | 2.49992394  |
| C  | -3.24893808 | 0.68458700  | 3.45639110  |
| H  | -5.02476215 | 0.83697802  | 2.23523593  |
| C  | -0.36114699 | -3.14435196 | -0.79200298 |
| H  | -1.09357095 | -3.97030592 | -2.63502192 |
| C  | 0.22689401  | -2.14274311 | 1.44430494  |
| C  | -1.97810102 | 0.14345200  | 3.54445004  |
| C  | -0.18058001 | -1.30202198 | 2.53895402  |
| H  | -3.65030003 | 1.30406201  | 4.24483204  |
| H  | 0.60417402  | -3.62594199 | -0.86057001 |
| N  | 1.40059304  | -2.78514791 | 1.46756005  |
| H  | -1.35844302 | 0.32707101  | 4.41085720  |
| N  | 0.58977002  | -1.11861300 | 3.60647607  |
| C  | 2.17829490  | -2.64471197 | 2.57826900  |
| C  | 1.76980102  | -1.80426300 | 3.66111803  |
| C  | 3.40531993  | -3.33726501 | 2.67279601  |
| C  | 2.59434605  | -1.69047105 | 4.80045319  |
| C  | 4.19035912  | -3.21002603 | 3.79998708  |
| H  | 3.70503211  | -3.97399306 | 1.85093606  |
| C  | 3.78488493  | -2.38376594 | 4.86669779  |
| H  | 2.27221799  | -1.03446805 | 5.59900093  |
| H  | 5.13028002  | -3.74456406 | 3.86236691  |
| H  | 4.41576481  | -2.29049706 | 5.74201012  |
| N  | 4.58927679  | -1.00267398 | 0.36454999  |
| N  | 3.18061805  | -1.16683495 | -1.93251705 |
| C  | 5.31565714  | -0.93199003 | 1.48205900  |
| C  | 3.37766910  | -0.38008401 | 0.32111600  |
| C  | 2.60363412  | -0.51127201 | -0.88768899 |
| C  | 2.47662401  | -1.36804903 | -3.04849195 |
| C  | 4.90665579  | -0.19532500 | 2.58987403  |
| H  | 6.25659513  | -1.46401596 | 1.48055196  |
| C  | 2.89714694  | 0.37952599  | 1.39809895  |
| C  | 1.31276500  | 0.04099400  | -0.98081899 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.17195702  | -0.89350498 | -3.19704103 |
| H  | 2.97305799  | -1.90450394 | -3.84470391 |
| C  | 3.69882703  | 0.47071400  | 2.54641104  |
| H  | 5.53484297  | -0.15713200 | 3.46729898  |
| C  | 1.59823895  | 1.03726101  | 1.28591800  |
| C  | 0.60199898  | -0.16599099 | -2.17310095 |
| C  | 0.78732502  | 0.83116198  | 0.12142000  |
| H  | 0.63838500  | -1.08000898 | -4.11830616 |
| H  | 3.36954904  | 1.05584800  | 3.38971710  |
| N  | 1.18338597  | 1.81187296  | 2.27742910  |
| H  | -0.38823301 | 0.24728800  | -2.27785993 |
| N  | -0.41870701 | 1.38526404  | 0.00362600  |
| C  | -0.04461900 | 2.38135600  | 2.18149900  |
| C  | -0.86286598 | 2.15635991  | 1.02749395  |
| C  | -0.51399899 | 3.20721412  | 3.22918105  |
| C  | -2.13704395 | 2.76878691  | 0.96970397  |
| C  | -1.75956404 | 3.78149700  | 3.14166594  |
| H  | 0.11675900  | 3.35028195  | 4.09501696  |
| C  | -2.56985688 | 3.56016493  | 2.00634003  |
| H  | -2.76878095 | 2.62978292  | 0.10676300  |
| H  | -2.12506604 | 4.40675116  | 3.94667101  |
| H  | -3.54817200 | 4.01818323  | 1.94842100  |
| H  | -8.55181408 | -2.63454604 | 0.20549300  |
| C  | 5.17353916  | 3.47726798  | -0.96210301 |
| C  | 4.49251986  | 2.89884210  | -2.03169394 |
| C  | 6.08406782  | 2.67570710  | -0.27059999 |
| C  | 4.69432116  | 1.55855799  | -2.33305311 |
| H  | 3.78790402  | 3.47270799  | -2.61952209 |
| C  | 6.24706793  | 1.35499406  | -0.64021200 |
| H  | 6.64461708  | 3.06615806  | 0.56765902  |
| N  | 5.54013681  | 0.78276801  | -1.63548994 |
| H  | 4.15016603  | 1.08390903  | -3.13804698 |
| H  | 6.94393396  | 0.72024399  | -0.11216700 |
| C  | -3.67853093 | 2.68766403  | -3.21372008 |
| C  | -2.66609812 | 1.99575901  | -2.55072904 |
| C  | -4.96932220 | 2.15534496  | -3.15124607 |
| C  | -2.98027897 | 0.90740699  | -1.76475406 |
| H  | -1.63868105 | 2.32932901  | -2.58113003 |
| C  | -5.21752787 | 1.04929805  | -2.36918211 |
| H  | -5.79186201 | 2.62658405  | -3.67258096 |
| N  | -4.24234676 | 0.45442799  | -1.64196706 |
| H  | -2.21963191 | 0.42941299  | -1.17030704 |
| H  | -6.21007395 | 0.63636798  | -2.28386903 |
| Re | 5.38687801  | -1.61690700 | -1.66095805 |
| C  | 5.09008789  | -3.50129199 | -1.47988701 |
| O  | 4.88237000  | -4.63249683 | -1.34970295 |
| C  | 5.84902477  | -1.82402599 | -3.53442907 |
| O  | 6.09342718  | -1.92140198 | -4.65617800 |
| C  | 7.25379419  | -1.84144998 | -1.18517101 |
| O  | 8.35645485  | -1.96969795 | -0.87468398 |
| H  | -4.51975203 | 5.67560816  | -3.28289509 |
| C  | -1.76448703 | 5.23964310  | -1.46034598 |
| H  | -2.32224703 | 5.08293676  | -0.53485399 |
| H  | -1.53072298 | 4.24390984  | -1.84191406 |
| H  | 4.28720713  | 5.91663885  | 1.10021102  |
| H  | 4.81723499  | 3.99008894  | 2.12972093  |
| O  | 5.04996204  | 3.45425797  | 2.93303490  |
| H  | 5.77902079  | 3.92806911  | 3.34709001  |
| H  | -4.58777714 | 4.29329205  | -1.28527200 |
| O  | -4.94456387 | 3.85206103  | -0.48068300 |
| H  | -5.09416485 | 4.57364321  | 0.13872001  |
| H  | 2.20042706  | 2.69883895  | 3.55391788  |
| O  | 2.67939496  | 3.06646609  | 4.32313013  |
| H  | 3.57301998  | 3.25477099  | 3.96610093  |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 0.80975097 | 0.47645500  | 4.84840107  |
| O | 0.93835199 | 1.10000706  | 5.58349323  |
| H | 1.62570298 | 1.71376896  | 5.27720499  |
| H | 1.94144905 | -4.31002283 | 0.46162400  |
| O | 2.12932110 | -5.12664604 | -0.04295000 |
| H | 2.97445011 | -4.96673012 | -0.47586501 |

## S19.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | 7.79680000   | 1.80550000   | 0.00000000      |
| 2    | 16.63020000  | 1.89300000   | 0.00000000      |
| 3    | 20.56070000  | 1.91100000   | 0.00000000      |
| 4    | 25.50580000  | 0.82850000   | 0.00000000      |
| 5    | 30.37020000  | 1.12330000   | 0.00000000      |
| 6    | 33.63300000  | 1.08870000   | 0.00000000      |
| 7    | 38.78840000  | 2.96440000   | 0.00000000      |
| 8    | 40.92930000  | 3.37290000   | 0.00000000      |
| 9    | 41.16180000  | 1.65690000   | 0.00000000      |
| 10   | 46.05500000  | 6.63910000   | 0.00000000      |
| 11   | 48.56740000  | 0.76070000   | 0.00000000      |
| 12   | 49.68890000  | 0.52630000   | 0.00000000      |
| 13   | 55.28180000  | 5.01560000   | 0.00000000      |
| 14   | 58.49450000  | 1.61370000   | 0.00000000      |
| 15   | 59.40760000  | 7.99860000   | 0.00000000      |
| 16   | 61.81800000  | 1.72320000   | 0.00000000      |
| 17   | 62.43560000  | 2.93330000   | 0.00000000      |
| 18   | 66.26970000  | 16.42430000  | 0.00000000      |
| 19   | 68.30150000  | 1.45230000   | 0.00000000      |
| 20   | 69.58730000  | 1.62030000   | 0.00000000      |
| 21   | 74.36650000  | 0.36270000   | 0.00000000      |
| 22   | 77.83650000  | 3.13880000   | 0.00000000      |
| 23   | 80.37500000  | 1.44230000   | 0.00000000      |
| 24   | 80.94960000  | 0.54490000   | 0.00000000      |
| 25   | 83.97310000  | 5.43720000   | 0.00000000      |
| 26   | 89.24030000  | 0.72310000   | 0.00000000      |
| 27   | 90.54350000  | 10.54170000  | 0.00000000      |
| 28   | 90.93980000  | 0.49830000   | 0.00000000      |
| 29   | 92.99450000  | 0.08530000   | 0.00000000      |
| 30   | 93.65750000  | 16.56440000  | 0.00000000      |
| 31   | 94.90550000  | 6.81510000   | 0.00000000      |
| 32   | 97.02780000  | 8.59140000   | 0.00000000      |
| 33   | 99.84190000  | 19.53600000  | 0.00000000      |
| 34   | 101.94160000 | 16.20600000  | 0.00000000      |
| 35   | 106.99150000 | 2.50390000   | 0.00000000      |
| 36   | 110.25850000 | 1.89110000   | 0.00000000      |
| 37   | 113.37450000 | 3.98510000   | 0.00000000      |
| 38   | 120.79830000 | 7.68600000   | 0.00000000      |
| 39   | 121.33660000 | 3.02100000   | 0.00000000      |
| 40   | 123.48640000 | 0.39530000   | 0.00000000      |
| 41   | 128.82630000 | 2.62290000   | 0.00000000      |
| 42   | 131.41520000 | 2.06130000   | 0.00000000      |
| 43   | 135.54210000 | 3.07080000   | 0.00000000      |
| 44   | 136.25620000 | 5.20440000   | 0.00000000      |
| 45   | 138.07860000 | 14.99480000  | 0.00000000      |
| 46   | 139.87550000 | 8.64110000   | 0.00000000      |
| 47   | 140.61710000 | 2.17980000   | 0.00000000      |
| 48   | 144.53960000 | 8.94380000   | 0.00000000      |
| 49   | 145.90860000 | 3.22740000   | 0.00000000      |
| 50   | 150.10000000 | 1.69500000   | 0.00000000      |
| 51   | 154.11190000 | 2.64580000   | 0.00000000      |
| 52   | 154.75650000 | 12.57090000  | 0.00000000      |
| 53   | 156.29530000 | 7.26250000   | 0.00000000      |
| 54   | 160.45500000 | 6.20980000   | 0.00000000      |
| 55   | 162.38950000 | 1.08090000   | 0.00000000      |
| 56   | 165.23420000 | 2.52440000   | 0.00000000      |
| 57   | 171.30020000 | 0.76100000   | 0.00000000      |
| 58   | 173.71640000 | 2.15140000   | 0.00000000      |
| 59   | 181.10920000 | 1.29560000   | 0.00000000      |
| 60   | 182.07500000 | 7.97400000   | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 183.20890000 | 4.55260000   | 0.00000000 |
| 62  | 186.63780000 | 3.70670000   | 0.00000000 |
| 63  | 192.20050000 | 4.72540000   | 0.00000000 |
| 64  | 193.51540000 | 1.89670000   | 0.00000000 |
| 65  | 195.76330000 | 11.97300000  | 0.00000000 |
| 66  | 196.52690000 | 2.02330000   | 0.00000000 |
| 67  | 199.08790000 | 6.08950000   | 0.00000000 |
| 68  | 202.18240000 | 4.76200000   | 0.00000000 |
| 69  | 206.09720000 | 7.86780000   | 0.00000000 |
| 70  | 216.24210000 | 3.16920000   | 0.00000000 |
| 71  | 217.71530000 | 7.00240000   | 0.00000000 |
| 72  | 219.08650000 | 10.59890000  | 0.00000000 |
| 73  | 236.35910000 | 41.12430000  | 0.00000000 |
| 74  | 242.86930000 | 15.93220000  | 0.00000000 |
| 75  | 245.22710000 | 10.59810000  | 0.00000000 |
| 76  | 249.16940000 | 201.15450000 | 0.00000000 |
| 77  | 253.04990000 | 12.17390000  | 0.00000000 |
| 78  | 254.82600000 | 14.76930000  | 0.00000000 |
| 79  | 259.35520000 | 105.37190000 | 0.00000000 |
| 80  | 263.42870000 | 32.60540000  | 0.00000000 |
| 81  | 277.39870000 | 15.79750000  | 0.00000000 |
| 82  | 280.11110000 | 63.87690000  | 0.00000000 |
| 83  | 282.91880000 | 57.49140000  | 0.00000000 |
| 84  | 292.49730000 | 71.33760000  | 0.00000000 |
| 85  | 300.26000000 | 33.22010000  | 0.00000000 |
| 86  | 307.40360000 | 14.53620000  | 0.00000000 |
| 87  | 317.80640000 | 12.61390000  | 0.00000000 |
| 88  | 323.46700000 | 11.26240000  | 0.00000000 |
| 89  | 329.34100000 | 9.72840000   | 0.00000000 |
| 90  | 331.95260000 | 7.14220000   | 0.00000000 |
| 91  | 337.09770000 | 8.26310000   | 0.00000000 |
| 92  | 338.58520000 | 5.02610000   | 0.00000000 |
| 93  | 339.94760000 | 19.46280000  | 0.00000000 |
| 94  | 340.79780000 | 5.76110000   | 0.00000000 |
| 95  | 343.23810000 | 20.37990000  | 0.00000000 |
| 96  | 349.40200000 | 9.30440000   | 0.00000000 |
| 97  | 362.21140000 | 5.16940000   | 0.00000000 |
| 98  | 367.88330000 | 6.33360000   | 0.00000000 |
| 99  | 375.42020000 | 41.87120000  | 0.00000000 |
| 100 | 379.87230000 | 33.00270000  | 0.00000000 |
| 101 | 386.97350000 | 3.66780000   | 0.00000000 |
| 102 | 391.31470000 | 5.24040000   | 0.00000000 |
| 103 | 391.88680000 | 0.15090000   | 0.00000000 |
| 104 | 400.65940000 | 2.14530000   | 0.00000000 |
| 105 | 402.01470000 | 0.70420000   | 0.00000000 |
| 106 | 410.32850000 | 72.96940000  | 0.00000000 |
| 107 | 411.54030000 | 5.06110000   | 0.00000000 |
| 108 | 413.37540000 | 74.27950000  | 0.00000000 |
| 109 | 417.00690000 | 30.58240000  | 0.00000000 |
| 110 | 421.83600000 | 7.19420000   | 0.00000000 |
| 111 | 433.77130000 | 58.86770000  | 0.00000000 |
| 112 | 438.13240000 | 79.26640000  | 0.00000000 |
| 113 | 446.23670000 | 76.14150000  | 0.00000000 |
| 114 | 452.84960000 | 2.12030000   | 0.00000000 |
| 115 | 463.54690000 | 10.36000000  | 0.00000000 |
| 116 | 473.54150000 | 31.51110000  | 0.00000000 |
| 117 | 476.67290000 | 8.15620000   | 0.00000000 |
| 118 | 481.20080000 | 9.30060000   | 0.00000000 |
| 119 | 485.75490000 | 16.96520000  | 0.00000000 |
| 120 | 488.41110000 | 45.47760000  | 0.00000000 |
| 121 | 489.91810000 | 53.78550000  | 0.00000000 |
| 122 | 495.08650000 | 5.28020000   | 0.00000000 |
| 123 | 499.29530000 | 19.17860000  | 0.00000000 |
| 124 | 501.98630000 | 8.92450000   | 0.00000000 |



|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 505.33590000 | 12.70290000  | 0.00000000 |
| 126 | 508.00070000 | 40.19510000  | 0.00000000 |
| 127 | 510.70210000 | 50.04210000  | 0.00000000 |
| 128 | 511.26740000 | 42.46850000  | 0.00000000 |
| 129 | 511.97050000 | 39.43210000  | 0.00000000 |
| 130 | 514.99270000 | 8.05070000   | 0.00000000 |
| 131 | 526.07490000 | 18.66190000  | 0.00000000 |
| 132 | 528.85320000 | 29.23660000  | 0.00000000 |
| 133 | 534.00870000 | 2.01430000   | 0.00000000 |
| 134 | 549.84790000 | 0.77240000   | 0.00000000 |
| 135 | 555.95130000 | 21.62440000  | 0.00000000 |
| 136 | 559.53130000 | 22.23180000  | 0.00000000 |
| 137 | 559.93460000 | 27.81890000  | 0.00000000 |
| 138 | 570.65470000 | 9.49160000   | 0.00000000 |
| 139 | 571.81540000 | 8.02420000   | 0.00000000 |
| 140 | 575.95480000 | 11.35730000  | 0.00000000 |
| 141 | 576.72080000 | 6.44650000   | 0.00000000 |
| 142 | 580.02170000 | 12.45030000  | 0.00000000 |
| 143 | 592.29680000 | 209.89090000 | 0.00000000 |
| 144 | 595.43420000 | 122.85840000 | 0.00000000 |
| 145 | 597.28740000 | 0.72140000   | 0.00000000 |
| 146 | 599.57910000 | 28.28820000  | 0.00000000 |
| 147 | 599.75790000 | 117.35750000 | 0.00000000 |
| 148 | 608.49470000 | 28.92600000  | 0.00000000 |
| 149 | 615.83600000 | 49.53670000  | 0.00000000 |
| 150 | 617.92360000 | 26.13620000  | 0.00000000 |
| 151 | 628.90000000 | 373.50310000 | 0.00000000 |
| 152 | 630.83200000 | 34.12220000  | 0.00000000 |
| 153 | 632.20880000 | 20.31490000  | 0.00000000 |
| 154 | 637.71360000 | 116.33840000 | 0.00000000 |
| 155 | 645.99580000 | 1.05000000   | 0.00000000 |
| 156 | 651.04620000 | 110.18960000 | 0.00000000 |
| 157 | 653.53540000 | 4.91790000   | 0.00000000 |
| 158 | 653.85470000 | 14.70540000  | 0.00000000 |
| 159 | 657.79990000 | 17.22720000  | 0.00000000 |
| 160 | 665.56410000 | 10.60010000  | 0.00000000 |
| 161 | 670.40330000 | 2.66890000   | 0.00000000 |
| 162 | 673.23610000 | 2.40080000   | 0.00000000 |
| 163 | 674.08660000 | 177.13390000 | 0.00000000 |
| 164 | 680.70390000 | 5.63670000   | 0.00000000 |
| 165 | 684.05490000 | 6.87210000   | 0.00000000 |
| 166 | 701.89390000 | 114.20150000 | 0.00000000 |
| 167 | 706.63260000 | 43.48350000  | 0.00000000 |
| 168 | 725.47500000 | 144.96150000 | 0.00000000 |
| 169 | 728.14300000 | 138.70960000 | 0.00000000 |
| 170 | 729.49620000 | 85.00780000  | 0.00000000 |
| 171 | 735.31300000 | 77.21070000  | 0.00000000 |
| 172 | 736.97990000 | 41.14660000  | 0.00000000 |
| 173 | 740.07790000 | 40.16440000  | 0.00000000 |
| 174 | 742.92990000 | 30.20850000  | 0.00000000 |
| 175 | 743.92500000 | 25.44200000  | 0.00000000 |
| 176 | 746.96350000 | 105.42990000 | 0.00000000 |
| 177 | 748.88250000 | 70.19720000  | 0.00000000 |
| 178 | 750.92560000 | 5.32050000   | 0.00000000 |
| 179 | 759.26900000 | 16.87440000  | 0.00000000 |
| 180 | 762.57900000 | 24.23840000  | 0.00000000 |
| 181 | 765.27170000 | 58.79640000  | 0.00000000 |
| 182 | 770.25430000 | 117.70920000 | 0.00000000 |
| 183 | 773.55870000 | 76.95760000  | 0.00000000 |
| 184 | 776.30120000 | 92.37060000  | 0.00000000 |
| 185 | 777.82820000 | 127.12770000 | 0.00000000 |
| 186 | 779.86290000 | 44.38730000  | 0.00000000 |
| 187 | 781.76360000 | 253.16850000 | 0.00000000 |
| 188 | 788.42980000 | 49.04930000  | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 189 | 789.78120000  | 34.79610000  | 0.00000000 |
| 190 | 793.79350000  | 71.47660000  | 0.00000000 |
| 191 | 794.26410000  | 67.32470000  | 0.00000000 |
| 192 | 796.51110000  | 77.73300000  | 0.00000000 |
| 193 | 797.25510000  | 75.74240000  | 0.00000000 |
| 194 | 801.81320000  | 36.92760000  | 0.00000000 |
| 195 | 803.13100000  | 31.06580000  | 0.00000000 |
| 196 | 805.60620000  | 1.57680000   | 0.00000000 |
| 197 | 814.43400000  | 36.94320000  | 0.00000000 |
| 198 | 818.74380000  | 168.07200000 | 0.00000000 |
| 199 | 821.66760000  | 186.07190000 | 0.00000000 |
| 200 | 822.85450000  | 36.02440000  | 0.00000000 |
| 201 | 828.06360000  | 16.18550000  | 0.00000000 |
| 202 | 833.06380000  | 70.48960000  | 0.00000000 |
| 203 | 836.22090000  | 0.75460000   | 0.00000000 |
| 204 | 842.93330000  | 16.86940000  | 0.00000000 |
| 205 | 851.96900000  | 0.65340000   | 0.00000000 |
| 206 | 871.92350000  | 62.19270000  | 0.00000000 |
| 207 | 874.23760000  | 168.59340000 | 0.00000000 |
| 208 | 875.72930000  | 50.24690000  | 0.00000000 |
| 209 | 879.88710000  | 7.68560000   | 0.00000000 |
| 210 | 880.14620000  | 17.97800000  | 0.00000000 |
| 211 | 884.46320000  | 50.05700000  | 0.00000000 |
| 212 | 887.75350000  | 0.90900000   | 0.00000000 |
| 213 | 888.55900000  | 14.88230000  | 0.00000000 |
| 214 | 889.02190000  | 7.35490000   | 0.00000000 |
| 215 | 889.33080000  | 5.92210000   | 0.00000000 |
| 216 | 895.70450000  | 23.83330000  | 0.00000000 |
| 217 | 898.27060000  | 5.60140000   | 0.00000000 |
| 218 | 910.02030000  | 29.52610000  | 0.00000000 |
| 219 | 916.78370000  | 4.37670000   | 0.00000000 |
| 220 | 918.38560000  | 8.79860000   | 0.00000000 |
| 221 | 934.91280000  | 151.84060000 | 0.00000000 |
| 222 | 935.90600000  | 23.83820000  | 0.00000000 |
| 223 | 937.06390000  | 2.25770000   | 0.00000000 |
| 224 | 940.44230000  | 0.96590000   | 0.00000000 |
| 225 | 941.51470000  | 0.16450000   | 0.00000000 |
| 226 | 944.83110000  | 1.24980000   | 0.00000000 |
| 227 | 949.93060000  | 0.75080000   | 0.00000000 |
| 228 | 966.79390000  | 8.83760000   | 0.00000000 |
| 229 | 969.41590000  | 3.06160000   | 0.00000000 |
| 230 | 974.12220000  | 3.92880000   | 0.00000000 |
| 231 | 974.69240000  | 1.71160000   | 0.00000000 |
| 232 | 975.56770000  | 9.02160000   | 0.00000000 |
| 233 | 976.84260000  | 13.41640000  | 0.00000000 |
| 234 | 978.55960000  | 4.56820000   | 0.00000000 |
| 235 | 984.89030000  | 21.60110000  | 0.00000000 |
| 236 | 986.51340000  | 0.94070000   | 0.00000000 |
| 237 | 989.00380000  | 9.47720000   | 0.00000000 |
| 238 | 993.78440000  | 2.36890000   | 0.00000000 |
| 239 | 1001.24350000 | 6.15790000   | 0.00000000 |
| 240 | 1003.68860000 | 0.56580000   | 0.00000000 |
| 241 | 1004.66630000 | 13.00760000  | 0.00000000 |
| 242 | 1006.27340000 | 6.44850000   | 0.00000000 |
| 243 | 1008.34180000 | 2.30250000   | 0.00000000 |
| 244 | 1009.66060000 | 1.68700000   | 0.00000000 |
| 245 | 1010.93930000 | 2.05660000   | 0.00000000 |
| 246 | 1014.36090000 | 4.67650000   | 0.00000000 |
| 247 | 1014.83980000 | 19.19310000  | 0.00000000 |
| 248 | 1019.84060000 | 25.85240000  | 0.00000000 |
| 249 | 1020.22750000 | 34.12420000  | 0.00000000 |
| 250 | 1022.34250000 | 1.75410000   | 0.00000000 |
| 251 | 1023.76890000 | 87.33070000  | 0.00000000 |
| 252 | 1026.34210000 | 19.59870000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1031.03800000 | 13.93970000   | 0.00000000 |
| 254 | 1036.82330000 | 5.84660000    | 0.00000000 |
| 255 | 1047.94520000 | 3.73540000    | 0.00000000 |
| 256 | 1048.56670000 | 2.65060000    | 0.00000000 |
| 257 | 1051.35760000 | 28.13840000   | 0.00000000 |
| 258 | 1060.56140000 | 70.73970000   | 0.00000000 |
| 259 | 1063.93810000 | 110.92950000  | 0.00000000 |
| 260 | 1065.67620000 | 3.01330000    | 0.00000000 |
| 261 | 1065.85400000 | 6.17230000    | 0.00000000 |
| 262 | 1071.46690000 | 2.55420000    | 0.00000000 |
| 263 | 1072.02860000 | 3.20780000    | 0.00000000 |
| 264 | 1077.53510000 | 364.85800000  | 0.00000000 |
| 265 | 1080.57110000 | 146.82780000  | 0.00000000 |
| 266 | 1085.97470000 | 93.86160000   | 0.00000000 |
| 267 | 1088.82710000 | 30.63740000   | 0.00000000 |
| 268 | 1091.92890000 | 29.10870000   | 0.00000000 |
| 269 | 1100.82400000 | 2.27740000    | 0.00000000 |
| 270 | 1103.30030000 | 44.50420000   | 0.00000000 |
| 271 | 1105.92660000 | 46.33460000   | 0.00000000 |
| 272 | 1110.36630000 | 23.91170000   | 0.00000000 |
| 273 | 1114.14550000 | 348.02350000  | 0.00000000 |
| 274 | 1122.38210000 | 36.94940000   | 0.00000000 |
| 275 | 1126.53220000 | 15.94030000   | 0.00000000 |
| 276 | 1128.41410000 | 47.59160000   | 0.00000000 |
| 277 | 1130.67990000 | 45.86530000   | 0.00000000 |
| 278 | 1134.56010000 | 107.37520000  | 0.00000000 |
| 279 | 1135.98270000 | 79.29930000   | 0.00000000 |
| 280 | 1137.60940000 | 5.19180000    | 0.00000000 |
| 281 | 1140.95430000 | 158.97480000  | 0.00000000 |
| 282 | 1145.09590000 | 121.93050000  | 0.00000000 |
| 283 | 1152.08210000 | 110.43560000  | 0.00000000 |
| 284 | 1154.27800000 | 41.90490000   | 0.00000000 |
| 285 | 1157.55040000 | 33.34010000   | 0.00000000 |
| 286 | 1164.13570000 | 618.45560000  | 0.00000000 |
| 287 | 1165.67000000 | 286.07100000  | 0.00000000 |
| 288 | 1168.24110000 | 639.04310000  | 0.00000000 |
| 289 | 1172.37020000 | 19.66530000   | 0.00000000 |
| 290 | 1176.04490000 | 19.97550000   | 0.00000000 |
| 291 | 1197.41240000 | 0.65610000    | 0.00000000 |
| 292 | 1203.48060000 | 1488.90710000 | 0.00000000 |
| 293 | 1208.41770000 | 179.56480000  | 0.00000000 |
| 294 | 1217.32060000 | 238.13740000  | 0.00000000 |
| 295 | 1218.45200000 | 20.56500000   | 0.00000000 |
| 296 | 1231.35920000 | 24.91350000   | 0.00000000 |
| 297 | 1235.00080000 | 55.80580000   | 0.00000000 |
| 298 | 1235.76810000 | 62.69380000   | 0.00000000 |
| 299 | 1241.05790000 | 44.29630000   | 0.00000000 |
| 300 | 1245.42990000 | 223.83470000  | 0.00000000 |
| 301 | 1249.85590000 | 1886.89180000 | 0.00000000 |
| 302 | 1250.41310000 | 267.31310000  | 0.00000000 |
| 303 | 1254.70720000 | 226.45870000  | 0.00000000 |
| 304 | 1262.64910000 | 59.50750000   | 0.00000000 |
| 305 | 1263.09620000 | 74.44220000   | 0.00000000 |
| 306 | 1266.11080000 | 95.63350000   | 0.00000000 |
| 307 | 1269.26480000 | 398.98180000  | 0.00000000 |
| 308 | 1270.16960000 | 0.50250000    | 0.00000000 |
| 309 | 1273.45860000 | 112.47440000  | 0.00000000 |
| 310 | 1280.82090000 | 124.48570000  | 0.00000000 |
| 311 | 1281.58150000 | 24.24690000   | 0.00000000 |
| 312 | 1283.10250000 | 131.67790000  | 0.00000000 |
| 313 | 1297.92280000 | 400.59410000  | 0.00000000 |
| 314 | 1302.76490000 | 360.79920000  | 0.00000000 |
| 315 | 1303.77370000 | 31.31480000   | 0.00000000 |
| 316 | 1306.60750000 | 39.66090000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1308.28910000 | 158.57020000  | 0.00000000 |
| 318 | 1309.54620000 | 340.93860000  | 0.00000000 |
| 319 | 1317.54100000 | 28.56530000   | 0.00000000 |
| 320 | 1318.54570000 | 55.82880000   | 0.00000000 |
| 321 | 1320.84860000 | 151.80250000  | 0.00000000 |
| 322 | 1325.47080000 | 146.16090000  | 0.00000000 |
| 323 | 1326.16100000 | 471.93360000  | 0.00000000 |
| 324 | 1328.75770000 | 4.34680000    | 0.00000000 |
| 325 | 1331.61000000 | 253.58670000  | 0.00000000 |
| 326 | 1332.92030000 | 10.93460000   | 0.00000000 |
| 327 | 1335.49600000 | 1.62280000    | 0.00000000 |
| 328 | 1339.67660000 | 3.91580000    | 0.00000000 |
| 329 | 1347.45080000 | 30.37910000   | 0.00000000 |
| 330 | 1349.44190000 | 163.33940000  | 0.00000000 |
| 331 | 1358.51540000 | 11.76500000   | 0.00000000 |
| 332 | 1362.39340000 | 60.41590000   | 0.00000000 |
| 333 | 1364.49070000 | 48.38060000   | 0.00000000 |
| 334 | 1369.17340000 | 53.30270000   | 0.00000000 |
| 335 | 1371.06150000 | 183.45690000  | 0.00000000 |
| 336 | 1373.49280000 | 142.29770000  | 0.00000000 |
| 337 | 1373.87080000 | 253.83570000  | 0.00000000 |
| 338 | 1378.83790000 | 74.97400000   | 0.00000000 |
| 339 | 1381.13200000 | 3.32490000    | 0.00000000 |
| 340 | 1382.48060000 | 7.13790000    | 0.00000000 |
| 341 | 1383.87370000 | 121.98910000  | 0.00000000 |
| 342 | 1389.18170000 | 402.70070000  | 0.00000000 |
| 343 | 1393.51390000 | 7.84820000    | 0.00000000 |
| 344 | 1399.11200000 | 12.05520000   | 0.00000000 |
| 345 | 1402.47830000 | 4.19500000    | 0.00000000 |
| 346 | 1408.20100000 | 110.88140000  | 0.00000000 |
| 347 | 1409.29940000 | 28.35500000   | 0.00000000 |
| 348 | 1410.30390000 | 18.18310000   | 0.00000000 |
| 349 | 1416.37010000 | 14.05940000   | 0.00000000 |
| 350 | 1419.15330000 | 8.24610000    | 0.00000000 |
| 351 | 1429.56250000 | 72.33020000   | 0.00000000 |
| 352 | 1436.96690000 | 115.59810000  | 0.00000000 |
| 353 | 1443.69320000 | 354.75430000  | 0.00000000 |
| 354 | 1444.43100000 | 91.29680000   | 0.00000000 |
| 355 | 1456.50510000 | 1045.31490000 | 0.00000000 |
| 356 | 1457.65800000 | 55.80510000   | 0.00000000 |
| 357 | 1466.49400000 | 580.84790000  | 0.00000000 |
| 358 | 1470.14660000 | 804.76620000  | 0.00000000 |
| 359 | 1471.74550000 | 22.68010000   | 0.00000000 |
| 360 | 1473.53280000 | 100.96230000  | 0.00000000 |
| 361 | 1475.13350000 | 306.68760000  | 0.00000000 |
| 362 | 1481.17210000 | 11.90430000   | 0.00000000 |
| 363 | 1482.36460000 | 7.93930000    | 0.00000000 |
| 364 | 1483.65480000 | 55.31580000   | 0.00000000 |
| 365 | 1486.47410000 | 52.35240000   | 0.00000000 |
| 366 | 1489.95920000 | 54.29530000   | 0.00000000 |
| 367 | 1490.76820000 | 2.38390000    | 0.00000000 |
| 368 | 1492.79540000 | 246.78240000  | 0.00000000 |
| 369 | 1495.39040000 | 64.41360000   | 0.00000000 |
| 370 | 1495.87970000 | 20.21480000   | 0.00000000 |
| 371 | 1498.24740000 | 6.05660000    | 0.00000000 |
| 372 | 1500.26530000 | 3.21150000    | 0.00000000 |
| 373 | 1500.68280000 | 1.46420000    | 0.00000000 |
| 374 | 1505.32430000 | 3.50150000    | 0.00000000 |
| 375 | 1509.59570000 | 231.14510000  | 0.00000000 |
| 376 | 1510.99210000 | 200.82910000  | 0.00000000 |
| 377 | 1517.35190000 | 113.00200000  | 0.00000000 |
| 378 | 1517.83870000 | 84.47570000   | 0.00000000 |
| 379 | 1518.63680000 | 125.98460000  | 0.00000000 |
| 380 | 1520.61370000 | 360.72110000  | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 1528.20200000 | 45.51300000   | 0.00000000 |
| 382 | 1532.29850000 | 127.33910000  | 0.00000000 |
| 383 | 1538.72970000 | 7.05120000    | 0.00000000 |
| 384 | 1543.00440000 | 61.18820000   | 0.00000000 |
| 385 | 1553.60350000 | 34.94010000   | 0.00000000 |
| 386 | 1557.74240000 | 3.39500000    | 0.00000000 |
| 387 | 1573.10830000 | 802.33720000  | 0.00000000 |
| 388 | 1574.21770000 | 272.24350000  | 0.00000000 |
| 389 | 1581.40860000 | 77.25250000   | 0.00000000 |
| 390 | 1593.62120000 | 119.40320000  | 0.00000000 |
| 391 | 1594.82790000 | 42.91660000   | 0.00000000 |
| 392 | 1595.24870000 | 149.00770000  | 0.00000000 |
| 393 | 1598.39840000 | 194.02210000  | 0.00000000 |
| 394 | 1602.04530000 | 117.17570000  | 0.00000000 |
| 395 | 1615.30500000 | 25.77660000   | 0.00000000 |
| 396 | 1618.60840000 | 33.59540000   | 0.00000000 |
| 397 | 1623.04140000 | 49.60210000   | 0.00000000 |
| 398 | 1626.18260000 | 22.40240000   | 0.00000000 |
| 399 | 1638.88120000 | 16.90860000   | 0.00000000 |
| 400 | 1648.69370000 | 49.62990000   | 0.00000000 |
| 401 | 1649.05330000 | 87.41090000   | 0.00000000 |
| 402 | 1650.62570000 | 31.60170000   | 0.00000000 |
| 403 | 1662.33430000 | 332.93120000  | 0.00000000 |
| 404 | 1667.36840000 | 214.01060000  | 0.00000000 |
| 405 | 1675.71760000 | 63.09800000   | 0.00000000 |
| 406 | 1677.46760000 | 76.93940000   | 0.00000000 |
| 407 | 1724.82340000 | 36.89190000   | 0.00000000 |
| 408 | 1847.32350000 | 65.08820000   | 0.00000000 |
| 409 | 1942.63650000 | 2433.73230000 | 0.00000000 |
| 410 | 1967.52060000 | 2253.04470000 | 0.00000000 |
| 411 | 2080.46570000 | 1997.09040000 | 0.00000000 |
| 412 | 2969.50870000 | 139.85500000  | 0.00000000 |
| 413 | 3003.74090000 | 60.16820000   | 0.00000000 |
| 414 | 3010.03240000 | 2.47580000    | 0.00000000 |
| 415 | 3017.16320000 | 88.00880000   | 0.00000000 |
| 416 | 3025.47850000 | 183.92600000  | 0.00000000 |
| 417 | 3030.83650000 | 24.91100000   | 0.00000000 |
| 418 | 3040.10850000 | 69.19860000   | 0.00000000 |
| 419 | 3043.34980000 | 9.22090000    | 0.00000000 |
| 420 | 3048.99830000 | 67.82420000   | 0.00000000 |
| 421 | 3061.88090000 | 77.34150000   | 0.00000000 |
| 422 | 3064.44120000 | 28.42880000   | 0.00000000 |
| 423 | 3066.97550000 | 61.08390000   | 0.00000000 |
| 424 | 3082.78290000 | 82.83800000   | 0.00000000 |
| 425 | 3087.26670000 | 25.02060000   | 0.00000000 |
| 426 | 3101.04350000 | 26.91100000   | 0.00000000 |
| 427 | 3106.11130000 | 86.17690000   | 0.00000000 |
| 428 | 3179.19260000 | 5.54560000    | 0.00000000 |
| 429 | 3188.21930000 | 4.44640000    | 0.00000000 |
| 430 | 3188.30400000 | 13.66270000   | 0.00000000 |
| 431 | 3190.08050000 | 14.96730000   | 0.00000000 |
| 432 | 3196.31650000 | 2.46050000    | 0.00000000 |
| 433 | 3197.87060000 | 86.62830000   | 0.00000000 |
| 434 | 3199.54570000 | 23.60540000   | 0.00000000 |
| 435 | 3207.05060000 | 84.74020000   | 0.00000000 |
| 436 | 3207.63780000 | 1.17620000    | 0.00000000 |
| 437 | 3207.78390000 | 2.19550000    | 0.00000000 |
| 438 | 3207.92030000 | 34.86490000   | 0.00000000 |
| 439 | 3212.70460000 | 22.87000000   | 0.00000000 |
| 440 | 3213.08910000 | 97.54620000   | 0.00000000 |
| 441 | 3213.76760000 | 39.40470000   | 0.00000000 |
| 442 | 3214.49580000 | 4.47790000    | 0.00000000 |
| 443 | 3214.69640000 | 0.75590000    | 0.00000000 |
| 444 | 3215.82060000 | 1367.09720000 | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 445 | 3219.64540000 | 11.65410000   | 0.00000000 |
| 446 | 3220.69080000 | 22.20070000   | 0.00000000 |
| 447 | 3221.97900000 | 36.07050000   | 0.00000000 |
| 448 | 3222.95970000 | 8.73320000    | 0.00000000 |
| 449 | 3226.66710000 | 2.85520000    | 0.00000000 |
| 450 | 3229.43410000 | 5.09020000    | 0.00000000 |
| 451 | 3230.61530000 | 4.45550000    | 0.00000000 |
| 452 | 3243.65140000 | 2.88810000    | 0.00000000 |
| 453 | 3244.90740000 | 10.89600000   | 0.00000000 |
| 454 | 3245.42430000 | 3.41950000    | 0.00000000 |
| 455 | 3248.09440000 | 0.24460000    | 0.00000000 |
| 456 | 3248.35580000 | 15.80870000   | 0.00000000 |
| 457 | 3251.85520000 | 60.35790000   | 0.00000000 |
| 458 | 3258.45820000 | 7.40400000    | 0.00000000 |
| 459 | 3262.80320000 | 0.59530000    | 0.00000000 |
| 460 | 3266.18060000 | 1.25240000    | 0.00000000 |
| 461 | 3269.48870000 | 31.81940000   | 0.00000000 |
| 462 | 3272.85680000 | 2.05120000    | 0.00000000 |
| 463 | 3272.97210000 | 23.31730000   | 0.00000000 |
| 464 | 3286.94410000 | 7.78850000    | 0.00000000 |
| 465 | 3288.12890000 | 8.96990000    | 0.00000000 |
| 466 | 3288.42720000 | 5.44580000    | 0.00000000 |
| 467 | 3400.70610000 | 855.31740000  | 0.00000000 |
| 468 | 3492.54720000 | 1241.26770000 | 0.00000000 |
| 469 | 3501.55360000 | 2137.45210000 | 0.00000000 |
| 470 | 3505.84620000 | 5.40390000    | 0.00000000 |
| 471 | 3513.54110000 | 1882.52760000 | 0.00000000 |
| 472 | 3552.58390000 | 13.57350000   | 0.00000000 |
| 473 | 3620.98670000 | 735.78580000  | 0.00000000 |
| 474 | 3698.48610000 | 514.21400000  | 0.00000000 |
| 475 | 3847.85540000 | 229.03990000  | 0.00000000 |
| 476 | 3850.77190000 | 76.64740000   | 0.00000000 |
| 477 | 3857.67070000 | 63.83790000   | 0.00000000 |

