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A dinuclear osmium(II) complex near-infrared nanoscopy probe for nuclear DNA.

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Contents

1 Additional Experimental Data

1.1 Experimental Details

All chemicals and reagents were purchased from standard suppliers (Sigma Aldrich, Merck, Alfa Aesar) and used without further purification. Calf thymus DNA was purchased from Sigma Aldrich (DNA from calf thymus, sodium salt, fibres, Type I) and was modified by sonification, as stated below. The ligands TAP (1,4,5,8-tetraazaphenanthrene), and tpphz (tetrapyrido[3,2-a:2′,3′-c:3″,2″-h:2‴,3‴-j]phenazine) and complex $[\{Ru(TAP)_2\}_2(\mu - \text{tpphz})](Cl)_4$, $[\mathbf{1}]Cl_4$ were synthesised according to literature methods.[1]

1.2 Instrumentation

Microwave syntheses were conducted on a CEM Discover-SP microwave synthesiser using either 10 mL or 35 mL snap-cap vials with a maximum power of 200 W under argon atmosphere. NMR spectra were recorded on a Bruker Avance 400 or Avance III HD 400, both operating at resonance frequencies of 400 MHz. Mass spectroscopy was conducted mostly via matrix-assisted laser desorption mass spectrometry (MALDI MS) or direct-injection electrospray (ES) MS in positive mode. MALDI measurements were recorded on a Bruker Reflex III MALDI-ToF (time-of-flight) instrument. Electrospray analyses were carried out on a Waters LCT ES-ToF instrument for mass-to-charge ratios up to m/z = 2500.

For x-ray single crystal diffraction, a suitable crystal of the corresponding crystal was selected and mounted on a MITIGEN holder in oil on a Bruker APEX-II CCD diffractometer. The crystal was kept at 100 K during data collection. Using Olex2, the structure was solved with ShelXT structure solution program using Intrinsic Phasing and refined with the XL refinement package using Least Squares minimisation.

2 Spectroscopy

2.1 Sample Preparation

Experiments were conducted in Tris HCl buffer solution (Tris, 25 mM NaCl, 5 mM tris(hydroxymethyl)-aminomethane in deionised water, pH 7.40, adjusted using 1 M HCl, filtered with 0.22 µm Nylon filter). Sample integrity in the laser spectroscopy experiments was ensured by recording steady state UV-Vis spectra before and after each measurement. Here, no alterations of the resulting absorption spectra were observed.

2.2 Steady state spectroscopy

UV-Vis spectra were recorded on a Jasco V780 double-beam spectrophotometer in the wavelength interval of 200-850 nm using a scan rate of 200 nm min^{-1} and a slit width of $\Delta\lambda = 2$ nm. Emission spectra were recorded in 90° geometry on an Edinburgh Instruments FLS980 emission spectrometer with an excitation wavelength of 425 nm in the emission wavelength interval of 500-830 nm (or 500-1200 nm using an NIR-sensitive PMT).

2.3 Resonance Raman spectroscopy

For resonance Raman experiments, two different setups, were employed. Spectra were recorded either using a rotating cuvette setup with a continuous wave (cw) Argon ion laser (458, 476, 496, 514 nm, 60 mW at sample position) in a 90° geometry or in a 1 mm quartz cuvette employing commercial diode pumped solid state lasers (405, 473 nm, 3 mW at sample position) and forward scattering (0°) geometry. Spectra were processed by means of numerical background correction by a custom R script from the *baselineWavelet* package which used the continuous wavelet transform algorithm for peak detection and peak width estimation before fitting the background via a modified penalised least squares algorithm.

2.4 Femtosecond time resolved transient absorption spectroscopy

Femtosecond time resolved transient absorption spectroscopy is conducted on a setup described elsewhere.[2] The sample was pumped using the second harmonic of the amplifier output at 403 nm. The excited state dynamics were probed using a white-light supercontinuum generated by passing a minor part of the Ti:Sapphire amplifier output through a rotating calcium fluoride (CaF_2) window. Excitation laser powers were adjusted to around 150 µW at sample position. Sample analysis was conducted by chirp correction and subsequent global fitting to a sum of exponential decay functions. The temporal solution achieved in these experiments is reduced to 300 fs due to strong coherent artefact signals residing in the data.

2.5 Nanosecond time resolved transient absorption spectroscopy

Excited state lifetimes on the nanosecond timescale were determined using nanosecond time resolved absorption spectroscopy. The corresponding setup is described elsewhere.[3] Samples with a path length of 10 mm were excited at 410 nm. Excitation pulses had a peak widths of around 5-10 ns. The excitation energy at the sample position was adjusted to around 0.1 mJ. Experiments were conducted in air-equilibrated solvents. The obtained data was analysed using a custom built global fit routine in the programming language Python [PythonRM] based on the SciPy[4] function *scipy.optimize.leastsq* using mono- and biexponential decay models with and without infinite lifetime components. The data is modelled for delay times larger than 50 ns.

3 Syntheses

3.1 Synthesis of $[Os(TAP)_2Cl_2]$

OsCl3 trihydrate (395 mg, 1 eq., 1.13 mmol), TAP (400 mg, 1.99 eq, 2.20 mmol) and lithium chloride (240 mg, 5 eq., 5.5 mmol) are suspended in 16 mL of a mixture of ethanol and deionised water (1:1, v:v), de-aerated and heated under microwave conditions to 140 °C for 3 h. The black, microcrystalline precipitate is filtered, washed with water (100 mL) and diethyl ether (100 mL) and dried in vacuo. Residual ethanol in the aqueous fraction of the filtrate is evaporated and the dark brown solution is extracted with dichloromethane (5 x 30 mL). The combined extracts are evaporated, dried in vacuo and combined with the crystalline precipitate to yield pure [(tap)2OsCl2] as black solid (670 mg, 95 % (Os)). 1H-NMR (DMSO–d6, 400MHz, 140 °C, TMS): δ = 9.95 (d, J = 9.49 Hz 2H), 9.13 (d, J = 3.12 Hz, 2H), 8.58 (d, J = 9.40 Hz, 2H), 8.47 (d, J = 9.28 Hz, 2H), 8.22 ppm (s, 4H). ESI-MS (ES-ToF pos. in ACN/MeOH) m/z: 646 [(M+Na)+], 632 [(M-Cl—+ACN)+], 591 [(M-Cl—)+].

3.2 Synthesis of $[\{Os(TAP)_2\}_2(\mu\text{-tpphz})](Cl)_4$ $[4]Cl_4$

[(tap)2OsCl2] (400 mg, 4 eq., 0.640 mmol) and tpphz (61.3 mg, 1 eq., 0.160 mmol) are suspended in 15 mL of a mixture of ethanol and deionised water (1:1, v:v). The suspension is purged with argon for 20 min and heated at 140 °C for 9 h under microwave conditions. After cooling, the ethanol is evaporated, and the dark suspension is filtered through a glass sinter funnel. After thorough washing of the black residue with water (60-100 mL), the combined dark brown filtrate is transferred to a separatory funnel and extracted with dichloromethane (8 x 30 mL, until the organic layer is colourless). (8 x 30 mL, until the organic layer is colourless). The residual dark brown aqueous phase is extracted with Na+tfpb— in order to convert cationic complexes in the aqueous layer to the corresponding tfpb— salts. Column chromatography on basic aluminium oxide is conducted using a mixture of acetonitrile and water (9:1, v:v) as starting eluent. In order to elute brown fractions, the polarity is increased by adding aqueous saturated potassium nitrate solution to a final ratio (9 : 1) : 0.2 [(ACN : H2O) : KNO3]. The brown fractions are collected, combined and solvents evaporated. The dark residual solid is dissolved in water and cationic complexes are extracted using Na+tfpb— and dichloromethane before reconversion to the chloride salts. For final purification, ion exchange chromatography on Sephadex-SP C25 was employed. The desired product was eluted with 0.4 mol L^{-1} aqueous sodium chloride solution. The fractions containing the product were then extracted with Na+tfpb− into dichloromethane, evaporated and converted back to the chloride salt. Pure **1** is obtained as a black solid (30 mg, 6 %). 1H-NMR (D2O, 400 MHz, 25 °C, TMS): δ = 9.90 (dd, J = 8.34, 1.16 Hz, 4H), 8.78 (m, 8H), 8.61 (d, J = 8.34, 1.73 Hz, 8H), 8.41 (dd, J = 2.92, 2.37 Hz, 4H), 8.30 (d, J = 2.72 Hz, 4H), 8.15 (dd, J = 5.52, 1.13 Hz, 4H), 7.90 ppm (dd, J = 8.34, 5.55 Hz, 4H). ESI-MS (ES-ToF pos. in MeOH/H2O) m/z: 1601 $[(M-Cl^-)^+]$, 782 $[(M-2Cl^-)^{2+}]$, 510 $[(M-3Cl^-)^{3+}]$, 373 $[(M-4Cl^-)^{4+}]$.

4 X-ray Crystallography Data

X-ray quality crystals of $[Os(TAP)_3]^{2+}$ were grown by vapor diffusion of water into a DMSO solution of its tfpb$^-$ salt. The resulting, optimized molecular structure of the complex is depicted in Figure S1A.

