**Supplementary Information**

The compounds Ru(CO)3(dpae) **1** and Ru(CO)2(PPh3)(dpae), **2**, were prepared and purified as described below. Appropriate IR (νCO), NMR and FAB mass spectral data are provided in Table S1. The dominant ligand arrangements of the three compounds are shown in Scheme S1.



Scheme S1. Structures of **1** and **2**.

**Preparation of Ru(CO)3(dpae) (1):** The compound Ru(CO)3(dpae) was prepared by adapting the literature procedure for the preparation of Ru(CO)3(dppe). In a typical experiment, Ru3(CO)12 (100 mg, 0.16 mmol), dpae (230 mg, 0.47 mmol) and benzene (25 mL) were place in a stainless steel autoclave (1). The autoclave was flushed with CO three times before being pressurised to 80 atm with CO and heated to 373 K for 16 hours. After cooling to room temperature, the excess pressure was released and the pale yellow solution reduced to half volume before cooling to 273 K for 4 hours; this gave Ru(CO)3(dpae) as a yellow microcrystalline material. The complex was washed with benzene and light petroleum and dried in vacuo. Yield: 420 mg (95%). Analysis C: 52.51% (51.88% Theoretical) and H 3.50% (3.60% Theoretical). The characterization data for this complex are given in Table S1.

**Preparation of Ru(CO)2(dpae)(PPh3) (2):** To prepare this complex, Ru(CO)3(PPh3)2 (100 mg, 0.14 mmol) and dpae (69 mg, 0.14 mmol) were refluxed in toluene (10 mL) under a continuous flow of N2 for 4 hours. The sample was then left to stand at room temperature for 12 hours, yielding a yellow microcrystalline precipitate of Ru(CO)2(PPh3)(dpae), which was then recrystallized from THF/pentane (1 : 2). Yield: 87 mg (68%). Analysis C: 68.10% (67.6% Theoretical) and H 4.93% (4.81% Theoretical). The characterization data for this compound are given in Table S1.

**Table S1.** Spectroscopic data for **1** and **2**. IR spectra were recorded in hexane, 13C NMR spectra in CD2Cl2 and all other NMR spectra in C6D6 at 295 K.

|  |  |  |
| --- | --- | --- |
| Compound | Ru(CO)3(dpae) (**1**) | Ru(CO)2(dpae)(PPh3) (**2**) |
| IR (νCO) / cm–1 | 2000 (m), 1970 (s), 1872 (m) | 2028 (s), 1896 (m) |
| 1H NMR | 1.92 (s)  7.10-7.30 (m)  7.65-7.75 (m) | 2.00 (s), 7.00 (m), 7.15 (m), 7.62 (m), 7.80 (m) |
| 31P {1H} NMR | N/A | 62.5 s |
| 13C {1H} NMR | 27.2 (CH2)  129.3 (meta-Ph)  130.4 (para-Ph)  132.0 (ortho-Ph)  137.8 (ipso-Ph)  211.4 (CO) | 30.1 (CH2)  127.9 (P-Ph, meta)  128.7 (As-Ph, meta)  129.3 (As-Ph, para)  129.5 (P- Ph, para)  132.4 (As-Ph, ortho)  132.9 (P-Ph, ortho)  134.0 (As-Ph, ipso)  134.8 (d, JCP = 24 Hz, P-Ph, ipso)  214.5 (br, CO) |

**NMR methods.** All NMR solvents (C6D6, THF-d8, and toluene-d8 Apollo Scientific) were dried and degassed prior to use. NMR measurements were made using NMR tubes fitted with J. Young valves and solvents were added by vacuum transfer. For the PHIP experiments, hydrogen enriched in the *para* spin state was prepared by cooling H2 to 18 K over a paramagnetic catalyst (activated charcoal) as described previously (2). All the NMR studies were carried out with sample concentrations of approximately 1 mM and NMR spectra were recorded on either a Bruker DMX-400 or DRX-400 spectrometer with 1H at 400.1, 31P at 161.9 and 13C at 100.0 MHz, respectively. 1H NMR chemical shifts are reported in ppm relative to residual 1H signals in the deuterated solvents (toluene-d7,  2.13 and C6D6, 7.16), 13C NMR shifts are relative to toluene-d8,  21.3 and C6D6,  128.4 with 31P NMR shifts in ppm downfield of an external 85% solution of phosphoric acid. Modified COSY, HMQC and EXSY pulse sequences were used as previously described (3). 1H EXSY spectra used to obtain kinetic data were processed using literature methods and analysed as described (4).

**In-situ photolysis.** This was achieved using a modified NMR probe, as described previously (5). A Kimmon IK3202R-D 325 nm He–Cd 27 mW continuous wave (CW) laser was used as the light source.

In the case of complex **1**, the IR data are directly comparable to those of the known phosphine analogue Ru(CO)3(dppe), which exhibited three ν(CO) bands at 1997, 1942 and 1885 cm–1. The observation of only one 13C signal for the three distinct CO groups in the proposed structure indicates that rapid exchange of the carbonyl ligands occurs at 295 K, giving a time-averaged NMR signal for the associated 13C nuclei. Such processes are common in mononuclear ruthenium(0) carbonyl complexes.1 For compound **2**, only two bands were observed in the carbonyl region of the IR spectrum, and a single 31P resonance was detected, which was unaffected by cooling to 183 K. Compound **2** therefore exists predominantly in a geometrical arrangement that matches that of **1** illustrated in Scheme 2. The 13C NMR for **2** data also supports this deduction.

|  |  |  |  |
| --- | --- | --- | --- |
| **Table S2.** Key NMR data for the complexes detected in this study by PHIP. | | | |
| Compound, solvent | *δ 1H* | *δ 31P* | *δ 13C* |
| **3**,C6D6 | –7.21 (H, d, JHH = –5 Hz)  –7.61 (H d, JHH = –5 Hz, JHC = 16 Hz)  2.05 and 1.88 (CH2)  7.02 – 7.54 (m, Ph) |  | 26.2 and 26.9 (CH2)  130.9 (*meta* -Ph)  131.7 (*para*-Ph)  132.2 (*ortho* -Ph)  133.2 (*ipso* -Ph)  202.2 (CO - Ca)  187.1 (CO - Cb) |
| **4a**, C6D6 | –3.48 and –5.39 |  |  |
| **4b**, THF-*d*8 | –3.95 and –6.21 |  |  |
| **4c**, toluene-*d*8 | –3.48 and –5.39 |  |  |
| **5**, toluene-*d*8 | –7.0 (d, JHP = 22 Hz) | 59.7 |  |
| **6**, toluene-*d*8 | –6.55 (JPH = 26 Hz)  –8.47 (JPH = 30 Hz)where JHH is -9.3 Hz | 57.6 |  |
| **7a**, toluene-*d*8 | –7.52 (H, dd, JHP = 21 Hz, JHH = –5 Hz)  –8.22 (H, dd, JHP = 24 Hz, JHH = –5 Hz) | 66.2 |  |
| **7b**, toluene-*d*8 | –7.74 (H, dd, JHP = 17 Hz, JHH = –5 Hz)  –9.13 (H, dd, JHP = 66 Hz, JHH = –5 Hz) | 49.8 |  |
| **8**, toluene-*d*8 | 2.88 (H, d, JHH = 15.3 Hz)  2.64 (H, d, JHH = 15.3 Hz) |  | 37.1  38.5 |
| **9a**, toluene-*d*8 | –6.26 (d, JHH = +2.9 Hz)  4.04 (CHPh, m, JHH = 2.9 Hz)  3.98, 4.26 (CH2Ph) |  | 26.8 (CH)  52.6 (CH2) |
| **9b**, toluene-*d*8 | –11.34 (d, JHH = + 5.6 Hz)  3.18 (CHPh)  4.19, 4.06 (CH2Ph) |  |  |
| **10**, toluene-*d*8 | 6.40 (Ha, dd, JHC = 166 Hz, JHH = +8 Hz)  1.56 (Hb, dd, JHC = 152 Hz, JHH = +8 Hz) |  | 64.2 (CH=, bound)  45.0 (CH=, free) |