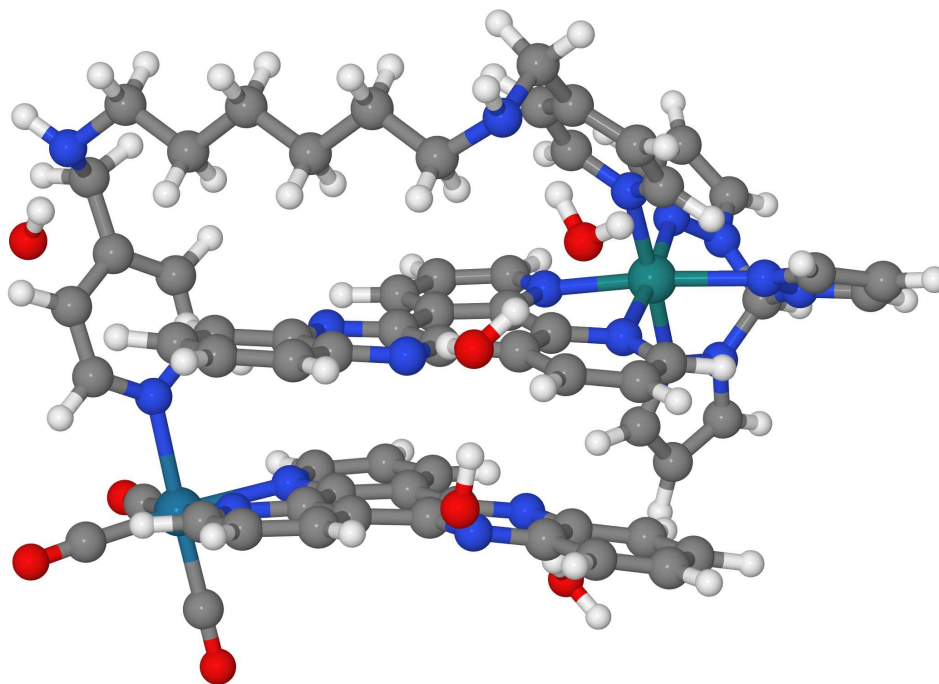
S20. CALCULATIONS ON ALTERNATIVE CONFORMER OF  $2w^{3+}$  ( $^1A$ )

FIG. S30. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+][6[Ru]578(n9ccc[n+][9C([n+]
            : 1n7ccc1)[n+][1n8ccc1)[n+][1ccc(cc1)CNCCCCCNc1cc[n+](cc1)[Re]
            : 1([n+][2cccc3c2c2[n+][1cccc2c1c3nc2cccc2n1])([C][O])([C][O])[C][O].O.O.O.O.O
Formula    : C67H66N18O8ReRu3+
Charge     : 3
Multiplicity : 1
Energy     : -4354.96766440
Gibbs Energy : -4353.81741300
Number of imaginary frequencies : 1

```

a.u.

a.u.

## S20.1. Cartesian Co-ordinates (XYZ format)

161