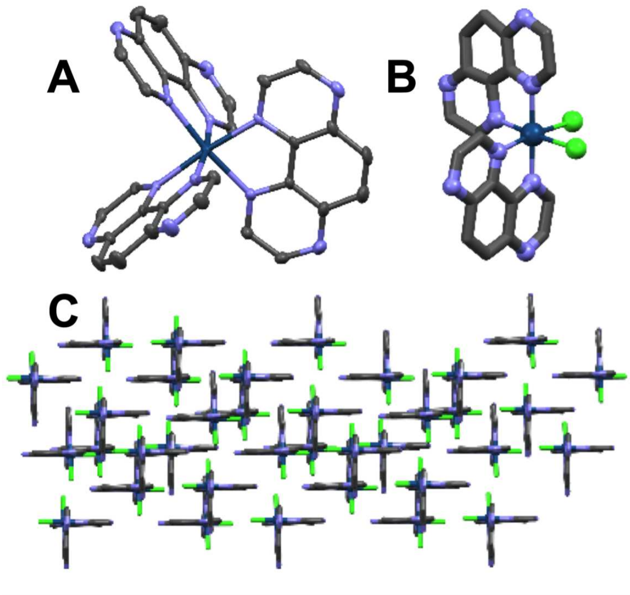
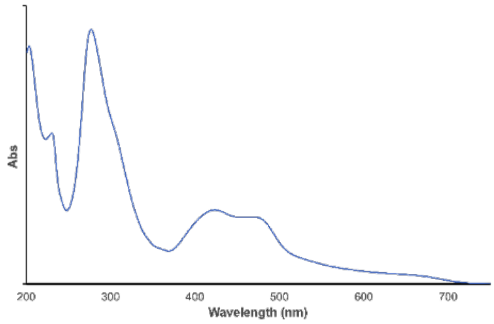


Figure S1: X-ray crystal structures of $[Os(TAP)_3]^{2+}$ and $[Os(TAP)_2Cl_2]$ A. Thermal ellipsoid depiction of $[Os(TAP)_3]^{2+}$ B. Structure of $[Os(TAP)_2Cl_2]$. C. Packing of $[Os(TAP)_2Cl_2]$ driven by $\pi - \pi$ interactions of coordinated TAP ligands

The asymmetric unit is composed of half an osmium complex, one tfpb–anion and half a dichloromethane molecule (from the solvent extraction of the salt) with the rest of the structure generated through rotation of this unit along the main C2 axis. As a consequence, two sets of Os-N bond lengths, measuring 2:064(3) and 2:076(3) Å, are observed; values that are very close to reported complexes such as $[Os(phen)_3](PF_6)_2$ with bong lengths ranging from 2:047(3) - 2:072(4) Å and 2:040(7)-2:076(7) Å respectively. Similar to related literature structures, the coordination sphere is slightly distorted away from an idealized octahedral geometry. The crystals of $[Os(TAP)_2Cl_2]$ produced in its microwave-based synthesis diffracted X-ray and, although the quality of the solution is not high enough to provide accurate bond distances and angles, the structure confirms the connectivity of the complex and reveals that individual complexes are packed together through extended $\pi - \pi$ interactions involving coordinated TAP ligands – Fig S1B and C.

5 UV-Vis and Luminescent spectra of $[4]Cl_4$



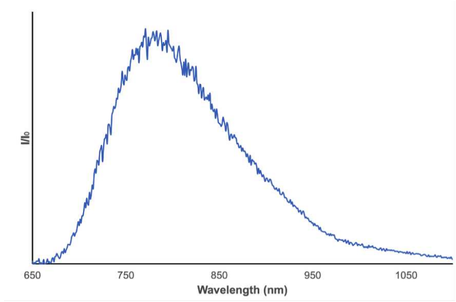


Figure S2: Left: UV-Vis spectrum of the complexes [4]Cl4 in Tris buffer solution. Right: emission spectrum λ_{ex} = 415 nm with excitation and emission slit widths of 10 nm and 30 nm, respectively

Table S1: Summary of steady-state UV-Vis data, extinction coefficients and emission maximum in water and buffer solution.

Solvent	Ext. max/ nm (ext. coeff/10^4 M^{-1})	Em. Max
Water	278 (10.0), 366 (1.3), 415 (2.9),	
	476 (2.6), 650 (0.4, ca.)	780
Tris-buffer	277 (9.8), 360 (1.4), 423 (2.9),	
	470 (2.6), 650 (0.4, ca)	780

6 Cell studies

6.1 Cell Culture

A2780 cell lines were cultured in RPMI-1640 growth medium supplemented with 10% fetal bovine serum (FBS), 2 mM L-glutamine, 100 IU mL^{-1} penicillin and 100 μg mL^{-1} streptomycin. Cultures were incubated at 37 degC in an atmosphere of 5 CO_2 and passaged regularly to maintain health and optimal growth.

6.2 Preparation of Complex Solution for Cell Studies

The solution of OsOsTAP was first dissolved in phosphate buffered saline (PBS) and then diluted in RPMI growth medium to the appropriate concentration. The complex solution was sterile filtered through a 0.22 μm filter before cell treatment.

6.3 Cytotoxicity (MTT Assay)

A2780 cells were seeded in a 48 well plate at a density of 5 x 104 cells per well and after 24 hours were treated with the corresponding concentrations of OsOsTAP in triplicate. After 48 hours of compound exposure, the media was carefully aspirated from wells and replaced with MTT (0.5 mg mL^{-1} in serum free media). After 30-45 minutes incubation, the MTT was removed and the purple coloured formazan product was eluted and dissolved in 130 μL iso-propanol per well. 100 μL from each well was transferred into a 96 well plate and the absorbance read on a plate reader spectrophotometer at 595 nm. An average absorbance was calculated for each concentration and the cell viability determined as a percentage of the untreated control well. The percentage cell viability was plotted against complex concentration and the IC50 determined by interpolation.

6.4 Phototoxicity

A2780 cells were seeded in four 48 well plates at a density of 5 x 104 cells per well and after 24 hours incubation were treated with the corresponding concentrations of OsOsTAP in triplicate. After 24 hours exposure to the compound, the media was removed and replaced with fresh media prior to irradiation. One plate was kept in the dark in the incubator whilst the other three plates were irradiated with white light for either 5 minutes, 15 minutes, 30 minutes corresponding to light doses of 8, 24 or 48 J cm^{-2} respectively. The plates were then incubated for a further 24 hours after irradiation, after which the media was removed and replaced with MTT (0.5 mg mL^{-1} in serum free media). After a 30-45 minute incubation period the formazan product was dissolved in 130 μL iso-propanol per well. 100 μL from each well was then transferred into a 96 well plate and the absorbance measured on a plate reader spectrophotometer. Cell viability was then calculated as a percentage of the untreated control wells for each plate.

7 Microscopy

7.1 Live Cell Imaging

MCF-7 cells were seeded at a density of 6×10^4 onto a 35 mm imaging μ-dish with an ibidi polymer coverslip bottom and were incubated for 24 hours. The media was removed, the cells washed once with PBS and the corresponding concentration of $\mathbf{4}^{4+}$ added and incubated for 24 hours. Prior to imaging, media was removed and the cells washed thrice with PBS before replacing with fresh media. Samples were then imaged immediately. Imaging was performed using an Airyscan confocal laser scanning inverted microscope ZEISS LSM 880 with an environmental control chamber. Images were taken with an oil immersion 63 x objective using 518 F immersion media. The 405 nm excitation laser was used to excite the compound and luminescent images were collected between 700-800 nm. Detector gain and laser power were adjusted to avoid saturation. Images were processed and analysed with FIJI Image J software.

7.2 Fixed Cell Preparation for STED Microscopy

Glass cover slips (22 mm x 22 mm) were sterilised and placed into six well plates. A2780 cells were then seeded onto coverslips with RPMI media and incubated for 24 hours. Cells were treated with the relevant concentration of $\mathbf{4}^{4+}$ and incubated further for the corresponding time point. Cells were then washed thrice with PBS and fixed with 4% PFA (paraformaldehyde) for 20 minutes. The PFA was removed and any remaining PFA was quenched by washing with ammonium chloride solution (50 mM). Before mounting, cells were washed once more with PBS and then coverslips were mounted onto glass slides using mounting medium (ProLong Gold Antifade). Coverslips were sealed using nail varnish and imaged on a LEICA SP8 3X gSTED SMD confocal microscope.

7.3 Stimulated Emission Depletion (STED) nanoscopy and image deconvolution

STED images were acquired on a LEICA SP8 3X gSTED SMD confocal microscope (Leica Microsystems, Manheim, 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. Excitation laser is a pulsed (80 MHz) super-continuum laser. We used clean-up notch filters in the optical pathway. The objective employed was a Leica 100x/1.4NA oil objective. The pinhole was set at one Airy unit. The dye was excited at 470 nm, and STED depleted at 775 nm; the emission was collected from 600 to 710 nm and a gating between 2 and 6.5 ns was used. For the 3D STED images the depletion lasers were split in two, the second vortex was set at 50%. To enhance the signal to noise ratio at the images obtained 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. The surface rendered images, and intensity images have been processed using Huygens Professional, LAX software (Leica SP8). Origin Pro (OriginLab Corporation, Northampton, MA, U.S.A.) was used as a software to represent the line profiles and the figures organised and presented using the free open-source software Inkscape (www.inkscape.org).

7.4 Quantum Yield Determination

The quantum yield of $\mathbf{4}^{4+}$ was obtained in water through the relative comparison method using tris(2,2'-bipyridyl)ruthenium(II) chloride as the standard (Φ_p, 0.04).[5, 6] The emission spectra of solutions of $\mathbf{4}^{4+}$ and $[Ru(bpy)_3]^{2+}$ were recorded over a range of known absorbance values between 0 and 0.1 at the excitation wavelength. The integrated fluorescence intensity was plotted as a function of solution absorbance and the quantum yield obtained using the gradients.