**Thermal reactions of Ru(CO)3(dpae),** **1, with *p*-H2: Characterization of 3**.

When this spectrum was acquired with a large number of transients, the resonance at δ–7.61 exhibited visible 13C satellites from which a *trans* JHC coupling of 16 Hz could be deduced. The resonance for the carbonyl carbon providing this splitting was detected at δ 202.2 via a 1H-13C HMQC experiment. Upon optimization of the HMQC experiment for a *cis* 1H-13C arrangement, a second carbonyl carbon signal was located at δ 187.1, although the associated 2*J*HC coupling was now hidden within the line width of the hydride signal. The hydride resonating at δ –7.21 also connected with each of these carbonyl environments, but the JHCcoupling was again hidden within the line width of the hydride resonance. Hence, a *cis* arrangement between the hydride ligand giving rise to the δ –7.21 signal and both carbonyl groups can be deduced, i.e. this hydride ligand is *trans* to arsine.

**Table S3.** Rates and activation parameters determined in toluene-*d*8 solution for hydride site exchange in **3** and H2 elimination in **7a**.

|  |  |  |  |
| --- | --- | --- | --- |
| Temp (K) | Rate (/s) **3** | Temp (K) | Rate (/s) **7a** |
| 308 | 0.32 | 338 | 0.14 |
| 313 | 0.77 | 343 | 0.42 |
| 318 | 1.42 | 348 | 0.60 |
| 323 | 2.03 | 353 | 1.00 |
| 328 | 3.70 | 363 | 2.73 |
| ΔH≠ kJ mol-1 | 94 ± 6 | ΔH≠ kJ mol-1 | 109 ± 12 |
| ΔS≠ J K-1 mol-1 | 55 ± 20 | ΔS≠ J K-1 mol-1 | 65 ± 34 |

**Further evidence of the identity of 5 and 6.**

The addition of either CO or dpae to solutions of **2** and *p*-H2 quenches the observation of the solvent complexes Rh(H)2(CO)(dpae)(sol) at 295 K. Signals for **3** are, however, clearly visible in the associated NMR spectra recorded between 318 K and 335 K. Weak signals for **5** and **6** appear at 338 K. Addition of CO reduces the size of the signals for **6** thereby suggesting that they arise fromRu(H)2(CO)(1-dpae)2(PPh3). The characteristics of **5** require it to have a (H)2Ru(CO)2 core, where coupling to a single phosphine provides the 22 Hz splitting. The remaining ligand is 1-dpae. These hydride signals of **6** both couple to a single *cis*-phosphine ligand and appear at  -6.55 (JPH = 26 Hz) and  -8.47 (JPH = 30 Hz)where JHH is -9.3 Hz. In the corresponding 2D 1H-31P HMQC experiment, the phosphine resonance of **6** was locatedat 57.6 while that of **5** proved toappear at  59.7.

It should be noted that Ru(H)2(CO)(PPh3)2 yields a hydride signal with similar spectral characteristics to **5** at  -6.31, but contains a 31P centre that resonates at  56.5. This known material is observed when PPh3 is added to these samples.

When 348 K is reached the signals for **3** are again dominant, with those for **6** appearing and those for **7a** vanishing.The ratio of the enhanced hydride signals for **3** : **6** at 348 K in the absence of CO was 1 : 0.02, and with 2 atm. CO and 1 atm. p-H2 became 1 : 0.006 while when a 5 fold excess of dpae was added they became 1 : 0.13. This confirms that the proportion of **6** is dramatically increased by the addition of dpae to the solution and thereby suggests that a suitable structure for **6** would be *cis*-Ru(H)2(CO)(1-dpae)2(PPh3). These data suggest that the arsine ligand can unhook at temperatures in excess of 348 K. The identity of **5** as Ru(H)2(CO)(1-dpae)(PPh3)2 is consistent with this deduction; both **5** and **6** can be formed from **2** via the common 16-electron intermediate Ru(H)2(CO)(1-dpae)(PPh3).

**Reaction in d8-THF**

It should be noted, that in d8-THF reaction, the signals for **4b** disappear at 318 K where those for **3** begin to dominate. Weak signals for the species **7a** (at δ –8.16 and –9.01) and **7b** (at δ –8.5 and –9.94) are also visible in these spectra at this point. These observations confirm that there is a sizeable solvent dependence on the initial H2 addition reaction; these species are identified in the photochemical work where they are dominant. Upon warming to 353 K the signals for **7**. Signals for **3** remain,and very weak signals due to **5** and **6**now appearing. When this sample is cooled back down to 298 K, only signals for **3** (93 %) and **7a** (7 %) remain visible.

**Formation of 7.**

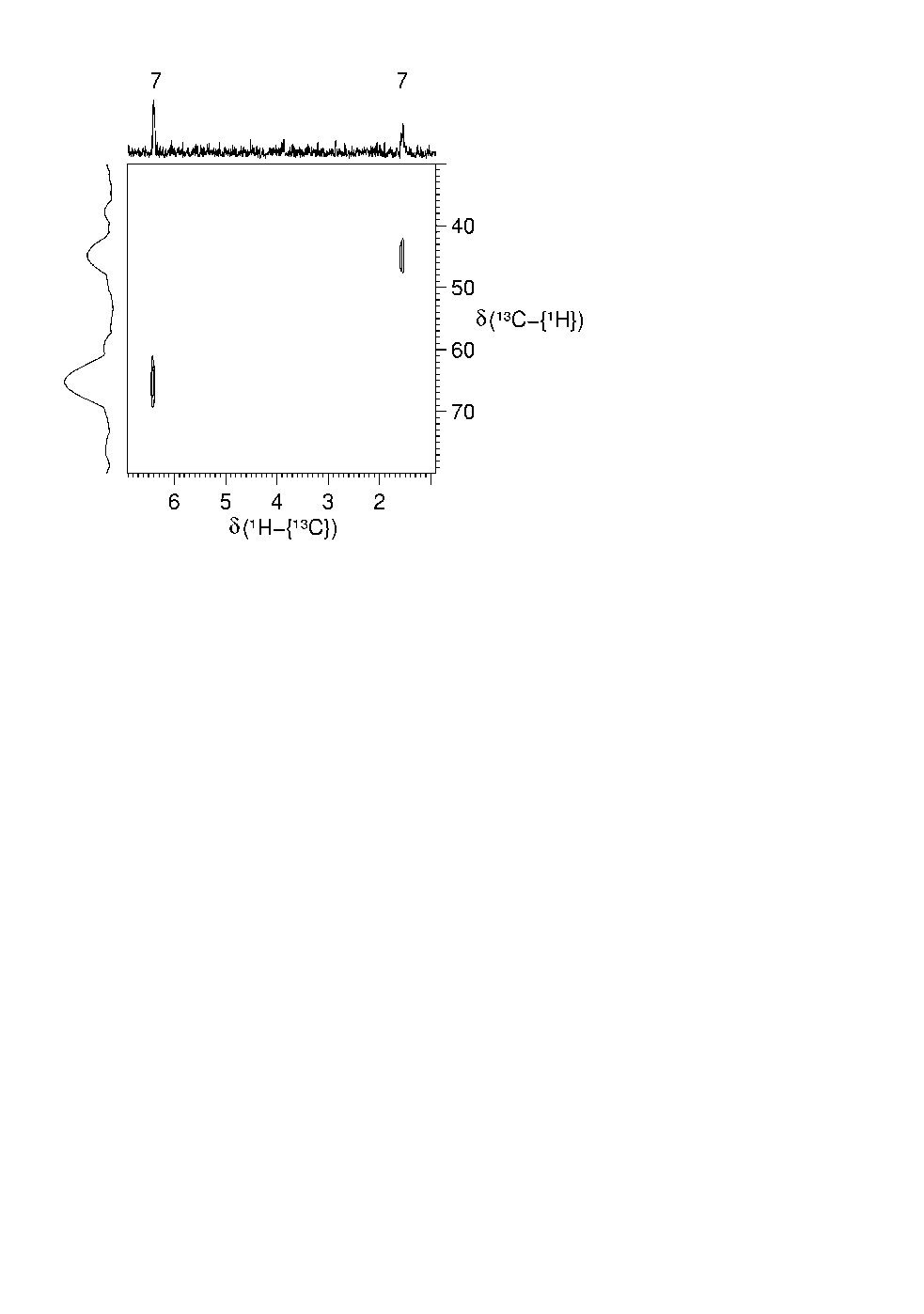
No isomer of **7**, where the hydride ligands both lie *trans* to the NMR silent arsenic centre was observed in these experiments. We note, however, that such a species would not be expected to show any PHIP enhancement and hence its signals would not be enhanced.