```

C   0.87155700  4.99361897  0.79914701
H   0.32188699  4.88033915  1.73735404
H   1.14381003  3.98456907  0.47585800
C  -0.02709700  5.65159988 -0.24911501
H   0.52723300  5.80195999 -1.18057799
H  -0.32228699  6.64660978  0.10374300
C  -1.27014303  4.81490278 -0.55040097
H  -1.84599304  4.66568279  0.36969000
H  -0.95823401  3.82016802 -0.88766098
C  -2.17293310  5.43917704 -1.61486602
H  -1.58618999  5.62102795 -2.52342391
H  -2.51900792  6.42024994 -1.26819098

```

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.27949810 | 5.19459677  | -3.00981998 |
| H | -3.71123409 | 5.35140419  | -3.93891907 |
| H | -4.60953999 | 6.17754793  | -2.66200805 |
| N | 2.12151194  | 5.70831299  | 1.12072802  |
| C | -5.24835396 | 3.14830089  | -4.00052118 |
| H | -4.34399986 | 3.21779895  | -4.61655378 |
| H | -6.08543205 | 2.98396707  | -4.68449593 |
| N | -5.49573898 | 4.39825916  | -3.26389599 |
| C | 3.05413103  | 5.87135887  | -0.01396700 |
| H | 2.59099698  | 6.36040306  | -0.87693697 |
| H | 3.87084103  | 6.51027107  | 0.32689300  |
| C | 6.84219885  | -2.12471008 | -2.06899190 |
| N | 6.41277885  | -1.29371703 | -3.17132401 |
| N | 7.40767479  | -1.30782294 | -1.01488996 |
| N | 5.74932098  | -2.92024493 | -1.56049204 |
| N | 5.46671009  | -0.34145901 | -2.95677996 |
| C | 6.88729715  | -1.24552596 | -4.44459915 |
| N | 6.64981079  | -0.36084101 | -0.38905799 |
| C | 8.65939903  | -1.37601101 | -0.49092799 |
| N | 4.67953777  | -2.28853393 | -1.01518095 |
| C | 5.62202311  | -4.27330685 | -1.46961796 |
| C | 5.34003878  | 0.30894101  | -4.11335087 |
| C | 6.21145487  | -0.22722299 | -5.07895899 |
| H | 7.64892006  | -1.92731404 | -4.78363609 |
| C | 7.45217514  | 0.16752800  | 0.53724003  |
| C | 8.72123909  | -0.43548101 | 0.51126403  |
| H | 9.38626575  | -2.07489610 | -0.86988401 |
| C | 3.86410689  | -3.24681306 | -0.58315301 |
| C | 4.41595984  | -4.51420879 | -0.84906298 |
| H | 6.38608789  | -4.93140984 | -1.84764898 |
| N | -2.95694208 | -2.61745310 | -0.73841900 |
| N | -4.17523718 | -1.34129000 | 1.28049695  |
| H | 4.64473391  | 1.12488794  | -4.20991707 |
| H | 6.32756281  | 0.09062600  | -6.10050583 |
| H | 7.10943985  | 0.94921100  | 1.19123495  |
| H | 9.56390190  | -0.20813499 | 1.14067101  |
| H | 2.94025898  | -2.98903990 | -0.09566300 |
| H | 3.96849394  | -5.46051979 | -0.60447699 |
| C | -2.38125396 | -3.24099708 | -1.77366805 |
| C | -2.18693709 | -2.26884508 | 0.32585099  |
| C | -2.84039998 | -1.55992699 | 1.40675497  |
| C | -4.80281401 | -0.63845998 | 2.22825694  |
| C | -1.02279902 | -3.54898000 | -1.79639399 |
| H | -3.02542305 | -3.50557399 | -2.60006094 |
| C | -0.82316798 | -2.58863711 | 0.39558300  |
| C | -2.11675406 | -1.13250196 | 2.52890205  |
| C | -4.14094114 | -0.13928799 | 3.34884691  |
| H | -5.86315918 | -0.48128200 | 2.09517789  |
| C | -0.24033500 | -3.23832393 | -0.70195001 |
| H | -0.60383898 | -4.04055977 | -2.66290498 |
| C | -0.08256300 | -2.26888299 | 1.61289406  |
| C | -2.79552603 | -0.39975399 | 3.51513910  |
| C | -0.71364301 | -1.51684201 | 2.65751505  |
| H | -4.69348907 | 0.43542999  | 4.07798004  |
| H | 0.80648100  | -3.49867511 | -0.68660200 |
| N | 1.16102397  | -2.70937109 | 1.74542701  |
| H | -2.26616693 | -0.04092700 | 4.38688183  |
| N | -0.06137200 | -1.21034205 | 3.76932311  |
| C | 1.82253599  | -2.44277406 | 2.89159608  |
| C | 1.19595897  | -1.67242098 | 3.92728305  |
| C | 3.13949299  | -2.93013811 | 3.08497190  |
| C | 1.90402901  | -1.40896106 | 5.12798119  |
| C | 3.79264593  | -2.66651893 | 4.26095295  |
| H | 3.60043192  | -3.51178098 | 2.29804492  |



|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.17178106  | -1.90432096 | 5.28626204  |
| H  | 1.42042601  | -0.80693799 | 5.88650799  |
| H  | 4.79752302  | -3.03908706 | 4.41355085  |
| H  | 3.71604800  | -1.70925605 | 6.20152378  |
| N  | 3.64600611  | 0.01404900  | 0.78907901  |
| N  | 2.64055109  | -0.26836699 | -1.63673699 |
| C  | 4.19432592  | 0.11748100  | 2.00352597  |
| C  | 2.34911704  | 0.39282301  | 0.62886798  |
| C  | 1.78263104  | 0.17397299  | -0.67908299 |
| C  | 2.14500594  | -0.62173200 | -2.82847595 |
| C  | 3.51155996  | 0.68549198  | 3.07581997  |
| H  | 5.20902920  | -0.23886900 | 2.10659409  |
| C  | 1.58891797  | 0.95333701  | 1.66278100  |
| C  | 0.42102599  | 0.37347600  | -0.92407697 |
| C  | 0.78885901  | -0.49116099 | -3.13171911 |
| H  | 2.85500312  | -0.99280202 | -3.55375791 |
| C  | 2.21152091  | 1.12517405  | 2.90704393  |
| H  | 4.00784111  | 0.77913302  | 4.03041792  |
| C  | 0.19959900  | 1.31940305  | 1.38651705  |
| C  | -0.07580400 | 0.03668400  | -2.18959188 |
| C  | -0.39926600 | 0.96517801  | 0.12865201  |
| H  | 0.43669701  | -0.78330302 | -4.11124992 |
| H  | 1.68027496  | 1.58467996  | 3.72487903  |
| N  | -0.50066501 | 1.96526599  | 2.30629706  |
| H  | -1.12179804 | 0.19541200  | -2.40409493 |
| N  | -1.67539597 | 1.20631897  | -0.12210000 |
| C  | -1.79133296 | 2.26700211  | 2.04783297  |
| C  | -2.39710808 | 1.85136795  | 0.81629300  |
| C  | -2.55415702 | 3.00336194  | 2.98892498  |
| C  | -3.75074697 | 2.17741394  | 0.56865603  |
| C  | -3.86055493 | 3.31253910  | 2.70633411  |
| H  | -2.08213305 | 3.31146502  | 3.91258407  |
| C  | -4.46362019 | 2.89998388  | 1.48912394  |
| H  | -4.18345118 | 1.87856197  | -0.37178701 |
| H  | -4.44393301 | 3.88177299  | 3.41905999  |
| H  | -5.48134518 | 3.18789291  | 1.25875199  |
| H  | 7.61493301  | -2.79563189 | -2.42944193 |
| C  | 3.60707092  | 4.53067207  | -0.42678201 |
| C  | 4.53827190  | 3.87270403  | 0.37626499  |
| C  | 3.17896104  | 3.86916590  | -1.57601202 |
| C  | 4.94559383  | 2.59672308  | 0.04285500  |
| H  | 4.91865778  | 4.33023214  | 1.27921402  |
| C  | 3.61914396  | 2.57897091  | -1.83381402 |
| H  | 2.47441101  | 4.32914305  | -2.25672102 |
| N  | 4.46849918  | 1.92144299  | -1.02229595 |
| H  | 5.64301491  | 2.07334900  | 0.67251199  |
| H  | 3.24346995  | 2.03664994  | -2.68841791 |
| C  | -5.15851212 | 1.93043697  | -3.11004210 |
| C  | -4.10636806 | 1.02229500  | -3.20460296 |
| C  | -6.16450214 | 1.64183998  | -2.18597603 |
| C  | -4.10034323 | -0.11465200 | -2.41162491 |
| H  | -3.28870010 | 1.18940902  | -3.89396596 |
| C  | -6.09619904 | 0.48597100  | -1.43317604 |
| H  | -7.00354004 | 2.30818391  | -2.04763389 |
| N  | -5.08137608 | -0.40057701 | -1.53650403 |
| H  | -3.29265094 | -0.82628101 | -2.48038197 |
| H  | -6.87623692 | 0.25551000  | -0.72388899 |
| H  | -6.13832808 | 4.96419001  | -3.80594301 |
| C  | -3.37859988 | 4.56318092  | -1.95423198 |
| H  | -3.97135997 | 4.37740517  | -1.05604196 |
| H  | -3.02291894 | 3.58698893  | -2.29975200 |
| H  | 1.89248598  | 6.63303709  | 1.47523904  |
| Ru | 4.62163877  | -0.22127900 | -1.04731095 |
| Re | -5.14426279 | -2.36349106 | -0.43270400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.14975023 | -4.06099987 | 0.51459002  |
| O | -5.14529800 | -5.06770277 | 1.07240403  |
| C | -5.75516510 | -3.23498297 | -2.05700707 |
| O | -6.09181976 | -3.74063897 | -3.03568292 |
| C | -6.98705101 | -2.10013509 | 0.10264700  |
| O | -8.07457161 | -1.95674503 | 0.45973700  |
| H | 2.69734097  | 4.82727718  | 2.59469008  |
| O | 2.89091396  | 4.28832817  | 3.40663695  |
| H | 3.50572705  | 4.81952620  | 3.92343807  |
| H | -6.27136612 | 4.37966394  | -1.53013003 |
| O | -6.61921310 | 4.41188717  | -0.61036003 |
| H | -6.25838423 | 5.22762489  | -0.24820501 |
| H | 0.17404500  | 3.01794100  | 3.71873403  |
| O | 0.51458198  | 3.43230510  | 4.53327322  |
| H | 1.38165998  | 3.80212092  | 4.25837803  |
| H | -0.29806700 | 0.39342001  | 5.03461790  |
| O | -0.38750300 | 1.01942694  | 5.76855993  |
| H | -0.00373700 | 1.85553396  | 5.44811201  |
| H | 1.57637596  | -4.55608606 | 1.12785900  |
| O | 1.77365696  | -5.41409922 | 0.71928102  |
| H | 2.18206906  | -5.92825890 | 1.42369103  |

## S20.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -2.49430000  | 1.09040000   | 0.00000000      |
| 2    | 9.10430000   | 0.13660000   | 0.00000000      |
| 3    | 18.67740000  | 0.79660000   | 0.00000000      |
| 4    | 23.04480000  | 0.71660000   | 0.00000000      |
| 5    | 25.08040000  | 0.73190000   | 0.00000000      |
| 6    | 28.98400000  | 1.00570000   | 0.00000000      |
| 7    | 35.36520000  | 0.05300000   | 0.00000000      |
| 8    | 36.87700000  | 2.35540000   | 0.00000000      |
| 9    | 40.60150000  | 1.72020000   | 0.00000000      |
| 10   | 43.70560000  | 5.66540000   | 0.00000000      |
| 11   | 44.85210000  | 0.43330000   | 0.00000000      |
| 12   | 47.20930000  | 3.55660000   | 0.00000000      |
| 13   | 49.70820000  | 8.41430000   | 0.00000000      |
| 14   | 52.71000000  | 0.73290000   | 0.00000000      |
| 15   | 54.44000000  | 0.82680000   | 0.00000000      |
| 16   | 55.14790000  | 7.01500000   | 0.00000000      |
| 17   | 57.13700000  | 10.94170000  | 0.00000000      |
| 18   | 59.15220000  | 16.41810000  | 0.00000000      |
| 19   | 62.62340000  | 1.15960000   | 0.00000000      |
| 20   | 64.39380000  | 4.67330000   | 0.00000000      |
| 21   | 68.56510000  | 2.09670000   | 0.00000000      |
| 22   | 70.15530000  | 4.81140000   | 0.00000000      |
| 23   | 70.51450000  | 1.14730000   | 0.00000000      |
| 24   | 74.73160000  | 4.08440000   | 0.00000000      |
| 25   | 77.05080000  | 4.34900000   | 0.00000000      |
| 26   | 81.10460000  | 4.97250000   | 0.00000000      |
| 27   | 84.58410000  | 0.31610000   | 0.00000000      |
| 28   | 85.37150000  | 5.78200000   | 0.00000000      |
| 29   | 89.09360000  | 1.35740000   | 0.00000000      |
| 30   | 90.89970000  | 3.60240000   | 0.00000000      |
| 31   | 92.36220000  | 0.74580000   | 0.00000000      |
| 32   | 96.18640000  | 5.26010000   | 0.00000000      |
| 33   | 96.54160000  | 16.20660000  | 0.00000000      |
| 34   | 101.45050000 | 1.37830000   | 0.00000000      |
| 35   | 102.51030000 | 45.54510000  | 0.00000000      |
| 36   | 103.03460000 | 14.34080000  | 0.00000000      |
| 37   | 103.87560000 | 13.01240000  | 0.00000000      |
| 38   | 108.11310000 | 3.03790000   | 0.00000000      |
| 39   | 113.54200000 | 11.07400000  | 0.00000000      |
| 40   | 117.01070000 | 3.37700000   | 0.00000000      |
| 41   | 120.70800000 | 5.95030000   | 0.00000000      |
| 42   | 123.31310000 | 3.91770000   | 0.00000000      |
| 43   | 129.12030000 | 3.94730000   | 0.00000000      |
| 44   | 130.31580000 | 4.17870000   | 0.00000000      |
| 45   | 132.95220000 | 8.70240000   | 0.00000000      |
| 46   | 134.84190000 | 5.31430000   | 0.00000000      |
| 47   | 139.88260000 | 6.11290000   | 0.00000000      |
| 48   | 142.53850000 | 1.86600000   | 0.00000000      |
| 49   | 145.23250000 | 3.97070000   | 0.00000000      |
| 50   | 147.13580000 | 3.25780000   | 0.00000000      |
| 51   | 148.60450000 | 12.11030000  | 0.00000000      |
| 52   | 152.52800000 | 38.58210000  | 0.00000000      |
| 53   | 156.48160000 | 35.83310000  | 0.00000000      |
| 54   | 159.00420000 | 39.99220000  | 0.00000000      |
| 55   | 162.94400000 | 5.81640000   | 0.00000000      |
| 56   | 165.41510000 | 1.64020000   | 0.00000000      |
| 57   | 168.66750000 | 7.79590000   | 0.00000000      |
| 58   | 170.18470000 | 13.20380000  | 0.00000000      |
| 59   | 173.05440000 | 3.13850000   | 0.00000000      |
| 60   | 175.86310000 | 0.93780000   | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 177.24240000 | 2.14760000   | 0.00000000 |
| 62  | 179.31990000 | 5.08810000   | 0.00000000 |
| 63  | 184.49920000 | 6.22190000   | 0.00000000 |
| 64  | 187.13650000 | 5.80350000   | 0.00000000 |
| 65  | 190.20780000 | 1.31640000   | 0.00000000 |
| 66  | 193.31110000 | 13.13370000  | 0.00000000 |
| 67  | 194.87100000 | 0.58190000   | 0.00000000 |
| 68  | 199.04120000 | 19.11280000  | 0.00000000 |
| 69  | 203.46730000 | 7.52200000   | 0.00000000 |
| 70  | 207.85880000 | 28.96570000  | 0.00000000 |
| 71  | 212.91490000 | 51.98980000  | 0.00000000 |
| 72  | 218.92780000 | 89.79970000  | 0.00000000 |
| 73  | 222.81870000 | 21.08040000  | 0.00000000 |
| 74  | 227.92800000 | 4.88600000   | 0.00000000 |
| 75  | 229.38250000 | 6.67580000   | 0.00000000 |
| 76  | 234.01170000 | 24.23230000  | 0.00000000 |
| 77  | 238.80010000 | 2.51180000   | 0.00000000 |
| 78  | 254.48890000 | 101.26810000 | 0.00000000 |
| 79  | 256.75980000 | 3.09400000   | 0.00000000 |
| 80  | 262.25270000 | 1.28380000   | 0.00000000 |
| 81  | 265.83210000 | 3.59970000   | 0.00000000 |
| 82  | 275.65320000 | 3.27650000   | 0.00000000 |
| 83  | 279.71730000 | 2.78870000   | 0.00000000 |
| 84  | 290.92800000 | 10.70170000  | 0.00000000 |
| 85  | 301.95680000 | 3.99450000   | 0.00000000 |
| 86  | 311.36090000 | 2.04200000   | 0.00000000 |
| 87  | 314.79050000 | 2.87580000   | 0.00000000 |
| 88  | 321.38180000 | 1.46980000   | 0.00000000 |
| 89  | 327.14390000 | 0.77990000   | 0.00000000 |
| 90  | 329.06700000 | 10.49660000  | 0.00000000 |
| 91  | 329.58170000 | 3.64070000   | 0.00000000 |
| 92  | 333.91390000 | 4.53200000   | 0.00000000 |
| 93  | 338.93830000 | 14.90370000  | 0.00000000 |
| 94  | 342.30220000 | 3.54630000   | 0.00000000 |
| 95  | 343.79950000 | 1.19190000   | 0.00000000 |
| 96  | 359.23000000 | 7.74250000   | 0.00000000 |
| 97  | 365.08450000 | 49.43410000  | 0.00000000 |
| 98  | 368.09660000 | 6.08100000   | 0.00000000 |
| 99  | 372.39570000 | 104.48600000 | 0.00000000 |
| 100 | 380.48090000 | 4.42850000   | 0.00000000 |
| 101 | 381.43310000 | 1.23920000   | 0.00000000 |
| 102 | 389.43330000 | 3.85020000   | 0.00000000 |
| 103 | 391.65100000 | 7.71200000   | 0.00000000 |
| 104 | 395.06330000 | 3.01340000   | 0.00000000 |
| 105 | 396.70860000 | 1.17510000   | 0.00000000 |
| 106 | 406.39240000 | 1.17950000   | 0.00000000 |
| 107 | 407.60170000 | 0.54350000   | 0.00000000 |
| 108 | 417.82280000 | 3.24790000   | 0.00000000 |
| 109 | 421.52710000 | 0.76200000   | 0.00000000 |
| 110 | 427.36060000 | 1.36520000   | 0.00000000 |
| 111 | 434.31660000 | 10.31930000  | 0.00000000 |
| 112 | 442.87520000 | 4.29080000   | 0.00000000 |
| 113 | 443.77080000 | 4.09420000   | 0.00000000 |
| 114 | 445.20740000 | 28.78510000  | 0.00000000 |
| 115 | 454.30930000 | 11.97130000  | 0.00000000 |
| 116 | 472.80870000 | 27.18060000  | 0.00000000 |
| 117 | 474.40850000 | 17.97950000  | 0.00000000 |
| 118 | 478.48570000 | 0.11260000   | 0.00000000 |
| 119 | 479.41490000 | 1.15200000   | 0.00000000 |
| 120 | 480.92240000 | 101.70360000 | 0.00000000 |
| 121 | 486.79700000 | 21.94640000  | 0.00000000 |
| 122 | 492.69290000 | 51.47780000  | 0.00000000 |
| 123 | 494.53650000 | 7.29340000   | 0.00000000 |
| 124 | 496.16000000 | 23.01260000  | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 499.41120000 | 3.71980000   | 0.00000000 |
| 126 | 502.70020000 | 16.26770000  | 0.00000000 |
| 127 | 505.68580000 | 6.79410000   | 0.00000000 |
| 128 | 511.42730000 | 31.97760000  | 0.00000000 |
| 129 | 514.62520000 | 7.92410000   | 0.00000000 |
| 130 | 517.86020000 | 64.65070000  | 0.00000000 |
| 131 | 519.66950000 | 12.57980000  | 0.00000000 |
| 132 | 533.28710000 | 19.73750000  | 0.00000000 |
| 133 | 535.31260000 | 14.72080000  | 0.00000000 |
| 134 | 537.28950000 | 11.49300000  | 0.00000000 |
| 135 | 541.42020000 | 24.62380000  | 0.00000000 |
| 136 | 546.44260000 | 146.00820000 | 0.00000000 |
| 137 | 559.84200000 | 5.41180000   | 0.00000000 |
| 138 | 563.20370000 | 2.20580000   | 0.00000000 |
| 139 | 576.16250000 | 42.12540000  | 0.00000000 |
| 140 | 576.79250000 | 7.78440000   | 0.00000000 |
| 141 | 577.28620000 | 13.23710000  | 0.00000000 |
| 142 | 578.63600000 | 15.17670000  | 0.00000000 |
| 143 | 583.51750000 | 77.05160000  | 0.00000000 |
| 144 | 594.23420000 | 15.40490000  | 0.00000000 |
| 145 | 596.62600000 | 33.58250000  | 0.00000000 |
| 146 | 602.85820000 | 22.32650000  | 0.00000000 |
| 147 | 604.20220000 | 1.36820000   | 0.00000000 |
| 148 | 605.24110000 | 4.78140000   | 0.00000000 |
| 149 | 616.72800000 | 11.10930000  | 0.00000000 |
| 150 | 617.56530000 | 23.45850000  | 0.00000000 |
| 151 | 621.30740000 | 25.78980000  | 0.00000000 |
| 152 | 624.70160000 | 36.56130000  | 0.00000000 |
| 153 | 624.86960000 | 23.15330000  | 0.00000000 |
| 154 | 631.40210000 | 29.30590000  | 0.00000000 |
| 155 | 646.32840000 | 34.90520000  | 0.00000000 |
| 156 | 648.06900000 | 38.35000000  | 0.00000000 |
| 157 | 650.13240000 | 84.97130000  | 0.00000000 |
| 158 | 653.50690000 | 33.28320000  | 0.00000000 |
| 159 | 655.37690000 | 6.53120000   | 0.00000000 |
| 160 | 658.69990000 | 8.71530000   | 0.00000000 |
| 161 | 662.47490000 | 34.12680000  | 0.00000000 |
| 162 | 667.52620000 | 0.59900000   | 0.00000000 |
| 163 | 676.23390000 | 56.28710000  | 0.00000000 |
| 164 | 678.40290000 | 0.53550000   | 0.00000000 |
| 165 | 681.93160000 | 0.27620000   | 0.00000000 |
| 166 | 685.20470000 | 0.98060000   | 0.00000000 |
| 167 | 686.41070000 | 0.44760000   | 0.00000000 |
| 168 | 694.90830000 | 113.51100000 | 0.00000000 |
| 169 | 738.09360000 | 48.23490000  | 0.00000000 |
| 170 | 740.69610000 | 17.75810000  | 0.00000000 |
| 171 | 741.22300000 | 20.64140000  | 0.00000000 |
| 172 | 742.58780000 | 11.65630000  | 0.00000000 |
| 173 | 744.38830000 | 40.22980000  | 0.00000000 |
| 174 | 746.26730000 | 13.44320000  | 0.00000000 |
| 175 | 746.78090000 | 94.30340000  | 0.00000000 |
| 176 | 747.52760000 | 176.43950000 | 0.00000000 |
| 177 | 749.20640000 | 7.85220000   | 0.00000000 |
| 178 | 750.74190000 | 11.78200000  | 0.00000000 |
| 179 | 755.60270000 | 12.58390000  | 0.00000000 |
| 180 | 756.13330000 | 56.94710000  | 0.00000000 |
| 181 | 758.20730000 | 25.89660000  | 0.00000000 |
| 182 | 759.06220000 | 74.15140000  | 0.00000000 |
| 183 | 760.54910000 | 80.73520000  | 0.00000000 |
| 184 | 761.28540000 | 105.62120000 | 0.00000000 |
| 185 | 768.78400000 | 25.32090000  | 0.00000000 |
| 186 | 779.86060000 | 108.51210000 | 0.00000000 |
| 187 | 781.76640000 | 86.36870000  | 0.00000000 |
| 188 | 783.89720000 | 147.41060000 | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 189 | 786.93530000  | 28.01000000  | 0.00000000 |
| 190 | 793.59250000  | 73.03030000  | 0.00000000 |
| 191 | 799.08800000  | 85.57630000  | 0.00000000 |
| 192 | 800.08120000  | 54.83200000  | 0.00000000 |
| 193 | 801.46630000  | 110.62680000 | 0.00000000 |
| 194 | 810.94040000  | 10.98580000  | 0.00000000 |
| 195 | 813.33760000  | 6.63270000   | 0.00000000 |
| 196 | 815.44260000  | 12.73560000  | 0.00000000 |
| 197 | 817.34100000  | 128.15080000 | 0.00000000 |
| 198 | 821.72780000  | 17.88900000  | 0.00000000 |
| 199 | 822.73850000  | 107.03110000 | 0.00000000 |
| 200 | 825.87250000  | 4.41880000   | 0.00000000 |
| 201 | 832.04800000  | 53.88470000  | 0.00000000 |
| 202 | 836.50640000  | 58.15840000  | 0.00000000 |
| 203 | 848.40150000  | 60.63260000  | 0.00000000 |
| 204 | 849.56640000  | 51.83050000  | 0.00000000 |
| 205 | 860.78980000  | 23.19130000  | 0.00000000 |
| 206 | 865.16420000  | 6.85140000   | 0.00000000 |
| 207 | 866.09320000  | 1.98890000   | 0.00000000 |
| 208 | 867.29640000  | 5.97950000   | 0.00000000 |
| 209 | 868.70190000  | 18.31740000  | 0.00000000 |
| 210 | 873.47010000  | 34.83260000  | 0.00000000 |
| 211 | 875.65850000  | 59.96350000  | 0.00000000 |
| 212 | 879.65370000  | 1.63770000   | 0.00000000 |
| 213 | 885.84860000  | 12.23170000  | 0.00000000 |
| 214 | 887.69340000  | 57.40400000  | 0.00000000 |
| 215 | 889.33660000  | 24.40460000  | 0.00000000 |
| 216 | 890.79060000  | 65.87830000  | 0.00000000 |
| 217 | 895.54200000  | 1.41090000   | 0.00000000 |
| 218 | 900.27230000  | 87.22110000  | 0.00000000 |
| 219 | 915.68220000  | 2.75890000   | 0.00000000 |
| 220 | 917.18710000  | 1.00670000   | 0.00000000 |
| 221 | 918.21940000  | 25.04140000  | 0.00000000 |
| 222 | 922.01440000  | 2.32150000   | 0.00000000 |
| 223 | 923.63340000  | 1.21600000   | 0.00000000 |
| 224 | 931.40180000  | 121.20440000 | 0.00000000 |
| 225 | 943.92940000  | 1.12520000   | 0.00000000 |
| 226 | 944.94580000  | 2.00180000   | 0.00000000 |
| 227 | 948.93760000  | 0.48320000   | 0.00000000 |
| 228 | 954.54130000  | 0.85450000   | 0.00000000 |
| 229 | 968.96180000  | 8.44970000   | 0.00000000 |
| 230 | 970.90800000  | 0.53290000   | 0.00000000 |
| 231 | 974.73330000  | 11.43880000  | 0.00000000 |
| 232 | 978.85950000  | 1.37140000   | 0.00000000 |
| 233 | 983.31200000  | 3.23760000   | 0.00000000 |
| 234 | 989.54040000  | 8.46160000   | 0.00000000 |
| 235 | 990.67830000  | 9.27210000   | 0.00000000 |
| 236 | 992.45620000  | 2.51880000   | 0.00000000 |
| 237 | 992.77990000  | 11.12700000  | 0.00000000 |
| 238 | 998.13050000  | 2.50850000   | 0.00000000 |
| 239 | 1000.39890000 | 0.73130000   | 0.00000000 |
| 240 | 1000.71870000 | 8.14850000   | 0.00000000 |
| 241 | 1003.92270000 | 9.63770000   | 0.00000000 |
| 242 | 1009.34860000 | 10.33930000  | 0.00000000 |
| 243 | 1010.07620000 | 9.53890000   | 0.00000000 |
| 244 | 1010.56710000 | 1.10380000   | 0.00000000 |
| 245 | 1011.18720000 | 4.40370000   | 0.00000000 |
| 246 | 1012.57340000 | 17.75300000  | 0.00000000 |
| 247 | 1014.83100000 | 2.33090000   | 0.00000000 |
| 248 | 1017.25870000 | 27.61340000  | 0.00000000 |
| 249 | 1017.82330000 | 0.08120000   | 0.00000000 |
| 250 | 1019.98780000 | 2.38970000   | 0.00000000 |
| 251 | 1023.15340000 | 7.10390000   | 0.00000000 |
| 252 | 1026.68580000 | 0.39750000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1029.88520000 | 10.44440000  | 0.00000000 |
| 254 | 1034.08350000 | 0.48540000   | 0.00000000 |
| 255 | 1035.38650000 | 0.59170000   | 0.00000000 |
| 256 | 1037.01780000 | 0.32700000   | 0.00000000 |
| 257 | 1047.06620000 | 1.22020000   | 0.00000000 |
| 258 | 1049.04980000 | 4.11480000   | 0.00000000 |
| 259 | 1050.83980000 | 14.04100000  | 0.00000000 |
| 260 | 1069.30540000 | 24.97470000  | 0.00000000 |
| 261 | 1069.55010000 | 38.72530000  | 0.00000000 |
| 262 | 1070.10500000 | 5.51880000   | 0.00000000 |
| 263 | 1072.38470000 | 0.89920000   | 0.00000000 |
| 264 | 1074.02940000 | 39.88380000  | 0.00000000 |
| 265 | 1074.06410000 | 1.12270000   | 0.00000000 |
| 266 | 1079.74400000 | 17.78420000  | 0.00000000 |
| 267 | 1081.24850000 | 80.44470000  | 0.00000000 |
| 268 | 1089.62970000 | 1.78130000   | 0.00000000 |
| 269 | 1091.53300000 | 6.85830000   | 0.00000000 |
| 270 | 1094.51960000 | 24.11990000  | 0.00000000 |
| 271 | 1107.67690000 | 27.03300000  | 0.00000000 |
| 272 | 1108.03530000 | 42.22740000  | 0.00000000 |
| 273 | 1120.18870000 | 46.60900000  | 0.00000000 |
| 274 | 1120.92530000 | 77.62240000  | 0.00000000 |
| 275 | 1122.59470000 | 65.52810000  | 0.00000000 |
| 276 | 1124.52390000 | 45.02160000  | 0.00000000 |
| 277 | 1125.63010000 | 59.89840000  | 0.00000000 |
| 278 | 1126.57220000 | 14.52110000  | 0.00000000 |
| 279 | 1129.71680000 | 8.71400000   | 0.00000000 |
| 280 | 1131.19030000 | 10.14920000  | 0.00000000 |
| 281 | 1141.31770000 | 21.58870000  | 0.00000000 |
| 282 | 1145.90210000 | 40.56180000  | 0.00000000 |
| 283 | 1147.73260000 | 6.02930000   | 0.00000000 |
| 284 | 1149.94110000 | 12.55540000  | 0.00000000 |
| 285 | 1159.33350000 | 4.13200000   | 0.00000000 |
| 286 | 1162.75630000 | 0.19290000   | 0.00000000 |
| 287 | 1164.41010000 | 19.56000000  | 0.00000000 |
| 288 | 1168.84140000 | 29.41460000  | 0.00000000 |
| 289 | 1174.12800000 | 12.47380000  | 0.00000000 |
| 290 | 1178.42300000 | 4.23410000   | 0.00000000 |
| 291 | 1180.24210000 | 2.50580000   | 0.00000000 |
| 292 | 1201.69930000 | 4.96410000   | 0.00000000 |
| 293 | 1211.72310000 | 3.33250000   | 0.00000000 |
| 294 | 1214.05940000 | 0.88100000   | 0.00000000 |
| 295 | 1217.82790000 | 9.44050000   | 0.00000000 |
| 296 | 1225.07950000 | 1.91260000   | 0.00000000 |
| 297 | 1234.56820000 | 11.22980000  | 0.00000000 |
| 298 | 1237.26670000 | 4.25700000   | 0.00000000 |
| 299 | 1240.38320000 | 1.58030000   | 0.00000000 |
| 300 | 1247.29010000 | 10.65600000  | 0.00000000 |
| 301 | 1247.69260000 | 35.59550000  | 0.00000000 |
| 302 | 1250.21560000 | 2.29600000   | 0.00000000 |
| 303 | 1250.80970000 | 1.54230000   | 0.00000000 |
| 304 | 1258.05650000 | 17.15130000  | 0.00000000 |
| 305 | 1263.93230000 | 11.72450000  | 0.00000000 |
| 306 | 1268.55010000 | 71.61730000  | 0.00000000 |
| 307 | 1269.16910000 | 30.24870000  | 0.00000000 |
| 308 | 1272.84350000 | 2.25070000   | 0.00000000 |
| 309 | 1275.84360000 | 111.91250000 | 0.00000000 |
| 310 | 1276.01220000 | 4.42100000   | 0.00000000 |
| 311 | 1278.07510000 | 6.36610000   | 0.00000000 |
| 312 | 1281.99480000 | 6.62680000   | 0.00000000 |
| 313 | 1282.34530000 | 1.59750000   | 0.00000000 |
| 314 | 1301.23240000 | 8.32300000   | 0.00000000 |
| 315 | 1304.12890000 | 3.67170000   | 0.00000000 |
| 316 | 1305.71830000 | 7.58370000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 317 | 1309.97850000 | 12.44580000  | 0.00000000 |
| 318 | 1312.53400000 | 3.73670000   | 0.00000000 |
| 319 | 1312.55170000 | 11.53430000  | 0.00000000 |
| 320 | 1318.48160000 | 10.94250000  | 0.00000000 |
| 321 | 1320.94900000 | 25.99800000  | 0.00000000 |
| 322 | 1324.13080000 | 87.52530000  | 0.00000000 |
| 323 | 1326.34300000 | 123.12650000 | 0.00000000 |
| 324 | 1328.85170000 | 1.47000000   | 0.00000000 |
| 325 | 1332.58650000 | 0.67020000   | 0.00000000 |
| 326 | 1336.96070000 | 0.41080000   | 0.00000000 |
| 327 | 1337.35300000 | 0.03350000   | 0.00000000 |
| 328 | 1342.17590000 | 3.21550000   | 0.00000000 |
| 329 | 1346.00000000 | 7.55880000   | 0.00000000 |
| 330 | 1350.19400000 | 10.75390000  | 0.00000000 |
| 331 | 1351.40890000 | 16.86030000  | 0.00000000 |
| 332 | 1351.74790000 | 2.47370000   | 0.00000000 |
| 333 | 1367.92210000 | 0.86540000   | 0.00000000 |
| 334 | 1371.33930000 | 219.71680000 | 0.00000000 |
| 335 | 1374.06550000 | 1.01890000   | 0.00000000 |
| 336 | 1374.40630000 | 6.48280000   | 0.00000000 |
| 337 | 1375.62740000 | 48.42800000  | 0.00000000 |
| 338 | 1377.13590000 | 12.87930000  | 0.00000000 |
| 339 | 1377.72570000 | 175.83440000 | 0.00000000 |
| 340 | 1381.07190000 | 4.60010000   | 0.00000000 |
| 341 | 1381.79570000 | 4.56300000   | 0.00000000 |
| 342 | 1390.37000000 | 10.35510000  | 0.00000000 |
| 343 | 1391.85000000 | 14.72420000  | 0.00000000 |
| 344 | 1406.70910000 | 8.34140000   | 0.00000000 |
| 345 | 1410.66540000 | 7.76620000   | 0.00000000 |
| 346 | 1412.05380000 | 15.32400000  | 0.00000000 |
| 347 | 1416.91930000 | 11.95850000  | 0.00000000 |
| 348 | 1426.30650000 | 9.12060000   | 0.00000000 |
| 349 | 1430.05960000 | 6.11980000   | 0.00000000 |
| 350 | 1431.61560000 | 10.83340000  | 0.00000000 |
| 351 | 1436.31120000 | 62.57390000  | 0.00000000 |
| 352 | 1438.64290000 | 49.59250000  | 0.00000000 |
| 353 | 1443.59250000 | 172.83100000 | 0.00000000 |
| 354 | 1454.87850000 | 36.87660000  | 0.00000000 |
| 355 | 1455.67250000 | 99.86020000  | 0.00000000 |
| 356 | 1455.88660000 | 119.57440000 | 0.00000000 |
| 357 | 1464.08060000 | 42.51400000  | 0.00000000 |
| 358 | 1472.82930000 | 88.69310000  | 0.00000000 |
| 359 | 1475.05060000 | 11.73870000  | 0.00000000 |
| 360 | 1476.15250000 | 21.04320000  | 0.00000000 |
| 361 | 1476.82410000 | 16.60620000  | 0.00000000 |
| 362 | 1479.31650000 | 70.28920000  | 0.00000000 |
| 363 | 1481.92140000 | 2.97850000   | 0.00000000 |
| 364 | 1483.59540000 | 2.05280000   | 0.00000000 |
| 365 | 1492.81160000 | 3.02020000   | 0.00000000 |
| 366 | 1494.89380000 | 2.30530000   | 0.00000000 |
| 367 | 1495.71950000 | 32.57070000  | 0.00000000 |
| 368 | 1497.01390000 | 1.39660000   | 0.00000000 |
| 369 | 1500.78140000 | 10.93260000  | 0.00000000 |
| 370 | 1501.89340000 | 4.92510000   | 0.00000000 |
| 371 | 1502.86430000 | 19.35190000  | 0.00000000 |
| 372 | 1507.03240000 | 6.19280000   | 0.00000000 |
| 373 | 1507.76010000 | 1.75830000   | 0.00000000 |
| 374 | 1510.81160000 | 3.48020000   | 0.00000000 |
| 375 | 1512.95970000 | 6.10590000   | 0.00000000 |
| 376 | 1520.30620000 | 28.57500000  | 0.00000000 |
| 377 | 1525.21580000 | 26.45280000  | 0.00000000 |
| 378 | 1525.44810000 | 34.68470000  | 0.00000000 |
| 379 | 1529.72580000 | 43.46610000  | 0.00000000 |
| 380 | 1531.70100000 | 151.16650000 | 0.00000000 |



|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 1538.31990000 | 7.02050000    | 0.00000000 |
| 382 | 1544.17470000 | 16.62740000   | 0.00000000 |
| 383 | 1552.41040000 | 10.94010000   | 0.00000000 |
| 384 | 1553.43070000 | 9.24660000    | 0.00000000 |
| 385 | 1558.03770000 | 12.67240000   | 0.00000000 |
| 386 | 1573.91270000 | 5.98460000    | 0.00000000 |
| 387 | 1575.95610000 | 6.33890000    | 0.00000000 |
| 388 | 1584.47950000 | 25.11200000   | 0.00000000 |
| 389 | 1585.26800000 | 9.76360000    | 0.00000000 |
| 390 | 1597.83380000 | 5.52930000    | 0.00000000 |
| 391 | 1599.83340000 | 5.14300000    | 0.00000000 |
| 392 | 1609.88280000 | 7.08030000    | 0.00000000 |
| 393 | 1614.31460000 | 22.51990000   | 0.00000000 |
| 394 | 1622.25570000 | 5.11780000    | 0.00000000 |
| 395 | 1623.21690000 | 0.69480000    | 0.00000000 |
| 396 | 1624.54860000 | 2.16290000    | 0.00000000 |
| 397 | 1625.07750000 | 2.64890000    | 0.00000000 |
| 398 | 1637.99910000 | 4.44420000    | 0.00000000 |
| 399 | 1639.12220000 | 3.49260000    | 0.00000000 |
| 400 | 1656.16710000 | 163.08680000  | 0.00000000 |
| 401 | 1659.61430000 | 18.70410000   | 0.00000000 |
| 402 | 1659.92550000 | 33.56540000   | 0.00000000 |
| 403 | 1660.83310000 | 78.09680000   | 0.00000000 |
| 404 | 1662.91560000 | 102.23290000  | 0.00000000 |
| 405 | 1663.22920000 | 46.96090000   | 0.00000000 |
| 406 | 1677.20690000 | 51.06060000   | 0.00000000 |
| 407 | 1691.15190000 | 76.94720000   | 0.00000000 |
| 408 | 1716.05300000 | 54.62400000   | 0.00000000 |
| 409 | 1965.49450000 | 2266.19950000 | 0.00000000 |
| 410 | 1974.75810000 | 2308.16010000 | 0.00000000 |
| 411 | 2087.16730000 | 2038.49940000 | 0.00000000 |
| 412 | 2966.16410000 | 130.49250000  | 0.00000000 |
| 413 | 3003.00830000 | 41.47850000   | 0.00000000 |
| 414 | 3010.33230000 | 72.29380000   | 0.00000000 |
| 415 | 3013.40490000 | 2.96990000    | 0.00000000 |
| 416 | 3019.18090000 | 48.40590000   | 0.00000000 |
| 417 | 3026.19930000 | 37.10850000   | 0.00000000 |
| 418 | 3027.78410000 | 144.50660000  | 0.00000000 |
| 419 | 3034.56570000 | 26.48520000   | 0.00000000 |
| 420 | 3040.73970000 | 45.61840000   | 0.00000000 |
| 421 | 3046.78680000 | 49.83170000   | 0.00000000 |
| 422 | 3058.59910000 | 68.13020000   | 0.00000000 |
| 423 | 3063.36030000 | 49.88650000   | 0.00000000 |
| 424 | 3069.70860000 | 15.84560000   | 0.00000000 |
| 425 | 3082.75560000 | 93.56880000   | 0.00000000 |
| 426 | 3088.64430000 | 23.41940000   | 0.00000000 |
| 427 | 3091.80630000 | 86.97880000   | 0.00000000 |
| 428 | 3180.35830000 | 1.09000000    | 0.00000000 |
| 429 | 3190.41630000 | 4.36140000    | 0.00000000 |
| 430 | 3190.46530000 | 10.56110000   | 0.00000000 |
| 431 | 3196.69950000 | 2.89530000    | 0.00000000 |
| 432 | 3198.67420000 | 2.89360000    | 0.00000000 |
| 433 | 3199.28880000 | 5.80780000    | 0.00000000 |
| 434 | 3202.38960000 | 2.15440000    | 0.00000000 |
| 435 | 3206.84770000 | 9.45350000    | 0.00000000 |
| 436 | 3208.27360000 | 1436.30250000 | 0.00000000 |
| 437 | 3208.98350000 | 87.19510000   | 0.00000000 |
| 438 | 3211.95400000 | 37.48640000   | 0.00000000 |
| 439 | 3213.02760000 | 22.03280000   | 0.00000000 |
| 440 | 3213.48010000 | 0.01140000    | 0.00000000 |
| 441 | 3215.76110000 | 15.76680000   | 0.00000000 |
| 442 | 3217.65910000 | 0.15300000    | 0.00000000 |
| 443 | 3220.49240000 | 0.60800000    | 0.00000000 |
| 444 | 3221.11370000 | 0.06850000    | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 445 | 3224.06740000 | 11.23990000  | 0.00000000 |
| 446 | 3226.16950000 | 3.24340000   | 0.00000000 |
| 447 | 3227.67770000 | 5.09900000   | 0.00000000 |
| 448 | 3229.17960000 | 2.05570000   | 0.00000000 |
| 449 | 3232.69730000 | 6.07640000   | 0.00000000 |
| 450 | 3234.03110000 | 1.01960000   | 0.00000000 |
| 451 | 3234.75450000 | 15.67650000  | 0.00000000 |
| 452 | 3236.48100000 | 3.03330000   | 0.00000000 |
| 453 | 3242.69040000 | 2.61800000   | 0.00000000 |
| 454 | 3247.28320000 | 6.28910000   | 0.00000000 |
| 455 | 3247.98890000 | 31.75310000  | 0.00000000 |
| 456 | 3263.95070000 | 5.34320000   | 0.00000000 |
| 457 | 3267.15030000 | 6.71540000   | 0.00000000 |
| 458 | 3267.90880000 | 5.23710000   | 0.00000000 |
| 459 | 3271.20940000 | 1.00580000   | 0.00000000 |
| 460 | 3272.60640000 | 3.86830000   | 0.00000000 |
| 461 | 3273.61070000 | 29.79150000  | 0.00000000 |
| 462 | 3276.73320000 | 4.81220000   | 0.00000000 |
| 463 | 3282.01310000 | 5.07660000   | 0.00000000 |
| 464 | 3287.37180000 | 2.61000000   | 0.00000000 |
| 465 | 3291.22270000 | 1.91940000   | 0.00000000 |
| 466 | 3296.08940000 | 14.17100000  | 0.00000000 |
| 467 | 3401.60350000 | 887.41040000 | 0.00000000 |
| 468 | 3475.57230000 | 872.15030000 | 0.00000000 |
| 469 | 3507.28060000 | 5.82220000   | 0.00000000 |
| 470 | 3540.88010000 | 9.71300000   | 0.00000000 |
| 471 | 3563.12000000 | 988.07860000 | 0.00000000 |
| 472 | 3615.88840000 | 334.83220000 | 0.00000000 |
| 473 | 3662.03840000 | 623.03390000 | 0.00000000 |
| 474 | 3716.06870000 | 694.77530000 | 0.00000000 |
| 475 | 3853.00730000 | 81.09410000  | 0.00000000 |
| 476 | 3855.41540000 | 64.92150000  | 0.00000000 |
| 477 | 3858.94430000 | 136.07190000 | 0.00000000 |

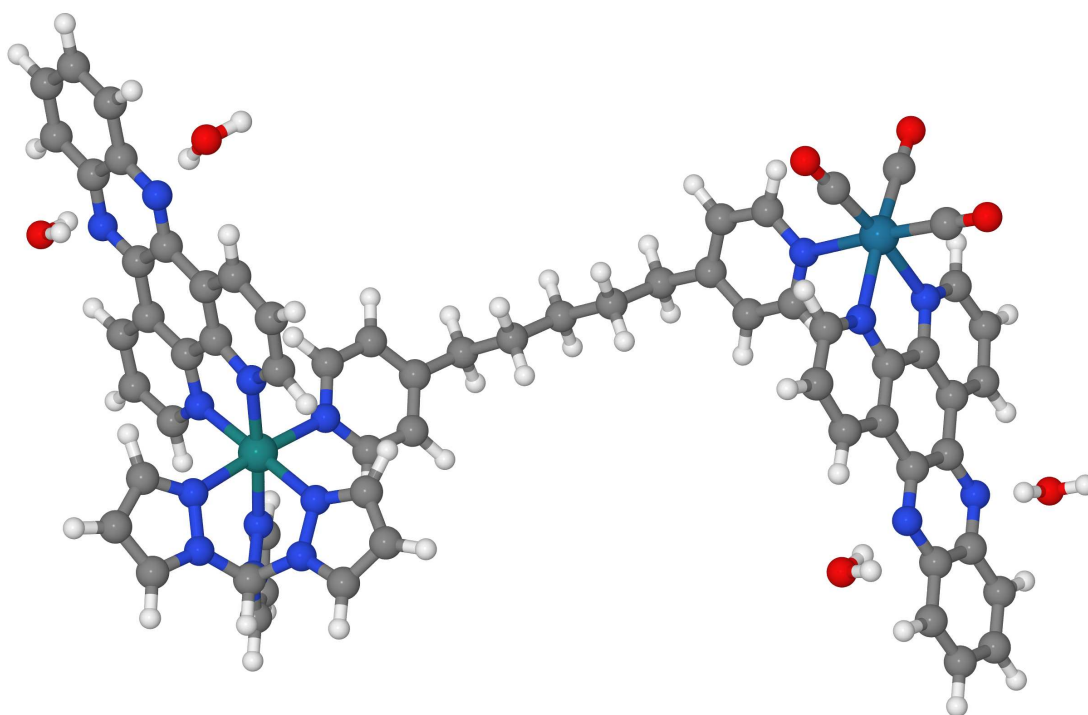
S21. CALCULATIONS ON EXTENDED CONFORMER OF  $1w^{3+}$  ( $^1A$ )

FIG. S31. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
SMILES     : aldispersion=gd3bj int=ultrafine pop=regular
            : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+](6[Ru]578(n9ccc[n+](9C([n+](
            : 1n7ccc1)[n+](1n8ccc1)[n+](1ccc(cc1)CCCCCc1cc[n+](cc1)[Re]
            : 1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1)([C][O])([C][O])([C][O]).O.O.O.O
Formula    : C64H56N16O7ReRu3+
Charge     : 3
Multiplicity : 1
Energy     : -4049.71947075 a.u.
Gibbs Energy : -4048.71491000 a.u.
Number of imaginary frequencies : 4

```

## S21.1. Cartesian Co-ordinates (XYZ format)

145

```

C    2.93233705 -1.97130203 3.44809198
H    3.19103599 -1.23728299 4.21628809
H    2.65025091 -2.89642310 3.95764303
C    1.73482597 -1.44971704 2.63096189
H    1.47157800 -2.19048190 1.86813700
H    2.03650594 -0.54289597 2.09558392
C    0.51628202 -1.14804995 3.50369596
H    0.79192400 -0.41312900 4.26913595
H    0.21423900 -2.05626392 4.03807783
C   -1.88103795 -0.27478999 3.57631993
H   -1.58305597 0.46346799 4.32659292

```

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | -2.20629501  | -1.17140496 | 4.11047411  |
| C  | -6.76603889  | 5.04023695  | -0.95986497 |
| N  | -5.53232098  | 4.46847391  | -1.46122801 |
| N  | -7.91180611  | 4.34282684  | -1.49809802 |
| N  | -6.77778912  | 5.01110888  | 0.48892301  |
| N  | -5.22168398  | 3.17912006  | -1.15784800 |
| C  | -4.52591991  | 5.07122803  | -2.14998388 |
| N  | -8.07003212  | 3.01937795  | -1.23619103 |
| C  | -8.92133904  | 4.81689787  | -2.27804208 |
| N  | -6.69348001  | 3.81596398  | 1.13346195  |
| C  | -6.77009106  | 6.04901600  | 1.36822498  |
| Ru | -6.62883186  | 2.09028006  | -0.05121900 |
| C  | -4.00593519  | 2.96955991  | -1.66281295 |
| C  | -3.53096104  | 4.13079405  | -2.30032897 |
| H  | -4.60252905  | 6.09678221  | -2.46985507 |
| C  | -9.18991184  | 2.65338707  | -1.85601902 |
| C  | -9.76052666  | 3.75328588  | -2.52524996 |
| H  | -8.95411205  | 5.84929419  | -2.58316112 |
| C  | -6.63394594  | 4.10691500  | 2.43306398  |
| C  | -6.68383884  | 5.49964094  | 2.62821102  |
| H  | -6.82847500  | 7.06954384  | 1.02948797  |
| N  | -6.70192480  | 0.37729400  | -1.22955000 |
| N  | -8.09366035  | 0.98602200  | 0.92794698  |
| H  | -3.52689004  | 2.01222992  | -1.53988695 |
| H  | -2.58764195  | 4.26044416  | -2.80187511 |
| H  | -9.53458691  | 1.63427496  | -1.79818797 |
| H  | -10.66437626 | 3.76411009  | -3.10941291 |
| H  | -6.54729319  | 3.31678510  | 3.16056895  |
| H  | -6.65973806  | 6.02845478  | 3.56519890  |
| C  | -6.00872993  | 0.14449900  | -2.34737992 |
| C  | -7.57754517  | -0.57125199 | -0.79614300 |
| C  | -8.34082222  | -0.23710400 | 0.38349301  |
| C  | -8.81133175  | 1.37156498  | 1.98665500  |
| C  | -6.13381481  | -1.04487896 | -3.06182599 |
| H  | -5.34473896  | 0.92993599  | -2.67565107 |
| C  | -7.75782585  | -1.79313695 | -1.45897698 |
| C  | -9.29496098  | -1.11967397 | 0.90849698  |
| C  | -9.77890205  | 0.55188000  | 2.56318092  |
| H  | -8.60778809  | 2.35843492  | 2.37407708  |
| C  | -7.00306797  | -2.02510309 | -2.61939096 |
| H  | -5.54580688  | -1.18705595 | -3.95814204 |
| C  | -8.72173309  | -2.75086904 | -0.91559702 |
| C  | -10.02269077 | -0.70204699 | 2.03361297  |
| C  | -9.48574924  | -2.41582990 | 0.25661901  |
| H  | -10.32985497 | 0.90875000  | 3.42244697  |
| H  | -7.10097313  | -2.95154905 | -3.16740298 |
| N  | -8.88086987  | -3.92005801 | -1.51844501 |
| H  | -10.76949787 | -1.34391606 | 2.47906303  |
| N  | -10.36727715 | -3.26823592 | 0.75881398  |
| C  | -9.77318954  | -4.79780912 | -1.01268494 |
| C  | -10.53554153 | -4.46341610 | 0.15408701  |
| C  | -9.96371460  | -6.06025410 | -1.63300705 |
| C  | -11.46870422 | -5.40030384 | 0.67030799  |
| C  | -10.87321377 | -6.94127178 | -1.10935497 |
| H  | -9.38231754  | -6.29861307 | -2.51437902 |
| C  | -11.62867069 | -6.60997677 | 0.04685200  |
| H  | -12.03864479 | -5.13402796 | 1.55116498  |
| H  | -11.02207565 | -7.90504599 | -1.57993197 |
| H  | -12.33984661 | -7.32716084 | 0.43716100  |
| N  | 7.49958086   | -1.03450298 | -1.46850705 |
| N  | 9.15980816   | -1.55507100 | 0.55853701  |
| C  | 6.62652397   | -0.81875700 | -2.45752692 |
| C  | 8.17341995   | 0.02306600  | -0.94379902 |
| C  | 9.07929897   | -0.26015699 | 0.15140900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 9.95644760  | -1.86091006 | 1.58755898  |
| C  | 6.38967323  | 0.45311001  | -2.97179890 |
| H  | 6.10987091  | -1.68393195 | -2.84666705 |
| C  | 7.99093103  | 1.33315694  | -1.41028094 |
| C  | 9.80731392  | 0.76602900  | 0.77089298  |
| C  | 10.71134663 | -0.89763600 | 2.25134706  |
| H  | 9.99136543  | -2.89945197 | 1.88256204  |
| C  | 7.07389688  | 1.53566396  | -2.45372105 |
| H  | 5.67369795  | 0.57641798  | -3.77241492 |
| C  | 8.75044155  | 2.41999888  | -0.79267401 |
| C  | 10.64379406 | 0.42076901  | 1.84433496  |
| C  | 9.65621853  | 2.13755894  | 0.28554201  |
| H  | 11.34155083 | -1.19499004 | 3.07790399  |
| H  | 6.89875078  | 2.52639389  | -2.84863305 |
| N  | 8.58979893  | 3.65723491  | -1.23979104 |
| H  | 11.22757053 | 1.17512906  | 2.35283089  |
| N  | 10.35726738 | 3.10647798  | 0.85649699  |
| C  | 9.30037498  | 4.65219402  | -0.66838002 |
| C  | 10.20811081 | 4.36944914  | 0.40512699  |
| C  | 9.15615654  | 5.98796511  | -1.12677205 |
| C  | 10.94828796 | 5.42964602  | 0.99103701  |
| C  | 9.88557243  | 6.98757505  | -0.53873998 |
| H  | 8.46579170  | 6.18823481  | -1.93598998 |
| C  | 10.78527260 | 6.70734310  | 0.52421302  |
| H  | 11.62862015 | 5.20225716  | 1.80160606  |
| H  | 9.77862167  | 8.00771523  | -0.88559502 |
| H  | 11.34771633 | 7.51891518  | 0.96851897  |
| H  | -6.81607819 | 6.07516479  | -1.28127503 |
| C  | 4.12445021  | -2.21871090 | 2.56969094  |
| C  | 5.02257919  | -1.19672894 | 2.25708795  |
| C  | 4.35878801  | -3.46319509 | 1.97923994  |
| C  | 6.07641983  | -1.43983197 | 1.39438605  |
| H  | 4.90825081  | -0.20762600 | 2.68213010  |
| C  | 5.43352890  | -3.63457298 | 1.12671900  |
| H  | 3.70700502  | -4.30401802 | 2.17992496  |
| N  | 6.29342890  | -2.63905096 | 0.82127798  |
| H  | 6.76912212  | -0.64783698 | 1.15766299  |
| H  | 5.62339401  | -4.59399509 | 0.66722202  |
| C  | -3.01958990 | 0.27126899  | 2.76249695  |
| C  | -4.05829000 | -0.54275900 | 2.30708694  |
| C  | -3.06188297 | 1.61463797  | 2.38035393  |
| C  | -5.06433678 | -0.01054800 | 1.51931298  |
| H  | -4.09301805 | -1.59383595 | 2.56468201  |
| C  | -4.09537077 | 2.07972693  | 1.58838999  |
| H  | -2.29207993 | 2.30669308  | 2.69851494  |
| N  | -5.09720182 | 1.28569603  | 1.15308499  |
| H  | -5.86995316 | -0.63827801 | 1.17043602  |
| H  | -4.13853502 | 3.11518502  | 1.28657103  |
| Re | 7.98659897  | -3.01322198 | -0.61675400 |
| C  | 9.46289062  | -3.25014496 | -1.85757899 |
| O  | 10.34079647 | -3.37921309 | -2.59170294 |
| C  | 8.51379108  | -4.61395597 | 0.34593001  |
| O  | 8.83892441  | -5.54697990 | 0.94007099  |
| C  | 6.84160089  | -4.07499886 | -1.76738703 |
| O  | 6.15294695  | -4.67851114 | -2.46850491 |
| C  | -0.66604102 | -0.61539602 | 2.69354010  |
| H  | -0.96465999 | -1.35464394 | 1.94228601  |
| H  | -0.36054701 | 0.28211999  | 2.14469910  |
| H  | 11.65737820 | 3.09345293  | 2.29215503  |
| O  | 12.34546185 | 3.07741499  | 2.98293209  |
| H  | 13.15739918 | 2.91969800  | 2.48798490  |
| H  | 7.46215582  | 4.40003109  | -2.63200092 |
| O  | 6.94657516  | 4.76228094  | -3.37617993 |
| H  | 7.55411720  | 4.69687796  | -4.12177277 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | -11.54193401 | -3.15298605 | 2.28999710  |
| O | -12.09694767 | -3.12329888 | 3.09174895  |
| H | -11.51723385 | -3.47068596 | 3.77901006  |
| H | -8.02492523  | -4.69541121 | -3.06686401 |
| O | -7.56759882  | -5.11087513 | -3.82188606 |
| H | -6.80466509  | -5.53765678 | -3.41600704 |