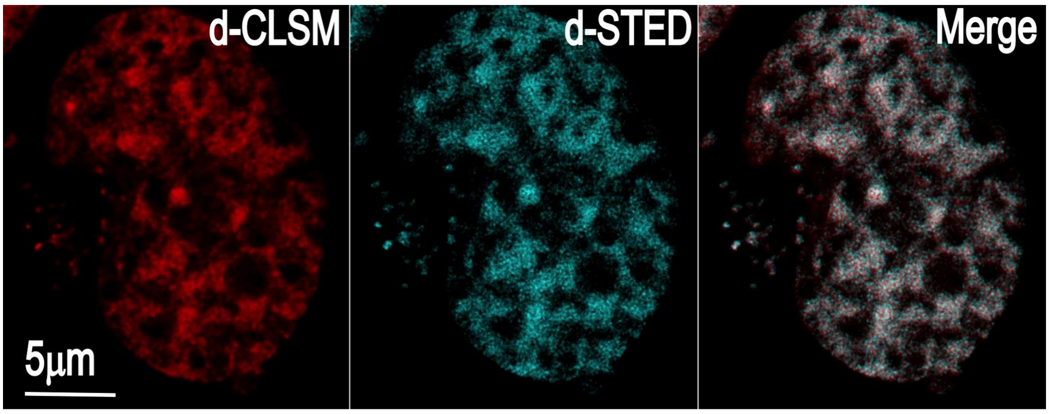


Figure S3: Comparison of d-CLSM and d-STED cell images using phototoxic $[Ru(TAP)_{22}(\mu\text{-tpphz})](Cl)_4$;$[1]Cl_4$

8 Computational Data

8.1 Computational Details

All calculations were performed with Gaussian 09 v. E.01[7] using density-functional theory. The functional used was B3LYP[8] with empirical dispersion corrections.[9] The basis set used consisted of SDD[10] on Ru and 6-311G(d,p)[11,12] on all other atoms. All bulk solvent was described using the PCM method[13,14] as implemented in Gaussian using the provided parameters for MeCN and water. For the calculations involving water, additional water molecules were placed around the complexes coordinated to the free nitrogen atoms. In the case of TAP, the initial orientation of the additional waters was chosen randomly, since for those moieties a negligible dependence of the energetics and final electronic structure on the precise orientation of the water molecules can be expected. For the water molecules coordinated to the central tpphz unit, the initial orientation was chosen to be with the waters functioning as hydrogen-bond donors. However, during the optimisation these water molecules rotated to become hydrogen-bond acceptors. For all optimised structures frequencies were calculated in the harmonic approximation. Only non-imaginary frequencies were obtained.

All absorption spectra were calculated with the TD-DFT method[15] as implemented. Additional keywords were used to perform the wavefunction analysis using the TheoDORE 1.7.2 program.[16] Briefly, this involves partition of the one-particle transition density matrices into atomic contributions using a Löwdin partitioning.[17,18] 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. 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.[19]

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

8.2 Additional Figures

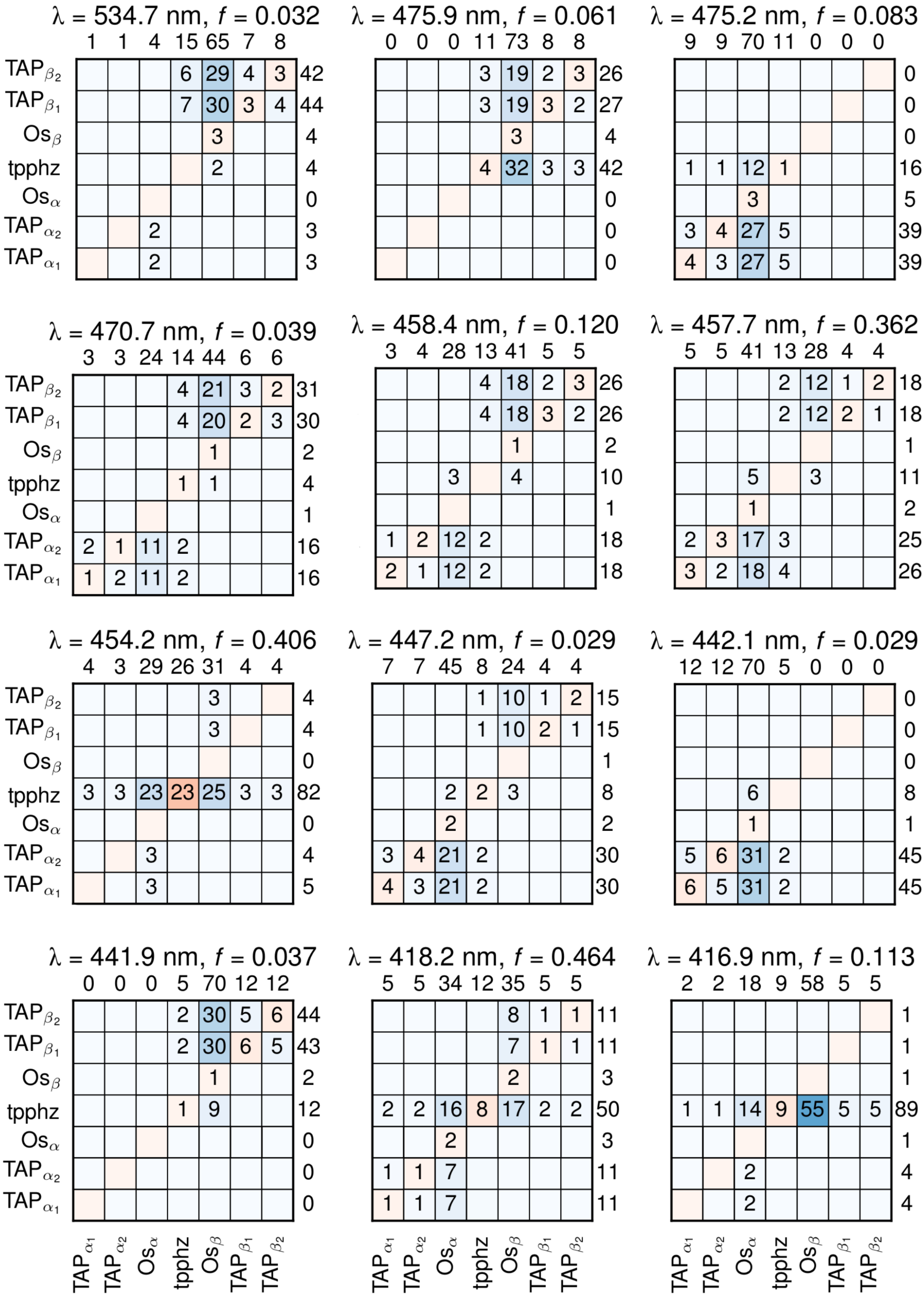


Figure S4: Electron-hole plots of the 12 strongest transitions for $\mathbf{4}^{4+}$.

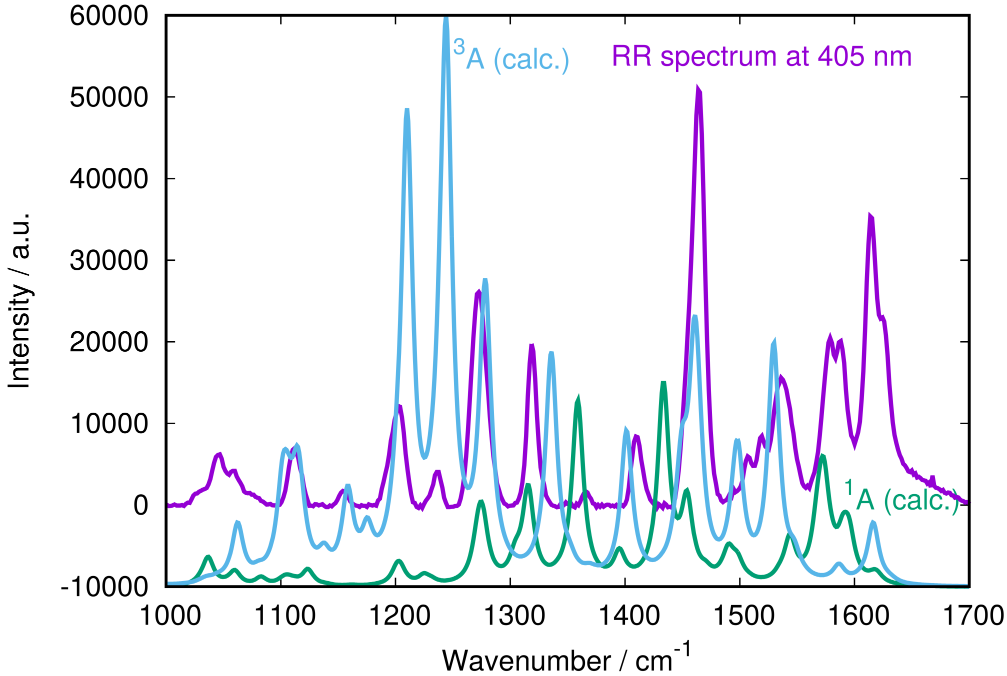
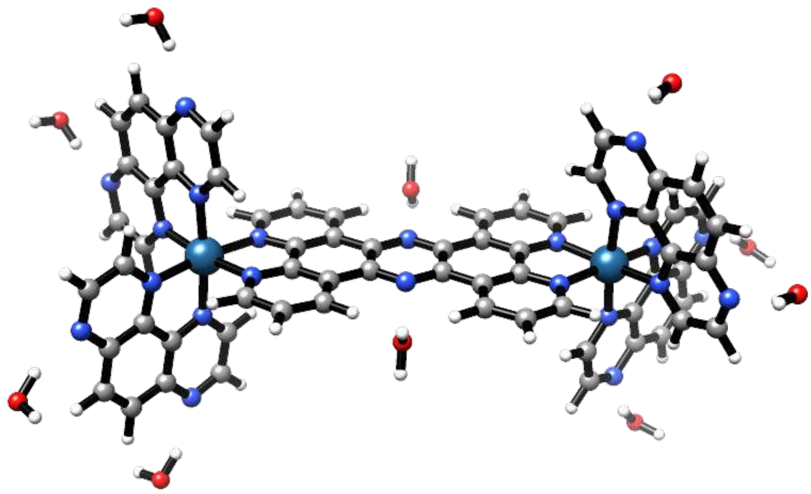


Figure S5: Comparison between experimental (purple trace) and calculated Raman spectra (green trace (^{1}A) and blue trace (^{3}A).