**Formation of 10.**

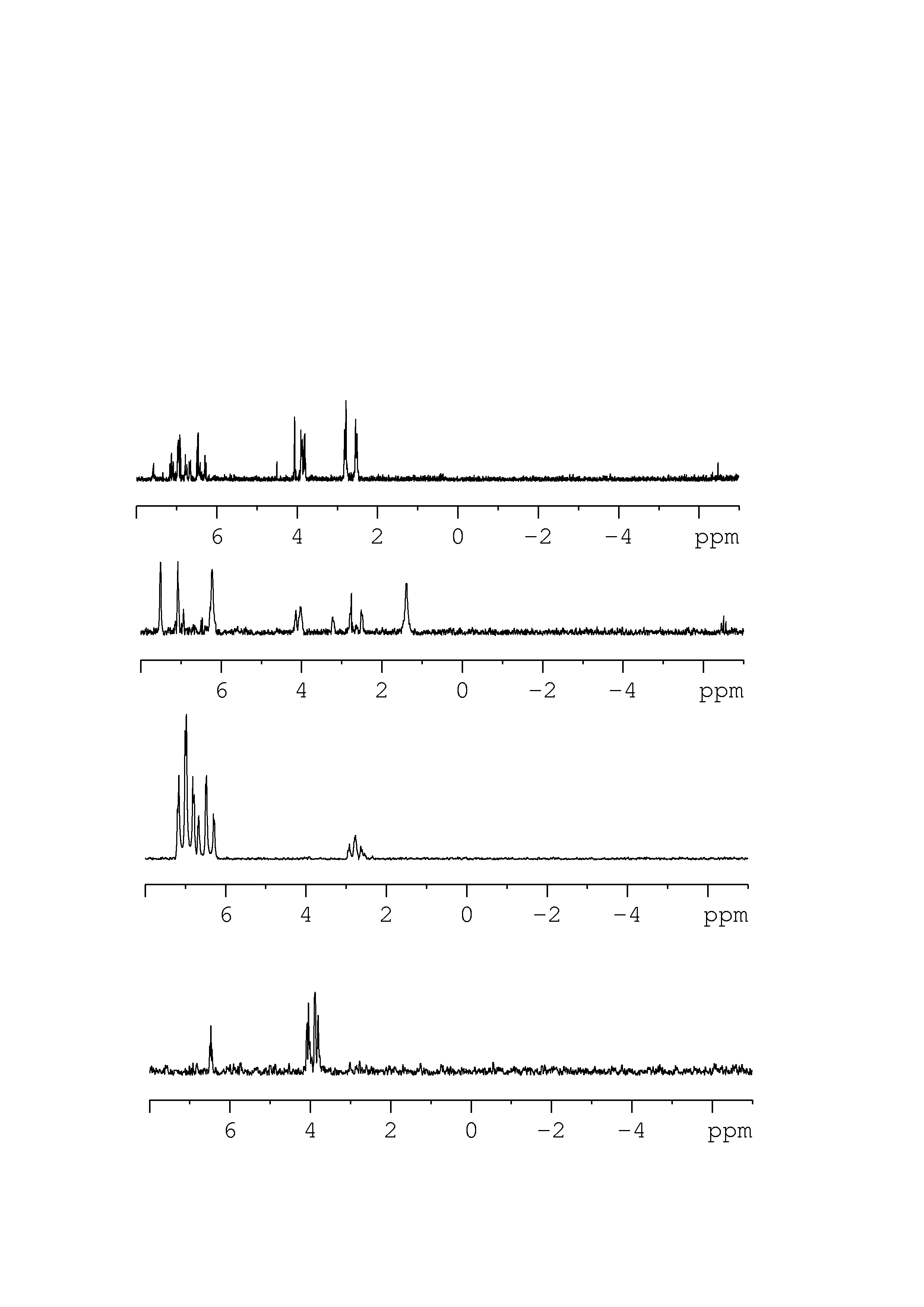
We concluded that **10** is 18 electron because it is seen in toluene-d8, THF-d8 and cyclohexane-d12, and the two corresponding PHIP polarised resonances always have essentially identical chemical shifts. Figure S1 details a HMQC measurement used to locate the two alkene like 13C signals for **10**.

It should be noted that the CO ligands of **10** could not be detected by NMR spectroscopy directly because of the need for *p*-H2 enhancement to observe this species. 1H-13C HMQC experiments, which attempted to locate these ligands via the associated weak three-bond coupling from **10**-Hb were unsuccessful even with a 13CO enriched sample.