## S21.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -9.79820000  | 0.06350000   | 0.00000000      |
| 2    | -8.80110000  | 0.55630000   | 0.00000000      |
| 3    | -7.81820000  | 0.47470000   | 0.00000000      |
| 4    | -4.61020000  | 0.42250000   | 0.00000000      |
| 5    | 4.99150000   | 0.51190000   | 0.00000000      |
| 6    | 10.15790000  | 0.78320000   | 0.00000000      |
| 7    | 13.33660000  | 0.03220000   | 0.00000000      |
| 8    | 17.46920000  | 1.19080000   | 0.00000000      |
| 9    | 21.64250000  | 2.74680000   | 0.00000000      |
| 10   | 23.76220000  | 0.96910000   | 0.00000000      |
| 11   | 27.98880000  | 2.09610000   | 0.00000000      |
| 12   | 28.60860000  | 1.30740000   | 0.00000000      |
| 13   | 35.08730000  | 0.17310000   | 0.00000000      |
| 14   | 43.28100000  | 0.85930000   | 0.00000000      |
| 15   | 45.81280000  | 0.79550000   | 0.00000000      |
| 16   | 47.12170000  | 0.22330000   | 0.00000000      |
| 17   | 52.21710000  | 0.10650000   | 0.00000000      |
| 18   | 56.24290000  | 1.79060000   | 0.00000000      |
| 19   | 57.01530000  | 1.29130000   | 0.00000000      |
| 20   | 59.00060000  | 0.76320000   | 0.00000000      |
| 21   | 62.06800000  | 0.88830000   | 0.00000000      |
| 22   | 65.03340000  | 0.24700000   | 0.00000000      |
| 23   | 66.68870000  | 1.46520000   | 0.00000000      |
| 24   | 69.43850000  | 2.74620000   | 0.00000000      |
| 25   | 70.24500000  | 0.57600000   | 0.00000000      |
| 26   | 73.03230000  | 1.98510000   | 0.00000000      |
| 27   | 73.43560000  | 2.10670000   | 0.00000000      |
| 28   | 78.38020000  | 0.13840000   | 0.00000000      |
| 29   | 83.14900000  | 1.66900000   | 0.00000000      |
| 30   | 83.88380000  | 2.24800000   | 0.00000000      |
| 31   | 88.72460000  | 1.10060000   | 0.00000000      |
| 32   | 90.50840000  | 7.35460000   | 0.00000000      |
| 33   | 91.06920000  | 1.00570000   | 0.00000000      |
| 34   | 95.74430000  | 14.21470000  | 0.00000000      |
| 35   | 97.24930000  | 0.80750000   | 0.00000000      |
| 36   | 98.34520000  | 3.66600000   | 0.00000000      |
| 37   | 99.11130000  | 0.20520000   | 0.00000000      |
| 38   | 101.84280000 | 9.90540000   | 0.00000000      |
| 39   | 110.12950000 | 0.55310000   | 0.00000000      |
| 40   | 119.04500000 | 0.03030000   | 0.00000000      |
| 41   | 133.42380000 | 0.74070000   | 0.00000000      |
| 42   | 139.40400000 | 0.08840000   | 0.00000000      |
| 43   | 142.45410000 | 0.23000000   | 0.00000000      |
| 44   | 143.11900000 | 0.25370000   | 0.00000000      |
| 45   | 143.70450000 | 0.57330000   | 0.00000000      |
| 46   | 144.69180000 | 0.25570000   | 0.00000000      |
| 47   | 147.01080000 | 0.00310000   | 0.00000000      |
| 48   | 155.73220000 | 0.13730000   | 0.00000000      |
| 49   | 156.39970000 | 1.32880000   | 0.00000000      |
| 50   | 157.14670000 | 0.79910000   | 0.00000000      |
| 51   | 159.45360000 | 1.33270000   | 0.00000000      |
| 52   | 167.26310000 | 4.86350000   | 0.00000000      |
| 53   | 168.69910000 | 4.01100000   | 0.00000000      |
| 54   | 170.67260000 | 10.33880000  | 0.00000000      |
| 55   | 174.74570000 | 1.02360000   | 0.00000000      |
| 56   | 177.82720000 | 1.69540000   | 0.00000000      |
| 57   | 178.81130000 | 4.12330000   | 0.00000000      |
| 58   | 182.67690000 | 1.39450000   | 0.00000000      |
| 59   | 186.11960000 | 1.89480000   | 0.00000000      |
| 60   | 189.73050000 | 11.08130000  | 0.00000000      |

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|-----|--------------|--------------|------------|
| 61  | 197.12520000 | 0.11740000   | 0.00000000 |
| 62  | 199.65540000 | 2.34740000   | 0.00000000 |
| 63  | 204.98070000 | 12.92010000  | 0.00000000 |
| 64  | 213.80290000 | 37.18840000  | 0.00000000 |
| 65  | 219.63460000 | 59.21580000  | 0.00000000 |
| 66  | 222.55620000 | 32.11330000  | 0.00000000 |
| 67  | 227.14450000 | 2.33800000   | 0.00000000 |
| 68  | 231.76090000 | 0.59820000   | 0.00000000 |
| 69  | 236.35320000 | 18.38120000  | 0.00000000 |
| 70  | 254.31090000 | 137.75280000 | 0.00000000 |
| 71  | 260.92510000 | 154.12740000 | 0.00000000 |
| 72  | 264.75560000 | 8.15380000   | 0.00000000 |
| 73  | 267.69070000 | 4.87110000   | 0.00000000 |
| 74  | 272.69940000 | 12.72050000  | 0.00000000 |
| 75  | 276.87490000 | 185.39490000 | 0.00000000 |
| 76  | 281.73240000 | 33.80240000  | 0.00000000 |
| 77  | 285.78970000 | 10.61520000  | 0.00000000 |
| 78  | 288.53530000 | 149.82040000 | 0.00000000 |
| 79  | 302.36090000 | 13.64000000  | 0.00000000 |
| 80  | 305.80330000 | 70.09990000  | 0.00000000 |
| 81  | 308.77360000 | 46.12440000  | 0.00000000 |
| 82  | 310.77970000 | 2.55660000   | 0.00000000 |
| 83  | 321.97550000 | 7.06630000   | 0.00000000 |
| 84  | 334.58670000 | 7.03180000   | 0.00000000 |
| 85  | 339.93600000 | 9.28970000   | 0.00000000 |
| 86  | 342.30460000 | 13.46290000  | 0.00000000 |
| 87  | 342.53350000 | 6.51470000   | 0.00000000 |
| 88  | 343.29830000 | 22.50410000  | 0.00000000 |
| 89  | 343.51380000 | 6.66570000   | 0.00000000 |
| 90  | 347.05060000 | 29.90780000  | 0.00000000 |
| 91  | 360.67540000 | 1.41740000   | 0.00000000 |
| 92  | 364.48250000 | 0.03920000   | 0.00000000 |
| 93  | 367.64340000 | 7.44000000   | 0.00000000 |
| 94  | 378.97320000 | 5.14560000   | 0.00000000 |
| 95  | 380.66750000 | 3.88950000   | 0.00000000 |
| 96  | 383.08930000 | 3.97350000   | 0.00000000 |
| 97  | 389.60440000 | 0.88890000   | 0.00000000 |
| 98  | 392.43660000 | 0.79680000   | 0.00000000 |
| 99  | 402.99440000 | 4.04360000   | 0.00000000 |
| 100 | 403.94530000 | 0.10070000   | 0.00000000 |
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| 102 | 412.89360000 | 0.21880000   | 0.00000000 |
| 103 | 417.00700000 | 0.93610000   | 0.00000000 |
| 104 | 435.18070000 | 9.77740000   | 0.00000000 |
| 105 | 442.17140000 | 3.52170000   | 0.00000000 |
| 106 | 451.10460000 | 33.68460000  | 0.00000000 |
| 107 | 451.49300000 | 21.56700000  | 0.00000000 |
| 108 | 456.05050000 | 3.95570000   | 0.00000000 |
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| 110 | 475.51900000 | 30.10660000  | 0.00000000 |
| 111 | 478.85300000 | 1.41800000   | 0.00000000 |
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| 113 | 488.00520000 | 4.99910000   | 0.00000000 |
| 114 | 494.23160000 | 2.81700000   | 0.00000000 |
| 115 | 496.98960000 | 0.39950000   | 0.00000000 |
| 116 | 506.61350000 | 0.72490000   | 0.00000000 |
| 117 | 509.34780000 | 2.83270000   | 0.00000000 |
| 118 | 509.43190000 | 1.96180000   | 0.00000000 |
| 119 | 517.07090000 | 2.49430000   | 0.00000000 |
| 120 | 531.07010000 | 24.06140000  | 0.00000000 |
| 121 | 533.78400000 | 24.24200000  | 0.00000000 |
| 122 | 544.79650000 | 16.23600000  | 0.00000000 |
| 123 | 561.66610000 | 19.64380000  | 0.00000000 |
| 124 | 562.53560000 | 1.08860000   | 0.00000000 |



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|-----|--------------|--------------|------------|
| 125 | 565.59410000 | 1.30230000   | 0.00000000 |
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| 127 | 576.90900000 | 3.65650000   | 0.00000000 |
| 128 | 579.79080000 | 0.62280000   | 0.00000000 |
| 129 | 581.10070000 | 0.39450000   | 0.00000000 |
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| 131 | 594.99320000 | 20.67730000  | 0.00000000 |
| 132 | 606.52250000 | 0.59010000   | 0.00000000 |
| 133 | 607.06570000 | 1.90580000   | 0.00000000 |
| 134 | 609.86770000 | 29.79730000  | 0.00000000 |
| 135 | 611.98710000 | 3.66580000   | 0.00000000 |
| 136 | 618.40080000 | 20.87830000  | 0.00000000 |
| 137 | 623.90200000 | 33.34870000  | 0.00000000 |
| 138 | 625.00810000 | 18.83510000  | 0.00000000 |
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| 140 | 636.52580000 | 10.67910000  | 0.00000000 |
| 141 | 646.38620000 | 80.91180000  | 0.00000000 |
| 142 | 652.06790000 | 5.16090000   | 0.00000000 |
| 143 | 652.12960000 | 6.13540000   | 0.00000000 |
| 144 | 654.64580000 | 5.04250000   | 0.00000000 |
| 145 | 655.44670000 | 2.98600000   | 0.00000000 |
| 146 | 658.95490000 | 0.29850000   | 0.00000000 |
| 147 | 666.43400000 | 0.49230000   | 0.00000000 |
| 148 | 669.39040000 | 3.44960000   | 0.00000000 |
| 149 | 678.23830000 | 3.05760000   | 0.00000000 |
| 150 | 685.25470000 | 0.06460000   | 0.00000000 |
| 151 | 686.39880000 | 0.26990000   | 0.00000000 |
| 152 | 686.58660000 | 0.60710000   | 0.00000000 |
| 153 | 736.94560000 | 8.11070000   | 0.00000000 |
| 154 | 738.27030000 | 10.81540000  | 0.00000000 |
| 155 | 739.85950000 | 4.56840000   | 0.00000000 |
| 156 | 741.04940000 | 14.66550000  | 0.00000000 |
| 157 | 741.79790000 | 1.89400000   | 0.00000000 |
| 158 | 750.21010000 | 0.01230000   | 0.00000000 |
| 159 | 752.04890000 | 0.15330000   | 0.00000000 |
| 160 | 757.31570000 | 103.39170000 | 0.00000000 |
| 161 | 759.40410000 | 92.87080000  | 0.00000000 |
| 162 | 761.04980000 | 0.70950000   | 0.00000000 |
| 163 | 763.18130000 | 86.53370000  | 0.00000000 |
| 164 | 763.74000000 | 79.49700000  | 0.00000000 |
| 165 | 764.31130000 | 132.71730000 | 0.00000000 |
| 166 | 765.82150000 | 3.73730000   | 0.00000000 |
| 167 | 767.19350000 | 0.58950000   | 0.00000000 |
| 168 | 778.66550000 | 76.03690000  | 0.00000000 |
| 169 | 778.99270000 | 80.15500000  | 0.00000000 |
| 170 | 787.77270000 | 75.57260000  | 0.00000000 |
| 171 | 787.79710000 | 73.57140000  | 0.00000000 |
| 172 | 798.92880000 | 99.43380000  | 0.00000000 |
| 173 | 802.92900000 | 86.55040000  | 0.00000000 |
| 174 | 804.07240000 | 84.10900000  | 0.00000000 |
| 175 | 804.38500000 | 17.64270000  | 0.00000000 |
| 176 | 806.84430000 | 319.11970000 | 0.00000000 |
| 177 | 808.95940000 | 224.16480000 | 0.00000000 |
| 178 | 820.16120000 | 0.79610000   | 0.00000000 |
| 179 | 821.74470000 | 0.99940000   | 0.00000000 |
| 180 | 822.23970000 | 0.23230000   | 0.00000000 |
| 181 | 830.46230000 | 1.18650000   | 0.00000000 |
| 182 | 835.17140000 | 30.00650000  | 0.00000000 |
| 183 | 839.14730000 | 41.53590000  | 0.00000000 |
| 184 | 839.94280000 | 61.70280000  | 0.00000000 |
| 185 | 842.68480000 | 23.61590000  | 0.00000000 |
| 186 | 844.92780000 | 66.18560000  | 0.00000000 |
| 187 | 859.44820000 | 0.36090000   | 0.00000000 |
| 188 | 860.87860000 | 30.24470000  | 0.00000000 |

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|-----|---------------|--------------|------------|
| 189 | 865.60380000  | 11.01800000  | 0.00000000 |
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| 192 | 874.47200000  | 4.80330000   | 0.00000000 |
| 193 | 875.17660000  | 4.76940000   | 0.00000000 |
| 194 | 875.95960000  | 22.02910000  | 0.00000000 |
| 195 | 877.00100000  | 0.05870000   | 0.00000000 |
| 196 | 878.32570000  | 5.60480000   | 0.00000000 |
| 197 | 879.17220000  | 56.57450000  | 0.00000000 |
| 198 | 881.31200000  | 0.63340000   | 0.00000000 |
| 199 | 906.00320000  | 0.08770000   | 0.00000000 |
| 200 | 906.02410000  | 0.07450000   | 0.00000000 |
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| 202 | 921.60110000  | 2.03410000   | 0.00000000 |
| 203 | 921.84050000  | 0.90050000   | 0.00000000 |
| 204 | 923.42360000  | 3.07340000   | 0.00000000 |
| 205 | 925.19730000  | 4.13150000   | 0.00000000 |
| 206 | 947.73710000  | 0.00310000   | 0.00000000 |
| 207 | 947.79020000  | 0.07750000   | 0.00000000 |
| 208 | 953.51200000  | 0.35130000   | 0.00000000 |
| 209 | 956.99590000  | 0.15980000   | 0.00000000 |
| 210 | 983.25280000  | 5.75440000   | 0.00000000 |
| 211 | 988.70210000  | 0.06540000   | 0.00000000 |
| 212 | 989.61360000  | 0.10260000   | 0.00000000 |
| 213 | 989.68520000  | 2.81560000   | 0.00000000 |
| 214 | 993.14170000  | 0.07900000   | 0.00000000 |
| 215 | 993.75390000  | 0.15240000   | 0.00000000 |
| 216 | 1000.23260000 | 13.19850000  | 0.00000000 |
| 217 | 1004.82370000 | 0.42640000   | 0.00000000 |
| 218 | 1007.16590000 | 0.33720000   | 0.00000000 |
| 219 | 1008.41110000 | 0.41320000   | 0.00000000 |
| 220 | 1009.55130000 | 0.90580000   | 0.00000000 |
| 221 | 1009.68230000 | 2.11500000   | 0.00000000 |
| 222 | 1009.70800000 | 7.41910000   | 0.00000000 |
| 223 | 1010.53320000 | 6.73190000   | 0.00000000 |
| 224 | 1010.88960000 | 24.99390000  | 0.00000000 |
| 225 | 1014.15990000 | 14.32820000  | 0.00000000 |
| 226 | 1031.86780000 | 0.88760000   | 0.00000000 |
| 227 | 1032.08760000 | 0.03860000   | 0.00000000 |
| 228 | 1032.65310000 | 0.02710000   | 0.00000000 |
| 229 | 1041.78970000 | 1.99320000   | 0.00000000 |
| 230 | 1042.20980000 | 0.50390000   | 0.00000000 |
| 231 | 1044.54100000 | 0.36810000   | 0.00000000 |
| 232 | 1046.07700000 | 0.31550000   | 0.00000000 |
| 233 | 1049.41390000 | 17.02100000  | 0.00000000 |
| 234 | 1052.23730000 | 0.10400000   | 0.00000000 |
| 235 | 1052.86510000 | 0.50320000   | 0.00000000 |
| 236 | 1053.77980000 | 0.35380000   | 0.00000000 |
| 237 | 1063.93820000 | 1.62250000   | 0.00000000 |
| 238 | 1071.12920000 | 0.76240000   | 0.00000000 |
| 239 | 1071.35010000 | 0.87680000   | 0.00000000 |
| 240 | 1073.91420000 | 4.34210000   | 0.00000000 |
| 241 | 1075.99550000 | 39.93070000  | 0.00000000 |
| 242 | 1076.53390000 | 52.14430000  | 0.00000000 |
| 243 | 1079.39830000 | 26.55860000  | 0.00000000 |
| 244 | 1080.27380000 | 0.53180000   | 0.00000000 |
| 245 | 1082.09720000 | 109.29900000 | 0.00000000 |
| 246 | 1088.03620000 | 1.01430000   | 0.00000000 |
| 247 | 1093.13070000 | 19.29470000  | 0.00000000 |
| 248 | 1093.30940000 | 9.54020000   | 0.00000000 |
| 249 | 1113.98650000 | 0.62190000   | 0.00000000 |
| 250 | 1120.32810000 | 100.26950000 | 0.00000000 |
| 251 | 1121.03690000 | 130.06440000 | 0.00000000 |
| 252 | 1121.78050000 | 45.50330000  | 0.00000000 |

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|-----|---------------|--------------|------------|
| 253 | 1126.94330000 | 25.20690000  | 0.00000000 |
| 254 | 1128.52990000 | 68.00610000  | 0.00000000 |
| 255 | 1136.18080000 | 3.25600000   | 0.00000000 |
| 256 | 1137.84660000 | 1.37660000   | 0.00000000 |
| 257 | 1148.63190000 | 16.68660000  | 0.00000000 |
| 258 | 1150.25100000 | 9.74650000   | 0.00000000 |
| 259 | 1154.57930000 | 3.02250000   | 0.00000000 |
| 260 | 1158.60850000 | 0.22240000   | 0.00000000 |
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| 262 | 1170.06720000 | 5.80710000   | 0.00000000 |
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| 264 | 1178.79630000 | 17.58560000  | 0.00000000 |
| 265 | 1183.46350000 | 6.82080000   | 0.00000000 |
| 266 | 1183.53970000 | 3.50270000   | 0.00000000 |
| 267 | 1212.56530000 | 1.03680000   | 0.00000000 |
| 268 | 1218.04450000 | 0.32740000   | 0.00000000 |
| 269 | 1227.17860000 | 26.03710000  | 0.00000000 |
| 270 | 1231.90450000 | 11.51370000  | 0.00000000 |
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| 273 | 1241.62100000 | 2.25530000   | 0.00000000 |
| 274 | 1242.49770000 | 1.04130000   | 0.00000000 |
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| 280 | 1269.45700000 | 96.87320000  | 0.00000000 |
| 281 | 1275.56700000 | 116.32720000 | 0.00000000 |
| 282 | 1278.44010000 | 3.42540000   | 0.00000000 |
| 283 | 1279.33130000 | 1.82560000   | 0.00000000 |
| 284 | 1282.13100000 | 0.04490000   | 0.00000000 |
| 285 | 1282.79980000 | 0.21940000   | 0.00000000 |
| 286 | 1283.90850000 | 3.28310000   | 0.00000000 |
| 287 | 1300.93610000 | 9.34700000   | 0.00000000 |
| 288 | 1304.94720000 | 0.97230000   | 0.00000000 |
| 289 | 1305.06380000 | 1.50220000   | 0.00000000 |
| 290 | 1311.19250000 | 4.25530000   | 0.00000000 |
| 291 | 1312.05850000 | 2.76920000   | 0.00000000 |
| 292 | 1314.01530000 | 0.26570000   | 0.00000000 |
| 293 | 1319.66670000 | 19.08270000  | 0.00000000 |
| 294 | 1320.05530000 | 49.50510000  | 0.00000000 |
| 295 | 1323.76290000 | 50.18400000  | 0.00000000 |
| 296 | 1329.73260000 | 109.59860000 | 0.00000000 |
| 297 | 1333.79720000 | 0.17860000   | 0.00000000 |
| 298 | 1335.17420000 | 0.07160000   | 0.00000000 |
| 299 | 1339.47570000 | 0.08440000   | 0.00000000 |
| 300 | 1342.23710000 | 0.99570000   | 0.00000000 |
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| 302 | 1351.93080000 | 4.36990000   | 0.00000000 |
| 303 | 1353.94440000 | 0.59100000   | 0.00000000 |
| 304 | 1372.60720000 | 208.35080000 | 0.00000000 |
| 305 | 1376.06210000 | 1.46960000   | 0.00000000 |
| 306 | 1376.88950000 | 2.30310000   | 0.00000000 |
| 307 | 1376.98040000 | 164.54620000 | 0.00000000 |
| 308 | 1379.03270000 | 5.50420000   | 0.00000000 |
| 309 | 1379.54100000 | 9.62240000   | 0.00000000 |
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| 311 | 1380.47300000 | 51.36640000  | 0.00000000 |
| 312 | 1380.90300000 | 9.07610000   | 0.00000000 |
| 313 | 1381.39360000 | 11.40670000  | 0.00000000 |
| 314 | 1400.15520000 | 1.71520000   | 0.00000000 |
| 315 | 1418.13650000 | 16.23380000  | 0.00000000 |
| 316 | 1421.40300000 | 24.09650000  | 0.00000000 |

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| 317 | 1430.89920000 | 7.14070000    | 0.00000000 |
| 318 | 1431.67020000 | 17.19050000   | 0.00000000 |
| 319 | 1437.77720000 | 53.75050000   | 0.00000000 |
| 320 | 1442.51200000 | 56.56110000   | 0.00000000 |
| 321 | 1443.76830000 | 132.32170000  | 0.00000000 |
| 322 | 1455.01600000 | 76.59290000   | 0.00000000 |
| 323 | 1455.99750000 | 105.55170000  | 0.00000000 |
| 324 | 1463.56150000 | 26.55540000   | 0.00000000 |
| 325 | 1464.74190000 | 31.19910000   | 0.00000000 |
| 326 | 1473.80680000 | 60.13660000   | 0.00000000 |
| 327 | 1475.39360000 | 0.91470000    | 0.00000000 |
| 328 | 1480.29770000 | 82.80430000   | 0.00000000 |
| 329 | 1481.01320000 | 3.99320000    | 0.00000000 |
| 330 | 1481.23340000 | 32.25500000   | 0.00000000 |
| 331 | 1481.31570000 | 13.24350000   | 0.00000000 |
| 332 | 1492.24350000 | 0.04950000    | 0.00000000 |
| 333 | 1492.48730000 | 7.49450000    | 0.00000000 |
| 334 | 1501.47300000 | 24.43120000   | 0.00000000 |
| 335 | 1503.15550000 | 27.70540000   | 0.00000000 |
| 336 | 1503.71180000 | 5.43320000    | 0.00000000 |
| 337 | 1507.09350000 | 1.21450000    | 0.00000000 |
| 338 | 1507.94330000 | 2.55490000    | 0.00000000 |
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| 340 | 1525.66160000 | 25.78090000   | 0.00000000 |
| 341 | 1526.28950000 | 29.52970000   | 0.00000000 |
| 342 | 1530.65540000 | 65.29850000   | 0.00000000 |
| 343 | 1532.38250000 | 137.43250000  | 0.00000000 |
| 344 | 1538.16000000 | 49.63400000   | 0.00000000 |
| 345 | 1541.58700000 | 27.74360000   | 0.00000000 |
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| 347 | 1553.19980000 | 13.10370000   | 0.00000000 |
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| 350 | 1575.54170000 | 7.12050000    | 0.00000000 |
| 351 | 1587.69540000 | 38.38490000   | 0.00000000 |
| 352 | 1588.19900000 | 10.50190000   | 0.00000000 |
| 353 | 1593.28150000 | 12.48260000   | 0.00000000 |
| 354 | 1595.44020000 | 11.33340000   | 0.00000000 |
| 355 | 1612.38330000 | 8.28020000    | 0.00000000 |
| 356 | 1615.56710000 | 17.73770000   | 0.00000000 |
| 357 | 1625.06450000 | 1.26280000    | 0.00000000 |
| 358 | 1625.73730000 | 2.40430000    | 0.00000000 |
| 359 | 1626.09830000 | 3.89560000    | 0.00000000 |
| 360 | 1627.02690000 | 6.70180000    | 0.00000000 |
| 361 | 1637.00720000 | 0.08140000    | 0.00000000 |
| 362 | 1639.83910000 | 3.02040000    | 0.00000000 |
| 363 | 1651.81330000 | 95.58110000   | 0.00000000 |
| 364 | 1652.74290000 | 111.16320000  | 0.00000000 |
| 365 | 1652.88620000 | 100.29260000  | 0.00000000 |
| 366 | 1652.99820000 | 82.98960000   | 0.00000000 |
| 367 | 1661.12800000 | 0.59240000    | 0.00000000 |
| 368 | 1661.30060000 | 107.97320000  | 0.00000000 |
| 369 | 1661.67500000 | 1.02310000    | 0.00000000 |
| 370 | 1662.30690000 | 106.54980000  | 0.00000000 |
| 371 | 1963.82400000 | 2385.60940000 | 0.00000000 |
| 372 | 1969.82950000 | 2313.41880000 | 0.00000000 |
| 373 | 2083.69960000 | 1987.20370000 | 0.00000000 |
| 374 | 3007.38540000 | 18.14580000   | 0.00000000 |
| 375 | 3014.79090000 | 0.93910000    | 0.00000000 |
| 376 | 3020.05010000 | 75.84750000   | 0.00000000 |
| 377 | 3030.74420000 | 1.18510000    | 0.00000000 |
| 378 | 3037.69930000 | 62.58460000   | 0.00000000 |
| 379 | 3040.52600000 | 72.20580000   | 0.00000000 |
| 380 | 3047.63980000 | 0.15800000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 3060.69340000 | 70.10110000   | 0.00000000 |
| 382 | 3083.67550000 | 54.29010000   | 0.00000000 |
| 383 | 3086.64960000 | 93.45420000   | 0.00000000 |
| 384 | 3186.10650000 | 7.03080000    | 0.00000000 |
| 385 | 3186.78820000 | 6.75660000    | 0.00000000 |
| 386 | 3188.93680000 | 1.05530000    | 0.00000000 |
| 387 | 3191.26090000 | 5.96100000    | 0.00000000 |
| 388 | 3193.89260000 | 4.90900000    | 0.00000000 |
| 389 | 3194.13210000 | 0.47900000    | 0.00000000 |
| 390 | 3195.02890000 | 0.61820000    | 0.00000000 |
| 391 | 3195.22050000 | 3.26250000    | 0.00000000 |
| 392 | 3195.89120000 | 3.37860000    | 0.00000000 |
| 393 | 3201.80410000 | 0.19720000    | 0.00000000 |
| 394 | 3202.88440000 | 0.26170000    | 0.00000000 |
| 395 | 3207.40890000 | 40.50560000   | 0.00000000 |
| 396 | 3208.20660000 | 39.50540000   | 0.00000000 |
| 397 | 3210.60190000 | 16.54690000   | 0.00000000 |
| 398 | 3211.16410000 | 15.45150000   | 0.00000000 |
| 399 | 3212.23890000 | 24.82880000   | 0.00000000 |
| 400 | 3213.17940000 | 17.99290000   | 0.00000000 |
| 401 | 3219.50870000 | 7.11750000    | 0.00000000 |
| 402 | 3220.44440000 | 37.91030000   | 0.00000000 |
| 403 | 3220.57130000 | 26.10720000   | 0.00000000 |
| 404 | 3221.27360000 | 42.75240000   | 0.00000000 |
| 405 | 3221.49460000 | 33.59110000   | 0.00000000 |
| 406 | 3231.44210000 | 4.92770000    | 0.00000000 |
| 407 | 3231.79930000 | 4.56520000    | 0.00000000 |
| 408 | 3231.83380000 | 9.90330000    | 0.00000000 |
| 409 | 3235.02580000 | 1.45090000    | 0.00000000 |
| 410 | 3237.48200000 | 7.48930000    | 0.00000000 |
| 411 | 3237.86080000 | 3.80620000    | 0.00000000 |
| 412 | 3245.98590000 | 3.19250000    | 0.00000000 |
| 413 | 3259.86430000 | 0.99900000    | 0.00000000 |
| 414 | 3260.30250000 | 1.06860000    | 0.00000000 |
| 415 | 3261.16540000 | 0.40420000    | 0.00000000 |
| 416 | 3269.26280000 | 7.15410000    | 0.00000000 |
| 417 | 3270.58230000 | 6.39470000    | 0.00000000 |
| 418 | 3271.35910000 | 6.93740000    | 0.00000000 |
| 419 | 3284.09750000 | 3.17970000    | 0.00000000 |
| 420 | 3284.85960000 | 4.59900000    | 0.00000000 |
| 421 | 3285.50920000 | 4.92470000    | 0.00000000 |
| 422 | 3558.97860000 | 1759.95030000 | 0.00000000 |
| 423 | 3564.69200000 | 139.47390000  | 0.00000000 |
| 424 | 3568.80000000 | 1726.60570000 | 0.00000000 |
| 425 | 3574.29340000 | 114.04760000  | 0.00000000 |
| 426 | 3841.22540000 | 96.43650000   | 0.00000000 |
| 427 | 3842.19050000 | 93.92590000   | 0.00000000 |
| 428 | 3842.39350000 | 93.33010000   | 0.00000000 |
| 429 | 3842.71750000 | 87.63140000   | 0.00000000 |

# S22. CALCULATIONS ON EXTENDED CONFORMER OF $1w^{3+}$ ( $^3A$ )

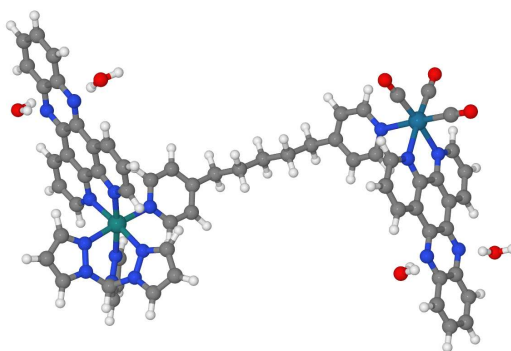


FIG. S32. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+](c4c6c(c3n2)ccc[n+])6[Ru]578(n9ccc[n+])9C([n+]
            : 1n7ccc1)[n+](n8ccc1)[n+](1ccc(cc1)CCCCC1cc[n+](cc1)[Re]
            : 1([n+](2cccc3c2c2[n+](1cccc2c1c3nc2cccc2n1))([C][O])([C][O])([C][O]).O.O.O.O
Formula    : C64H56N16O7ReRu3+,3
Charge     : 3
Multiplicity : 3
Energy     : -4049.65188059
Gibbs Energy : -4048.65289200
Number of imaginary frequencies : 4

```

a.u.

a.u.

## S22.1. Cartesian Co-ordinates (XYZ format)

145