8.3 Calculations on $[4]^{4+}$ (^{1}A)



Route	:	# freq=raman b3lyp/genecp
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	:	geom=connectivity empiricaldispersion=gd3bj
	:	int=ultrafine pop=regular
SMILES	:	c1cc2c3c(c4ccc[n+]5c4c2[n+](c1)[Os]567
	:	([n+]8ccnc9c8c1[n+]6ccnc1cc9)[n+]1ccnc2c1c1
	:	[n+]7ccnc1cc2)nc1c2ccc[n+]4c2c2c(c1n3)
	:	ccc[n+]2[Os]412([n+]3ccnc4c3c3[n+]1ccnc3cc4)
	:	[n+]1ccnc3c1c1[n+]
	:	2ccnc1cc3.O.O.O.O.O.O.O.O.O.O
Formula	:	$C_{64}H_{56}N_{22}O_{10}Os_2^{4+,1}$
Charge	:	4
Multiplicity	:	1
Energy	:	-4612.20156064 a.u.
Gibbs Energy	:	-4611.18477300 a.u.
Number of imaginary frequencies	:	0

8.3.1 Cartesian Co-ordinates (XYZ format)

154

N	4.808	0.09323	-1.33215
N	-0.00868	0.05516	-1.40147
N	-0.00886	-0.05982	1.38539
N	4.80779	-0.08439	1.31757
C	4.8574	0.16799	-2.66861
H	5.83997	0.20672	-3.11548
C	3.70467	0.20056	-3.452
H	3.8035	0.26125	-4.52709
C	2.45834	0.15688	-2.85281

H	1.55053	0.18227	-3.44648
C	2.39114	0.0785	-1.45311
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C	-1.15149	-0.0307	0.70322
C	1.13385	-0.03321	0.70317
C	2.3909	-0.07533	1.43776
C	2.45784	-0.15292	2.8375
H	1.54983	-0.17979	3.43083
C	3.70407	-0.19296	3.43715
H	3.80267	-0.25246	4.51233
C	4.85694	-0.15821	2.65409
H	5.83945	-0.19448	3.10129
C	3.58776	-0.03876	0.71164
C	3.58787	0.04469	-0.72665
C	7.44204	-2.4106	-1.28697
C	5.84891	-3.04764	0.23858
C	7.64694	-3.74637	-1.66997
C	8.18457	-1.37106	-1.89077
C	6.0586	-4.3821	-0.1574
H	5.13109	-2.79543	1.00482
C	9.14339	-1.66061	-2.87598
H	5.48211	-5.16796	0.3152
C	8.64441	0.87328	-2.043
C	9.60655	0.57081	-3.02535
H	8.4616	1.89137	-1.73232
H	10.17572	1.37756	-3.47075
N	7.92598	-0.09515	-1.47576
N	6.54007	-2.05645	-0.32314
C	8.1841	1.38091	1.87699
C	8.64274	-0.86358	2.03049
C	9.1423	1.67042	2.86283
C	7.44221	2.42049	1.27248
C	9.60419	-0.56117	3.01354
H	8.45959	-1.88171	1.72011
C	7.64792	3.75638	1.65457
H	10.17171	-1.36814	3.46064
C	5.84962	3.05746	-0.25366
C	6.06007	4.39207	0.14148
H	5.13174	2.80517	-1.01982
H	5.48408	5.17795	-0.33169
N	7.92526	0.10496	1.46225
N	6.54023	2.06624	0.30867
C	-4.87504	0.04212	-2.67382
C	-4.87558	-0.06503	2.65656

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H	-1.56907	-0.11311	3.43436
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N	-7.94201	-0.22176	1.4503
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C	-5.85358	3.01427	0.47159
C	-8.19474	-1.52569	1.77211
C	-8.66413	0.69963	2.08722
C	-7.45338	-2.51573	1.08905
C	-5.87106	-3.03345	-0.49143
C	-9.12575	1.88606	-2.76765
C	-9.61664	-0.32343	-3.0718
H	-8.49708	-1.7447	-1.86652
C	-7.62099	3.86546	-1.40283
C	-6.04676	4.37576	0.17042
H	-5.14668	2.70173	1.22556
C	-9.1507	-1.89024	2.73499
C	-9.62415	0.32214	3.04536
H	-8.48517	1.73846	1.85232
C	-7.656	-3.87704	1.36976
C	-6.07834	-4.39447	-0.19766
H	-5.15753	-2.72384	-1.24036
H	-10.19284	-1.09009	-3.57521
H	-5.46943	5.11993	0.70543
H	-10.19611	1.09177	3.5491
H	-5.50449	-5.1414	-0.73255
C	9.34282	3.03847	3.2476
H	10.08591	3.23332	4.01073
C	8.62435	4.04055	2.66747
H	8.76062	5.07836	2.94475
C	8.62298	-4.03044	-2.68327
H	8.75794	-5.06804	-2.96195
C	9.34326	-3.02856	-3.26149

H	10.08473	-3.22312	-4.02627
C	-8.62747	-4.23794	2.36275
H	-8.76539	-5.29404	2.55787
C	-9.3469	-3.2836	3.0173
H	-10.0893	-3.53655	3.76384
C	-8.58217	4.23057	-2.40427
H	-8.70378	5.28658	-2.61041
C	-9.30653	3.27976	-3.05855
H	-10.03696	3.5356	-3.81581
N	-6.90439	4.80483	-0.74017
N	-9.84725	0.93468	-3.40718
N	6.93339	4.74714	1.0689
N	9.85525	0.66832	3.43052
N	9.8572	-0.6586	-3.44276
N	6.93171	-4.73706	-1.08505
N	-9.86853	-0.93534	3.37338
N	-6.94525	-4.81994	0.70583
O	-0.00749	-0.16826	4.94908
O	-0.00536	0.22409	-4.9593
H	-0.02191	-0.88975	5.58776
H	0.02564	0.63162	5.48562
H	-0.05761	1.02682	-5.48997
H	0.00033	-0.49346	-5.60257
O	11.72177	-1.94797	-5.2829
O	7.91503	-7.22801	-2.24799
O	7.91632	7.23783	2.23285
O	11.53918	1.93465	5.45284
O	-11.64621	2.37202	-5.20553
O	-7.85176	7.38301	-1.73098
O	-11.55695	-2.35465	5.28975
O	-7.78455	-7.38887	1.81308
H	-10.91972	-2.46451	6.00397
H	-7.22331	-7.41489	2.59572
H	-12.35462	2.58544	-4.58846
H	-8.63648	7.4851	-1.18144
H	8.69139	-7.36602	-1.69445
H	10.89738	1.99254	6.16909
H	8.69289	7.37697	1.67987
H	12.41312	-2.19419	-4.65871
H	7.44016	6.52263	1.77452
H	11.15517	-1.34914	-4.76466
H	7.43822	-6.51257	-1.79072
H	11.10077	1.35282	4.80677
H	-7.38761	6.63135	-1.32123
H	-11.10454	1.73112	-4.71158
H	-7.42058	-6.64459	1.30129
H	-11.11648	-1.72468	4.69205
Os	-6.45657	-0.00818	-0.00848

Os	6.43902	0.00489	-0.00706

8.3.2 Frequencies

Mode	IR frequency	IR intensity
1	6.747	0.5696
2	7.6244	0.0655
3	10.4895	0.4554
4	14.6783	0.444
5	15.8362	5.8659
6	18.6792	4.495
7	19.9292	2.2991
8	21.0901	4.0574
9	22.5343	4.6643
10	23.7683	0.7945
11	26.182	1.1078
12	27.9426	0.1966
13	30.3934	0.4613
14	41.0347	0.4948
15	44.6876	5.4085
16	44.9863	3.4039
17	46.7819	0.7547
18	48.0359	9.5703
19	48.8468	2.6957
20	51.852	4.3492
21	52.5957	1.2222
22	54.2824	3.0645
23	55.4145	2.7948
24	56.5271	0.3758
25	63.314	364.0888
26	65.2841	0.2597
27	65.8686	1.5071
28	67.1466	7.9069
29	67.575	1.0197
30	69.5574	109.881
31	69.9727	123.2255
32	71.0564	106.7895
33	76.2103	0.0126
34	81.9189	9.1111
35	84.3898	0.1258
36	85.2727	7.1393
37	86.2357	9.8314
38	90.6555	34.0931
39	91.6116	7.4734
40	93.1482	18.6094
41	96.603	13.8342
42	97.7459	10.3442
43	99.5856	8.1303

44	100.1106	6.721
45	112.9379	2.0285
46	116.3235	8.0299
47	129.8231	2.0483
48	131.7505	0.0674
49	132.9928	0.1131
50	137.42	0.2341
51	138.8485	5.619
52	139.5213	0.64
53	143.9038	7.3191
54	144.4387	1.3793
55	145.6291	3.5579
56	146.949	2.7408
57	151.9864	213.2407
58	156.1228	1.0873
59	176.9341	3.4565
60	180.5795	0.9367
61	181.5838	0.2069
62	182.2663	5.4712
63	184.8938	0.6502
64	185.6984	1.8631
65	186.6329	9.5754
66	189.5813	0.9149
67	195.55	0.567
68	196.5823	3.5333
69	199.317	1.2243
70	204.4547	0.9855
71	205.6685	15.1407
72	210.6548	2.3716
73	212.8408	25.0115
74	214.92	10.8885
75	216.2868	3.5661
76	217.9062	85.092
77	218.5917	4.4205
78	219.6471	8.6194
79	227.1651	2.3999
80	228.3674	0.1264
81	235.0804	0.2269
82	241.5577	333.1196
83	243.4041	263.0474
84	245.211	57.1191
85	245.504	255.0286
86	248.0066	5.0108
87	251.6992	1.8852
88	252.3734	0.7453
89	258.6023	12.336
90	260.7135	10.0189
91	261.465	44.6159