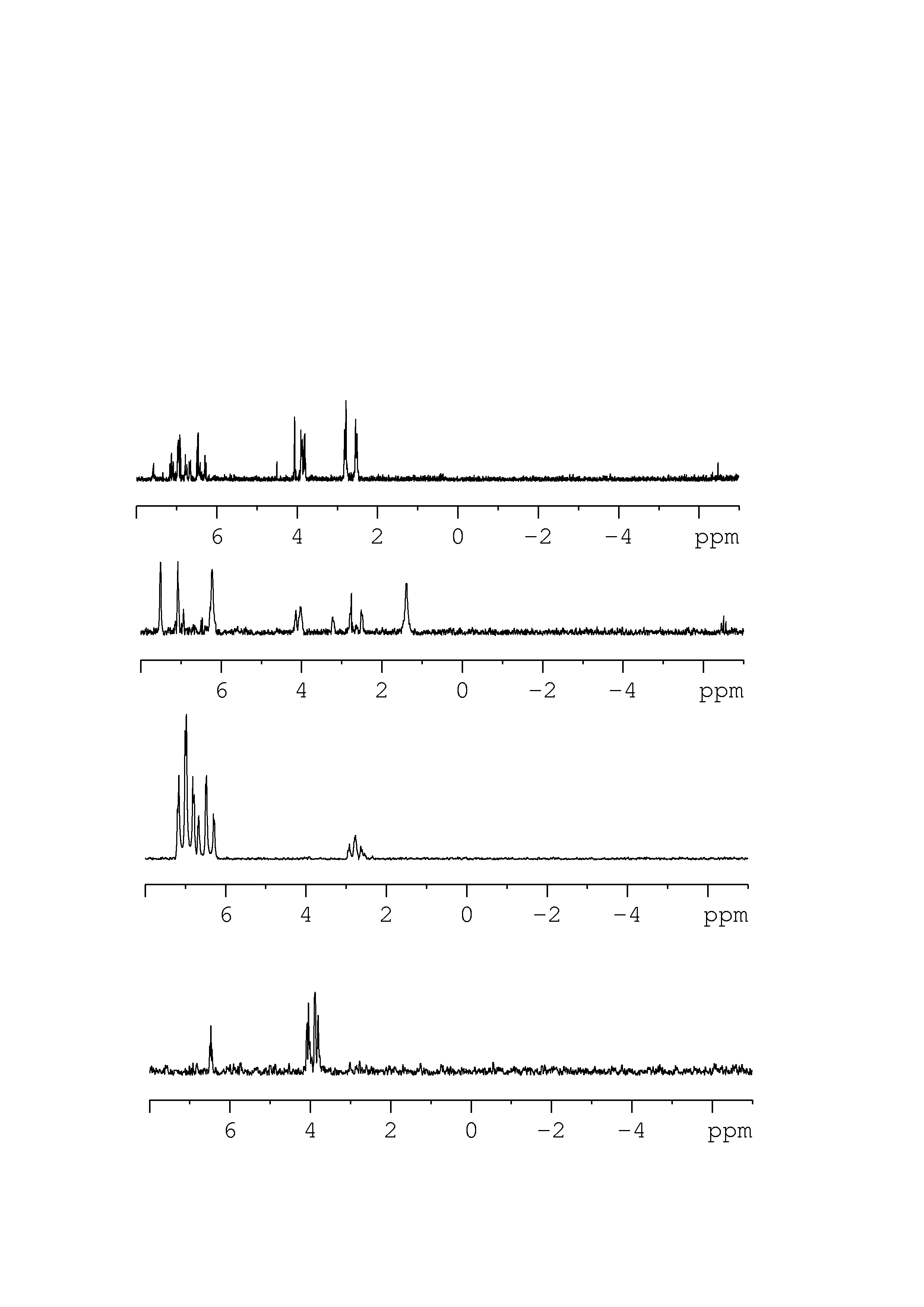
A series of EXSY experiments were carried out at 295 K in the presence of UV irradiation, with selective excitation of each of the two enhanced resonances of **10**. No magnetisation transfer was observed from these sites and consequently we conclude that **10** is inert on the NMR time-scale at 295 K. We also note that no signals could be seen for **10** upon cooling the sample below 290 K, or warming it above 305 K.



**Figure S1**. 1H-13C HMQC NMR spectrum obtained during irradiation of **1** at 295 K with *p*-H2 and Ph-13C≡C-Ph-d10 in C6D6 showing signals for **10.**

****

**Figure S2**. 1H-NMR spectrum showing how the hydrogenation products *trans-* and *cis* stilbene and diphenlyethane become hyperpolarized when their C2-13C centres are labelled.

****

**Figure S3.** Under irradiation at 295 K, hydrogenation of C6D6CCC6D5 by Ru(CO)2(dpae)(PPh3) leads to a number of hyperpolarized signals (attributed in the manuscript).

**Thermally initiated hydrogenation by 1 and 2 in the presence of CO, H2 and diphenylacetylene.**

Repeating these experiments with **1** or **2,** the alkyne, CO and *p*-H2 under thermal conditions results in the quenching of all the enhanced signals except for those of **3** and the suppression of hydrogenation catalysis.

**1,2-diphenylethane.**

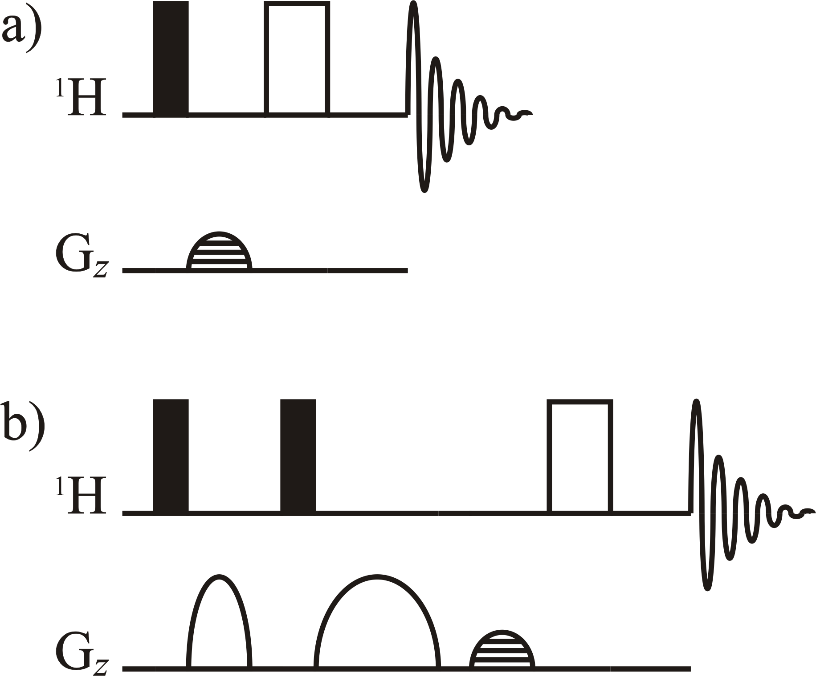
It should also be noted that the ethane bridge proton resonance of 1,2-diphenylethane, is observed atδ2.88 and can be obscured by signals for **8**. This signal becomes much stronger when a sample of Ph-13C≡C-Ph-d10 is utilized as the catalytic substrate, as evidenced by the OPSY spectroscopy. The 13CH2 signal for this material was located atδ 38.0 by employing an HMQC methodology and matches with that obtained separately from an authentic sample of 1,2-diphenyl ethane.

**Methods for Chemical Shift Imaging (CSI) and OPSY-Filtered CSI experiments for simultaneous monitoring of thermal and photochemically initiated reactions.**

In order to measure chemical shift information and position within a sample at the same time the technique of Chemical Shift Imaging (CSI) was employed. This approach uses an incrementing magnetic field gradient, here applied along the Z axis, to change the phase of the detected signals. Subsequent Fourier transformation of the 2-dimensional data gives a chemical shift resolved NMR spectrum in F2 and position in F1.

The pulse sequence used for collection of this data is shown in Figure S4a. The maximum gradient strength used is set according to the number of increments and the length and shape of the gradient pulse. For 1H experiments, we used a 1 *ms* Gaussian gradient pulse with a maximum strength of 2.95 and 5.99 *gauss* / *cm* respectively for the 32 and 64 data point measurements in the second dimension. This reflected a field of view of approximately 2 cm.

Modification of this standard sequence to include the OPSY filter was achieved by replacement of the initial excitation pulse with a pulse-gradient-pulse-gradient block typical of the OPSY experiment. A gradient ratio 1:2 was used here to achieve the double quantum coherence selection associated with the *para*hydrogen derived signals in order to remove all other signals. The associated pulse sequence is shown in Figure S4b. The phase encoding gradient used the same number of increments and gradient strengths as that of the standard 1H-CSI experiment described above.



**Figure S4**. Pulse sequences for (a) the spatial phase-encoding of chemical shift in one dimension and (b) the OPSY-filtered equivalent experiment.