```

C      2.88828111 -1.70300603 3.68542194
H      3.17863393 -0.93621600 4.40895605
H      2.60912490 -2.59810090 4.24739122
C      1.67543495 -1.20500696 2.87635207
H      1.38653195 -1.97577298 2.15366411
H      1.97180498 -0.32569301 2.29427409
C      0.48035699 -0.85409403 3.76329207
H      0.77773499 -0.08931800 4.48997593
H      0.18095800 -1.73581696 4.34130907
C     -1.91731906 0.02188800 3.84026408
H     -1.61936796 0.79677200 4.55112696
H     -2.22864103 -0.85545897 4.41272020
C     -6.95225716 5.04466486 -0.91902697
N     -5.63484287 4.59708023 -1.31938601
N     -7.97650194 4.21555424 -1.52235901
N     -7.06631517 5.02336502 0.52399302
N     -5.22185898 3.34785509 -0.97748500
C     -4.64805698 5.28098392 -1.95247102
N     -8.01523590 2.88381791 -1.23933494
C     -8.97012138 4.55399179 -2.37438607
N     -6.91016722 3.84930110 1.19281995
C     -7.24730015 6.05584812 1.38582504
Ru     -6.59984493 2.10820794 0.03510300
C     -3.96026802 3.24531603 -1.40118802

```

|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -3.55910397  | 4.43808413  | -2.02175593 |
| H | -4.79936409  | 6.28956699  | -2.29878211 |
| C | -9.04959869  | 2.38199711  | -1.92616796 |
| C | -9.67750263  | 3.39665508  | -2.65280199 |
| H | -9.09631348  | 5.56932878  | -2.71171188 |
| C | -6.99505711  | 4.14930677  | 2.49078989  |
| C | -7.20775318  | 5.52600479  | 2.65809798  |
| H | -7.39033079  | 7.06247997  | 1.02993500  |
| N | -6.44028187  | 0.42961800  | -1.16682696 |
| N | -8.02743816  | 0.88686299  | 0.90761298  |
| H | -3.40032697  | 2.33990908  | -1.23366594 |
| H | -2.60130405  | 4.65243387  | -2.46261096 |
| H | -9.28416157  | 1.33237195  | -1.86251903 |
| H | -10.53409958 | 3.30403996  | -3.29728007 |
| H | -6.88793898  | 3.37967801  | 3.23744988  |
| H | -7.31859922  | 6.05952692  | 3.58585310  |
| C | -5.65626812  | 0.27724400  | -2.22892594 |
| C | -7.28887892  | -0.58786100 | -0.79596299 |
| C | -8.12980461  | -0.34579501 | 0.30461100  |
| C | -8.82640743  | 1.18758297  | 1.92567098  |
| C | -5.64782906  | -0.91095001 | -2.96711397 |
| H | -5.03039122  | 1.11287296  | -2.50296211 |
| C | -7.33337307  | -1.82445800 | -1.49205399 |
| C | -9.04708099  | -1.33167195 | 0.75404602  |
| C | -9.75718307  | 0.26900300  | 2.42232203  |
| H | -8.73338509  | 2.17613292  | 2.34892392  |
| C | -6.47366619  | -1.95668495 | -2.59745789 |
| H | -4.99022579  | -0.99322599 | -3.82105303 |
| C | -8.24504948  | -2.86298800 | -1.04768801 |
| C | -9.86267281  | -0.98328000 | 1.84578896  |
| C | -9.10439873  | -2.61588907 | 0.07978800  |
| H | -10.38405418 | 0.55541998  | 3.25504899  |
| H | -6.46133614  | -2.87563205 | -3.16797400 |
| N | -8.27193928  | -4.03270197 | -1.70024598 |
| H | -10.58129215 | -1.69235098 | 2.23429704  |
| N | -9.96193695  | -3.54678297 | 0.51874101  |
| C | -9.14095497  | -4.99558115 | -1.25554705 |
| C | -9.99286079  | -4.75066900 | -0.13669100 |
| C | -9.20041275  | -6.24562407 | -1.90343499 |
| C | -10.87213421 | -5.76492691 | 0.29235399  |
| C | -10.07394600 | -7.22601795 | -1.46214998 |
| H | -8.55015945  | -6.41702080 | -2.75258303 |
| C | -10.91138744 | -6.98524189 | -0.36200199 |
| H | -11.51421070 | -5.56494904 | 1.14150298  |
| H | -10.10964584 | -8.18266869 | -1.96967804 |
| H | -11.59235477 | -7.75633621 | -0.02180900 |
| N | 7.28698206   | -1.07497704 | -1.42297900 |
| N | 9.01462078   | -1.50853598 | 0.56767601  |
| C | 6.38007021   | -0.90117002 | -2.38944292 |
| C | 7.98668814   | 0.00139300  | -0.97618401 |
| C | 8.92922211   | -0.23500000 | 0.09897700  |
| C | 9.84300423   | -1.76967001 | 1.58381796  |
| C | 6.13272190   | 0.34578401  | -2.95704603 |
| H | 5.84397078   | -1.78032005 | -2.71591210 |
| C | 7.79452896   | 1.28866100  | -1.49883902 |
| C | 9.68458080   | 0.81452799  | 0.64187098  |
| C | 10.62593079  | -0.78085601 | 2.17347908  |
| H | 9.88018036   | -2.79253197 | 1.92920697  |
| C | 6.84155321   | 1.44708002  | -2.51743293 |
| H | 5.38910484   | 0.43558100  | -3.73664308 |
| C | 8.58163261   | 2.39858007  | -0.96201402 |
| C | 10.55369282  | 0.51624501  | 1.70351100  |
| C | 9.52511597   | 2.16172600  | 0.09464100  |
| H | 11.28090954  | -1.04188001 | 2.99304891  |

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | 6.65752983   | 2.41882300  | -2.95339108 |
| N  | 8.41016388   | 3.61431098  | -1.46110106 |
| H  | 11.15902615  | 1.29017305  | 2.15424895  |
| N  | 10.25295162  | 3.15168810  | 0.59095103  |
| C  | 9.14563370   | 4.63074780  | -0.96378303 |
| C  | 10.09276581  | 4.39292383  | 0.08627600  |
| C  | 8.98949146   | 5.94460678  | -1.47812903 |
| C  | 10.86036682  | 5.47441387  | 0.59259701  |
| C  | 9.74541759   | 6.96598387  | -0.96585900 |
| H  | 8.26933861   | 6.11118078  | -2.26881599 |
| C  | 10.68490887  | 6.72998714  | 0.07317600  |
| H  | 11.57119179  | 5.28036308  | 1.38553703  |
| H  | 9.62938976   | 7.96954489  | -1.35550594 |
| H  | 11.26793385  | 7.55786324  | 0.45668799  |
| H  | -7.09102583  | 6.06441307  | -1.26196301 |
| C  | 4.05024195   | -2.01023793 | 2.78552008  |
| C  | 4.94123983   | -1.01413095 | 2.38196802  |
| C  | 4.25956821   | -3.28926897 | 2.26365709  |
| C  | 5.96258020   | -1.31454301 | 1.49861205  |
| H  | 4.84597778   | -0.00066700 | 2.75079489  |
| C  | 5.30313110   | -3.51759291 | 1.38586795  |
| H  | 3.61212397   | -4.11281586 | 2.53689003  |
| N  | 6.15445185   | -2.54686809 | 0.99026000  |
| H  | 6.64919519   | -0.54209399 | 1.19063103  |
| H  | 5.47345018   | -4.50415182 | 0.97927600  |
| C  | -3.06072688  | 0.51404101  | 3.00626898  |
| C  | -4.02062702  | -0.36488301 | 2.49318600  |
| C  | -3.17838097  | 1.86290395  | 2.65323210  |
| C  | -5.02100182  | 0.10638100  | 1.66912997  |
| H  | -3.99072909  | -1.41979098 | 2.73238993  |
| C  | -4.20083714  | 2.27332711  | 1.82407200  |
| H  | -2.47333598  | 2.59688807  | 3.02097011  |
| N  | -5.11671591  | 1.41024101  | 1.32632995  |
| H  | -5.76559877  | -0.56231600 | 1.26698804  |
| H  | -4.30514002  | 3.30851197  | 1.53768003  |
| Re | 7.78932619   | -3.01194191 | -0.48930201 |
| C  | 9.21621323   | -3.32353306 | -1.77056098 |
| O  | 10.06519794  | -3.49589300 | -2.52936006 |
| C  | 8.34357071   | -4.56523991 | 0.53371298  |
| O  | 8.68780422   | -5.46788120 | 1.16301095  |
| C  | 6.59403896   | -4.11990118 | -1.54173696 |
| O  | 5.87537003   | -4.75126123 | -2.18582702 |
| C  | -0.71179402  | -0.34739500 | 2.95110011  |
| H  | -1.02048302  | -1.11171496 | 2.23006392  |
| H  | -0.41472501  | 0.53161800  | 2.36923790  |
| H  | 11.62144470  | 3.19090390  | 1.95628798  |
| O  | 12.33710575  | 3.20000601  | 2.61874008  |
| H  | 13.12547302  | 2.99912906  | 2.10182905  |
| H  | 7.23254681   | 4.29793692  | -2.84283996 |
| O  | 6.68896723   | 4.62730408  | -3.58233190 |
| H  | 7.26599598   | 4.52373314  | -4.34757280 |
| H  | -11.16681480 | -3.54431510 | 1.91591799  |
| O  | -11.77210426 | -3.56073904 | 2.69245195  |
| H  | -11.21273708 | -3.89471412 | 3.40245795  |
| H  | -7.32092381  | -4.64967203 | -3.15628409 |
| O  | -6.77539206  | -4.99932384 | -3.89773893 |
| H  | -6.02378321  | -5.40194416 | -3.44882202 |



## S22.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -11.14430000 | 1.33830000   | 0.00000000      |
| 2    | -8.89430000  | 0.58240000   | 0.00000000      |
| 3    | -8.26850000  | 1.53490000   | 0.00000000      |
| 4    | -7.72660000  | 1.39920000   | 0.00000000      |
| 5    | 2.13020000   | 3.17290000   | 0.00000000      |
| 6    | 8.74840000   | 0.56020000   | 0.00000000      |
| 7    | 13.38520000  | 0.68820000   | 0.00000000      |
| 8    | 14.79630000  | 0.91110000   | 0.00000000      |
| 9    | 19.97160000  | 1.75700000   | 0.00000000      |
| 10   | 21.51970000  | 2.57280000   | 0.00000000      |
| 11   | 25.57540000  | 0.56310000   | 0.00000000      |
| 12   | 26.78680000  | 2.47000000   | 0.00000000      |
| 13   | 33.14770000  | 0.37450000   | 0.00000000      |
| 14   | 38.45640000  | 0.18560000   | 0.00000000      |
| 15   | 45.86690000  | 0.70440000   | 0.00000000      |
| 16   | 46.44620000  | 1.26320000   | 0.00000000      |
| 17   | 52.98900000  | 1.30740000   | 0.00000000      |
| 18   | 55.97210000  | 1.53980000   | 0.00000000      |
| 19   | 57.85890000  | 2.38990000   | 0.00000000      |
| 20   | 59.43620000  | 0.41610000   | 0.00000000      |
| 21   | 60.47420000  | 1.57350000   | 0.00000000      |
| 22   | 63.15930000  | 2.28060000   | 0.00000000      |
| 23   | 66.68900000  | 1.57860000   | 0.00000000      |
| 24   | 68.96940000  | 0.41400000   | 0.00000000      |
| 25   | 69.79690000  | 2.77880000   | 0.00000000      |
| 26   | 70.25460000  | 1.14070000   | 0.00000000      |
| 27   | 70.71510000  | 0.07470000   | 0.00000000      |
| 28   | 72.55100000  | 3.23090000   | 0.00000000      |
| 29   | 82.69580000  | 1.73760000   | 0.00000000      |
| 30   | 83.76580000  | 3.81530000   | 0.00000000      |
| 31   | 89.41340000  | 2.73700000   | 0.00000000      |
| 32   | 90.69520000  | 3.50470000   | 0.00000000      |
| 33   | 91.15980000  | 1.40700000   | 0.00000000      |
| 34   | 96.60750000  | 4.55720000   | 0.00000000      |
| 35   | 98.17500000  | 5.63280000   | 0.00000000      |
| 36   | 101.18710000 | 2.58430000   | 0.00000000      |
| 37   | 104.14890000 | 4.65190000   | 0.00000000      |
| 38   | 107.07070000 | 3.28810000   | 0.00000000      |
| 39   | 111.79210000 | 0.19700000   | 0.00000000      |
| 40   | 119.79220000 | 0.48510000   | 0.00000000      |
| 41   | 130.65040000 | 0.92460000   | 0.00000000      |
| 42   | 137.91750000 | 0.01910000   | 0.00000000      |
| 43   | 142.40640000 | 1.28470000   | 0.00000000      |
| 44   | 144.68670000 | 0.62130000   | 0.00000000      |
| 45   | 145.46910000 | 0.95220000   | 0.00000000      |
| 46   | 148.06460000 | 0.19890000   | 0.00000000      |
| 47   | 154.41060000 | 1.03160000   | 0.00000000      |
| 48   | 155.47250000 | 1.00000000   | 0.00000000      |
| 49   | 156.64810000 | 0.76210000   | 0.00000000      |
| 50   | 160.96010000 | 13.15570000  | 0.00000000      |
| 51   | 164.54680000 | 0.69640000   | 0.00000000      |
| 52   | 165.94290000 | 9.94880000   | 0.00000000      |
| 53   | 167.60660000 | 3.07380000   | 0.00000000      |
| 54   | 169.04230000 | 8.72770000   | 0.00000000      |
| 55   | 171.39300000 | 2.28400000   | 0.00000000      |
| 56   | 177.09320000 | 5.90230000   | 0.00000000      |
| 57   | 178.49630000 | 6.92980000   | 0.00000000      |
| 58   | 180.39950000 | 7.79120000   | 0.00000000      |
| 59   | 185.19880000 | 0.75990000   | 0.00000000      |
| 60   | 187.73000000 | 1.83330000   | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 189.26050000 | 4.25090000   | 0.00000000 |
| 62  | 196.86710000 | 4.60710000   | 0.00000000 |
| 63  | 203.10070000 | 16.72980000  | 0.00000000 |
| 64  | 213.19050000 | 69.11430000  | 0.00000000 |
| 65  | 215.47490000 | 24.64140000  | 0.00000000 |
| 66  | 218.60210000 | 6.82710000   | 0.00000000 |
| 67  | 225.62690000 | 3.29970000   | 0.00000000 |
| 68  | 231.73350000 | 0.38580000   | 0.00000000 |
| 69  | 238.57630000 | 94.19610000  | 0.00000000 |
| 70  | 252.35810000 | 151.68340000 | 0.00000000 |
| 71  | 254.30320000 | 96.54020000  | 0.00000000 |
| 72  | 259.33700000 | 27.09940000  | 0.00000000 |
| 73  | 261.22040000 | 40.72180000  | 0.00000000 |
| 74  | 266.31030000 | 16.93250000  | 0.00000000 |
| 75  | 279.49940000 | 150.37930000 | 0.00000000 |
| 76  | 283.94010000 | 41.38920000  | 0.00000000 |
| 77  | 287.64930000 | 8.04730000   | 0.00000000 |
| 78  | 296.83240000 | 13.85150000  | 0.00000000 |
| 79  | 299.19630000 | 83.08010000  | 0.00000000 |
| 80  | 303.80930000 | 29.40730000  | 0.00000000 |
| 81  | 306.84010000 | 43.11570000  | 0.00000000 |
| 82  | 312.84620000 | 1.86530000   | 0.00000000 |
| 83  | 319.73830000 | 14.18030000  | 0.00000000 |
| 84  | 324.36860000 | 5.22700000   | 0.00000000 |
| 85  | 337.86960000 | 5.15310000   | 0.00000000 |
| 86  | 340.36850000 | 41.33480000  | 0.00000000 |
| 87  | 341.29750000 | 26.70120000  | 0.00000000 |
| 88  | 342.48390000 | 7.73370000   | 0.00000000 |
| 89  | 360.88390000 | 0.04510000   | 0.00000000 |
| 90  | 363.22270000 | 6.63020000   | 0.00000000 |
| 91  | 364.22610000 | 0.52050000   | 0.00000000 |
| 92  | 366.78550000 | 22.22480000  | 0.00000000 |
| 93  | 380.44700000 | 3.75030000   | 0.00000000 |
| 94  | 383.19340000 | 100.45780000 | 0.00000000 |
| 95  | 383.44460000 | 10.04510000  | 0.00000000 |
| 96  | 384.22560000 | 3.60400000   | 0.00000000 |
| 97  | 389.93300000 | 2.58810000   | 0.00000000 |
| 98  | 391.19730000 | 2.04410000   | 0.00000000 |
| 99  | 400.96150000 | 10.39380000  | 0.00000000 |
| 100 | 403.93950000 | 0.07540000   | 0.00000000 |
| 101 | 405.69010000 | 1.15350000   | 0.00000000 |
| 102 | 407.65300000 | 2.34980000   | 0.00000000 |
| 103 | 414.95850000 | 120.23130000 | 0.00000000 |
| 104 | 424.27450000 | 47.26470000  | 0.00000000 |
| 105 | 435.20910000 | 10.01100000  | 0.00000000 |
| 106 | 447.66150000 | 0.72830000   | 0.00000000 |
| 107 | 450.22230000 | 31.67570000  | 0.00000000 |
| 108 | 455.63420000 | 3.47460000   | 0.00000000 |
| 109 | 462.76500000 | 6.08920000   | 0.00000000 |
| 110 | 475.44970000 | 33.97610000  | 0.00000000 |
| 111 | 475.68500000 | 23.80020000  | 0.00000000 |
| 112 | 483.22160000 | 6.68910000   | 0.00000000 |
| 113 | 488.06670000 | 5.63410000   | 0.00000000 |
| 114 | 493.50030000 | 1.12030000   | 0.00000000 |
| 115 | 494.06730000 | 3.70310000   | 0.00000000 |
| 116 | 499.50780000 | 10.52110000  | 0.00000000 |
| 117 | 508.45710000 | 2.02560000   | 0.00000000 |
| 118 | 508.63930000 | 2.64110000   | 0.00000000 |
| 119 | 516.43450000 | 3.08090000   | 0.00000000 |
| 120 | 531.53250000 | 22.65050000  | 0.00000000 |
| 121 | 533.67610000 | 32.87760000  | 0.00000000 |
| 122 | 545.41210000 | 25.79880000  | 0.00000000 |
| 123 | 551.14610000 | 0.37380000   | 0.00000000 |
| 124 | 562.38150000 | 1.33480000   | 0.00000000 |

|     |              |               |            |
|-----|--------------|---------------|------------|
| 125 | 563.00050000 | 16.89620000   | 0.00000000 |
| 126 | 571.97260000 | 0.30210000    | 0.00000000 |
| 127 | 576.58360000 | 2.10540000    | 0.00000000 |
| 128 | 576.94930000 | 3.72660000    | 0.00000000 |
| 129 | 580.93100000 | 0.59330000    | 0.00000000 |
| 130 | 586.13640000 | 1181.82240000 | 0.00000000 |
| 131 | 592.03800000 | 2.10730000    | 0.00000000 |
| 132 | 594.23340000 | 18.12510000   | 0.00000000 |
| 133 | 599.91590000 | 0.21660000    | 0.00000000 |
| 134 | 605.92910000 | 3.21800000    | 0.00000000 |
| 135 | 609.86880000 | 36.42380000   | 0.00000000 |
| 136 | 612.00000000 | 43.30520000   | 0.00000000 |
| 137 | 617.84050000 | 35.93150000   | 0.00000000 |
| 138 | 624.98610000 | 10.68700000   | 0.00000000 |
| 139 | 633.94590000 | 43.73910000   | 0.00000000 |
| 140 | 634.69440000 | 687.75750000  | 0.00000000 |
| 141 | 637.53700000 | 17.13220000   | 0.00000000 |
| 142 | 646.09080000 | 1.60150000    | 0.00000000 |
| 143 | 646.64500000 | 80.53520000   | 0.00000000 |
| 144 | 651.95990000 | 5.36180000    | 0.00000000 |
| 145 | 653.77750000 | 12.23800000   | 0.00000000 |
| 146 | 655.30130000 | 2.95250000    | 0.00000000 |
| 147 | 665.99590000 | 11.59360000   | 0.00000000 |
| 148 | 667.89830000 | 0.03970000    | 0.00000000 |
| 149 | 669.66240000 | 3.58460000    | 0.00000000 |
| 150 | 672.59130000 | 3.19270000    | 0.00000000 |
| 151 | 680.08870000 | 3.30630000    | 0.00000000 |
| 152 | 686.13520000 | 0.63760000    | 0.00000000 |
| 153 | 724.62330000 | 113.01150000  | 0.00000000 |
| 154 | 728.49800000 | 0.38750000    | 0.00000000 |
| 155 | 737.42360000 | 8.45770000    | 0.00000000 |
| 156 | 738.43510000 | 11.81980000   | 0.00000000 |
| 157 | 741.15660000 | 21.35660000   | 0.00000000 |
| 158 | 744.39880000 | 388.03530000  | 0.00000000 |
| 159 | 745.14280000 | 45.53140000   | 0.00000000 |
| 160 | 751.49440000 | 0.28910000    | 0.00000000 |
| 161 | 762.00870000 | 5.15280000    | 0.00000000 |
| 162 | 762.31310000 | 78.55260000   | 0.00000000 |
| 163 | 764.06650000 | 1.32360000    | 0.00000000 |
| 164 | 767.30170000 | 0.82480000    | 0.00000000 |
| 165 | 768.98570000 | 1053.30360000 | 0.00000000 |
| 166 | 770.72950000 | 93.50910000   | 0.00000000 |
| 167 | 772.73780000 | 107.92080000  | 0.00000000 |
| 168 | 775.78140000 | 132.61430000  | 0.00000000 |
| 169 | 778.82500000 | 72.29700000   | 0.00000000 |
| 170 | 780.04570000 | 66.35650000   | 0.00000000 |
| 171 | 780.80910000 | 35.10490000   | 0.00000000 |
| 172 | 787.37300000 | 73.96400000   | 0.00000000 |
| 173 | 794.75700000 | 1.54730000    | 0.00000000 |
| 174 | 795.49490000 | 101.35340000  | 0.00000000 |
| 175 | 799.80460000 | 100.16310000  | 0.00000000 |
| 176 | 804.61910000 | 98.73040000   | 0.00000000 |
| 177 | 810.28750000 | 211.07040000  | 0.00000000 |
| 178 | 817.57040000 | 61.76230000   | 0.00000000 |
| 179 | 821.60940000 | 1.63350000    | 0.00000000 |
| 180 | 827.14550000 | 0.20860000    | 0.00000000 |
| 181 | 830.18760000 | 1.37200000    | 0.00000000 |
| 182 | 835.95220000 | 36.66610000   | 0.00000000 |
| 183 | 841.67670000 | 26.56460000   | 0.00000000 |
| 184 | 843.80090000 | 21.02280000   | 0.00000000 |
| 185 | 844.50490000 | 61.05050000   | 0.00000000 |
| 186 | 862.14540000 | 42.90540000   | 0.00000000 |
| 187 | 863.22330000 | 924.38420000  | 0.00000000 |
| 188 | 870.59780000 | 66.61590000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 189 | 874.51470000  | 37.38860000   | 0.00000000 |
| 190 | 874.91640000  | 110.71140000  | 0.00000000 |
| 191 | 875.24250000  | 1.77190000    | 0.00000000 |
| 192 | 877.46050000  | 6.56130000    | 0.00000000 |
| 193 | 881.02990000  | 0.33630000    | 0.00000000 |
| 194 | 884.88640000  | 0.17780000    | 0.00000000 |
| 195 | 888.10670000  | 5.45330000    | 0.00000000 |
| 196 | 893.35250000  | 6.33780000    | 0.00000000 |
| 197 | 894.48270000  | 2.37170000    | 0.00000000 |
| 198 | 897.21030000  | 1.48900000    | 0.00000000 |
| 199 | 905.74310000  | 0.10170000    | 0.00000000 |
| 200 | 907.12300000  | 61.92890000   | 0.00000000 |
| 201 | 921.69400000  | 2.38390000    | 0.00000000 |
| 202 | 923.02160000  | 6.32370000    | 0.00000000 |
| 203 | 937.83620000  | 2.11670000    | 0.00000000 |
| 204 | 940.75380000  | 2.70970000    | 0.00000000 |
| 205 | 940.78870000  | 0.93730000    | 0.00000000 |
| 206 | 943.75020000  | 0.98640000    | 0.00000000 |
| 207 | 947.42410000  | 0.79680000    | 0.00000000 |
| 208 | 952.28210000  | 0.41260000    | 0.00000000 |
| 209 | 958.26900000  | 1.05190000    | 0.00000000 |
| 210 | 968.31260000  | 5.25220000    | 0.00000000 |
| 211 | 970.59950000  | 0.34900000    | 0.00000000 |
| 212 | 971.23680000  | 6.09680000    | 0.00000000 |
| 213 | 984.81680000  | 24.33780000   | 0.00000000 |
| 214 | 992.85650000  | 0.00290000    | 0.00000000 |
| 215 | 993.59650000  | 0.43180000    | 0.00000000 |
| 216 | 993.99380000  | 4.13370000    | 0.00000000 |
| 217 | 994.05880000  | 3.01320000    | 0.00000000 |
| 218 | 1000.05420000 | 33.02260000   | 0.00000000 |
| 219 | 1002.91330000 | 11.02080000   | 0.00000000 |
| 220 | 1006.55920000 | 1.04780000    | 0.00000000 |
| 221 | 1009.47900000 | 1.99640000    | 0.00000000 |
| 222 | 1010.55420000 | 6.84700000    | 0.00000000 |
| 223 | 1012.68190000 | 0.25340000    | 0.00000000 |
| 224 | 1020.54180000 | 439.86370000  | 0.00000000 |
| 225 | 1021.66690000 | 26.14170000   | 0.00000000 |
| 226 | 1022.90110000 | 172.88190000  | 0.00000000 |
| 227 | 1030.34530000 | 19.48600000   | 0.00000000 |
| 228 | 1032.36790000 | 0.02840000    | 0.00000000 |
| 229 | 1040.48630000 | 5651.37950000 | 0.00000000 |
| 230 | 1041.54500000 | 1.00690000    | 0.00000000 |
| 231 | 1048.49310000 | 19.26020000   | 0.00000000 |
| 232 | 1049.21270000 | 30.98120000   | 0.00000000 |
| 233 | 1049.91500000 | 6.41960000    | 0.00000000 |
| 234 | 1051.54150000 | 0.16380000    | 0.00000000 |
| 235 | 1053.51230000 | 0.37820000    | 0.00000000 |
| 236 | 1054.43290000 | 224.35980000  | 0.00000000 |
| 237 | 1057.21060000 | 13.66140000   | 0.00000000 |
| 238 | 1062.70050000 | 2.19780000    | 0.00000000 |
| 239 | 1065.49960000 | 1773.24010000 | 0.00000000 |
| 240 | 1071.34650000 | 1.03390000    | 0.00000000 |
| 241 | 1072.03590000 | 1.52630000    | 0.00000000 |
| 242 | 1080.41800000 | 0.62030000    | 0.00000000 |
| 243 | 1082.05810000 | 107.55530000  | 0.00000000 |
| 244 | 1085.70040000 | 187.86150000  | 0.00000000 |
| 245 | 1087.53830000 | 10.71100000   | 0.00000000 |
| 246 | 1088.27420000 | 88.56030000   | 0.00000000 |
| 247 | 1092.22810000 | 22.08510000   | 0.00000000 |
| 248 | 1095.94360000 | 1779.03860000 | 0.00000000 |
| 249 | 1103.12520000 | 246.40250000  | 0.00000000 |
| 250 | 1114.31530000 | 3.89890000    | 0.00000000 |
| 251 | 1125.62780000 | 8.66420000    | 0.00000000 |
| 252 | 1128.49670000 | 69.65120000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 253 | 1130.28750000 | 134.90680000  | 0.00000000 |
| 254 | 1131.25660000 | 383.83450000  | 0.00000000 |
| 255 | 1134.88700000 | 33.24650000   | 0.00000000 |
| 256 | 1135.44280000 | 195.49930000  | 0.00000000 |
| 257 | 1137.91830000 | 1.29270000    | 0.00000000 |
| 258 | 1151.04050000 | 3.77890000    | 0.00000000 |
| 259 | 1151.27640000 | 5.67060000    | 0.00000000 |
| 260 | 1154.50960000 | 1.55530000    | 0.00000000 |
| 261 | 1161.35540000 | 1.43240000    | 0.00000000 |
| 262 | 1169.42870000 | 12.11080000   | 0.00000000 |
| 263 | 1169.88530000 | 6.21320000    | 0.00000000 |
| 264 | 1175.22200000 | 320.69400000  | 0.00000000 |
| 265 | 1178.44590000 | 19.76400000   | 0.00000000 |
| 266 | 1183.21680000 | 4.71950000    | 0.00000000 |
| 267 | 1186.04400000 | 2357.54240000 | 0.00000000 |
| 268 | 1202.80610000 | 124.54580000  | 0.00000000 |
| 269 | 1211.16450000 | 70.67370000   | 0.00000000 |
| 270 | 1214.72810000 | 31.51410000   | 0.00000000 |
| 271 | 1231.84260000 | 11.99370000   | 0.00000000 |
| 272 | 1235.53060000 | 82.59090000   | 0.00000000 |
| 273 | 1238.15200000 | 18.91950000   | 0.00000000 |
| 274 | 1241.75390000 | 4.25880000    | 0.00000000 |
| 275 | 1246.79980000 | 32.99450000   | 0.00000000 |
| 276 | 1247.48110000 | 22.96690000   | 0.00000000 |
| 277 | 1247.95590000 | 4.30890000    | 0.00000000 |
| 278 | 1258.58430000 | 1938.27600000 | 0.00000000 |
| 279 | 1261.52200000 | 137.13220000  | 0.00000000 |
| 280 | 1263.06330000 | 52.78100000   | 0.00000000 |
| 281 | 1265.01880000 | 10.91210000   | 0.00000000 |
| 282 | 1275.62330000 | 122.56050000  | 0.00000000 |
| 283 | 1279.31430000 | 2.41670000    | 0.00000000 |
| 284 | 1279.44940000 | 119.50570000  | 0.00000000 |
| 285 | 1282.04150000 | 0.03720000    | 0.00000000 |
| 286 | 1286.51660000 | 1.08060000    | 0.00000000 |
| 287 | 1290.75580000 | 1.11030000    | 0.00000000 |
| 288 | 1301.53300000 | 1342.54540000 | 0.00000000 |
| 289 | 1304.84580000 | 1.58370000    | 0.00000000 |
| 290 | 1306.44020000 | 7.49750000    | 0.00000000 |
| 291 | 1308.57150000 | 22.50670000   | 0.00000000 |
| 292 | 1310.91340000 | 5.89670000    | 0.00000000 |
| 293 | 1318.74210000 | 25.63800000   | 0.00000000 |
| 294 | 1319.76830000 | 21.00630000   | 0.00000000 |
| 295 | 1323.52530000 | 2.30200000    | 0.00000000 |
| 296 | 1323.80320000 | 167.38910000  | 0.00000000 |
| 297 | 1324.38390000 | 18.84140000   | 0.00000000 |
| 298 | 1326.49460000 | 156.33370000  | 0.00000000 |
| 299 | 1335.10760000 | 0.24710000    | 0.00000000 |
| 300 | 1335.56490000 | 0.19060000    | 0.00000000 |
| 301 | 1342.64000000 | 0.85710000    | 0.00000000 |
| 302 | 1348.31490000 | 20.76700000   | 0.00000000 |
| 303 | 1354.47370000 | 0.74340000    | 0.00000000 |
| 304 | 1360.43590000 | 51.39190000   | 0.00000000 |
| 305 | 1372.95740000 | 0.24100000    | 0.00000000 |
| 306 | 1376.89030000 | 163.77540000  | 0.00000000 |
| 307 | 1377.74030000 | 6.68090000    | 0.00000000 |
| 308 | 1378.06970000 | 9.99940000    | 0.00000000 |
| 309 | 1379.27120000 | 10.95840000   | 0.00000000 |
| 310 | 1379.76470000 | 4.81730000    | 0.00000000 |
| 311 | 1380.45900000 | 75.51500000   | 0.00000000 |
| 312 | 1380.51380000 | 67.22350000   | 0.00000000 |
| 313 | 1381.01810000 | 122.11730000  | 0.00000000 |
| 314 | 1384.05240000 | 329.16810000  | 0.00000000 |
| 315 | 1399.05840000 | 41.78230000   | 0.00000000 |
| 316 | 1399.60860000 | 2.44200000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 317 | 1404.59510000 | 24.99680000   | 0.00000000 |
| 318 | 1413.18160000 | 24.43040000   | 0.00000000 |
| 319 | 1431.68890000 | 16.26940000   | 0.00000000 |
| 320 | 1435.72170000 | 93.59740000   | 0.00000000 |
| 321 | 1439.37780000 | 18.62760000   | 0.00000000 |
| 322 | 1442.10660000 | 708.31160000  | 0.00000000 |
| 323 | 1447.17340000 | 1400.55660000 | 0.00000000 |
| 324 | 1452.77190000 | 328.09000000  | 0.00000000 |
| 325 | 1456.25860000 | 104.30890000  | 0.00000000 |
| 326 | 1463.42330000 | 32.40300000   | 0.00000000 |
| 327 | 1472.93040000 | 48.69660000   | 0.00000000 |
| 328 | 1475.79190000 | 1.95150000    | 0.00000000 |
| 329 | 1478.51510000 | 10.50540000   | 0.00000000 |
| 330 | 1481.24930000 | 13.34840000   | 0.00000000 |
| 331 | 1481.45050000 | 5.44270000    | 0.00000000 |
| 332 | 1484.34480000 | 61.21790000   | 0.00000000 |
| 333 | 1486.16130000 | 39.07190000   | 0.00000000 |
| 334 | 1488.26350000 | 58.24390000   | 0.00000000 |
| 335 | 1493.35000000 | 0.42010000    | 0.00000000 |
| 336 | 1501.33070000 | 1.57700000    | 0.00000000 |
| 337 | 1503.01680000 | 27.54220000   | 0.00000000 |
| 338 | 1504.62190000 | 6.87630000    | 0.00000000 |
| 339 | 1507.93600000 | 2.19790000    | 0.00000000 |
| 340 | 1510.28610000 | 15.43000000   | 0.00000000 |
| 341 | 1515.81390000 | 28.49940000   | 0.00000000 |
| 342 | 1522.96710000 | 278.10890000  | 0.00000000 |
| 343 | 1525.93080000 | 29.69490000   | 0.00000000 |
| 344 | 1532.34550000 | 137.67350000  | 0.00000000 |
| 345 | 1535.97800000 | 12.35780000   | 0.00000000 |
| 346 | 1540.67560000 | 27.28290000   | 0.00000000 |
| 347 | 1544.10740000 | 85.56840000   | 0.00000000 |
| 348 | 1555.24300000 | 33.92610000   | 0.00000000 |
| 349 | 1559.02800000 | 9.39910000    | 0.00000000 |
| 350 | 1571.04400000 | 115.17080000  | 0.00000000 |
| 351 | 1574.91780000 | 236.65940000  | 0.00000000 |
| 352 | 1575.14690000 | 7.44870000    | 0.00000000 |
| 353 | 1581.37090000 | 160.40450000  | 0.00000000 |
| 354 | 1585.75480000 | 8.01490000    | 0.00000000 |
| 355 | 1588.04980000 | 10.31250000   | 0.00000000 |
| 356 | 1595.21580000 | 11.37370000   | 0.00000000 |
| 357 | 1613.61030000 | 67.04770000   | 0.00000000 |
| 358 | 1615.31530000 | 19.91430000   | 0.00000000 |
| 359 | 1617.90980000 | 63.64950000   | 0.00000000 |
| 360 | 1625.58740000 | 1.64910000    | 0.00000000 |
| 361 | 1626.50210000 | 41.59650000   | 0.00000000 |
| 362 | 1627.00170000 | 6.61930000    | 0.00000000 |
| 363 | 1639.62180000 | 3.00020000    | 0.00000000 |
| 364 | 1651.75780000 | 106.90200000  | 0.00000000 |
| 365 | 1652.29510000 | 87.31740000   | 0.00000000 |
| 366 | 1656.50550000 | 412.00800000  | 0.00000000 |
| 367 | 1661.13990000 | 89.81770000   | 0.00000000 |
| 368 | 1661.48900000 | 5.31340000    | 0.00000000 |
| 369 | 1661.74600000 | 107.49490000  | 0.00000000 |
| 370 | 1661.97930000 | 125.68610000  | 0.00000000 |
| 371 | 1963.93560000 | 2391.46960000 | 0.00000000 |
| 372 | 1970.09600000 | 2306.53220000 | 0.00000000 |
| 373 | 2083.78720000 | 1995.88500000 | 0.00000000 |
| 374 | 3010.09000000 | 16.10810000   | 0.00000000 |
| 375 | 3016.87590000 | 3.33200000    | 0.00000000 |
| 376 | 3022.44250000 | 76.43030000   | 0.00000000 |
| 377 | 3034.05370000 | 0.71310000    | 0.00000000 |
| 378 | 3041.39790000 | 59.91600000   | 0.00000000 |
| 379 | 3045.52140000 | 54.34930000   | 0.00000000 |
| 380 | 3050.57840000 | 0.56830000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 3064.25490000 | 73.63500000   | 0.00000000 |
| 382 | 3087.47410000 | 63.03770000   | 0.00000000 |
| 383 | 3092.89760000 | 62.94370000   | 0.00000000 |
| 384 | 3170.30350000 | 5.50810000    | 0.00000000 |
| 385 | 3180.96510000 | 9.33660000    | 0.00000000 |
| 386 | 3186.71580000 | 6.72550000    | 0.00000000 |
| 387 | 3187.87890000 | 5.86220000    | 0.00000000 |
| 388 | 3189.52200000 | 12.14140000   | 0.00000000 |
| 389 | 3194.98790000 | 0.67520000    | 0.00000000 |
| 390 | 3195.30960000 | 3.33180000    | 0.00000000 |
| 391 | 3195.62080000 | 104.63280000  | 0.00000000 |
| 392 | 3195.83340000 | 3.11330000    | 0.00000000 |
| 393 | 3202.67750000 | 1.70240000    | 0.00000000 |
| 394 | 3202.86740000 | 0.13410000    | 0.00000000 |
| 395 | 3203.73720000 | 4.56330000    | 0.00000000 |
| 396 | 3203.85880000 | 78.95350000   | 0.00000000 |
| 397 | 3204.61960000 | 1.72210000    | 0.00000000 |
| 398 | 3208.18610000 | 39.45830000   | 0.00000000 |
| 399 | 3212.00920000 | 27.00700000   | 0.00000000 |
| 400 | 3213.13520000 | 19.94040000   | 0.00000000 |
| 401 | 3216.98140000 | 8.22760000    | 0.00000000 |
| 402 | 3217.37810000 | 1.72700000    | 0.00000000 |
| 403 | 3219.32660000 | 7.41330000    | 0.00000000 |
| 404 | 3220.44160000 | 25.68120000   | 0.00000000 |
| 405 | 3221.54350000 | 33.31340000   | 0.00000000 |
| 406 | 3232.11360000 | 4.89770000    | 0.00000000 |
| 407 | 3232.49840000 | 3.65140000    | 0.00000000 |
| 408 | 3238.21300000 | 0.13620000    | 0.00000000 |
| 409 | 3238.98330000 | 6.49890000    | 0.00000000 |
| 410 | 3239.21040000 | 5.67460000    | 0.00000000 |
| 411 | 3242.90190000 | 42.06520000   | 0.00000000 |
| 412 | 3243.48330000 | 3.11060000    | 0.00000000 |
| 413 | 3260.98340000 | 1.16520000    | 0.00000000 |
| 414 | 3262.32250000 | 0.87150000    | 0.00000000 |
| 415 | 3266.76810000 | 6.17070000    | 0.00000000 |
| 416 | 3272.37660000 | 9.40450000    | 0.00000000 |
| 417 | 3273.19270000 | 25.00870000   | 0.00000000 |
| 418 | 3273.72060000 | 17.99600000   | 0.00000000 |
| 419 | 3287.90090000 | 8.46160000    | 0.00000000 |
| 420 | 3288.25560000 | 9.53320000    | 0.00000000 |
| 421 | 3288.68450000 | 7.17750000    | 0.00000000 |
| 422 | 3373.52070000 | 2924.64840000 | 0.00000000 |
| 423 | 3376.45150000 | 1378.47030000 | 0.00000000 |
| 424 | 3567.69130000 | 1652.07360000 | 0.00000000 |
| 425 | 3573.95490000 | 201.35960000  | 0.00000000 |
| 426 | 3840.53270000 | 96.68420000   | 0.00000000 |
| 427 | 3840.54990000 | 75.94370000   | 0.00000000 |
| 428 | 3841.03570000 | 75.78840000   | 0.00000000 |
| 429 | 3842.19380000 | 94.82350000   | 0.00000000 |

### S23. CALCULATIONS ON EXTENDED CONFORMER OF 2w<sup>3+</sup> (<sup>1</sup>A)

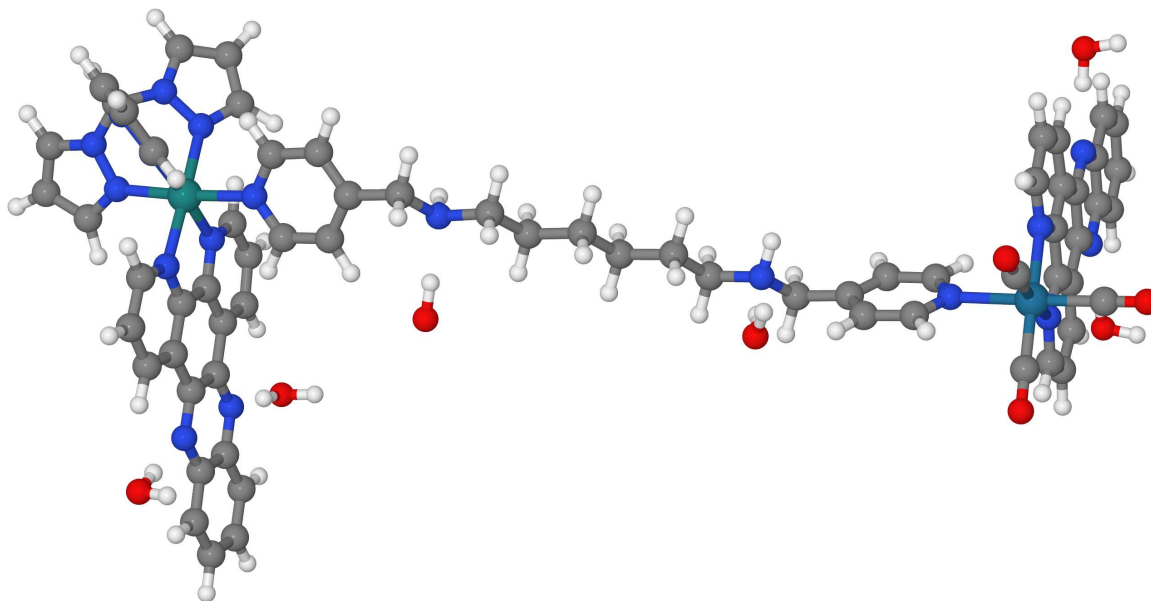


FIG. S33. Molecule