92	262.9141	25.2902
93	264.8179	12.8088
94	266.8373	135.1502
95	267.2252	2.6894
96	268.763	42.0991
97	284.0018	3.7342
98	285.8268	11.1932
99	299.9886	15.3555
100	301.4591	15.8434
101	302.8401	28.932
102	304.409	7.2494
103	308.5705	2.6311
104	328.5542	19.433
105	341.1381	84.9182
106	342.8734	29.4078
107	343.517	20.7418
108	344.1494	108.1353
109	344.4721	6.8715
110	346.4065	97.1303
111	346.5567	84.5054
112	347.5842	218.6744
113	349.7463	50.797
114	350.8772	24.5651
115	352.641	44.8549
116	354.3384	102.6693
117	357.2638	21.5251
118	390.342	0.5431
119	393.5976	0.5028
120	442.9745	4.4332
121	446.5109	0.0143
122	448.2431	1.0021
123	448.5527	2.4517
124	449.0983	7.6313
125	451.5657	1.4779
126	451.8307	0.3203
127	458.9782	19.2478
128	461.1315	1.2878
129	464.3855	1.1653
130	469.772	1.2021
131	469.993	4.7172
132	472.7452	0.5173
133	476.4111	0.7645
134	483.1457	2.1444
135	488.5232	7.2643
136	489.3029	27.7987
137	489.3652	18.1612
138	491.1498	1.8968
139	500.3379	0.0551

140	503.3948	4.6625
141	508.1974	0.3778
142	508.718	5.7141
143	514.091	0.019
144	537.2105	14.5322
145	560.8444	0.1715
146	563.817	14.6442
147	564.2123	1.9902
148	564.4	13.018
149	564.7907	13.0741
150	567.453	0.4703
151	570.4388	1.8186
152	574.0646	0.0884
153	574.7195	0.2135
154	577.7719	0.5461
155	580.3353	0.5958
156	586.5986	91.8059
157	586.9533	84.8003
158	589.8301	0.1588
159	590.0653	45.7261
160	596.8488	5.3388
161	598.301	0.5835
162	598.7799	0.2841
163	599.3906	0.6689
164	600.0977	5.9971
165	602.6934	8.5375
166	627.5867	0.0243
167	650.3238	0.2676
168	651.0933	1.4634
169	654.0298	0.1594
170	654.3142	0.0099
171	662.7598	0.0023
172	663.5602	0.5388
173	666.3824	37.1913
174	667.7842	65.6868
175	672.4524	11.0469
176	673.3884	136.3668
177	674.0338	90.2342
178	675.0455	70.338
179	682.1712	82.7802
180	683.7909	50.3828
181	683.796	80.9732
182	686.1511	54.3336
183	688.7721	829.7459
184	690.2639	784.6237
185	690.8464	196.2115
186	692.2805	286.6186
187	722.706	0.3902

188	736.7122	0.0138
189	744.325	0.0089
190	747.641	41.7813
191	753.4967	4.559
192	753.6428	0.439
193	753.651	0.2564
194	753.7194	0.1731
195	757.1243	135.0558
196	757.5883	261.2209
197	763.6659	130.5321
198	767.1321	41.5521
199	767.7751	3.3576
200	771.7312	6.7362
201	772.5816	1.9488
202	772.8075	3.481
203	773.1361	40.9117
204	773.5775	0.6908
205	773.9286	48.1064
206	826.5236	0.0908
207	827.5035	0.0123
208	833.2035	0.0337
209	834.9359	0.1531
210	846.751	153.6069
211	849.6966	0.6663
212	858.7987	0.1242
213	859.3702	0.9749
214	859.6135	0.3632
215	860.1721	0.1184
216	869.6614	29.7289
217	869.9179	22.4126
218	869.9622	33.2574
219	871.2919	34.7355
220	873.8865	0.0653
221	875.8331	22.7751
222	880.3653	0.5104
223	881.6694	1.8049
224	881.6951	0.0056
225	881.7396	0.3223
226	891.6363	0.1048
227	920.5405	73.0424
228	920.7987	73.8904
229	920.9677	74.3245
230	921.4181	76.5625
231	927.0712	3.6563
232	927.3328	0.693
233	930.4055	1.6386
234	930.6703	1.1282
235	949.6669	0.7288

236	951.953	1.7015
237	953.3443	0.1316
238	954.7819	0.9309
239	954.9577	2.0704
240	993.1844	0.0336
241	993.3352	0.0153
242	993.5416	0.0806
243	994.3723	0.0242
244	997.6885	0.201
245	997.8048	0.3418
246	998.1677	0.1315
247	998.4442	0.4223
248	1000.0087	0.411
249	1000.0752	0.3877
250	1000.774	0.3334
251	1001.0801	0.547
252	1051.3205	1.58
253	1057.5172	3.0038
254	1058.4064	1.537
255	1058.8383	0.0049
256	1059.6654	0.0189
257	1065.4412	0.005
258	1066.0036	0.2691
259	1071.5469	5.2904
260	1075.8777	1.6402
261	1077.7578	0.1286
262	1078.3314	4.5758
263	1079.0799	0.0783
264	1079.3301	0.7134
265	1079.8478	0.1004
266	1079.8616	0.7469
267	1080.2377	0.7419
268	1087.5413	10.1709
269	1088.5306	10.2254
270	1089.0513	3.0121
271	1089.5397	0.7741
272	1093.083	37.8042
273	1112.7751	0.1099
274	1131.0945	11.1337
275	1131.551	29.1093
276	1132.2744	25.3665
277	1133.1181	47.3301
278	1133.8599	60.3543
279	1134.8383	4.6316
280	1136.0306	1.3681
281	1136.3964	0.783
282	1137.7995	0.4864
283	1142.3716	0.3182

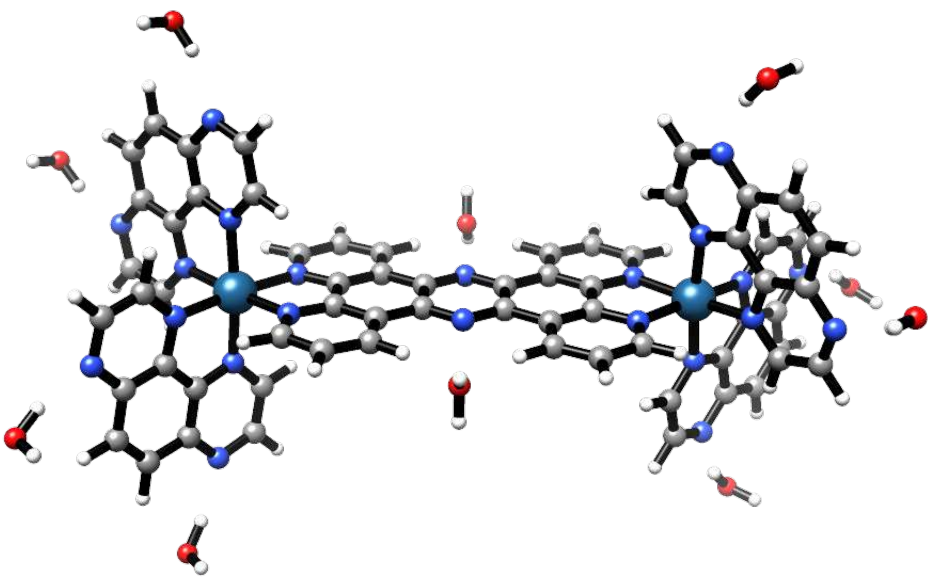
284	1144.9245	10.4048
285	1154.8078	0.1004
286	1158.196	245.7067
287	1166.9847	20.3905
288	1170.6871	0.197
289	1193.2908	0.4926
290	1193.4306	0.5542
291	1194.4086	0.2139
292	1194.5938	0.0696
293	1217.6578	38.6926
294	1232.3278	9.8435
295	1234.3245	23.7115
296	1234.5129	21.2812
297	1235.5364	0.2621
298	1236.9659	7.0828
299	1237.7531	0.2596
300	1258.3902	0.1556
301	1258.5794	0.1085
302	1258.9654	0.1516
303	1259.0786	0.3461
304	1264.9566	40.1853
305	1265.1943	16.3446
306	1265.3414	27.2874
307	1265.6508	14.2689
308	1265.8928	18.7645
309	1289.6516	5.0468
310	1305.8177	0.0228
311	1307.5	313.6392
312	1307.5592	152.4633
313	1310.7935	95.3124
314	1310.927	62.9364
315	1311.7418	149.2562
316	1311.7585	126.5831
317	1312.1209	48.6178
318	1312.2641	20.0954
319	1314.2305	0.052
320	1320.8156	0.3353
321	1322.1133	21.8071
322	1340.5779	0.0655
323	1344.101	2.3428
324	1352.1034	0.0038
325	1359.1841	15.1443
326	1378.0108	0.3559
327	1378.7177	0.6526
328	1378.7968	0.3855
329	1379.4957	0.36
330	1390.4442	334.604
331	1396.4675	0.5467