The approaches described above were used to obtain the data presented in Figure S5 and Figure 4 which detail the differentiation between signal strengths for the indicated products as a function of thermal and photochemical conditions. Consequently, the difference in signal intensities can be used to identify the route by which with the products form and thereby differentiate the underlying reaction pathways.

**Figure S5**. The photochemical formation of the hydride products is monitored in-situ by plotting signal intensity as a function of both chemical shift and position within the NMR tube at 333 K for **2** with the distinction between thermal and photochemical reaction pathways being illustrated.



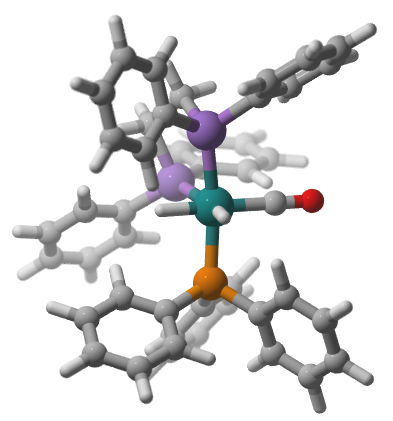
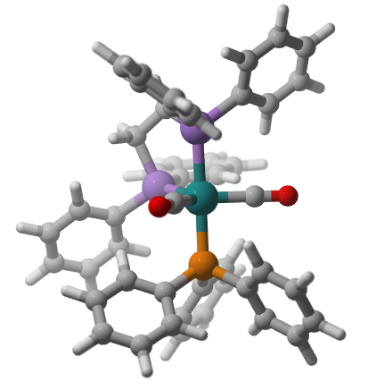
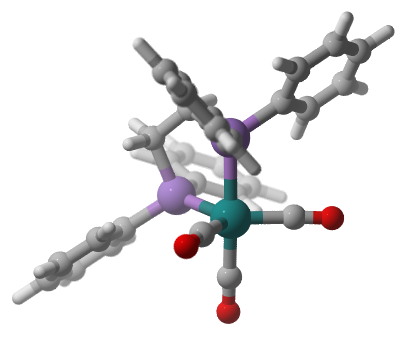
**Figure S6**. OPSY NMR spectrum at 358 K during diphenyl acetylene hydrogenation by **1** over the region 4.8 – 1 ppm.

**Theoretical Modelling**

The compounds Ru(CO)3(dpae) (**1**) and Ru(CO)2(PPh3)(dpae), **2**, were modeled by performing DFT calculations where the phenyl substituents of the arsine and phosphine ligands are included.

Two isomers of Ru(CO)3(dpae), **1**, were considered. When the fac- and mer- trigonal bipyramidal Ru(CO)3(dpae) initial structures were freely optimized, both converged to the same slightly distorted trigonal bipyramidal geometry with the three CO ligands coordinated *fac* to the metal centre (see Chart S1).

Similarly, two minima were located corresponding to two isomers of Ru(CO)2(PPh3)(dpae) (**eq-2 and ax-2**). In these, the CO and PPh3 ligands are coordinated in a “fac-“ fashion with the bis-arsine ligand occupying the remaining two sites of the trigonal bipyramidal coordination environment of Ru. The PPh3 ligand is coordinated either in one of the equatorial (**eq-2**) or axial positions (**ax-2**). (Two more isomers, with the arsine ligand coordinated in the equatorial plane, and the CO ligands coordinated *cis* and *trans* to each other respectively were considered but the initial structures converged to the geometries previously described).



**ChartS1.** DFT-optimized structures for complexes **1**, **ax\_2** and **7a**.

In the second set of two isomers considered, the CO and PPh3 ligands are coordinated in a facial fashion with the PPh3 ligand coordinated in the equatorial plane (**eq-2**) and the remaining axial position (**ax-2**) in each case. The equatorial isomer is predicted to be 9.6 kJ mol-1 less stable than the axial isomer, in agreement with experimental evidence. This difference is consistent with the predicted orbital interactions; good π–acceptors are preferred in the equatorial positions in trigonal bipyramidal geometries. This results in CO being coordinated preferentially in the equatorial position and the PPh3 ligand in the axial site.

In order to study the formation of the hydride complexes **3** and **7,** restricted (closed shell) DFT calculations were performed to optimize the 16e complexes that result from CO and phosphine dissociation from **1** and **2** respectively.

Dissociation of one of the equatorial COs in **1** leads to a 16e complex (**SP4**-**1’**), which exhibits a distorted square planar geometry with an As-Ru-As angle of 82.38° and a CO-Ru-CO angle of 90.90°. The formation of **SP4**-**1’** from **1** is endothermic by 94.1 kJ mol-1. Dissociation of the axial phosphine in **2** results in complex (**TP-1’**) where the CO ligands are mutually *trans* and lie approximately perpendicular to the plane defined by the As and Ru atoms. The formation of this complex is also endothermic, but by 176.9 kJ mol-1. This result indicates that dissociation of one of the equatorial CO ligands in **1** will be more facile than phosphine loss in **2** which correlates nicely with the experimental observations that higher reaction temperatures are needed to observe dihydride **3** than **7** by NMR under thermal exchange.

When a continuum solvent model (IEFPCM) is used to probe the effect of toluene (single point calculations from the gas phase-optimized structures), the energies required to remove one equatorial or axial CO from **1** are 92.5 and 170.3 kJ mol-1, respectively. This means that solvation stabilizes the products, respectively, by just 1.6 and 6.6 kJ mol-1.

Dihydrogen addition to the distorted square planar complex **SP4-1’** yields *cis-cis*-Ru(H)2(CO)2(dpae) (***cis-cis*-3**) with an energy return of 65.8 kJ mol-1. According to the calculations, the overall formation of the ***cis-cis***-**3** form **1** is therefore endothermic by 28.3 kJ/mol.

The alternative isomer resulting from dihydrogen addition to TP\_1’ results in a complex where both hydride ligands lie opposite to dpae (***trans-cis*-3**). This isomer is 9.0 kJ mol-1 higher in energy than ***cis-cis*-3**. The corresponding *trans-cis*- Ru(H)2(CO)2(dpae) isomer will not be detected by PHIP-MNR due to its magnetically equivalent hydride ligands.

Dissociation of any of the CO ligands from **2** ultimately gives the same 16e distorted four coordinate complex Ru(CO)(PPh3)(dpae) (**SP4-2’**). The formation of this complex via ***ax*** or ***eq*** ligand loss is endothermic by 112.7 and 105.7 kJ mol-1 respectively. PPh3 dissociation from **2** yields **TP-1’** (ΔE = 115.4 kJ mol-1). The facile rearrangement of both CO loss products results in the generation of ***cis-cis*-3** with H2 in a process that is endothermic by 22.0 kJ mol-1. These results agree with the experimental observations that **3** is preferred over **7** at higher temperatures.

Pairwise hydrogen oxidative addition along the As-Ru-CO axis of **SP4-2’** gives ***ax-cis-***Ru(CO)(PPh3)(dpae)(H)2, **7a**, while addition to the As-CO-P axis yields ***eq-cis-***Ru(CO)(PPh3)(dpae)(H)2, **7b**. The latter isomer, with the PPh3 ligand in an equatorial position, is less stable by 16.8 kJ mol-1. This is in agreement with the **7a** being more stable than **7b** in solution. It islikely that steric repulsion between the phenyl substituents of the arsine and phosphine ligands play a role in this. The overall formation of these species from **2** is predicted to be exothermic by 81.3 and 64.5 kJ mol-1 respectively in agreement with the ready detection of both **7a** and **7b** in the photochemical reaction of **2** with H2.