```

Route      : # opt freq b3lyp/genecp scrf=(solvent=water) geom=connectivity empiric
            : aldispersion=gd3bj int=ultrafine pop=regular
SMILES     : c1ccc2c(c1)nc3c4ccc[n+]5c4c6c(c3n2)ccc[n+]6[Ru]578(n9ccc[n+]9C([n+]
            : 1n7ccc1)[n+]1n8ccc1)[n+]1ccc(cc1)CNCNCCCCNCCc1cc[n+](cc1)[Re]
            : 1([n+]2cccc3c2c2[n+]1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O].O.O.O.O.O.O
Formula    : C67H68N18O9ReRu3+
Charge     : 3
Multiplicity : 1
Energy     : -4431.37419254 a.u.
Gibbs Energy : -4430.22060800 a.u.
Number of imaginary frequencies : 4

```

#### S23.1. Cartesian Co-ordinates (XYZ format)

164

```

C    3.15440011  0.46022099 -0.39880499
H    2.87946105  1.48968899 -0.14638700
H    3.11683106 -0.11970300  0.53573501
C    2.15884209 -0.10816000 -1.40484798
H    2.45713806 -1.12969100 -1.67131495
H    2.20477891  0.48532799 -2.32343888
C    0.72800201 -0.11956700 -0.86426401
H    0.43841001  0.90125400 -0.58689302
H    0.68934703 -0.71237600  0.05754500
C   -0.28849101 -0.67418498 -1.86418104
H   -0.01187300 -1.70083296 -2.13254094
H   -0.24044301 -0.08855000 -2.79017305
C   -2.73724699 -1.19279206 -2.32386088
H   -2.47151804 -2.22005892 -2.61579704

```



|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | -2.72066808  | -0.58713299 | -3.23598695 |
| N  | 4.51840019   | 0.49056101  | -0.95252001 |
| C  | -5.10544920  | -1.68301797 | -2.69119406 |
| H  | -4.85538578  | -2.70407510 | -3.00859308 |
| H  | -5.10966396  | -1.06210101 | -3.59378695 |
| N  | -4.10129881  | -1.12933099 | -1.77396202 |
| C  | 5.49907303   | 0.98739398  | 0.01953000  |
| H  | 5.22546577   | 2.01846194  | 0.26989901  |
| H  | 5.47549295   | 0.41703001  | 0.95751899  |
| C  | -12.84430695 | -4.19697094 | -0.10523400 |
| N  | -11.62059498 | -4.53915787 | 0.59196401  |
| N  | -13.52801609 | -3.11198092 | 0.56118202  |
| N  | -12.55451965 | -3.85652804 | -1.48362195 |
| N  | -10.62662601 | -3.61551404 | 0.68897998  |
| C  | -11.24180698 | -5.73180199 | 1.12478805  |
| N  | -12.91041946 | -1.90798903 | 0.67925400  |
| C  | -14.75965118 | -3.09455490 | 1.13952804  |
| N  | -11.72416019 | -2.81322598 | -1.75417697 |
| C  | -12.91770554 | -4.50766516 | -2.62145209 |
| Ru | -10.99682045 | -1.72008097 | -0.12266500 |
| C  | -9.61144447  | -4.23574877 | 1.29044604  |
| C  | -9.95492744  | -5.56763601 | 1.58753598  |
| H  | -11.90774536 | -6.57812595 | 1.13057005  |
| C  | -13.76049137 | -1.12113094 | 1.33536994  |
| C  | -14.93926907 | -1.82634795 | 1.64565206  |
| H  | -15.38944530 | -3.96813607 | 1.14009702  |
| C  | -11.56756020 | -2.80670404 | -3.07792807 |
| C  | -12.30392647 | -3.85213804 | -3.66566610 |
| H  | -13.57178020 | -5.36286211 | -2.59173489 |
| N  | -10.39159012 | -0.56165397 | 1.49560201  |
| N  | -11.42928028 | 0.19390801  | -0.80976301 |
| H  | -8.68854427  | -3.70985603 | 1.47124898  |
| H  | -9.34235764  | -6.30657387 | 2.07426000  |
| H  | -13.49656773 | -0.09960000 | 1.55404401  |
| H  | -15.80307961 | -1.45483506 | 2.16921306  |
| H  | -10.93475533 | -2.06922793 | -3.54364896 |
| H  | -12.37487507 | -4.09207010 | -4.71236277 |
| C  | -9.92378044  | -1.00364304 | 2.66614294  |
| C  | -10.52504730 | 0.78087401  | 1.31188297  |
| C  | -11.09249401 | 1.19451106  | 0.04990600  |
| C  | -12.01067066 | 0.51454902  | -1.96879697 |
| C  | -9.54348278  | -0.13497700 | 3.68669796  |
| H  | -9.85748672  | -2.07449007 | 2.78651404  |
| C  | -10.16036129 | 1.71754205  | 2.28880692  |
| C  | -11.29974365 | 2.54846001  | -0.24761701 |
| C  | -12.25365162 | 1.83692896  | -2.33354092 |
| H  | -12.28872108 | -0.30637300 | -2.61258411 |
| C  | -9.65119267  | 1.23133194  | 3.50299811  |
| H  | -9.16532516  | -0.54305202 | 4.61395216  |
| C  | -10.33292866 | 3.14080405  | 1.99543095  |
| C  | -11.89249420 | 2.86350799  | -1.48028004 |
| C  | -10.89608192 | 3.55282092  | 0.73720700  |
| H  | -12.72255993 | 2.04461503  | -3.28553700 |
| H  | -9.35274506  | 1.91019702  | 4.28922510  |
| N  | -9.96529102  | 4.03626299  | 2.90033889  |
| H  | -12.07296276 | 3.89155197  | -1.76091504 |
| N  | -11.05869389 | 4.83703899  | 0.45418799  |
| C  | -10.12302399 | 5.34756517  | 2.62086201  |
| C  | -10.68288708 | 5.75798321  | 1.36689603  |
| C  | -9.73355961  | 6.33169079  | 3.56681895  |
| C  | -10.83886433 | 7.14168596  | 1.09135497  |
| C  | -9.89826393  | 7.65909100  | 3.26932907  |
| H  | -9.31325245  | 6.00754404  | 4.51019192  |
| C  | -10.45306301 | 8.06571960  | 2.02668500  |

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | -11.26471806 | 7.43697023  | 0.14102399  |
| H  | -9.60283947  | 8.41284466  | 3.98837709  |
| H  | -10.57075310 | 9.12218285  | 1.82049704  |
| N  | 12.27568436  | 1.55660403  | -0.23231199 |
| N  | 11.96242237  | -0.85591501 | -1.33629203 |
| C  | 12.37837315  | 2.78317690  | 0.28907400  |
| C  | 12.60757256  | 0.48527199  | 0.53602600  |
| C  | 12.44025803  | -0.82337898 | -0.06382200 |
| C  | 11.75838661  | -2.04075599 | -1.92053199 |
| C  | 12.81990719  | 2.99937797  | 1.59159505  |
| H  | 12.10356808  | 3.60789108  | -0.35213801 |
| C  | 13.06149864  | 0.62259102  | 1.85596895  |
| C  | 12.73324013  | -1.99104202 | 0.65572000  |
| C  | 12.02605724  | -3.24252892 | -1.27050900 |
| H  | 11.37530994  | -2.02514505 | -2.93040109 |
| C  | 13.16765308  | 1.92031598  | 2.38107896  |
| H  | 12.88569641  | 4.01063299  | 1.96815205  |
| C  | 13.39229584  | -0.57859999 | 2.62236309  |
| C  | 12.51855087  | -3.22429991 | 0.02006200  |
| C  | 13.23283386  | -1.87510002 | 2.02555394  |
| H  | 11.84485722  | -4.17561817 | -1.78561699 |
| H  | 13.51302624  | 2.07888508  | 3.39301109  |
| N  | 13.83445930  | -0.45174101 | 3.86526990  |
| H  | 12.73076630  | -4.15243387 | 0.53193998  |
| N  | 13.52723217  | -2.97609711 | 2.70189905  |
| C  | 14.13829231  | -1.56555200 | 4.56411791  |
| C  | 13.98237419  | -2.85989308 | 3.96699905  |
| C  | 14.61603069  | -1.46488500 | 5.89711905  |
| C  | 14.30980015  | -4.01925611 | 4.71791887  |
| C  | 14.92179775  | -2.60411310 | 6.59406519  |
| H  | 14.72659492  | -0.48203799 | 6.33681393  |
| C  | 14.76844025  | -3.88626194 | 6.00205898  |
| H  | 14.18647194  | -4.99000406 | 4.25529385  |
| H  | 15.28606796  | -2.53172898 | 7.61115599  |
| H  | 15.01875973  | -4.76793909 | 6.57858801  |
| H  | -13.49476814 | -5.06516409 | -0.09807900 |
| C  | 6.90366793   | 0.98360002  | -0.52816498 |
| C  | 7.96029377   | 0.46973199  | 0.22025600  |
| C  | 7.21074390   | 1.51257896  | -1.78578901 |
| C  | 9.24955559   | 0.50772202  | -0.28574699 |
| H  | 7.79284477   | 0.03616900  | 1.19773698  |
| C  | 8.52102375   | 1.51281595  | -2.22462296 |
| H  | 6.43840790   | 1.92177999  | -2.42475510 |
| N  | 9.54565811   | 1.02210999  | -1.49223197 |
| H  | 10.06522083  | 0.10977300  | 0.29696500  |
| H  | 8.77445984   | 1.92064595  | -3.19260406 |
| C  | -6.48561811  | -1.67440498 | -2.08365703 |
| C  | -7.02208710  | -0.52832502 | -1.49010301 |
| C  | -7.28762817  | -2.81427312 | -2.10209703 |
| C  | -8.29555225  | -0.56782198 | -0.95326501 |
| H  | -6.45393610  | 0.39166099  | -1.43506706 |
| C  | -8.55644417  | -2.77922297 | -1.54718494 |
| H  | -6.93287992  | -3.73768401 | -2.54196405 |
| N  | -9.06842709  | -1.67349803 | -0.97052300 |
| H  | -8.71484470  | 0.31361899  | -0.49371001 |
| H  | -9.18707275  | -3.65525889 | -1.55224204 |
| Re | 11.64655018  | 1.10552001  | -2.30065608 |
| C  | 13.48752689  | 1.14284801  | -2.92097402 |
| O  | 14.58234024  | 1.15938902  | -3.27760696 |
| C  | 11.06086731  | 0.45166299  | -4.03127718 |
| O  | 10.71312809  | 0.03292500  | -5.04775190 |
| C  | 11.39758682  | 2.93489289  | -2.89874792 |
| O  | 11.25885391  | 4.03226709  | -3.22415996 |
| H  | -4.12750578  | -1.65994704 | -0.90608001 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | 4.78036213   | -0.45408601 | -1.22552001 |
| C | -1.71950996  | -0.65240800 | -1.32448101 |
| H | -1.99836898  | 0.37151301  | -1.05598998 |
| H | -1.76942003  | -1.24613094 | -0.40328199 |
| H | -4.33722687  | 0.64877701  | -1.39332497 |
| O | -4.47371006  | 1.60788500  | -1.19957304 |
| H | -4.53971910  | 1.63354003  | -0.23887700 |
| H | 4.35378599   | 1.50614202  | -2.47185802 |
| O | 4.27641296   | 2.05563903  | -3.28880501 |
| H | 4.45634413   | 1.42772305  | -3.99690008 |
| H | 13.46577930  | -4.84902000 | 2.21763992  |
| O | 13.47516823  | -5.78855991 | 1.95641601  |
| H | 14.35145378  | -5.90699291 | 1.57275999  |
| H | 14.16534424  | 1.10388005  | 4.96977711  |
| O | 14.37987423  | 1.88961101  | 5.50608110  |
| H | 15.30000496  | 2.07005811  | 5.28264809  |
| H | -11.75649834 | 5.73128605  | -1.11049104 |
| O | -12.06616783 | 6.19060707  | -1.91354704 |
| H | -11.26714706 | 6.27662897  | -2.44573689 |
| H | -9.18574715  | 3.84549093  | 4.65917921  |
| O | -8.74470043  | 3.75758505  | 5.52490091  |
| H | -7.80762815  | 3.74829197  | 5.29936790  |

**S23.2. Frequencies**

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -12.39110000 | 0.60180000   | 0.00000000      |
| 2    | -9.61240000  | 0.16200000   | 0.00000000      |
| 3    | -8.95220000  | 0.59300000   | 0.00000000      |
| 4    | -5.28550000  | 0.53830000   | 0.00000000      |
| 5    | 0.47200000   | 0.45010000   | 0.00000000      |
| 6    | 9.03830000   | 1.08990000   | 0.00000000      |
| 7    | 10.67960000  | 1.32740000   | 0.00000000      |
| 8    | 11.37760000  | 0.86560000   | 0.00000000      |
| 9    | 14.31740000  | 1.68760000   | 0.00000000      |
| 10   | 16.61600000  | 2.99330000   | 0.00000000      |
| 11   | 18.80700000  | 1.03260000   | 0.00000000      |
| 12   | 24.06740000  | 0.55580000   | 0.00000000      |
| 13   | 26.75100000  | 1.69220000   | 0.00000000      |
| 14   | 27.46550000  | 1.17430000   | 0.00000000      |
| 15   | 28.99280000  | 0.81030000   | 0.00000000      |
| 16   | 32.16440000  | 0.85790000   | 0.00000000      |
| 17   | 38.06270000  | 1.40500000   | 0.00000000      |
| 18   | 41.58580000  | 1.91300000   | 0.00000000      |
| 19   | 44.59260000  | 0.61690000   | 0.00000000      |
| 20   | 46.98100000  | 0.31410000   | 0.00000000      |
| 21   | 51.97510000  | 0.52160000   | 0.00000000      |
| 22   | 53.25280000  | 0.81270000   | 0.00000000      |
| 23   | 57.36290000  | 2.18350000   | 0.00000000      |
| 24   | 60.24270000  | 2.26120000   | 0.00000000      |
| 25   | 62.69280000  | 1.76930000   | 0.00000000      |
| 26   | 65.15370000  | 1.37960000   | 0.00000000      |
| 27   | 66.53850000  | 0.56200000   | 0.00000000      |
| 28   | 68.48920000  | 2.09950000   | 0.00000000      |
| 29   | 69.47230000  | 3.42080000   | 0.00000000      |
| 30   | 73.32010000  | 1.97060000   | 0.00000000      |
| 31   | 73.97180000  | 2.39320000   | 0.00000000      |
| 32   | 74.48500000  | 0.75500000   | 0.00000000      |
| 33   | 78.14130000  | 0.19070000   | 0.00000000      |
| 34   | 82.07480000  | 9.95800000   | 0.00000000      |
| 35   | 83.39840000  | 0.93830000   | 0.00000000      |
| 36   | 85.79100000  | 0.21200000   | 0.00000000      |
| 37   | 90.53970000  | 6.02070000   | 0.00000000      |
| 38   | 90.80100000  | 0.57180000   | 0.00000000      |
| 39   | 91.87370000  | 2.29760000   | 0.00000000      |
| 40   | 94.21020000  | 14.48870000  | 0.00000000      |
| 41   | 96.62000000  | 3.44330000   | 0.00000000      |
| 42   | 97.62920000  | 1.19220000   | 0.00000000      |
| 43   | 98.78570000  | 3.29150000   | 0.00000000      |
| 44   | 99.46490000  | 15.72750000  | 0.00000000      |
| 45   | 103.36650000 | 7.01160000   | 0.00000000      |
| 46   | 107.64710000 | 2.31580000   | 0.00000000      |
| 47   | 110.14600000 | 2.34600000   | 0.00000000      |
| 48   | 121.70800000 | 0.15680000   | 0.00000000      |
| 49   | 126.84250000 | 0.39880000   | 0.00000000      |
| 50   | 130.51610000 | 3.01560000   | 0.00000000      |
| 51   | 140.24160000 | 0.37710000   | 0.00000000      |
| 52   | 141.91100000 | 0.64280000   | 0.00000000      |
| 53   | 143.89880000 | 0.57150000   | 0.00000000      |
| 54   | 144.90780000 | 0.65730000   | 0.00000000      |
| 55   | 147.68700000 | 0.22200000   | 0.00000000      |
| 56   | 148.00770000 | 0.03280000   | 0.00000000      |
| 57   | 152.40890000 | 0.56840000   | 0.00000000      |
| 58   | 155.54520000 | 0.47050000   | 0.00000000      |
| 59   | 157.88380000 | 1.54190000   | 0.00000000      |
| 60   | 158.68540000 | 2.19690000   | 0.00000000      |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 161.29050000 | 0.23950000   | 0.00000000 |
| 62  | 162.29310000 | 0.22480000   | 0.00000000 |
| 63  | 164.23460000 | 3.42330000   | 0.00000000 |
| 64  | 170.08720000 | 7.09780000   | 0.00000000 |
| 65  | 171.01950000 | 3.42550000   | 0.00000000 |
| 66  | 173.05010000 | 9.77300000   | 0.00000000 |
| 67  | 174.57730000 | 1.64770000   | 0.00000000 |
| 68  | 178.94020000 | 4.88200000   | 0.00000000 |
| 69  | 180.99890000 | 2.59220000   | 0.00000000 |
| 70  | 187.43320000 | 11.20200000  | 0.00000000 |
| 71  | 194.69480000 | 0.29160000   | 0.00000000 |
| 72  | 196.54220000 | 3.88090000   | 0.00000000 |
| 73  | 200.38180000 | 14.01510000  | 0.00000000 |
| 74  | 210.67630000 | 1.24410000   | 0.00000000 |
| 75  | 214.63210000 | 19.73260000  | 0.00000000 |
| 76  | 217.41460000 | 69.72260000  | 0.00000000 |
| 77  | 221.48710000 | 13.40990000  | 0.00000000 |
| 78  | 223.12770000 | 103.28010000 | 0.00000000 |
| 79  | 224.97040000 | 40.84030000  | 0.00000000 |
| 80  | 227.01030000 | 22.72510000  | 0.00000000 |
| 81  | 232.04850000 | 11.79450000  | 0.00000000 |
| 82  | 237.51260000 | 48.14900000  | 0.00000000 |
| 83  | 239.60240000 | 94.47670000  | 0.00000000 |
| 84  | 244.66870000 | 117.56000000 | 0.00000000 |
| 85  | 254.25870000 | 163.39380000 | 0.00000000 |
| 86  | 256.20530000 | 168.50090000 | 0.00000000 |
| 87  | 262.61170000 | 11.19600000  | 0.00000000 |
| 88  | 266.90510000 | 10.52740000  | 0.00000000 |
| 89  | 268.10840000 | 3.15390000   | 0.00000000 |
| 90  | 279.58900000 | 143.08920000 | 0.00000000 |
| 91  | 280.12330000 | 109.59830000 | 0.00000000 |
| 92  | 284.74120000 | 66.59900000  | 0.00000000 |
| 93  | 285.68740000 | 28.72530000  | 0.00000000 |
| 94  | 294.79950000 | 7.47310000   | 0.00000000 |
| 95  | 299.20840000 | 1.11960000   | 0.00000000 |
| 96  | 304.37880000 | 53.74790000  | 0.00000000 |
| 97  | 308.85930000 | 64.99320000  | 0.00000000 |
| 98  | 311.08700000 | 22.29440000  | 0.00000000 |
| 99  | 324.80350000 | 5.71880000   | 0.00000000 |
| 100 | 333.39430000 | 5.43310000   | 0.00000000 |
| 101 | 338.63150000 | 3.49250000   | 0.00000000 |
| 102 | 339.49200000 | 6.72810000   | 0.00000000 |
| 103 | 342.23870000 | 24.76490000  | 0.00000000 |
| 104 | 342.86250000 | 6.35870000   | 0.00000000 |
| 105 | 343.16620000 | 1.56830000   | 0.00000000 |
| 106 | 344.20010000 | 20.06290000  | 0.00000000 |
| 107 | 348.39510000 | 26.82330000  | 0.00000000 |
| 108 | 359.73960000 | 2.08020000   | 0.00000000 |
| 109 | 367.88620000 | 7.64600000   | 0.00000000 |
| 110 | 372.10390000 | 3.56940000   | 0.00000000 |
| 111 | 380.42250000 | 3.65650000   | 0.00000000 |
| 112 | 388.43000000 | 1.42990000   | 0.00000000 |
| 113 | 392.53070000 | 0.43590000   | 0.00000000 |
| 114 | 403.11820000 | 4.60780000   | 0.00000000 |
| 115 | 405.54090000 | 0.43110000   | 0.00000000 |
| 116 | 407.50350000 | 0.34340000   | 0.00000000 |
| 117 | 411.74320000 | 0.11850000   | 0.00000000 |
| 118 | 414.69930000 | 1.14980000   | 0.00000000 |
| 119 | 431.19010000 | 4.65190000   | 0.00000000 |
| 120 | 435.26990000 | 9.60850000   | 0.00000000 |
| 121 | 442.55640000 | 2.93300000   | 0.00000000 |
| 122 | 451.05760000 | 32.90290000  | 0.00000000 |
| 123 | 451.88880000 | 21.61330000  | 0.00000000 |
| 124 | 456.28660000 | 5.56430000   | 0.00000000 |

|     |              |              |            |
|-----|--------------|--------------|------------|
| 125 | 461.19410000 | 34.15480000  | 0.00000000 |
| 126 | 461.81580000 | 107.38000000 | 0.00000000 |
| 127 | 475.46710000 | 33.67260000  | 0.00000000 |
| 128 | 475.62370000 | 28.17540000  | 0.00000000 |
| 129 | 478.53570000 | 2.31570000   | 0.00000000 |
| 130 | 481.48350000 | 4.59180000   | 0.00000000 |
| 131 | 487.26210000 | 9.11490000   | 0.00000000 |
| 132 | 491.96780000 | 2.09580000   | 0.00000000 |
| 133 | 494.69870000 | 0.66050000   | 0.00000000 |
| 134 | 496.49040000 | 2.84980000   | 0.00000000 |
| 135 | 499.13290000 | 6.66570000   | 0.00000000 |
| 136 | 506.65360000 | 0.55360000   | 0.00000000 |
| 137 | 509.22070000 | 2.75680000   | 0.00000000 |
| 138 | 510.25140000 | 1.93810000   | 0.00000000 |
| 139 | 518.06610000 | 0.19020000   | 0.00000000 |
| 140 | 532.38100000 | 13.73740000  | 0.00000000 |
| 141 | 534.03490000 | 29.14250000  | 0.00000000 |
| 142 | 545.86330000 | 9.00170000   | 0.00000000 |
| 143 | 558.21970000 | 11.58310000  | 0.00000000 |
| 144 | 563.41050000 | 0.55130000   | 0.00000000 |
| 145 | 565.01320000 | 0.34400000   | 0.00000000 |
| 146 | 576.22580000 | 1.92840000   | 0.00000000 |
| 147 | 577.20670000 | 3.98310000   | 0.00000000 |
| 148 | 579.51390000 | 0.60910000   | 0.00000000 |
| 149 | 581.42890000 | 0.55850000   | 0.00000000 |
| 150 | 594.13450000 | 18.07420000  | 0.00000000 |
| 151 | 594.91760000 | 20.27720000  | 0.00000000 |
| 152 | 606.46350000 | 0.28920000   | 0.00000000 |
| 153 | 607.24590000 | 3.89950000   | 0.00000000 |
| 154 | 611.48940000 | 5.22120000   | 0.00000000 |
| 155 | 618.96030000 | 23.27110000  | 0.00000000 |
| 156 | 623.13400000 | 33.38350000  | 0.00000000 |
| 157 | 624.17320000 | 27.48640000  | 0.00000000 |
| 158 | 634.02830000 | 36.45030000  | 0.00000000 |
| 159 | 637.14890000 | 5.70360000   | 0.00000000 |
| 160 | 640.36280000 | 8.84270000   | 0.00000000 |
| 161 | 646.93680000 | 83.36380000  | 0.00000000 |
| 162 | 652.13680000 | 5.07980000   | 0.00000000 |
| 163 | 652.38720000 | 5.71760000   | 0.00000000 |
| 164 | 654.68330000 | 5.24290000   | 0.00000000 |
| 165 | 655.70660000 | 2.95940000   | 0.00000000 |
| 166 | 658.95370000 | 0.36880000   | 0.00000000 |
| 167 | 666.55220000 | 0.52940000   | 0.00000000 |
| 168 | 669.79300000 | 3.58540000   | 0.00000000 |
| 169 | 678.13240000 | 3.15340000   | 0.00000000 |
| 170 | 684.82020000 | 1.14010000   | 0.00000000 |
| 171 | 685.42820000 | 0.33980000   | 0.00000000 |
| 172 | 685.66760000 | 0.23900000   | 0.00000000 |
| 173 | 738.65210000 | 11.11570000  | 0.00000000 |
| 174 | 739.06480000 | 7.94390000   | 0.00000000 |
| 175 | 740.06820000 | 4.83670000   | 0.00000000 |
| 176 | 741.51940000 | 14.40480000  | 0.00000000 |
| 177 | 742.12040000 | 1.50960000   | 0.00000000 |
| 178 | 750.42810000 | 0.08450000   | 0.00000000 |
| 179 | 752.42230000 | 0.02770000   | 0.00000000 |
| 180 | 756.32130000 | 8.48410000   | 0.00000000 |
| 181 | 756.97760000 | 91.81250000  | 0.00000000 |
| 182 | 757.15700000 | 2.29040000   | 0.00000000 |
| 183 | 761.15870000 | 90.92110000  | 0.00000000 |
| 184 | 763.20950000 | 4.26330000   | 0.00000000 |
| 185 | 763.66350000 | 89.61880000  | 0.00000000 |
| 186 | 763.72760000 | 92.66400000  | 0.00000000 |
| 187 | 765.32320000 | 118.85330000 | 0.00000000 |
| 188 | 779.35600000 | 66.76230000  | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 189 | 780.09030000  | 60.64600000  | 0.00000000 |
| 190 | 787.61110000  | 75.87560000  | 0.00000000 |
| 191 | 788.07660000  | 72.86470000  | 0.00000000 |
| 192 | 800.15700000  | 109.42210000 | 0.00000000 |
| 193 | 800.95980000  | 90.42190000  | 0.00000000 |
| 194 | 806.61620000  | 54.29510000  | 0.00000000 |
| 195 | 808.61280000  | 35.03730000  | 0.00000000 |
| 196 | 809.52030000  | 259.91970000 | 0.00000000 |
| 197 | 810.19750000  | 30.23220000  | 0.00000000 |
| 198 | 810.23640000  | 283.30130000 | 0.00000000 |
| 199 | 820.63220000  | 1.53510000   | 0.00000000 |
| 200 | 821.86030000  | 0.57410000   | 0.00000000 |
| 201 | 822.38930000  | 0.16890000   | 0.00000000 |
| 202 | 831.25740000  | 4.45430000   | 0.00000000 |
| 203 | 833.32690000  | 80.06830000  | 0.00000000 |
| 204 | 835.54210000  | 65.51460000  | 0.00000000 |
| 205 | 839.75440000  | 70.67920000  | 0.00000000 |
| 206 | 844.98890000  | 70.02190000  | 0.00000000 |
| 207 | 859.43050000  | 0.12310000   | 0.00000000 |
| 208 | 867.08300000  | 5.73430000   | 0.00000000 |
| 209 | 868.30420000  | 11.87590000  | 0.00000000 |
| 210 | 869.78320000  | 81.90820000  | 0.00000000 |
| 211 | 870.29470000  | 35.08930000  | 0.00000000 |
| 212 | 870.82150000  | 79.70040000  | 0.00000000 |
| 213 | 872.35880000  | 66.45110000  | 0.00000000 |
| 214 | 874.72090000  | 24.01570000  | 0.00000000 |
| 215 | 876.40310000  | 0.27670000   | 0.00000000 |
| 216 | 877.08850000  | 9.53120000   | 0.00000000 |
| 217 | 879.00290000  | 50.22550000  | 0.00000000 |
| 218 | 880.35490000  | 77.72490000  | 0.00000000 |
| 219 | 882.82130000  | 110.58010000 | 0.00000000 |
| 220 | 888.89060000  | 141.57920000 | 0.00000000 |
| 221 | 906.30680000  | 0.08850000   | 0.00000000 |
| 222 | 906.37830000  | 0.06360000   | 0.00000000 |
| 223 | 907.16690000  | 87.98940000  | 0.00000000 |
| 224 | 908.75260000  | 46.81460000  | 0.00000000 |
| 225 | 913.86110000  | 40.33530000  | 0.00000000 |
| 226 | 917.18710000  | 1.42600000   | 0.00000000 |
| 227 | 921.75790000  | 2.07930000   | 0.00000000 |
| 228 | 921.81560000  | 0.67130000   | 0.00000000 |
| 229 | 924.52130000  | 3.36160000   | 0.00000000 |
| 230 | 926.73800000  | 4.24690000   | 0.00000000 |
| 231 | 947.00010000  | 0.26180000   | 0.00000000 |
| 232 | 947.99610000  | 0.00770000   | 0.00000000 |
| 233 | 953.26330000  | 0.35950000   | 0.00000000 |
| 234 | 978.68330000  | 0.60180000   | 0.00000000 |
| 235 | 988.25760000  | 0.03390000   | 0.00000000 |
| 236 | 988.51200000  | 0.03050000   | 0.00000000 |
| 237 | 990.19600000  | 74.96020000  | 0.00000000 |
| 238 | 994.32220000  | 0.33630000   | 0.00000000 |
| 239 | 995.24370000  | 0.11800000   | 0.00000000 |
| 240 | 996.35760000  | 24.36790000  | 0.00000000 |
| 241 | 999.80750000  | 9.32030000   | 0.00000000 |
| 242 | 1002.19390000 | 4.38710000   | 0.00000000 |
| 243 | 1008.09730000 | 0.69890000   | 0.00000000 |
| 244 | 1008.45600000 | 5.77120000   | 0.00000000 |
| 245 | 1009.86290000 | 2.47210000   | 0.00000000 |
| 246 | 1010.14160000 | 2.88090000   | 0.00000000 |
| 247 | 1010.54840000 | 6.33870000   | 0.00000000 |
| 248 | 1010.82850000 | 26.46850000  | 0.00000000 |
| 249 | 1011.21630000 | 26.51410000  | 0.00000000 |
| 250 | 1011.69660000 | 14.15410000  | 0.00000000 |