332	1424.4525	53.4171
333	1424.5464	55.4972
334	1424.7431	75.5898
335	1425.1773	46.5588
336	1433.5071	17.2677
337	1433.5998	75.8947
338	1433.7794	74.8123
339	1433.959	18.0589
340	1440.6616	238.7176
341	1442.284	122.3162
342	1443.3921	123.2404
343	1443.9925	33.7824
344	1444.6604	32.4016
345	1459.9073	0.1953
346	1473.2272	0.0277
347	1477.9011	46.0342
348	1486.9256	0.0664
349	1494.1749	0.1108
350	1494.3634	0.0266
351	1494.8139	0.6186
352	1494.9865	2.4656
353	1500.1364	41.5698
354	1511.1824	2.4149
355	1523.3476	108.4586
356	1524.443	220.1695
357	1524.8298	206.5458
358	1524.9652	63.2698
359	1525.4287	89.5198
360	1531.2953	250.9946
361	1531.6401	380.2805
362	1536.5318	50.3423
363	1539.1865	104.7693
364	1540.0954	88.1723
365	1549.5622	0.0123
366	1576.8369	23.6899
367	1577.0781	20.7565
368	1577.2495	23.7038
369	1577.3917	12.1051
370	1578.0827	121.0897
371	1578.412	112.7516
372	1579.1927	31.2129
373	1579.3185	17.6026
374	1586.5603	0.0555
375	1603.509	2.0989
376	1610.9601	0.0075
377	1614.1278	75.1734
378	1614.4593	87.4854
379	1615.0227	74.0476

380	1615.24	22.4328
381	1616.6862	11.3518
382	1617.0697	3.2895
383	1621.4772	31.6848
384	1621.6704	14.8396
385	1624.1922	0.3575
386	1634.0868	0.0141
387	1639.6242	0.0053
388	1648.3148	12.1905
389	1659.2467	170.0193
390	1660.1847	388.1936
391	1660.5162	107.8949
392	1660.5571	7.8965
393	1660.701	16.25
394	1661.9449	107.0426
395	1662.2064	168.6941
396	1663.1997	17.9013
397	1663.8709	19.679
398	1664.0511	70.0242
399	1665.1888	3.7662
400	1665.2208	11.1363
401	3163.9868	170.2504
402	3164.9776	209.4144
403	3170.1684	194.3084
404	3170.6307	95.6269
405	3192.9732	33.7693
406	3193.4298	33.8763
407	3193.7479	34.138
408	3193.8243	34.3753
409	3196.4293	6.6318
410	3196.4682	5.0795
411	3196.9857	7.045
412	3197.0262	5.8524
413	3197.12	6.0054
414	3197.2807	3.7211
415	3198.2741	8.9585
416	3198.3308	1.7995
417	3202.1333	9.0585
418	3202.7053	9.2262
419	3202.9876	9.2884
420	3203.0068	9.0728
421	3213.6398	1.0796
422	3213.7316	2.5469
423	3214.1405	0.1308
424	3214.1798	2.8753
425	3227.8417	7.6551
426	3227.9253	0.2493
427	3230.1643	6.9841

428	3230.2771	1.0023
429	3235.655	1.9858
430	3235.828	2.3093
431	3236.0371	1.9153
432	3236.1646	2.3202
433	3238.4091	3.8522
434	3239.0228	2.1219
435	3241.9617	5.0538
436	3242.1705	0.4965
437	3612.5878	1092.941
438	3612.7919	1207.3286
439	3612.7984	164.7319
440	3613.2346	297.4895
441	3613.8208	1507.0892
442	3614.43	1630.7968
443	3615.0386	1125.7173
444	3615.1973	805.3545
445	3800.1128	39.5746
446	3800.3695	38.1001
447	3846.8246	86.4667
448	3847.2612	79.8936
449	3847.5052	105.5978
450	3847.5288	22.1868
451	3847.5433	122.1685
452	3847.6177	99.8697
453	3847.6545	161.499
454	3848.2431	97.1993
455	3892.709	87.6648
456	3892.8611	89.1238

8.4 Calculations on $[4]^{4+}$ (^{3}A)



Route	:	# opt freq=raman ub3lyp/genecp
	:	scrf=(solvent=water) guess=read
	:	geom=connectivity empiricaldispersion=gd3bj
	:	int=ultrafine pop=regular
SMILES	:	c1cc2c3c(c4ccc[n+]5c4c2[n+](c1)[Os]567
	:	([n+]8ccnc9c8c1[n+]6ccnc1cc9)[n+]1ccnc2c1c1
	:	[n+]7ccnc1cc2)nc1c2ccc[n+]4c2c2c(c1n3)
	:	ccc[n+]2[Os]412([n+]3ccnc4c3c3[n+]1ccnc3cc4)
	:	[n+]1ccnc3c1c1[n+]
	:	2ccnc1cc3.O.O.O.O.O.O.O.O.O.O
Formula	:	$C_{64}H_{56}N_{22}O_{10}Os_2^{4+,3}$
Charge	:	4
Multiplicity	:	3
Energy	:	-4612.13492255 a.u.
Gibbs Energy	:	-4611.12113700 a.u.
Number of imaginary frequencies	:	0

8.4.1 Cartesian Co-ordinates (XYZ format)

154

N	4.84642410	0.11325900	-1.32962799
N	0.03227800	0.05857600	-1.41521001
N	0.02228500	-0.13863200	1.36803806
N	4.83956003	-0.13716400	1.31385696
C	4.89885521	0.22301400	-2.66375303
H	5.88220501	0.28118601	-3.10671210

C	3.74847889	0.26746699	-3.44982100
H	3.85028601	0.35655999	-4.52262783
C	2.50070596	0.20084199	-2.85577106
H	1.59386802	0.23702900	-3.45057702
C	2.43080091	0.08588600	-1.45883906
C	1.17200303	0.01637000	-0.72987002
C	-1.11192000	0.00652200	-0.73772597
C	-3.56319094	0.00562400	-0.75617301
C	-3.56867003	-0.06799000	0.67861098
C	-2.37814498	-0.12710001	1.41111505
C	-1.11733103	-0.08863200	0.68216401
C	1.16716599	-0.08980700	0.69098502
C	2.42245102	-0.14721100	1.42762697
C	2.48581791	-0.26479301	2.82465911
H	1.57598305	-0.31493899	3.41384006
C	3.73077297	-0.31647801	3.42621803
H	3.82705212	-0.40850601	4.49929380
C	4.88542318	-0.25137600	2.64775705
H	5.86708593	-0.29581100	3.09604907
C	3.62099195	-0.08282400	0.70607197
C	3.62513304	0.03993100	-0.72960401
C	7.51865482	-2.35244608	-1.34405804
C	5.93459511	-3.05613399	0.16172300
C	7.74561977	-3.67375112	-1.76284695
C	8.24468040	-1.28509295	-1.91858196
C	6.16669989	-4.37592983	-0.26965299
H	5.21212387	-2.83600903	0.93372399
C	9.20789337	-1.53158104	-2.91111708
H	5.60282993	-5.18363619	0.18082200
C	8.66632462	0.97007197	-2.01012897
C	9.63294315	0.71078998	-3.00047112
H	8.46564102	1.97600901	-1.67228794
H	10.18800831	1.53881395	-3.42407894
N	7.96459723	-0.02531500	-1.46975005
N	6.60958004	-2.03903103	-0.37286699
C	8.19275856	1.36471295	1.92268395
C	8.69596195	-0.87371099	2.00864697
C	9.14612389	1.64344394	2.91625500
C	7.43336821	2.40781999	1.34658504
C	9.65289688	-0.58183700	2.99932098
H	8.53276253	-1.88564205	1.66841900
C	7.61540985	3.73585892	1.76635206
H	10.23731709	-1.39040101	3.42105007
C	5.83477688	3.06049109	-0.16660000
C	6.02116108	4.38686323	0.26648799
H	5.12328100	2.81783891	-0.94189399
H	5.43314981	5.17585707	-0.18624701
N	7.95802784	0.09665600	1.47081697

N	6.54010677	2.06557798	0.37051699
C	-4.83334780	0.12371800	-2.70333409
C	-4.86008406	-0.18029299	2.61668396
C	-2.36548400	0.04985900	-1.47774196
C	-2.43305707	0.13462301	-2.87716508
H	-1.52431202	0.17471200	-3.46986008
C	-2.46071196	-0.21693601	2.80953097
H	-1.55783296	-0.26847199	3.41030097
C	-3.67815804	0.17081399	-3.48118997
C	-3.71184206	-0.24495199	3.40278792
H	-3.77322292	0.23636800	-4.55609703
H	-5.81557322	0.14646100	-3.15215802
H	-3.81613708	-0.31768900	4.47635412
H	-5.84912205	-0.19674000	3.05040908
N	-4.78049898	0.03762900	-1.36783099
N	-4.79081583	-0.08426800	1.28186905
N	-8.00537109	0.16366100	-1.41624796
N	-6.52103519	2.08750510	-0.29693800
N	-7.92177582	-0.16972700	1.41457105
N	-6.51535416	-2.08290005	0.17911500
C	-8.30254555	1.45584595	-1.73235905
C	-8.75342846	-0.78860599	-1.96535397
C	-7.51717901	2.47049308	-1.14492095
C	-5.76534891	3.04554701	0.23144300
C	-8.20478821	-1.48809302	1.73636997
C	-8.67080116	0.77432299	2.01871300
C	-7.47320700	-2.47786689	1.10110903
C	-5.77156305	-3.06204796	-0.37999400
C	-9.34718513	1.78487897	-2.61384106
C	-9.80080795	-0.44527900	-2.84449100
H	-8.53120804	-1.81733000	-1.72176301
C	-7.75848579	3.82217503	-1.44688594
C	-6.01727104	4.39731693	-0.07842400
H	-4.97060490	2.75928497	0.90460598
C	-9.21456146	-1.81009305	2.68106198
C	-9.65131474	0.42835900	2.93416905
H	-8.47052670	1.80818295	1.77618802
C	-7.67891502	-3.85011911	1.39805698
C	-5.99656677	-4.39053011	-0.06851800
H	-5.01166391	-2.77121210	-1.09093404
H	-10.40115738	-1.23318601	-3.28171992
H	-5.39592505	5.16508007	0.36527801
H	-10.23391914	1.20349705	3.41340399
H	-5.39893007	-5.15983915	-0.53852201
C	9.32138920	3.00320697	3.34062195
H	10.06070423	3.18942904	4.10954809
C	8.58530712	4.00836992	2.78863907
H	8.70230389	5.04002380	3.09599304