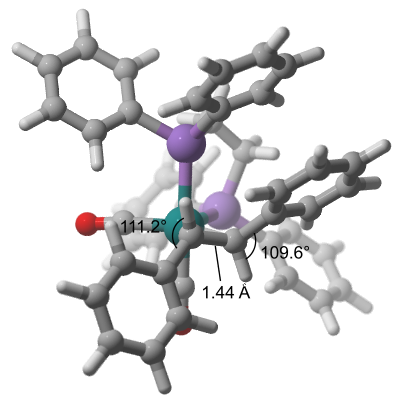
The geometry of the alkene complex **8**, Ru(CO)2(dpae)(PhCH=CHPh), **8-*trans***, has been optimized for *trans*-stilbene. In this geometry, the alkene ligand is η2-coordinated to the metal centre in the equatorial plane of the complex. The C=C distance in the coordinated ethylene is 1.441 Å. The C=C-H angles are close to 115°, while the H-C-Ph angles are 111.2° and 109.6° The difference in the H-C-Ph bond angles suggests some steric repulsion from the phenyl rings in the dpae ligand relative to that in the *trans*-stilbene ligand as illustrated in Figure S5. This suggests marked sp3 character in the C atoms of the *trans*-stilbene double bond in agreement with the experimentally determined value of JHC.

The structure of **9** was also evaluated. The relative stabilities of the four possible forms are detailed in Scheme S1.

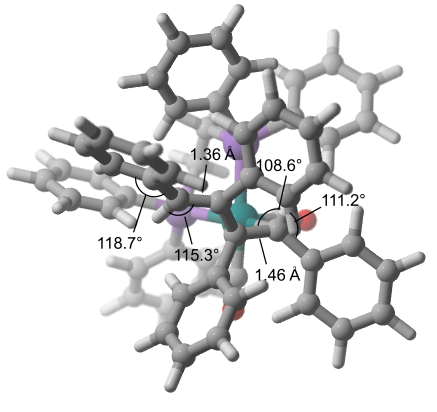


Scheme S1. Relative energies of Ru(H)(CHPhCH2Ph)(CO)2(dpae).

A similar analysis was applied to diene complex, **10**. This calculation shows that the geometry of the double bond of the diene ligand coordinated η2 to the Ru centre is very similar to that calculated for **8-*trans***, with a C=C bond length of 1.458 Å and C=C-H and H-C-Ph angles of 111.2 and 108.6° respectively. The remaining non-coordinated double bond has a shorter C=C distance of 1.36 Å and C=C-H and H-C-Ph angles of 115.3° and 113.1° respectively. This suggests a larger degree of sp2 character is present for the carbon centres forming the non-coordinated C=C double bond. The predictions again agree with the experimental values of JHC measured by NMR. This complex is illustrated in Figure S6.



**Figure S5**. **8\_*trans*** showing structural parameters for the η2 alkene coordination.



**Figure S6**. **10** showing structural parameters for the η2 alkene coordination.

Computational details.

All calculations were performed using the GAUSSIAN 09 series of programs (Frisch 2010) using the PBE0 functional (Perdew 1996+1997, Adamo 1999). An effective core potential and its associated LANL2TZ basis set (Hay 1985, Roy 2008) with additional f polarisation functions (Ehlers 1993) was used for the ruthenium atoms. All remaining atoms were assigned to the def2-SVP basis sets.(Schafer 1992, Weigend 2005) The calculations here employed the full ligand set to correctly account for steric interactions.. The structures of the reactants, intermediates, transition states, and products were fully optimized in gas phase without any symmetry restriction. Frequency calculations were performed on all optimized structures at the same level of theory to characterize the stationary points and the transitions states, as well as for the calculation of gas-phase zero-point energies (ZPE), enthalpies (H), entropies (S), and Gibbs energies (G) at 298.15 K..Single point calculations with the PBE0 functional along with the same LANL2TZ basis set for ruthenium were then used with the larger def2-TZVPP basis sets (Schafer 1992, Weigend 2005) to allow more accurate energies to be obtained. All energetics were counterpoise corrected for the effects of basis set superposition error.(Boys 1970, Simon 1996). Solvent effects were tested with the inclusion of the IEFPCM model into the single point calculations (Mennucci 1997, Cances 1997+1998).

**Tables of the optimized geometries (Cartesian coordinates, in Angstroms) for the calculated species.**

Energies (in a.u.) in parenthesis: (Energy in gas phase)