| 251 | 1028.67860000 | 6.57990000   | 0.00000000 |
| 252 | 1032.01150000 | 0.02090000   | 0.00000000 |

|     |               |              |            |
|-----|---------------|--------------|------------|
| 253 | 1032.82970000 | 0.02600000   | 0.00000000 |
| 254 | 1033.54980000 | 5.54060000   | 0.00000000 |
| 255 | 1041.47620000 | 5.54290000   | 0.00000000 |
| 256 | 1041.91250000 | 0.56560000   | 0.00000000 |
| 257 | 1042.22800000 | 2.18240000   | 0.00000000 |
| 258 | 1045.35600000 | 0.32780000   | 0.00000000 |
| 259 | 1046.14880000 | 0.33840000   | 0.00000000 |
| 260 | 1048.71660000 | 5.24070000   | 0.00000000 |
| 261 | 1052.39820000 | 1.02990000   | 0.00000000 |
| 262 | 1052.67840000 | 0.25070000   | 0.00000000 |
| 263 | 1054.46150000 | 0.34490000   | 0.00000000 |
| 264 | 1058.18260000 | 0.47990000   | 0.00000000 |
| 265 | 1066.04610000 | 4.88480000   | 0.00000000 |
| 266 | 1070.89910000 | 1.01050000   | 0.00000000 |
| 267 | 1071.27230000 | 0.87180000   | 0.00000000 |
| 268 | 1072.62870000 | 0.01720000   | 0.00000000 |
| 269 | 1074.07120000 | 58.14050000  | 0.00000000 |
| 270 | 1075.92750000 | 36.10880000  | 0.00000000 |
| 271 | 1079.38720000 | 34.65140000  | 0.00000000 |
| 272 | 1082.13020000 | 9.07840000   | 0.00000000 |
| 273 | 1082.24260000 | 104.75350000 | 0.00000000 |
| 274 | 1091.57970000 | 2.93080000   | 0.00000000 |
| 275 | 1093.25890000 | 11.89900000  | 0.00000000 |
| 276 | 1097.16530000 | 36.04170000  | 0.00000000 |
| 277 | 1117.32640000 | 68.31260000  | 0.00000000 |
| 278 | 1117.74400000 | 72.84170000  | 0.00000000 |
| 279 | 1117.83230000 | 16.27730000  | 0.00000000 |
| 280 | 1119.77940000 | 93.10030000  | 0.00000000 |
| 281 | 1120.24320000 | 169.04440000 | 0.00000000 |
| 282 | 1126.20700000 | 49.26660000  | 0.00000000 |
| 283 | 1128.88800000 | 68.52230000  | 0.00000000 |
| 284 | 1136.20100000 | 2.23710000   | 0.00000000 |
| 285 | 1138.18660000 | 1.18330000   | 0.00000000 |
| 286 | 1138.65690000 | 3.91430000   | 0.00000000 |
| 287 | 1150.70480000 | 22.20820000  | 0.00000000 |
| 288 | 1152.92850000 | 2.96980000   | 0.00000000 |
| 289 | 1153.64340000 | 1.90770000   | 0.00000000 |
| 290 | 1155.48720000 | 0.61310000   | 0.00000000 |
| 291 | 1169.11730000 | 7.23370000   | 0.00000000 |
| 292 | 1170.56090000 | 6.57040000   | 0.00000000 |
| 293 | 1171.98580000 | 15.33740000  | 0.00000000 |
| 294 | 1176.44850000 | 10.65820000  | 0.00000000 |
| 295 | 1179.50850000 | 16.83500000  | 0.00000000 |
| 296 | 1182.94530000 | 5.77950000   | 0.00000000 |
| 297 | 1183.80190000 | 3.84640000   | 0.00000000 |
| 298 | 1187.95690000 | 2.65650000   | 0.00000000 |
| 299 | 1214.21440000 | 0.31150000   | 0.00000000 |
| 300 | 1215.54100000 | 0.14920000   | 0.00000000 |
| 301 | 1227.72530000 | 26.00090000  | 0.00000000 |
| 302 | 1233.01500000 | 12.00540000  | 0.00000000 |
| 303 | 1233.72350000 | 8.93410000   | 0.00000000 |
| 304 | 1240.06820000 | 8.26870000   | 0.00000000 |
| 305 | 1242.08070000 | 13.49050000  | 0.00000000 |
| 306 | 1242.74510000 | 1.07920000   | 0.00000000 |
| 307 | 1248.31290000 | 3.42890000   | 0.00000000 |
| 308 | 1254.31690000 | 39.71560000  | 0.00000000 |
| 309 | 1254.35450000 | 6.59730000   | 0.00000000 |
| 310 | 1263.60480000 | 4.70850000   | 0.00000000 |
| 311 | 1265.25990000 | 15.30270000  | 0.00000000 |
| 312 | 1267.02760000 | 6.87760000   | 0.00000000 |
| 313 | 1269.19930000 | 99.23800000  | 0.00000000 |
| 314 | 1273.24020000 | 107.96070000 | 0.00000000 |
| 315 | 1278.64820000 | 2.02800000   | 0.00000000 |
| 316 | 1279.82000000 | 1.45540000   | 0.00000000 |



|     |               |              |            |
|-----|---------------|--------------|------------|
| 317 | 1281.31040000 | 2.53080000   | 0.00000000 |
| 318 | 1282.50090000 | 0.22010000   | 0.00000000 |
| 319 | 1282.69050000 | 0.00560000   | 0.00000000 |
| 320 | 1287.33950000 | 13.06000000  | 0.00000000 |
| 321 | 1304.89360000 | 3.41050000   | 0.00000000 |
| 322 | 1305.19340000 | 2.39110000   | 0.00000000 |
| 323 | 1305.32450000 | 0.78130000   | 0.00000000 |
| 324 | 1309.95590000 | 0.58390000   | 0.00000000 |
| 325 | 1310.85260000 | 6.39270000   | 0.00000000 |
| 326 | 1319.85530000 | 19.44500000  | 0.00000000 |
| 327 | 1320.37710000 | 36.21570000  | 0.00000000 |
| 328 | 1324.06280000 | 101.00150000 | 0.00000000 |
| 329 | 1324.49860000 | 29.65910000  | 0.00000000 |
| 330 | 1326.12570000 | 68.22980000  | 0.00000000 |
| 331 | 1331.39450000 | 0.73630000   | 0.00000000 |
| 332 | 1338.57520000 | 1.05660000   | 0.00000000 |
| 333 | 1338.70980000 | 0.34670000   | 0.00000000 |
| 334 | 1339.98590000 | 0.02350000   | 0.00000000 |
| 335 | 1342.93210000 | 1.54080000   | 0.00000000 |
| 336 | 1348.27680000 | 31.68390000  | 0.00000000 |
| 337 | 1351.98230000 | 0.56340000   | 0.00000000 |
| 338 | 1354.17150000 | 0.88800000   | 0.00000000 |
| 339 | 1365.21630000 | 0.52680000   | 0.00000000 |
| 340 | 1372.84340000 | 205.40000000 | 0.00000000 |
| 341 | 1376.26690000 | 0.75330000   | 0.00000000 |
| 342 | 1376.89740000 | 5.97370000   | 0.00000000 |
| 343 | 1377.12730000 | 149.82240000 | 0.00000000 |
| 344 | 1378.89300000 | 5.53620000   | 0.00000000 |
| 345 | 1380.19720000 | 10.33920000  | 0.00000000 |
| 346 | 1380.63650000 | 45.51190000  | 0.00000000 |
| 347 | 1380.74620000 | 45.38090000  | 0.00000000 |
| 348 | 1388.56090000 | 2.11160000   | 0.00000000 |
| 349 | 1397.05700000 | 41.56920000  | 0.00000000 |
| 350 | 1406.78140000 | 0.22230000   | 0.00000000 |
| 351 | 1415.35330000 | 6.31350000   | 0.00000000 |
| 352 | 1418.79080000 | 24.00560000  | 0.00000000 |
| 353 | 1426.85430000 | 1.00290000   | 0.00000000 |
| 354 | 1429.31150000 | 0.81470000   | 0.00000000 |
| 355 | 1430.94480000 | 7.54650000   | 0.00000000 |
| 356 | 1431.74300000 | 17.38670000  | 0.00000000 |
| 357 | 1437.73220000 | 46.27530000  | 0.00000000 |
| 358 | 1440.62720000 | 32.95660000  | 0.00000000 |
| 359 | 1443.04500000 | 164.49900000 | 0.00000000 |
| 360 | 1455.01210000 | 77.90030000  | 0.00000000 |
| 361 | 1456.02860000 | 106.95110000 | 0.00000000 |
| 362 | 1464.10780000 | 37.52410000  | 0.00000000 |
| 363 | 1464.21240000 | 31.16120000  | 0.00000000 |
| 364 | 1476.54290000 | 0.03020000   | 0.00000000 |
| 365 | 1476.94960000 | 67.73270000  | 0.00000000 |
| 366 | 1477.60020000 | 83.62580000  | 0.00000000 |
| 367 | 1481.41130000 | 12.21650000  | 0.00000000 |
| 368 | 1481.80830000 | 27.21780000  | 0.00000000 |
| 369 | 1483.39200000 | 0.27780000   | 0.00000000 |
| 370 | 1488.54480000 | 121.38170000 | 0.00000000 |
| 371 | 1488.64250000 | 11.58420000  | 0.00000000 |
| 372 | 1492.32720000 | 5.59920000   | 0.00000000 |
| 373 | 1492.76050000 | 0.17890000   | 0.00000000 |
| 374 | 1498.19640000 | 10.94850000  | 0.00000000 |
| 375 | 1500.47340000 | 1.76220000   | 0.00000000 |
| 376 | 1501.76980000 | 23.80330000  | 0.00000000 |
| 377 | 1503.07780000 | 27.07020000  | 0.00000000 |
| 378 | 1504.93660000 | 2.90070000   | 0.00000000 |
| 379 | 1506.98830000 | 1.29020000   | 0.00000000 |
| 380 | 1507.97300000 | 3.11430000   | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 381 | 1516.66270000 | 0.76080000    | 0.00000000 |
| 382 | 1518.24850000 | 15.64810000   | 0.00000000 |
| 383 | 1525.83240000 | 26.48730000   | 0.00000000 |
| 384 | 1526.27950000 | 29.88260000   | 0.00000000 |
| 385 | 1530.54290000 | 66.67980000   | 0.00000000 |
| 386 | 1532.57300000 | 138.29320000  | 0.00000000 |
| 387 | 1544.12680000 | 28.87720000   | 0.00000000 |
| 388 | 1545.50450000 | 14.90320000   | 0.00000000 |
| 389 | 1551.72400000 | 17.91920000   | 0.00000000 |
| 390 | 1551.95620000 | 10.09580000   | 0.00000000 |
| 391 | 1556.04380000 | 11.67570000   | 0.00000000 |
| 392 | 1575.18710000 | 7.64100000    | 0.00000000 |
| 393 | 1575.55790000 | 7.24280000    | 0.00000000 |
| 394 | 1587.78170000 | 38.99100000   | 0.00000000 |
| 395 | 1588.25700000 | 10.45340000   | 0.00000000 |
| 396 | 1594.81920000 | 6.72790000    | 0.00000000 |
| 397 | 1597.28040000 | 8.16130000    | 0.00000000 |
| 398 | 1612.66730000 | 8.24710000    | 0.00000000 |
| 399 | 1615.62960000 | 17.86390000   | 0.00000000 |
| 400 | 1625.21140000 | 1.24710000    | 0.00000000 |
| 401 | 1625.72790000 | 2.32370000    | 0.00000000 |
| 402 | 1626.15680000 | 3.76730000    | 0.00000000 |
| 403 | 1627.12240000 | 6.09020000    | 0.00000000 |
| 404 | 1637.29170000 | 0.05760000    | 0.00000000 |
| 405 | 1639.82570000 | 2.94000000    | 0.00000000 |
| 406 | 1651.39280000 | 113.66270000  | 0.00000000 |
| 407 | 1651.43990000 | 97.41150000   | 0.00000000 |
| 408 | 1651.53840000 | 77.07730000   | 0.00000000 |
| 409 | 1652.07680000 | 94.68310000   | 0.00000000 |
| 410 | 1661.05940000 | 0.48010000    | 0.00000000 |
| 411 | 1661.65230000 | 0.05540000    | 0.00000000 |
| 412 | 1663.93930000 | 31.01680000   | 0.00000000 |
| 413 | 1665.12670000 | 96.84240000   | 0.00000000 |
| 414 | 1682.20970000 | 78.11680000   | 0.00000000 |
| 415 | 1683.49030000 | 77.26800000   | 0.00000000 |
| 416 | 1964.48540000 | 2386.10050000 | 0.00000000 |
| 417 | 1970.64870000 | 2309.75010000 | 0.00000000 |
| 418 | 2084.15110000 | 1979.91530000 | 0.00000000 |
| 419 | 2963.25020000 | 173.01450000  | 0.00000000 |
| 420 | 2963.32960000 | 102.22640000  | 0.00000000 |
| 421 | 2990.19180000 | 111.40860000  | 0.00000000 |
| 422 | 2990.70010000 | 99.96660000   | 0.00000000 |
| 423 | 3000.86670000 | 2.27260000    | 0.00000000 |
| 424 | 3002.44200000 | 5.21300000    | 0.00000000 |
| 425 | 3007.43960000 | 8.68000000    | 0.00000000 |
| 426 | 3011.12480000 | 170.75960000  | 0.00000000 |
| 427 | 3022.37530000 | 11.66640000   | 0.00000000 |
| 428 | 3037.18810000 | 51.19670000   | 0.00000000 |
| 429 | 3039.59170000 | 57.46280000   | 0.00000000 |
| 430 | 3040.42550000 | 40.88200000   | 0.00000000 |
| 431 | 3041.00490000 | 14.09950000   | 0.00000000 |
| 432 | 3043.10720000 | 1.91870000    | 0.00000000 |
| 433 | 3062.17150000 | 4.14410000    | 0.00000000 |
| 434 | 3066.23300000 | 255.62570000  | 0.00000000 |
| 435 | 3186.13120000 | 6.85640000    | 0.00000000 |
| 436 | 3186.15900000 | 0.81650000    | 0.00000000 |
| 437 | 3186.70210000 | 6.65460000    | 0.00000000 |
| 438 | 3188.65700000 | 34.02310000   | 0.00000000 |
| 439 | 3188.97570000 | 27.16180000   | 0.00000000 |
| 440 | 3194.68680000 | 0.76930000    | 0.00000000 |
| 441 | 3194.83560000 | 0.51430000    | 0.00000000 |
| 442 | 3195.62320000 | 6.59760000    | 0.00000000 |
| 443 | 3198.50810000 | 3.52660000    | 0.00000000 |
| 444 | 3202.56600000 | 0.17170000    | 0.00000000 |

|     |               |               |            |
|-----|---------------|---------------|------------|
| 445 | 3202.64080000 | 0.26720000    | 0.00000000 |
| 446 | 3207.84510000 | 41.16080000   | 0.00000000 |
| 447 | 3208.06230000 | 39.70470000   | 0.00000000 |
| 448 | 3210.55150000 | 13.92080000   | 0.00000000 |
| 449 | 3210.69700000 | 15.82590000   | 0.00000000 |
| 450 | 3212.20260000 | 21.73710000   | 0.00000000 |
| 451 | 3212.59760000 | 21.32670000   | 0.00000000 |
| 452 | 3219.05160000 | 4.10580000    | 0.00000000 |
| 453 | 3220.65850000 | 27.32430000   | 0.00000000 |
| 454 | 3220.67840000 | 7.86780000    | 0.00000000 |
| 455 | 3220.73190000 | 73.36130000   | 0.00000000 |
| 456 | 3221.08330000 | 35.91480000   | 0.00000000 |
| 457 | 3231.96730000 | 4.92060000    | 0.00000000 |
| 458 | 3232.26120000 | 3.99890000    | 0.00000000 |
| 459 | 3233.28190000 | 7.37000000    | 0.00000000 |
| 460 | 3236.17520000 | 5.68030000    | 0.00000000 |
| 461 | 3237.44680000 | 4.90310000    | 0.00000000 |
| 462 | 3239.53490000 | 1.59230000    | 0.00000000 |
| 463 | 3245.77970000 | 3.52870000    | 0.00000000 |
| 464 | 3258.98360000 | 1.23380000    | 0.00000000 |
| 465 | 3259.71930000 | 1.06640000    | 0.00000000 |
| 466 | 3259.87550000 | 0.13470000    | 0.00000000 |
| 467 | 3270.21220000 | 4.54730000    | 0.00000000 |
| 468 | 3270.77660000 | 1.69930000    | 0.00000000 |
| 469 | 3270.91040000 | 14.23720000   | 0.00000000 |
| 470 | 3284.78900000 | 3.75370000    | 0.00000000 |
| 471 | 3285.06930000 | 3.50200000    | 0.00000000 |
| 472 | 3285.19210000 | 6.41610000    | 0.00000000 |
| 473 | 3317.15360000 | 1104.47430000 | 0.00000000 |
| 474 | 3324.46170000 | 1139.04520000 | 0.00000000 |
| 475 | 3486.97250000 | 2.73890000    | 0.00000000 |
| 476 | 3487.80020000 | 3.07440000    | 0.00000000 |
| 477 | 3559.74320000 | 1777.62380000 | 0.00000000 |
| 478 | 3565.32150000 | 119.83250000  | 0.00000000 |
| 479 | 3566.77300000 | 1716.11280000 | 0.00000000 |
| 480 | 3572.46310000 | 137.26250000  | 0.00000000 |
| 481 | 3841.68480000 | 99.35020000   | 0.00000000 |
| 482 | 3842.02330000 | 90.36970000   | 0.00000000 |
| 483 | 3842.22730000 | 93.19360000   | 0.00000000 |
| 484 | 3843.40980000 | 88.80370000   | 0.00000000 |
| 485 | 3843.44690000 | 52.11780000   | 0.00000000 |
| 486 | 3844.35170000 | 48.51640000   | 0.00000000 |

# S24. CALCULATIONS ON EXTENDED CONFORMER OF 2w<sup>3+</sup> (<sup>3</sup>A)

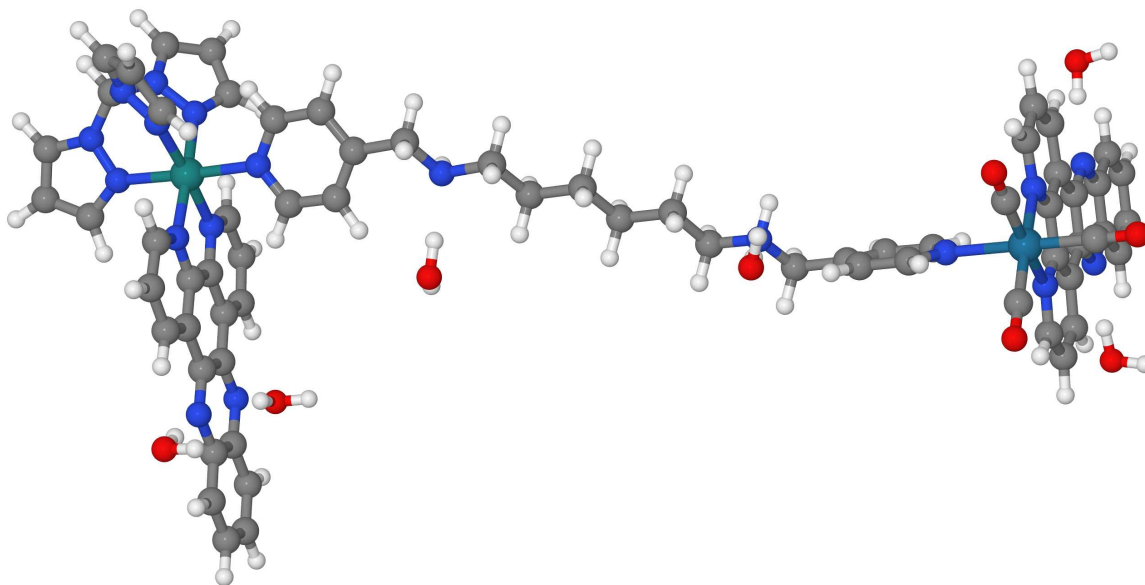


FIG. S34. Molecule

|                                 |  |      |
|---------------------------------|--|------|
| Route                           | : # opt freq ub3lyp/genecp scrf=(solvent=water) geom=connectivity empiri   |      |
|                                 | : calcdispersion=gd3bj int=ultrafine pop=regular   |      |
| SMILES                          | : c1ccc2c(c1)nc3c4ccc[n+]<br>5c4c6c(c3n2)ccc[n+]<br>6[Ru]578(n9ccc[n+]<br>9C([n+]<br>1n7ccc1)[n+]<br>1n8ccc1)[n+]<br>1ccc(cc1)CNCCCCCNCCc1cc[n+]<br>(cc1)[Re]<br>1([n+]<br>2cccc3c2c2[n+]<br>1cccc2c1c3nc2cccc2n1)([C][O])([C][O])[C][O].O.O.O.O.O.O |      |
| Formula                         | : C <sub>67</sub> H <sub>68</sub> N <sub>18</sub> O <sub>9</sub> ReRu <sup>3+,3</sup>  |      |
| Charge                          | : 3  |      |
| Multiplicity                    | : 3  |      |
| Energy                          | : -4431.30593560   | a.u. |
| Gibbs Energy                    | : -4430.15028500   | a.u. |
| Number of imaginary frequencies | : 5  |      |

## S24.1. Cartesian Co-ordinates (XYZ format)

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```

C    3.17356110  0.43408799 -0.47738600
H    2.89722896  1.49323201 -0.50855798
H    3.14151096  0.12542200  0.57845497
C    2.17592406 -0.38499400 -1.28978002
H    2.47890306 -1.43928897 -1.27692699
H    2.21386600 -0.05687400 -2.33339310
C    0.74788302 -0.25967601 -0.75625402
H    0.45087999  0.79603201 -0.76169801
H    0.71877003 -0.58308500  0.29120100
C   -0.26806501 -1.07048297 -1.56317198
H    0.01797700 -2.12899208 -1.54927802
H   -0.23140401 -0.75350600 -2.61237097
C   -2.71118307 -1.71583796 -1.84948802
H   -2.43444490 -2.78072691 -1.85590303

```

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | -2.70477605  | -1.37713695 | -2.89059305 |
| N  | 4.53489017   | 0.31608799  | -1.02557099 |
| C  | -5.06399012  | -2.32931089 | -2.05061507 |
| H  | -4.81098890  | -3.39782906 | -2.04839396 |
| H  | -5.05833197  | -2.00926709 | -3.09937191 |
| N  | -4.07622004  | -1.52324700 | -1.32897103 |
| C  | 5.52082682   | 1.04987395  | -0.22336100 |
| H  | 5.25285101   | 2.11170101  | -0.25698501 |
| H  | 5.49801207   | 0.75029802  | 0.83269697  |
| C  | -13.12077999 | -3.97059298 | 0.34902599  |
| N  | -11.98247528 | -4.29226112 | 1.18375599  |
| N  | -13.72861767 | -2.72516894 | 0.77373600  |
| N  | -12.71193027 | -3.89076400 | -1.03725505 |
| N  | -10.91241837 | -3.45390701 | 1.20480704  |
| C  | -11.74907684 | -5.40053606 | 1.93184602  |
| N  | -12.99847507 | -1.57607198 | 0.73740298  |
| C  | -14.97693062 | -2.48527002 | 1.23412895  |
| N  | -11.77643585 | -2.97629690 | -1.41010106 |
| C  | -13.07204819 | -4.67605591 | -2.08391190 |
| Ru | -11.05248833 | -1.66886795 | 0.08562600  |
| C  | -9.99683380  | -4.04056406 | 1.97864199  |
| C  | -10.48161888 | -5.26706982 | 2.45808911  |
| H  | -12.49073505 | -6.17546701 | 2.03144789  |
| C  | -13.80374432 | -0.60235697 | 1.18108797  |
| C  | -15.05628490 | -1.12949204 | 1.50426900  |
| H  | -15.70022678 | -3.27758598 | 1.33283806  |
| C  | -11.54999447 | -3.18819499 | -2.70847201 |
| C  | -12.34388447 | -4.24756098 | -3.17350006 |
| H  | -13.80491638 | -5.45733690 | -1.96984994 |
| N  | -10.49491215 | -0.33786899 | 1.56907797  |
| N  | -11.28858757 | 0.12702300  | -0.91854298 |
| H  | -9.04204082  | -3.56978703 | 2.14613509  |
| H  | -9.97227001  | -5.96058798 | 3.10404396  |
| H  | -13.44480419 | 0.41149801  | 1.24370098  |
| H  | -15.91033077 | -0.59696501 | 1.88463902  |
| H  | -10.82994556 | -2.59007597 | -3.24244308 |
| H  | -12.37937737 | -4.64414978 | -4.17306089 |
| C  | -10.15217209 | -0.63005197 | 2.81943893  |
| C  | -10.54192066 | 0.97689998  | 1.16558695  |
| C  | -10.96065998 | 1.22333205  | -0.15354900 |
| C  | -11.72922230 | 0.30113101  | -2.15967607 |
| C  | -9.80526543  | 0.36885300  | 3.73492408  |
| H  | -10.15961647 | -1.67195106 | 3.10150695  |
| C  | -10.19941235 | 2.04512095  | 2.03599691  |
| C  | -11.04788685 | 2.54797196  | -0.65715998 |
| C  | -11.84349918 | 1.57594895  | -2.72409201 |
| H  | -12.00296307 | -0.58403599 | -2.71351790 |
| C  | -9.82134914  | 1.69552505  | 3.34468699  |
| H  | -9.52828693  | 0.08570000  | 4.74069691  |
| C  | -10.26157188 | 3.41153502  | 1.55013394  |
| C  | -11.49918747 | 2.69056010  | -1.98154700 |
| C  | -10.68471718 | 3.66367888  | 0.19782101  |
| H  | -12.20186806 | 1.67001295  | -3.73953390 |
| H  | -9.54959774  | 2.46517611  | 4.05451918  |
| N  | -9.92692661  | 4.41397619  | 2.37319994  |
| H  | -11.58494186 | 3.67464805  | -2.42237091 |
| N  | -10.75647163 | 4.90989304  | -0.28782001 |
| C  | -9.99083996  | 5.69352198  | 1.88487804  |
| C  | -10.40828896 | 5.94351816  | 0.54294503  |
| C  | -9.64122963  | 6.78152895  | 2.70947409  |
| C  | -10.45981979 | 7.27205992  | 0.07568200  |
| C  | -9.70071602  | 8.07826042  | 2.22611904  |
| H  | -9.32922840  | 6.57776022  | 3.72647905  |
| C  | -10.11081696 | 8.32401276  | 0.90655798  |

|    |              |             |             |
|----|--------------|-------------|-------------|
| H  | -10.78044796 | 7.44735003  | -0.94399899 |
| H  | -9.42937088  | 8.90564632  | 2.87096691  |
| H  | -10.15526676 | 9.34076118  | 0.53472102  |
| N  | 12.30228233  | 1.41934097  | -0.62457001 |
| N  | 11.93912220  | -1.18535602 | -1.09255397 |
| C  | 12.43035984  | 2.73491502  | -0.42493200 |
| C  | 12.62086964  | 0.56680602  | 0.38543001  |
| C  | 12.42566776  | -0.84639603 | 0.13091999  |
| C  | 11.70901394  | -2.47414207 | -1.36260104 |
| C  | 12.88747120  | 3.25962400  | 0.78094399  |
| H  | 12.16433334  | 3.37952399  | -1.24991596 |
| C  | 13.08848953  | 1.01922095  | 1.62784505  |
| C  | 12.70220280  | -1.80358803 | 1.11792600  |
| C  | 11.95827103  | -3.48116398 | -0.43413401 |
| H  | 11.32013035  | -2.70235205 | -2.34420609 |
| C  | 13.22350788  | 2.40440512  | 1.81255603  |
| H  | 12.97463417  | 4.33127880  | 0.89361101  |
| C  | 13.40402985  | 0.04041300  | 2.66803408  |
| C  | 12.46009636  | -3.15180492 | 0.81010801  |
| C  | 13.21515942  | -1.36035204 | 2.41393995  |
| H  | 11.75644779  | -4.50943804 | -0.70015401 |
| H  | 13.58218956  | 2.80295110  | 2.75114894  |
| N  | 13.86026192  | 0.46378699  | 3.83805895  |
| H  | 12.65924740  | -3.92721796 | 1.53636897  |
| N  | 13.49569607  | -2.26406503 | 3.34175110  |
| C  | 14.15141201  | -0.44695500 | 4.79043198  |
| C  | 13.96593475  | -1.84580004 | 4.53545284  |
| C  | 14.64583874  | -0.02732600 | 6.05322409  |
| C  | 14.28119183  | -2.78815699 | 5.54922295  |
| C  | 14.93918991  | -0.96318501 | 7.00986385  |
| H  | 14.77962112  | 1.03158605  | 6.23312902  |
| C  | 14.75651073  | -2.34900498 | 6.75679588  |
| H  | 14.13604259  | -3.84083295 | 5.34322691  |
| H  | 15.31646919  | -0.64731598 | 7.97440481  |
| H  | 14.99796200  | -3.06433702 | 7.53292513  |
| H  | -13.85695553 | -4.76099491 | 0.44718400  |
| C  | 6.92233181   | 0.88950402  | -0.75512898 |
| C  | 7.97560310   | 0.55707502  | 0.09367600  |
| C  | 7.22862577   | 1.08632398  | -2.10540795 |
| C  | 9.26128197   | 0.44465300  | -0.41049400 |
| H  | 7.80808592   | 0.38212901  | 1.14857697  |
| C  | 8.53531742   | 0.95467299  | -2.53500605 |
| H  | 6.45765591   | 1.33758104  | -2.82299089 |
| N  | 9.55688381   | 0.64016801  | -1.70750701 |
| H  | 10.07469940  | 0.18683200  | 0.24892899  |
| H  | 8.78806019   | 1.10767901  | -3.57432508 |
| C  | -6.46214485  | -2.15185094 | -1.51833296 |
| C  | -6.95564795  | -0.90315998 | -1.12462699 |
| C  | -7.32864523  | -3.24433494 | -1.42890203 |
| C  | -8.25465107  | -0.79463500 | -0.67324501 |
| H  | -6.34069777  | -0.01379000 | -1.17304802 |
| C  | -8.61844540  | -3.06695509 | -0.97061801 |
| H  | -7.00460005  | -4.23739815 | -1.71075404 |
| N  | -9.08663368  | -1.85657799 | -0.59319597 |
| H  | -8.65166569  | 0.16088600  | -0.36873001 |
| H  | -9.30220699  | -3.89817595 | -0.89295501 |
| Re | 11.65358639  | 0.47950399  | -2.51532888 |
| C  | 13.49141979  | 0.32658699  | -3.12751794 |
| O  | 14.58421803  | 0.23352100  | -3.47845697 |
| C  | 11.04708195  | -0.57464701 | -4.02764893 |
| O  | 10.68636990  | -1.22786498 | -4.90667200 |
| C  | 11.43495464  | 2.10584593  | -3.55153799 |
| O  | 11.31483269  | 3.08886790  | -4.14197779 |
| H  | -4.08960915  | -1.79477298 | -0.34828401 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | 4.79575109   | -0.66733998 | -1.04192805 |
| C | -1.69639397  | -0.91783398 | -1.03737402 |
| H | -1.98349202  | 0.13828400  | -1.04970002 |
| H | -1.73532403  | -1.24455798 | 0.00917800  |
| H | -4.30765200  | 0.30601600  | -1.37325501 |
| O | -4.45895195  | 1.28059399  | -1.35391796 |
| H | -4.40381289  | 1.49490798  | -0.41621301 |
| H | 4.36767101   | 0.90945101  | -2.75278091 |
| O | 4.28813696   | 1.23850703  | -3.68058300 |
| H | 4.47051191   | 0.45532599  | -4.21101713 |
| H | 13.39854145  | -4.19759703 | 3.33810592  |
| O | 13.39143753  | -5.17257881 | 3.31763601  |
| H | 14.26121616  | -5.39657116 | 2.96766496  |
| H | 14.24325562  | 2.23753500  | 4.51539803  |
| O | 14.48806667  | 3.12580490  | 4.83473206  |
| H | 15.40765190  | 3.21737289  | 4.56052589  |
| H | -11.23638916 | 5.55453491  | -1.94902503 |
| O | -11.44420338 | 5.89436293  | -2.84949899 |
| H | -10.58831787 | 5.88753986  | -3.29213095 |
| H | -9.37100315  | 4.42531681  | 4.13487005  |
| O | -9.02167511  | 4.42785215  | 5.05540609  |
| H | -8.06742096  | 4.38062286  | 4.92984915  |