C	8.72647095	-3.91403103	-2.78293490
H	8.87768459	-4.94122410	-3.09034896
C	9.43013477	-2.88509607	-3.33356309
H	10.17404079	-3.04653692	-4.10366106
C	-8.70315361	-4.17604399	2.36030507
H	-8.85946560	-5.22648621	2.57198405
C	-9.43472385	-3.20564103	2.96996498
H	-10.20748043	-3.44110489	3.69114900
C	-8.82706261	4.14759779	-2.34773397
H	-8.99108028	5.19667816	-2.56034994
C	-9.59158611	3.16814399	-2.90765810
H	-10.40166759	3.39172506	-3.59063292
N	-6.98536921	4.78394318	-0.89111000
N	-10.09603977	0.80230898	-3.16590190
N	6.88534880	4.73031998	1.20672202
N	9.87930298	0.63914001	3.45349097
N	9.90411854	-0.50255698	-3.45079088
N	7.04597902	-4.69130802	-1.20583105
N	-9.92938709	-0.85357100	3.27476501
N	-6.94757080	-4.79818201	0.81054801
O	-0.01386100	-0.50719303	4.88286877
O	0.02336900	0.32592699	-4.94674778
H	0.00804200	0.03092100	5.68214893
H	-0.01197400	-1.41688097	5.20144987
H	0.05920700	-0.38468501	-5.59678078
H	0.01891500	1.13538396	-5.46979713
O	11.78269672	-1.70668399	-5.33388805
O	8.05111122	-7.13150787	-2.45614505
O	7.80612993	7.20279598	2.45909190
O	11.53753281	1.87748003	5.51376200
O	-12.12438011	2.20382190	-4.76828718
O	-8.12103653	7.31940985	-1.84964395
O	-11.69477654	-2.13589406	5.15185785
O	-7.78693295	-7.33729219	1.86793196
H	-11.07382679	-2.27478600	5.87504816
H	-7.28564501	-7.34302807	2.69042206
H	-12.76943493	2.39198494	-4.07767296
H	-8.82964516	7.43217802	-1.20653605
H	8.82815456	-7.28704405	-1.90826702
H	10.89510345	1.90240598	6.23134708
H	8.58123684	7.38176489	1.91566706
H	12.48199844	-1.95699501	-4.72028399
H	7.35031605	6.49299002	1.97260201
H	11.20797920	-1.13312399	-4.79637623
H	7.57040501	-6.43703222	-1.97146499
H	11.11016083	1.30624998	4.85105610
H	-7.57811689	6.61073112	-1.46418500
H	-11.52850246	1.55962300	-4.34946012

H	-7.42844200	-6.56112003	1.39371800
H	-11.19370365	-1.56728196	4.53468990
Os	-6.41786718	-0.01111700	-0.03504800
Os	6.47412586	0.01147900	-0.00227700

8.4.2 Frequencies

Mode	IR frequency	IR intensity
1	7.50850000	1.40620000
2	9.58020000	0.62500000
3	11.59480000	1.34200000
4	13.80870000	6.58830000
5	15.07600000	5.12920000
6	17.28220000	6.13690000
7	19.78300000	1.42950000
8	20.98910000	1.69630000
9	22.25230000	1.22150000
10	23.10540000	3.44010000
11	26.26930000	1.22650000
12	28.25780000	1.70580000
13	31.59210000	0.32870000
14	40.19450000	1.25630000
15	42.08130000	2.66520000
16	44.56840000	3.11820000
17	48.50670000	16.03680000
18	49.62020000	3.51480000
19	50.65070000	4.23910000
20	51.87970000	1.89430000
21	52.69030000	0.49710000
22	54.87040000	1.94520000
23	55.95940000	1.37440000
24	60.40730000	0.26220000
25	65.23090000	2.65750000
26	66.40140000	0.89030000
27	67.13330000	2.45730000
28	68.28950000	2.13100000
29	69.25120000	2.03030000
30	70.90300000	8.10450000
31	76.32180000	0.55910000
32	81.88060000	22.96250000
33	84.53880000	83.64440000
34	85.04280000	1.60120000
35	86.25850000	235.99220000
36	89.57300000	7.50610000
37	90.48900000	15.03310000
38	92.44240000	36.92360000
39	95.34410000	33.83400000
40	96.97700000	8.66840000

41	100.02880000	2.76690000
42	102.81400000	11.35850000
43	103.24400000	5.05220000
44	106.54090000	273.21590000
45	112.70840000	41.90090000
46	114.94600000	21.61080000
47	129.51020000	0.29620000
48	130.29260000	0.98630000
49	132.87080000	0.23250000
50	135.76520000	4.74540000
51	139.11470000	6.74310000
52	139.85260000	6.23560000
53	140.98050000	37.20190000
54	145.30600000	8.47300000
55	146.12190000	45.72170000
56	149.78590000	9.32500000
57	151.75070000	39.07450000
58	162.11770000	37.05840000
59	173.54890000	101.67000000
60	177.09720000	4.95050000
61	180.97830000	6.69570000
62	181.50040000	0.14350000
63	183.05540000	2.69110000
64	187.42310000	16.68790000
65	188.38610000	0.63890000
66	191.14730000	1.86730000
67	192.28260000	5.42160000
68	198.13430000	12.40090000
69	199.68510000	4.96130000
70	203.45160000	18.29570000
71	205.66080000	32.66060000
72	208.68900000	7.91270000
73	212.21120000	14.73220000
74	213.36880000	38.65350000
75	217.22790000	2.14220000
76	219.31030000	74.54260000
77	220.38440000	4.93170000
78	220.61220000	9.74790000
79	228.92960000	1.54130000
80	233.24610000	4.62740000
81	238.80980000	226.35470000
82	239.52530000	194.50530000
83	241.00070000	160.53590000
84	244.26330000	52.38760000
85	246.03860000	5.51210000
86	247.14320000	302.04280000
87	251.00370000	3.92370000
88	252.77110000	2.37060000

89	253.86120000	3.23570000
90	259.85630000	0.46090000
91	261.51780000	60.26520000
92	262.30820000	29.40310000
93	263.72240000	34.76210000
94	265.98430000	14.86370000
95	266.87460000	90.59740000
96	267.69930000	54.44120000
97	269.46580000	13.99840000
98	281.65490000	10.48910000
99	285.12570000	4.72040000
100	298.12310000	44.98030000
101	300.11250000	11.33010000
102	303.24290000	10.92790000
103	307.14160000	1.81860000
104	320.63770000	119.33380000
105	322.16720000	123.05370000
106	328.76650000	7.54450000
107	337.25910000	0.94160000
108	339.58300000	6.30330000
109	341.33450000	110.71570000
110	343.67640000	16.51060000
111	346.34380000	111.40160000
112	348.83720000	62.14580000
113	352.61100000	27.39740000
114	355.60200000	11.17930000
115	359.45740000	115.04860000
116	368.17340000	165.52600000
117	374.26780000	75.34940000
118	389.23640000	8.81450000
119	392.43450000	1.92120000
120	422.63490000	361.62940000
121	432.05410000	123.47750000
122	442.48130000	11.16040000
123	445.37480000	17.98290000
124	448.43110000	9.29170000
125	448.66790000	3.22490000
126	449.38110000	11.04680000
127	451.94200000	1.07320000
128	453.67250000	35.34020000
129	458.86740000	14.22490000
130	460.70210000	256.14140000
131	462.33060000	1.94890000
132	465.16570000	146.08750000
133	469.91080000	3.83990000
134	471.41550000	10.82270000
135	477.81150000	100.85090000
136	481.25550000	24.80810000

137	484.20030000	53.92150000
138	489.13980000	18.69300000
139	491.17290000	6.51220000
140	500.31140000	0.19570000
141	503.18400000	2.71080000
142	508.57740000	2.83860000
143	511.16940000	3.70340000
144	535.73260000	22.25700000
145	537.50760000	12.26540000
146	558.21290000	30.18420000
147	560.24120000	29.83110000
148	561.70850000	40.33790000
149	564.15000000	13.05700000
150	564.42350000	9.19330000
151	564.70990000	6.26500000
152	567.47660000	1.26420000
153	568.68290000	0.84790000
154	572.69820000	0.42680000
155	573.80050000	0.63100000
156	578.25720000	0.18440000
157	581.71820000	10.44300000
158	586.93960000	97.11790000
159	587.23760000	44.64750000
160	590.09720000	22.77360000
161	591.54350000	4.82860000
162	596.79400000	7.19510000
163	598.45350000	4.47190000
164	599.29580000	1.32110000
165	601.37850000	3.91770000
166	621.49860000	1.85870000
167	626.69470000	1.18110000
168	645.06780000	14.14320000
169	650.62590000	1.25330000
170	652.77960000	397.61220000
171	654.36650000	0.06680000
172	654.94930000	136.56560000
173	656.03000000	873.15210000
174	663.13350000	20.64220000
175	663.91010000	6.65920000
176	666.96030000	48.27970000
177	673.06510000	62.08750000
178	673.23690000	126.34880000
179	677.26610000	13.53150000
180	681.95570000	89.46190000
181	683.24120000	44.04390000
182	687.13040000	61.49820000
183	688.80010000	825.25150000
184	690.87000000	187.02710000