**Table S2. Ru(CO)3(dpae) (1)** (-5909.333188)

Ru 0.033520000 -0.374805000 1.458538000

C -0.417861000 -2.233714000 1.586095000

O -0.693714000 -3.340610000 1.750790000

C -0.834052000 0.937200000 2.546547000

O -1.380044000 1.664934000 3.256137000

C 1.430022000 -0.539304000 2.729640000

O 2.284628000 -0.632765000 3.490645000

As 1.661746000 -0.004711000 -0.352921000

As -1.610615000 0.008573000 -0.356949000

C -0.625950000 0.422613000 -2.018923000

C 0.716537000 -0.277615000 -2.065350000

H -0.498060000 1.516693000 -1.993486000

H -1.254778000 0.197802000 -2.893495000

H 1.339526000 0.090588000 -2.894899000

H 0.607582000 -1.367398000 -2.182546000

C -2.824251000 1.528729000 -0.292898000

C -4.176203000 1.418868000 -0.630613000

C -2.306148000 2.771568000 0.089328000

C -4.999740000 2.544477000 -0.589933000

H -4.593517000 0.452583000 -0.924238000

C -3.130181000 3.894349000 0.121227000

H -1.253450000 2.861312000 0.374339000

C -4.478869000 3.781828000 -0.216565000

H -6.056730000 2.450453000 -0.851357000

H -2.717972000 4.860504000 0.422249000

H -5.126661000 4.661305000 -0.183267000

C -2.818491000 -1.443904000 -0.821865000

C -3.043003000 -1.868884000 -2.135095000

C -3.489746000 -2.083057000 0.228057000

C -3.924558000 -2.919014000 -2.394187000

H -2.533637000 -1.388167000 -2.973318000

C -4.377675000 -3.124225000 -0.033650000

H -3.309482000 -1.769754000 1.260456000

C -4.594484000 -3.545812000 -1.345250000

H -4.087473000 -3.247306000 -3.423760000

H -4.894850000 -3.615071000 0.794245000

H -5.284302000 -4.368257000 -1.549782000

C 2.458460000 1.756618000 -0.636270000

C 3.148706000 2.098559000 -1.806682000

C 2.292909000 2.716271000 0.365911000

C 3.665448000 3.383324000 -1.967115000

H 3.295278000 1.360102000 -2.600304000

C 2.816341000 4.000217000 0.207545000

H 1.737854000 2.445660000 1.270799000

C 3.501225000 4.334666000 -0.959136000

H 4.200980000 3.643312000 -2.883816000

H 2.684844000 4.742001000 0.999295000

H 3.908417000 5.340860000 -1.086518000

C 3.179551000 -1.208679000 -0.558599000

C 4.505128000 -0.772239000 -0.640028000

C 2.907785000 -2.582675000 -0.562685000

C 5.542712000 -1.700012000 -0.745541000

H 4.736766000 0.295115000 -0.615397000

C 3.944253000 -3.505444000 -0.680612000

H 1.877683000 -2.935581000 -0.450816000

C 5.264951000 -3.065025000 -0.773196000

H 6.576372000 -1.349587000 -0.803348000

H 3.719988000 -4.574997000 -0.686512000

H 6.079545000 -3.788744000 -0.855976000

**Table S3. axial-Ru(CO)2(PPh3)(dpae) (ax\_2)** (-6831.680287)

Ru 0.349436000 -0.603020000 -0.157846000

C 0.448265000 -1.887418000 1.240449000

O 0.527897000 -2.730668000 2.029605000

C 0.724856000 -0.934060000 -1.986761000

O 0.969200000 -1.244767000 -3.077839000

As -0.112772000 1.688500000 0.656594000

As 2.670816000 0.034945000 0.277737000

C 2.727407000 1.908056000 0.906789000

C 1.480850000 2.259045000 1.692017000

H 2.790679000 2.504999000 -0.017378000

H 3.657684000 2.087785000 1.467047000

H 1.411209000 3.339407000 1.893409000

H 1.454689000 1.722256000 2.653075000

C 4.026968000 0.133174000 -1.123026000

C 5.349019000 -0.268366000 -0.904880000

C 3.670370000 0.666591000 -2.366427000

C 6.298960000 -0.137575000 -1.918256000

H 5.643845000 -0.688168000 0.059753000

C 4.622233000 0.800795000 -3.375192000

H 2.638617000 0.972499000 -2.554194000

C 5.938377000 0.397057000 -3.153641000

H 7.328481000 -0.457410000 -1.738132000

H 4.329995000 1.214954000 -4.343280000

H 6.683276000 0.495994000 -3.947207000

C 3.630951000 -0.966721000 1.643529000

C 4.174348000 -0.377404000 2.788702000

C 3.755284000 -2.350069000 1.463384000

C 4.837159000 -1.158410000 3.737035000

H 4.086458000 0.698420000 2.957592000

C 4.426889000 -3.126355000 2.404347000

H 3.311926000 -2.825148000 0.583307000

C 4.968416000 -2.531820000 3.544319000

H 5.253573000 -0.687157000 4.630939000

H 4.517814000 -4.204485000 2.251550000

H 5.488416000 -3.142202000 4.286771000

C -0.163663000 3.212189000 -0.587389000

C -0.473061000 4.513991000 -0.174044000

C 0.194217000 2.988537000 -1.918505000

C -0.425860000 5.570355000 -1.082749000

H -0.761810000 4.707869000 0.863122000

C 0.245942000 4.045562000 -2.828677000

H 0.428458000 1.964990000 -2.232480000

C -0.066455000 5.338129000 -2.411378000

H -0.671859000 6.582719000 -0.751521000

H 0.528778000 3.856759000 -3.867654000

H -0.030639000 6.168091000 -3.121681000

C -1.546303000 2.208352000 1.878305000

C -2.782147000 2.624514000 1.365777000

C -1.403008000 2.064045000 3.264259000

C -3.846135000 2.900405000 2.223407000

H -2.920751000 2.733249000 0.286381000

C -2.467768000 2.344244000 4.120815000

H -0.456937000 1.721332000 3.690860000

C -3.692407000 2.763321000 3.602441000

H -4.803998000 3.221529000 1.806391000

H -2.337364000 2.233548000 5.200494000

H -4.527321000 2.980506000 4.273271000

P -1.863970000 -1.291097000 -0.528437000

C -3.058023000 -0.017253000 -1.127077000

C -4.364194000 0.088579000 -0.634111000

C -2.634314000 0.869861000 -2.125076000

C -5.227064000 1.067538000 -1.128694000

H -4.709934000 -0.593229000 0.145720000

C -3.497344000 1.844891000 -2.619828000

H -1.612670000 0.797240000 -2.504809000

C -4.796462000 1.947763000 -2.120072000

H -6.242855000 1.141776000 -0.731964000

H -3.147891000 2.534402000 -3.392117000

H -5.472351000 2.716377000 -2.503505000

C -2.060839000 -2.621014000 -1.790447000

C -1.114448000 -3.653575000 -1.823792000

C -3.136437000 -2.653190000 -2.685941000

C -1.249885000 -4.704295000 -2.727743000

H -0.259064000 -3.614695000 -1.143608000

C -3.263166000 -3.701119000 -3.597802000

H -3.880959000 -1.854096000 -2.676548000

C -2.323037000 -4.729456000 -3.618569000

H -0.503896000 -5.502630000 -2.744098000

H -4.102797000 -3.710436000 -4.297395000

H -2.422162000 -5.548892000 -4.334994000

C -2.757512000 -2.003709000 0.919319000

C -3.503417000 -3.185534000 0.839972000

C -2.694492000 -1.321136000 2.141272000

C -4.173775000 -3.672721000 1.962830000

H -3.559557000 -3.736473000 -0.101112000

C -3.374216000 -1.802618000 3.256590000

H -2.104031000 -0.405943000 2.220263000

C -4.113814000 -2.982264000 3.171259000

H -4.744786000 -4.601657000 1.888781000

H -3.316839000 -1.253907000 4.199816000

H -4.638922000 -3.366529000 4.049432000

**Table S4. equatorial-Ru(CO)2(PPh3)(dpae) (eq\_2)** (-6831.678627)

Ru 0.242088000 0.094747000 -1.084964000

C 0.024182000 1.313814000 -2.500432000

O -0.114154000 2.061058000 -3.375753000

C 0.810634000 -1.196407000 -2.327072000

O 1.187829000 -1.975278000 -3.089616000

As 2.026187000 -0.619457000 0.445815000

As 0.177861000 2.027976000 0.457342000

C 0.969262000 1.489022000 2.181170000

C 2.225726000 0.675287000 1.941084000

H 0.195602000 0.906290000 2.706023000

H 1.190195000 2.389580000 2.775743000

H 2.542630000 0.127985000 2.842019000

H 3.059942000 1.326124000 1.636464000

C -1.448543000 2.956300000 0.994210000

C -2.430108000 3.156987000 0.016951000

C -1.680237000 3.407023000 2.300010000

C -3.624284000 3.799705000 0.338856000

H -2.267050000 2.792357000 -1.000556000

C -2.877722000 4.047511000 2.620596000

H -0.930559000 3.258337000 3.081154000