## S24.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|------|--------------|--------------|-----------------|
| 1    | -11.67840000 | 1.06940000   | 0.00000000      |
| 2    | -10.76170000 | 1.61960000   | 0.00000000      |
| 3    | -9.64230000  | 1.70520000   | 0.00000000      |
| 4    | -6.29200000  | 1.37390000   | 0.00000000      |
| 5    | -3.48810000  | 0.41250000   | 0.00000000      |
| 6    | 8.42970000   | 2.80450000   | 0.00000000      |
| 7    | 11.12730000  | 0.90300000   | 0.00000000      |
| 8    | 12.29440000  | 0.73780000   | 0.00000000      |
| 9    | 14.01530000  | 2.22840000   | 0.00000000      |
| 10   | 15.32580000  | 0.30440000   | 0.00000000      |
| 11   | 19.27340000  | 2.44760000   | 0.00000000      |
| 12   | 24.74050000  | 2.24000000   | 0.00000000      |
| 13   | 26.14530000  | 2.10470000   | 0.00000000      |
| 14   | 26.96850000  | 0.43550000   | 0.00000000      |
| 15   | 28.34360000  | 0.53150000   | 0.00000000      |
| 16   | 32.85630000  | 2.16300000   | 0.00000000      |
| 17   | 39.42720000  | 1.97780000   | 0.00000000      |
| 18   | 43.11100000  | 0.59070000   | 0.00000000      |
| 19   | 45.10330000  | 0.30140000   | 0.00000000      |
| 20   | 46.59650000  | 1.94290000   | 0.00000000      |
| 21   | 51.86910000  | 2.44630000   | 0.00000000      |
| 22   | 58.04070000  | 0.61910000   | 0.00000000      |
| 23   | 59.75710000  | 1.55990000   | 0.00000000      |
| 24   | 60.24940000  | 1.49930000   | 0.00000000      |
| 25   | 62.68920000  | 2.89640000   | 0.00000000      |
| 26   | 64.64690000  | 3.27130000   | 0.00000000      |
| 27   | 66.69620000  | 0.03300000   | 0.00000000      |
| 28   | 67.22590000  | 2.78100000   | 0.00000000      |
| 29   | 69.11340000  | 2.60050000   | 0.00000000      |
| 30   | 69.76770000  | 0.75810000   | 0.00000000      |
| 31   | 74.11980000  | 1.42900000   | 0.00000000      |
| 32   | 74.46180000  | 2.05110000   | 0.00000000      |
| 33   | 77.87000000  | 2.05880000   | 0.00000000      |
| 34   | 81.34790000  | 15.77730000  | 0.00000000      |
| 35   | 84.01700000  | 1.59480000   | 0.00000000      |
| 36   | 85.06970000  | 0.17770000   | 0.00000000      |
| 37   | 90.04680000  | 5.40560000   | 0.00000000      |
| 38   | 90.95800000  | 0.60050000   | 0.00000000      |
| 39   | 91.34180000  | 1.75520000   | 0.00000000      |
| 40   | 96.29390000  | 2.97430000   | 0.00000000      |
| 41   | 98.20760000  | 0.74210000   | 0.00000000      |
| 42   | 98.86700000  | 16.51560000  | 0.00000000      |
| 43   | 102.30220000 | 6.41130000   | 0.00000000      |
| 44   | 103.34750000 | 10.41750000  | 0.00000000      |
| 45   | 104.77240000 | 1.09400000   | 0.00000000      |
| 46   | 109.81690000 | 0.61220000   | 0.00000000      |
| 47   | 110.94080000 | 2.92730000   | 0.00000000      |
| 48   | 121.24880000 | 0.33750000   | 0.00000000      |
| 49   | 126.03370000 | 0.26570000   | 0.00000000      |
| 50   | 131.17060000 | 1.93800000   | 0.00000000      |
| 51   | 141.55900000 | 1.27050000   | 0.00000000      |
| 52   | 143.56630000 | 0.21440000   | 0.00000000      |
| 53   | 144.80210000 | 0.36270000   | 0.00000000      |
| 54   | 145.99920000 | 1.20770000   | 0.00000000      |
| 55   | 147.91360000 | 0.30480000   | 0.00000000      |
| 56   | 151.51140000 | 1.78040000   | 0.00000000      |
| 57   | 155.95460000 | 1.69100000   | 0.00000000      |
| 58   | 157.36940000 | 1.15630000   | 0.00000000      |
| 59   | 160.14460000 | 3.79660000   | 0.00000000      |
| 60   | 161.24090000 | 11.01830000  | 0.00000000      |



|     |              |              |            |
|-----|--------------|--------------|------------|
| 61  | 163.08050000 | 3.81760000   | 0.00000000 |
| 62  | 163.37030000 | 1.63160000   | 0.00000000 |
| 63  | 167.86890000 | 0.48670000   | 0.00000000 |
| 64  | 170.07600000 | 3.99150000   | 0.00000000 |
| 65  | 170.44210000 | 1.86850000   | 0.00000000 |
| 66  | 171.87300000 | 10.12300000  | 0.00000000 |
| 67  | 172.72600000 | 6.11810000   | 0.00000000 |
| 68  | 177.11560000 | 6.38940000   | 0.00000000 |
| 69  | 180.16510000 | 4.73610000   | 0.00000000 |
| 70  | 185.49530000 | 0.96720000   | 0.00000000 |
| 71  | 188.01440000 | 1.70640000   | 0.00000000 |
| 72  | 196.74250000 | 15.87270000  | 0.00000000 |
| 73  | 199.29650000 | 11.11880000  | 0.00000000 |
| 74  | 211.93200000 | 3.12580000   | 0.00000000 |
| 75  | 215.55930000 | 17.00050000  | 0.00000000 |
| 76  | 216.56700000 | 61.23430000  | 0.00000000 |
| 77  | 218.21130000 | 26.97700000  | 0.00000000 |
| 78  | 223.93620000 | 18.84200000  | 0.00000000 |
| 79  | 225.93870000 | 11.96240000  | 0.00000000 |
| 80  | 230.05970000 | 31.09860000  | 0.00000000 |
| 81  | 233.08750000 | 18.32870000  | 0.00000000 |
| 82  | 238.97310000 | 67.58830000  | 0.00000000 |
| 83  | 245.75620000 | 161.71190000 | 0.00000000 |
| 84  | 254.29400000 | 83.82810000  | 0.00000000 |
| 85  | 255.56250000 | 180.26770000 | 0.00000000 |
| 86  | 257.89590000 | 136.17620000 | 0.00000000 |
| 87  | 260.38090000 | 65.10770000  | 0.00000000 |
| 88  | 262.90110000 | 16.25060000  | 0.00000000 |
| 89  | 268.28750000 | 22.34900000  | 0.00000000 |
| 90  | 274.78880000 | 185.58040000 | 0.00000000 |
| 91  | 282.49650000 | 2.48120000   | 0.00000000 |
| 92  | 287.46130000 | 7.37260000   | 0.00000000 |
| 93  | 288.51450000 | 9.19600000   | 0.00000000 |
| 94  | 289.85900000 | 34.61160000  | 0.00000000 |
| 95  | 300.04830000 | 73.77650000  | 0.00000000 |
| 96  | 306.31310000 | 5.83640000   | 0.00000000 |
| 97  | 308.36980000 | 53.80270000  | 0.00000000 |
| 98  | 311.41930000 | 1.60680000   | 0.00000000 |
| 99  | 319.21050000 | 12.39700000  | 0.00000000 |
| 100 | 327.11430000 | 18.33230000  | 0.00000000 |
| 101 | 337.42560000 | 3.50140000   | 0.00000000 |
| 102 | 337.92360000 | 6.56720000   | 0.00000000 |
| 103 | 339.58530000 | 38.49590000  | 0.00000000 |
| 104 | 342.07650000 | 27.89290000  | 0.00000000 |
| 105 | 342.40980000 | 3.17490000   | 0.00000000 |
| 106 | 358.40950000 | 7.39110000   | 0.00000000 |
| 107 | 360.66410000 | 2.91520000   | 0.00000000 |
| 108 | 367.23510000 | 23.61080000  | 0.00000000 |
| 109 | 376.05340000 | 0.34900000   | 0.00000000 |
| 110 | 380.44430000 | 3.63060000   | 0.00000000 |
| 111 | 382.99880000 | 19.26350000  | 0.00000000 |
| 112 | 384.18330000 | 96.88490000  | 0.00000000 |
| 113 | 392.18150000 | 3.41810000   | 0.00000000 |
| 114 | 398.56260000 | 12.13200000  | 0.00000000 |
| 115 | 405.54980000 | 1.69740000   | 0.00000000 |
| 116 | 406.82890000 | 2.05130000   | 0.00000000 |
| 117 | 412.70700000 | 84.01750000  | 0.00000000 |
| 118 | 416.35060000 | 41.78030000  | 0.00000000 |
| 119 | 424.09880000 | 48.87400000  | 0.00000000 |
| 120 | 430.98630000 | 2.71320000   | 0.00000000 |
| 121 | 435.03880000 | 9.72290000   | 0.00000000 |
| 122 | 447.86770000 | 4.28790000   | 0.00000000 |
| 123 | 450.15720000 | 31.89300000  | 0.00000000 |
| 124 | 454.15470000 | 47.02350000  | 0.00000000 |

|     |              |               |            |
|-----|--------------|---------------|------------|
| 125 | 456.07280000 | 5.32300000    | 0.00000000 |
| 126 | 460.05960000 | 91.58120000   | 0.00000000 |
| 127 | 462.82140000 | 6.23390000    | 0.00000000 |
| 128 | 475.37850000 | 31.58820000   | 0.00000000 |
| 129 | 475.62300000 | 29.36350000   | 0.00000000 |
| 130 | 481.37420000 | 5.17890000    | 0.00000000 |
| 131 | 486.87070000 | 7.54710000    | 0.00000000 |
| 132 | 492.65520000 | 0.41000000    | 0.00000000 |
| 133 | 493.30420000 | 1.10480000    | 0.00000000 |
| 134 | 494.99460000 | 1.41290000    | 0.00000000 |
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| 136 | 499.34030000 | 3.65080000    | 0.00000000 |
| 137 | 508.55650000 | 1.44330000    | 0.00000000 |
| 138 | 508.81780000 | 2.69540000    | 0.00000000 |
| 139 | 517.97690000 | 0.43990000    | 0.00000000 |
| 140 | 531.72720000 | 12.00580000   | 0.00000000 |
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| 143 | 550.33710000 | 0.19440000    | 0.00000000 |
| 144 | 556.78780000 | 13.99240000   | 0.00000000 |
| 145 | 563.13520000 | 0.68170000    | 0.00000000 |
| 146 | 571.92430000 | 0.16880000    | 0.00000000 |
| 147 | 576.45360000 | 2.08050000    | 0.00000000 |
| 148 | 576.97330000 | 3.89650000    | 0.00000000 |
| 149 | 581.06830000 | 0.42140000    | 0.00000000 |
| 150 | 585.30740000 | 1263.13380000 | 0.00000000 |
| 151 | 591.62890000 | 1.16510000    | 0.00000000 |
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| 153 | 600.44240000 | 0.05910000    | 0.00000000 |
| 154 | 606.76980000 | 3.82630000    | 0.00000000 |
| 155 | 609.53130000 | 29.69480000   | 0.00000000 |
| 156 | 618.24960000 | 44.65130000   | 0.00000000 |
| 157 | 624.21000000 | 27.61680000   | 0.00000000 |
| 158 | 633.60450000 | 36.52160000   | 0.00000000 |
| 159 | 634.14240000 | 733.83820000  | 0.00000000 |
| 160 | 638.22330000 | 5.63050000    | 0.00000000 |
| 161 | 645.51930000 | 1.95990000    | 0.00000000 |
| 162 | 646.48850000 | 80.06250000   | 0.00000000 |
| 163 | 647.63340000 | 13.71140000   | 0.00000000 |
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| 166 | 655.40240000 | 3.04520000    | 0.00000000 |
| 167 | 666.28060000 | 13.07230000   | 0.00000000 |
| 168 | 668.16670000 | 0.11590000    | 0.00000000 |
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| 170 | 675.08390000 | 2.49060000    | 0.00000000 |
| 171 | 679.33200000 | 7.22010000    | 0.00000000 |
| 172 | 685.49140000 | 0.33850000    | 0.00000000 |
| 173 | 724.03280000 | 118.76010000  | 0.00000000 |
| 174 | 728.71370000 | 0.24030000    | 0.00000000 |
| 175 | 738.41220000 | 11.15670000   | 0.00000000 |
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| 177 | 741.23690000 | 14.33440000   | 0.00000000 |
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| 179 | 745.00910000 | 75.35820000   | 0.00000000 |
| 180 | 748.96710000 | 8.38290000    | 0.00000000 |
| 181 | 752.04510000 | 0.10870000    | 0.00000000 |
| 182 | 757.76570000 | 1.87470000    | 0.00000000 |
| 183 | 763.05480000 | 73.54230000   | 0.00000000 |
| 184 | 763.25700000 | 13.56090000   | 0.00000000 |
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| 188 | 774.39730000 | 168.16080000  | 0.00000000 |

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| 189 | 779.29120000  | 65.88710000  | 0.00000000 |
| 190 | 779.95090000  | 33.37620000  | 0.00000000 |
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| 192 | 787.59860000  | 73.07620000  | 0.00000000 |
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| 194 | 794.17470000  | 0.09700000   | 0.00000000 |
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| 198 | 810.68400000  | 4.80540000   | 0.00000000 |
| 199 | 816.11790000  | 61.89440000  | 0.00000000 |
| 200 | 821.56250000  | 0.97920000   | 0.00000000 |
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| 204 | 833.75960000  | 12.49430000  | 0.00000000 |
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| 206 | 862.62060000  | 937.44130000 | 0.00000000 |
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| 209 | 870.57030000  | 46.41000000  | 0.00000000 |
| 210 | 871.01520000  | 139.69380000 | 0.00000000 |
| 211 | 874.72800000  | 159.87940000 | 0.00000000 |
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| 213 | 877.72400000  | 98.35910000  | 0.00000000 |
| 214 | 884.71050000  | 0.11890000   | 0.00000000 |
| 215 | 886.53370000  | 230.87270000 | 0.00000000 |
| 216 | 888.42510000  | 2.89070000   | 0.00000000 |
| 217 | 890.40160000  | 43.11850000  | 0.00000000 |
| 218 | 891.89040000  | 4.82880000   | 0.00000000 |
| 219 | 895.59590000  | 0.42130000   | 0.00000000 |
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| 224 | 909.74330000  | 60.73190000  | 0.00000000 |
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| 228 | 938.13630000  | 2.29290000   | 0.00000000 |
| 229 | 941.82030000  | 0.82840000   | 0.00000000 |
| 230 | 943.35660000  | 1.54830000   | 0.00000000 |
| 231 | 944.80700000  | 1.75080000   | 0.00000000 |
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| 237 | 979.03410000  | 1.30660000   | 0.00000000 |
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| 240 | 994.52080000  | 0.14660000   | 0.00000000 |
| 241 | 994.89830000  | 0.21740000   | 0.00000000 |
| 242 | 996.47220000  | 48.04960000  | 0.00000000 |
| 243 | 1001.65530000 | 21.78070000  | 0.00000000 |
| 244 | 1001.75690000 | 8.92730000   | 0.00000000 |
| 245 | 1005.39270000 | 1.07600000   | 0.00000000 |
| 246 | 1009.84400000 | 1.99610000   | 0.00000000 |
| 247 | 1010.47400000 | 7.26130000   | 0.00000000 |
| 248 | 1012.21990000 | 37.68670000  | 0.00000000 |
| 249 | 1019.69390000 | 218.11400000 | 0.00000000 |
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| 252 | 1029.93680000 | 3.67540000   | 0.00000000 |

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| 253 | 1032.53500000 | 0.02760000    | 0.00000000 |
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| 257 | 1043.31110000 | 86.60040000   | 0.00000000 |
| 258 | 1048.53360000 | 23.15980000   | 0.00000000 |
| 259 | 1048.79940000 | 14.14830000   | 0.00000000 |
| 260 | 1049.03190000 | 15.67720000   | 0.00000000 |
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| 262 | 1053.13780000 | 0.31720000    | 0.00000000 |
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| 264 | 1057.02470000 | 11.67250000   | 0.00000000 |
| 265 | 1060.86870000 | 22.42940000   | 0.00000000 |
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| 267 | 1066.60920000 | 4.63980000    | 0.00000000 |
| 268 | 1071.14440000 | 0.89790000    | 0.00000000 |
| 269 | 1072.64510000 | 0.02250000    | 0.00000000 |
| 270 | 1077.29380000 | 100.94800000  | 0.00000000 |
| 271 | 1082.13490000 | 105.82410000  | 0.00000000 |
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| 273 | 1085.01760000 | 95.16840000   | 0.00000000 |
| 274 | 1090.99290000 | 119.20100000  | 0.00000000 |
| 275 | 1097.29080000 | 1751.10380000 | 0.00000000 |
| 276 | 1097.37310000 | 294.87580000  | 0.00000000 |
| 277 | 1102.33090000 | 72.64550000   | 0.00000000 |
| 278 | 1118.49140000 | 11.25690000   | 0.00000000 |
| 279 | 1122.24330000 | 144.38110000  | 0.00000000 |
| 280 | 1125.30100000 | 36.86280000   | 0.00000000 |
| 281 | 1127.35140000 | 112.26870000  | 0.00000000 |
| 282 | 1128.60600000 | 69.15620000   | 0.00000000 |
| 283 | 1131.37270000 | 199.26250000  | 0.00000000 |
| 284 | 1132.39190000 | 232.00480000  | 0.00000000 |
| 285 | 1136.22860000 | 109.08010000  | 0.00000000 |
| 286 | 1138.06650000 | 1.19240000    | 0.00000000 |
| 287 | 1139.24210000 | 5.47360000    | 0.00000000 |
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| 290 | 1155.25210000 | 0.78610000    | 0.00000000 |
| 291 | 1161.51340000 | 1.70910000    | 0.00000000 |
| 292 | 1168.45700000 | 3.33160000    | 0.00000000 |
| 293 | 1170.04140000 | 6.36460000    | 0.00000000 |
| 294 | 1172.99460000 | 32.04680000   | 0.00000000 |
| 295 | 1175.47470000 | 476.83370000  | 0.00000000 |
| 296 | 1178.94520000 | 16.75500000   | 0.00000000 |
| 297 | 1183.23560000 | 3.60000000    | 0.00000000 |
| 298 | 1184.44210000 | 2201.32760000 | 0.00000000 |
| 299 | 1189.45730000 | 3.03500000    | 0.00000000 |
| 300 | 1202.92840000 | 115.70020000  | 0.00000000 |
| 301 | 1209.86700000 | 68.11610000   | 0.00000000 |
| 302 | 1213.62770000 | 31.70190000   | 0.00000000 |
| 303 | 1232.31640000 | 11.60530000   | 0.00000000 |
| 304 | 1234.02930000 | 4.75860000    | 0.00000000 |
| 305 | 1237.57290000 | 48.16020000   | 0.00000000 |
| 306 | 1242.23400000 | 13.71980000   | 0.00000000 |
| 307 | 1247.03630000 | 22.42630000   | 0.00000000 |
| 308 | 1248.09970000 | 3.08250000    | 0.00000000 |
| 309 | 1255.36170000 | 9.48160000    | 0.00000000 |
| 310 | 1259.24980000 | 538.51140000  | 0.00000000 |
| 311 | 1259.72280000 | 1511.01940000 | 0.00000000 |
| 312 | 1264.96390000 | 22.27260000   | 0.00000000 |
| 313 | 1265.79800000 | 70.90790000   | 0.00000000 |
| 314 | 1268.98150000 | 10.60830000   | 0.00000000 |
| 315 | 1274.97840000 | 103.04210000  | 0.00000000 |
| 316 | 1276.47520000 | 91.70680000   | 0.00000000 |

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| 317 | 1279.44570000 | 1.68640000    | 0.00000000 |
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| 319 | 1284.43850000 | 5.30040000    | 0.00000000 |
| 320 | 1290.87170000 | 1.01530000    | 0.00000000 |
| 321 | 1294.79010000 | 12.94640000   | 0.00000000 |
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| 323 | 1305.09750000 | 1.46330000    | 0.00000000 |
| 324 | 1306.31280000 | 8.81240000    | 0.00000000 |
| 325 | 1307.94130000 | 49.36960000   | 0.00000000 |
| 326 | 1312.67050000 | 1.06500000    | 0.00000000 |
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| 347 | 1381.32680000 | 114.01930000  | 0.00000000 |
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| 349 | 1390.60500000 | 0.89540000    | 0.00000000 |
| 350 | 1398.72140000 | 34.55600000   | 0.00000000 |
| 351 | 1399.41270000 | 50.93750000   | 0.00000000 |
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| 353 | 1404.73570000 | 24.94860000   | 0.00000000 |
| 354 | 1407.54260000 | 0.64590000    | 0.00000000 |
| 355 | 1427.62020000 | 46.08970000   | 0.00000000 |
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| 357 | 1428.96580000 | 0.67540000    | 0.00000000 |
| 358 | 1431.81710000 | 17.35030000   | 0.00000000 |
| 359 | 1434.14870000 | 165.34730000  | 0.00000000 |
| 360 | 1441.45080000 | 614.72840000  | 0.00000000 |
| 361 | 1446.12060000 | 1473.43200000 | 0.00000000 |
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| 363 | 1456.10440000 | 104.47570000  | 0.00000000 |
| 364 | 1464.56210000 | 38.16420000   | 0.00000000 |
| 365 | 1472.23600000 | 54.91790000   | 0.00000000 |
| 366 | 1476.79090000 | 0.03930000    | 0.00000000 |
| 367 | 1479.09610000 | 12.37710000   | 0.00000000 |
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| 369 | 1481.93610000 | 48.85540000   | 0.00000000 |
| 370 | 1483.45480000 | 2.71760000    | 0.00000000 |
| 371 | 1486.48370000 | 46.33520000   | 0.00000000 |
| 372 | 1487.64320000 | 106.45870000  | 0.00000000 |
| 373 | 1487.80310000 | 36.06630000   | 0.00000000 |
| 374 | 1488.21830000 | 3.54840000    | 0.00000000 |
| 375 | 1493.13710000 | 26.88380000   | 0.00000000 |
| 376 | 1495.29160000 | 29.24200000   | 0.00000000 |
| 377 | 1499.46760000 | 6.32140000    | 0.00000000 |
| 378 | 1500.58710000 | 0.58680000    | 0.00000000 |
| 379 | 1503.02680000 | 27.17440000   | 0.00000000 |
| 380 | 1505.01080000 | 4.64270000    | 0.00000000 |

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| 381 | 1507.92130000 | 2.69460000    | 0.00000000 |
| 382 | 1515.85220000 | 24.82170000   | 0.00000000 |
| 383 | 1517.10880000 | 0.52720000    | 0.00000000 |
| 384 | 1518.58980000 | 15.55700000   | 0.00000000 |
| 385 | 1522.82870000 | 288.59680000  | 0.00000000 |
| 386 | 1526.25900000 | 29.69850000   | 0.00000000 |
| 387 | 1532.38300000 | 137.11930000  | 0.00000000 |
| 388 | 1541.90520000 | 0.17400000    | 0.00000000 |
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| 391 | 1551.45790000 | 40.50160000   | 0.00000000 |
| 392 | 1556.47020000 | 6.07360000    | 0.00000000 |
| 393 | 1570.34280000 | 113.72160000  | 0.00000000 |
| 394 | 1574.89700000 | 217.35680000  | 0.00000000 |
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| 396 | 1581.73530000 | 173.35000000  | 0.00000000 |
| 397 | 1587.70110000 | 4.39550000    | 0.00000000 |
| 398 | 1588.20280000 | 10.41720000   | 0.00000000 |
| 399 | 1597.45910000 | 8.49850000    | 0.00000000 |
| 400 | 1613.99170000 | 69.56770000   | 0.00000000 |
| 401 | 1615.51040000 | 17.85920000   | 0.00000000 |
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| 404 | 1626.78850000 | 41.24580000   | 0.00000000 |
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| 408 | 1653.31450000 | 96.64810000   | 0.00000000 |
| 409 | 1658.98710000 | 97.11050000   | 0.00000000 |
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| 411 | 1660.31180000 | 108.31810000  | 0.00000000 |
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| 413 | 1665.32300000 | 95.91150000   | 0.00000000 |
| 414 | 1679.66530000 | 84.00810000   | 0.00000000 |
| 415 | 1683.97340000 | 77.91710000   | 0.00000000 |
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| 417 | 1970.75470000 | 2306.98880000 | 0.00000000 |
| 418 | 2084.23660000 | 1984.57190000 | 0.00000000 |
| 419 | 2963.97280000 | 135.62570000  | 0.00000000 |
| 420 | 2965.90120000 | 130.03540000  | 0.00000000 |
| 421 | 2990.68080000 | 90.52130000   | 0.00000000 |
| 422 | 2991.15140000 | 100.72910000  | 0.00000000 |
| 423 | 3001.26520000 | 2.07890000    | 0.00000000 |
| 424 | 3002.79600000 | 4.39720000    | 0.00000000 |
| 425 | 3007.61200000 | 8.06550000    | 0.00000000 |
| 426 | 3011.31530000 | 174.46400000  | 0.00000000 |
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| 428 | 3033.54790000 | 26.10570000   | 0.00000000 |
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| 431 | 3041.17550000 | 31.89430000   | 0.00000000 |
| 432 | 3044.26050000 | 7.61080000    | 0.00000000 |
| 433 | 3062.76070000 | 3.40120000    | 0.00000000 |
| 434 | 3066.70430000 | 255.43520000  | 0.00000000 |
| 435 | 3170.25130000 | 5.33730000    | 0.00000000 |
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| 437 | 3183.75480000 | 4.46300000    | 0.00000000 |
| 438 | 3186.78580000 | 6.74890000    | 0.00000000 |
| 439 | 3187.71920000 | 32.50100000   | 0.00000000 |
| 440 | 3188.95410000 | 11.86000000   | 0.00000000 |
| 441 | 3191.81560000 | 54.38650000   | 0.00000000 |
| 442 | 3194.94400000 | 0.59640000    | 0.00000000 |
| 443 | 3195.33590000 | 107.52760000  | 0.00000000 |
| 444 | 3199.30310000 | 3.28850000    | 0.00000000 |

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| 445 | 3202.83000000 | 0.28420000    | 0.00000000 |
| 446 | 3203.50220000 | 32.60360000   | 0.00000000 |
| 447 | 3204.00630000 | 51.03390000   | 0.00000000 |
| 448 | 3204.85530000 | 1.54140000    | 0.00000000 |
| 449 | 3208.11510000 | 38.84920000   | 0.00000000 |
| 450 | 3212.27400000 | 22.23010000   | 0.00000000 |
| 451 | 3212.73820000 | 18.16460000   | 0.00000000 |
| 452 | 3216.67930000 | 9.37720000    | 0.00000000 |
| 453 | 3217.08860000 | 1.59430000    | 0.00000000 |
| 454 | 3218.71240000 | 4.58470000    | 0.00000000 |
| 455 | 3220.61970000 | 27.93440000   | 0.00000000 |
| 456 | 3221.34420000 | 37.25850000   | 0.00000000 |
| 457 | 3231.78710000 | 5.04730000    | 0.00000000 |
| 458 | 3231.90000000 | 3.48120000    | 0.00000000 |
| 459 | 3238.12250000 | 6.32450000    | 0.00000000 |
| 460 | 3238.82980000 | 4.90770000    | 0.00000000 |
| 461 | 3239.70450000 | 0.21220000    | 0.00000000 |
| 462 | 3243.52130000 | 39.48800000   | 0.00000000 |
| 463 | 3247.18670000 | 3.48010000    | 0.00000000 |
| 464 | 3262.22290000 | 0.85160000    | 0.00000000 |
| 465 | 3263.49850000 | 0.29970000    | 0.00000000 |
| 466 | 3267.59810000 | 7.54430000    | 0.00000000 |
| 467 | 3269.75480000 | 13.99320000   | 0.00000000 |
| 468 | 3271.52500000 | 18.06990000   | 0.00000000 |
| 469 | 3275.44250000 | 25.89970000   | 0.00000000 |
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| 473 | 3323.24420000 | 1135.34720000 | 0.00000000 |
| 474 | 3346.55810000 | 1026.67780000 | 0.00000000 |
| 475 | 3375.09860000 | 2727.18910000 | 0.00000000 |
| 476 | 3378.79650000 | 1590.84130000 | 0.00000000 |
| 477 | 3489.50730000 | 3.59220000    | 0.00000000 |
| 478 | 3490.33580000 | 2.88670000    | 0.00000000 |
| 479 | 3566.86340000 | 1741.64670000 | 0.00000000 |
| 480 | 3572.37910000 | 111.36650000  | 0.00000000 |
| 481 | 3840.58340000 | 76.32150000   | 0.00000000 |
| 482 | 3841.30530000 | 76.53780000   | 0.00000000 |
| 483 | 3841.37930000 | 96.10480000   | 0.00000000 |
| 484 | 3842.42680000 | 93.18540000   | 0.00000000 |
| 485 | 3842.56040000 | 51.98870000   | 0.00000000 |
| 486 | 3843.62380000 | 50.61360000   | 0.00000000 |

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[1] Theo Keane: <https://github.com/theochemtheo/chemscripts>.