185	720.89440000	77.82160000
186	724.40520000	6.77430000
187	733.14150000	683.96380000
188	736.32880000	14.76790000
189	737.12600000	588.10990000
190	745.31190000	35.48270000
191	748.61730000	164.88190000
192	750.62420000	10.74890000
193	753.25010000	0.57560000
194	753.69670000	3.29350000
195	753.97130000	0.20380000
196	757.57200000	187.42520000
197	762.36350000	99.37060000
198	764.24610000	202.09120000
199	768.28420000	4.94710000
200	769.40220000	55.45930000
201	771.48020000	9.42540000
202	772.43930000	2.26940000
203	773.01240000	1.14680000
204	773.31060000	50.49780000
205	773.66750000	1.31320000
206	809.45350000	0.50640000
207	816.92240000	43.76650000
208	822.63920000	1.98480000
209	826.99700000	0.37290000
210	827.64660000	3.04810000
211	834.06810000	0.31180000
212	835.43430000	1.25870000
213	847.71390000	122.85900000
214	851.91670000	16.49570000
215	857.16440000	0.84890000
216	858.39690000	1.07600000
217	860.00690000	0.16260000
218	867.83630000	32.55620000
219	869.08850000	29.18720000
220	870.08270000	28.74540000
221	876.32070000	52.82450000
222	876.41040000	10.13510000
223	879.85720000	1.67450000
224	880.06930000	3.50680000
225	882.35480000	2.01940000
226	893.51770000	2.54840000
227	904.47090000	59.22960000
228	918.30510000	1221.43390000
229	921.03800000	75.93610000
230	921.41010000	75.83430000
231	922.55540000	45.29210000
232	926.06210000	22.02590000

233	927.64740000	0.76950000
234	930.71300000	2.95890000
235	931.40850000	298.89750000
236	950.90130000	5.03500000
237	953.29380000	1.65280000
238	954.59020000	1.42780000
239	955.02930000	1.22840000
240	957.20350000	4.51750000
241	958.18070000	7.77360000
242	992.15440000	0.01890000
243	992.74160000	1859.11690000
244	994.82780000	0.01320000
245	996.70380000	0.50760000
246	998.04410000	0.35960000
247	998.41210000	9.69370000
248	1000.19310000	0.37030000
249	1000.39030000	4.05540000
250	1000.66160000	4.34620000
251	1000.96740000	0.31140000
252	1001.73100000	2.43290000
253	1051.39740000	1.37090000
254	1056.52410000	4.09710000
255	1058.70260000	2.75940000
256	1060.00130000	0.64400000
257	1065.36800000	3.37380000
258	1065.80190000	21.18720000
259	1068.97120000	0.84290000
260	1071.79910000	4.98750000
261	1079.72830000	2.32620000
262	1079.84430000	0.70440000
263	1080.36440000	0.08540000
264	1080.90580000	0.78900000
265	1081.10840000	0.72430000
266	1084.00360000	17.77870000
267	1088.89720000	7.91950000
268	1089.09810000	4.32070000
269	1090.04190000	0.72630000
270	1090.32240000	1.54470000
271	1093.71720000	81.49620000
272	1102.77060000	63.07140000
273	1113.65020000	11.97470000
274	1123.97140000	225.83110000
275	1128.45550000	633.88090000
276	1131.74220000	58.15690000
277	1132.58500000	49.93350000
278	1133.23500000	128.87660000
279	1134.57470000	109.22440000
280	1135.78760000	22.45640000

281	1136.88250000	9.90440000
282	1137.61300000	51.48800000
283	1140.81040000	17.26080000
284	1144.85920000	29.71440000
285	1155.91280000	27.85990000
286	1158.90940000	345.90530000
287	1160.97480000	1118.17300000
288	1168.45300000	22.28130000
289	1173.24670000	5.64140000
290	1182.02360000	138.93180000
291	1193.90810000	0.31770000
292	1195.31720000	0.16560000
293	1199.35250000	37.51240000
294	1218.66290000	7.13840000
295	1225.19940000	7.93830000
296	1232.62140000	6.99610000
297	1234.65840000	234.78340000
298	1234.74820000	22.48430000
299	1236.61080000	13.64470000
300	1238.32540000	2.71600000
301	1256.62000000	9.36790000
302	1259.12720000	0.21590000
303	1260.50390000	0.20580000
304	1263.69480000	2.23320000
305	1265.22440000	73.75510000
306	1265.42510000	12.12440000
307	1265.51820000	12.08810000
308	1265.74470000	33.58750000
309	1269.50330000	186.22280000
310	1270.22830000	68.28130000
311	1291.38730000	6.67640000
312	1304.19150000	397.12450000
313	1307.77470000	236.15930000
314	1310.23330000	11.42610000
315	1311.28310000	82.23560000
316	1311.44760000	102.99280000
317	1311.88170000	125.29830000
318	1312.28250000	59.55760000
319	1315.66350000	0.77020000
320	1322.07040000	0.23870000
321	1326.70790000	25.50990000
322	1341.87730000	0.43410000
323	1345.71010000	0.39800000
324	1353.22590000	9.39560000
325	1360.72350000	4.81950000
326	1363.07430000	36.90710000
327	1379.09750000	0.44690000
328	1379.29590000	2.08860000

329	1380.54090000	0.46310000
330	1390.67200000	260.92100000
331	1397.10810000	15.16880000
332	1401.84430000	321.67560000
333	1423.34160000	89.36680000
334	1424.84530000	63.92790000
335	1425.10340000	43.07310000
336	1429.85280000	155.24110000
337	1433.74020000	33.16720000
338	1434.11700000	59.85140000
339	1434.30800000	64.41890000
340	1436.59520000	688.97150000
341	1442.03130000	228.58110000
342	1443.97700000	102.67160000
343	1445.92480000	55.34510000
344	1447.34000000	53.78260000
345	1461.19150000	1.06380000
346	1472.95070000	579.67030000
347	1474.82790000	2.63350000
348	1479.12790000	337.33590000
349	1479.48340000	95.45320000
350	1487.62280000	11.12410000
351	1490.56620000	422.58670000
352	1494.11850000	228.13280000
353	1494.60210000	0.98630000
354	1495.15000000	11.53090000
355	1501.08230000	29.68910000
356	1511.54060000	7.47510000
357	1522.40350000	199.89270000
358	1523.32180000	556.83620000
359	1524.61000000	215.68410000
360	1524.94290000	201.99310000
361	1525.51760000	18.75390000
362	1528.80490000	92.01240000
363	1532.20780000	309.44070000
364	1536.46270000	335.95000000
365	1536.84180000	64.13180000
366	1540.53750000	100.83990000
367	1550.35580000	14.78420000
368	1560.86730000	61.28790000
369	1577.02640000	24.08420000
370	1577.49300000	22.97530000
371	1578.77380000	109.95560000
372	1579.12500000	63.07320000
373	1579.64690000	21.54330000
374	1582.91900000	44.30380000
375	1587.41110000	0.37950000
376	1603.04480000	23.59220000

377	1610.44990000	0.61920000
378	1613.97280000	74.14600000
379	1614.76140000	59.35050000
380	1616.78980000	48.37060000
381	1617.36910000	7.91150000
382	1618.79480000	18.01590000
383	1621.11210000	23.63100000
384	1621.72890000	21.64610000
385	1624.17300000	0.68430000
386	1634.22350000	5.89850000
387	1639.45900000	12.22690000
388	1648.30770000	30.83720000
389	1649.28410000	9.11130000
390	1659.26730000	160.48650000
391	1660.04450000	53.94340000
392	1660.08680000	362.36440000
393	1660.35870000	19.08270000
394	1660.63730000	24.51410000
395	1662.02340000	108.42290000
396	1662.42230000	25.29340000
397	1663.88350000	19.21730000
398	1665.25860000	5.48640000
399	1666.01500000	98.96330000
400	1666.99060000	161.02020000
401	3158.72960000	154.09820000
402	3159.29770000	241.94900000
403	3167.63690000	183.84450000
404	3168.24050000	126.32340000
405	3191.14470000	6.66840000
406	3192.71800000	42.20990000
407	3193.56660000	33.72670000
408	3193.86030000	34.08790000
409	3197.29860000	6.64570000
410	3197.45970000	6.22780000
411	3198.32450000	5.87490000
412	3198.68100000	4.80970000
413	3201.31480000	20.81910000
414	3201.52250000	0.48020000
415	3202.69350000	8.86010000
416	3203.00870000	9.00220000
417	3203.13500000	5.49860000
418	3203.32110000	3.89100000
419	3204.67710000	32.80000000
420	3204.91150000	18.45220000
421	3214.58550000	1.50140000
422	3214.96530000	1.81950000
423	3218.42940000	2.15730000
424	3218.71500000	3.44100000

425	3226.97690000	17.57520000
426	3230.54720000	18.13350000
427	3230.81300000	4.21690000
428	3232.76000000	3.59670000
429	3233.54410000	4.21200000
430	3234.00850000	4.50910000
431	3235.79030000	3.59090000
432	3237.43610000	2.11120000
433	3239.07900000	2.35450000
434	3239.77530000	2.17280000
435	3240.13300000	3.77860000
436	3241.08900000	2.22610000
437	3527.42510000	1754.92370000
438	3535.77930000	2403.52240000
439	3612.49470000	1387.16810000
440	3612.74580000	66.85960000
441	3614.17330000	1481.43550000
442	3615.10390000	996.85880000
443	3642.59240000	506.86500000
444	3643.45410000	1419.04150000
445	3799.80370000	41.89890000
446	3799.95240000	38.46170000
447	3846.74030000	41.02800000
448	3846.90730000	177.16960000
449	3847.01280000	73.66310000
450	3847.38780000	133.06810000
451	3847.62120000	13.75570000
452	3847.71310000	179.69170000
453	3847.99150000	97.11880000
454	3848.93620000	97.11760000
455	3891.28250000	89.57770000
456	3892.17210000	90.18310000

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