C -3.850346000 4.244286000 1.640998000

H -4.385421000 3.940744000 -0.432153000

H -3.050952000 4.393749000 3.642811000

H -4.789388000 4.742182000 1.895082000

C 1.324331000 3.549642000 0.007360000

C 1.148997000 4.807642000 0.595445000

C 2.377812000 3.351350000 -0.889122000

C 2.024598000 5.849924000 0.294944000

H 0.317588000 4.984294000 1.282977000

C 3.255675000 4.394565000 -1.184530000

H 2.496462000 2.371433000 -1.362171000

C 3.080798000 5.644158000 -0.593036000

H 1.877122000 6.831014000 0.753775000

H 4.076909000 4.228225000 -1.886151000

H 3.764916000 6.463294000 -0.828800000

C 1.997457000 -2.336897000 1.384604000

C 2.641078000 -3.457410000 0.843704000

C 1.229294000 -2.488712000 2.544587000

C 2.531095000 -4.702181000 1.463510000

H 3.239758000 -3.359346000 -0.066176000

C 1.126496000 -3.732436000 3.166875000

H 0.688126000 -1.637109000 2.967110000

C 1.777679000 -4.841667000 2.628814000

H 3.041922000 -5.567702000 1.033496000

H 0.524895000 -3.833318000 4.073572000

H 1.694785000 -5.816674000 3.115419000

C 3.871087000 -0.641844000 -0.207805000

C 4.132964000 -0.226369000 -1.514960000

C 4.936808000 -1.010508000 0.623471000

C 5.444734000 -0.180813000 -1.990426000

H 3.294542000 0.064573000 -2.156734000

C 6.246490000 -0.958156000 0.150178000

H 4.745853000 -1.349914000 1.645793000

C 6.501610000 -0.544138000 -1.158291000

H 5.638912000 0.139296000 -3.017252000

H 7.073235000 -1.245021000 0.805243000

H 7.529094000 -0.507768000 -1.529245000

P -1.765924000 -1.042777000 -0.466427000

C -3.347583000 -0.271679000 -1.048172000

C -4.553380000 -0.381471000 -0.342917000

C -3.344508000 0.413752000 -2.269926000

C -5.722152000 0.194037000 -0.841655000

H -4.584272000 -0.918822000 0.607282000

C -4.515328000 0.975979000 -2.775453000

H -2.407074000 0.513852000 -2.822418000

C -5.707739000 0.873717000 -2.058586000

H -6.651823000 0.105719000 -0.273555000

H -4.491346000 1.503261000 -3.732562000

H -6.625000000 1.322036000 -2.449038000

C -1.894232000 -2.732056000 -1.205558000

C -0.832119000 -3.627418000 -1.008118000

C -2.994609000 -3.152034000 -1.961980000

C -0.877365000 -4.913126000 -1.540278000

H 0.041500000 -3.315885000 -0.429474000

C -3.029844000 -4.435121000 -2.509663000

H -3.832622000 -2.473513000 -2.132478000

C -1.975553000 -5.320271000 -2.298134000

H -0.041115000 -5.595594000 -1.369523000

H -3.892702000 -4.742050000 -3.106291000

H -2.005600000 -6.324628000 -2.727937000

C -2.192517000 -1.395898000 1.304165000

C -2.324688000 -2.684771000 1.833404000

C -2.364088000 -0.301022000 2.165370000

C -2.603939000 -2.871393000 3.189229000

H -2.211293000 -3.556382000 1.186523000

C -2.651707000 -0.486580000 3.514528000

H -2.295020000 0.713875000 1.767501000

C -2.765198000 -1.777448000 4.035631000

H -2.701864000 -3.887168000 3.581271000

H -2.794327000 0.383915000 4.160449000

H -2.988682000 -1.927080000 5.094941000

**Table S5. TP4-Ru(CO)2(dpae) (TP-1’)** (-5796.012855)

Ru -0.066533000 -0.461842000 1.521761000

C -0.475578000 -2.317965000 1.498290000

O -0.746512000 -3.440513000 1.587969000

C -0.860957000 0.914663000 2.575512000

O -1.388643000 1.646430000 3.301506000

As 1.810875000 -0.094495000 -0.055757000

As -1.523449000 -0.051565000 -0.256435000

C -0.409705000 0.268030000 -1.863216000

C 0.933795000 -0.434634000 -1.799410000

H -0.278563000 1.361380000 -1.889164000

H -0.978932000 -0.003515000 -2.765100000

H 1.592631000 -0.100725000 -2.615888000

H 0.828202000 -1.527888000 -1.877289000

C -2.599863000 1.569385000 -0.243622000

C -3.976432000 1.543695000 -0.483607000

C -1.964278000 2.790917000 0.009248000

C -4.708963000 2.731384000 -0.474694000

H -4.483805000 0.595594000 -0.677112000

C -2.698381000 3.974362000 0.010959000

H -0.890855000 2.818469000 0.220221000

C -4.072308000 3.946189000 -0.230194000

H -5.785732000 2.703358000 -0.659367000

H -2.195011000 4.923581000 0.209946000

H -4.648380000 4.874790000 -0.222766000

C -2.833588000 -1.397472000 -0.761629000

C -3.151820000 -1.680522000 -2.094143000

C -3.506127000 -2.071986000 0.263698000

C -4.123794000 -2.633987000 -2.396529000

H -2.650305000 -1.158978000 -2.912537000

C -4.483389000 -3.017577000 -0.041260000

H -3.253395000 -1.859396000 1.306317000

C -4.790736000 -3.302634000 -1.371106000

H -4.360825000 -2.853513000 -3.440530000

H -5.000863000 -3.540196000 0.766756000

H -5.551286000 -4.050187000 -1.609761000

C 2.594442000 1.666278000 -0.404398000

C 3.356105000 1.955977000 -1.544340000

C 2.330144000 2.685227000 0.515469000

C 3.844177000 3.244523000 -1.756362000

H 3.580544000 1.171382000 -2.273074000

C 2.822654000 3.974433000 0.305815000

H 1.721542000 2.458010000 1.398068000

C 3.578681000 4.255022000 -0.830668000

H 4.436179000 3.461738000 -2.649275000

H 2.611882000 4.762154000 1.033669000

H 3.962849000 5.264363000 -0.998519000

C 3.356523000 -1.279903000 -0.196034000

C 4.680540000 -0.829145000 -0.198370000

C 3.104479000 -2.658311000 -0.208176000

C 5.734154000 -1.743841000 -0.238416000

H 4.897878000 0.241137000 -0.165447000

C 4.157552000 -3.568618000 -0.260649000

H 2.074321000 -3.025226000 -0.156238000

C 5.476113000 -3.112667000 -0.277165000

H 6.765045000 -1.380338000 -0.237873000

H 3.946834000 -4.640930000 -0.276060000

H 6.303049000 -3.826349000 -0.309923000

**Table S6. SP4-Ru(CO)2(dpae) (SP4-1’)** (-5796.042883)

Ru 0.028704000 -0.261095000 1.565797000

C 1.325385000 -1.027388000 2.671361000

O 2.115001000 -1.570290000 3.315318000

C -1.309734000 -0.657940000 2.810847000

O -2.150405000 -0.896500000 3.566290000

As -1.604120000 0.079401000 -0.273226000

As 1.664183000 0.145682000 -0.255459000

C 0.708603000 -0.050636000 -1.971495000

C -0.640787000 0.641306000 -1.906056000

H 0.596383000 -1.136722000 -2.120281000

H 1.329868000 0.329865000 -2.796783000

H -1.256636000 0.413655000 -2.790270000

H -0.518369000 1.735020000 -1.842627000

C 3.195450000 -1.016633000 -0.532078000

C 4.451833000 -0.552729000 -0.932062000

C 3.003698000 -2.384399000 -0.302895000

C 5.501145000 -1.453243000 -1.117605000

H 4.621420000 0.515076000 -1.090385000

C 4.052288000 -3.281204000 -0.496604000

H 2.030523000 -2.743973000 0.046707000

C 5.302167000 -2.816504000 -0.905539000

H 6.482582000 -1.083987000 -1.425710000

H 3.895230000 -4.347136000 -0.314354000

H 6.126990000 -3.518792000 -1.049429000

C 2.395173000 1.942986000 -0.379405000

C 2.852583000 2.506679000 -1.576981000

C 2.434521000 2.703398000 0.795846000

C 3.349955000 3.809196000 -1.595591000

H 2.828103000 1.932373000 -2.507137000

C 2.934414000 4.005176000 0.774951000

H 2.061347000 2.268587000 1.728760000

C 3.392847000 4.558405000 -0.419630000

H 3.705614000 4.241474000 -2.534321000

H 2.960814000 4.590581000 1.697222000

H 3.782183000 5.579409000 -0.436595000

C -2.439633000 -1.571386000 -0.884948000

C -3.462670000 -1.570496000 -1.839854000

C -1.975594000 -2.783400000 -0.365134000

C -4.006989000 -2.775883000 -2.279213000

H -3.849691000 -0.626378000 -2.234699000

C -2.523218000 -3.988139000 -0.808105000

H -1.187463000 -2.763020000 0.397054000

C -3.536244000 -3.985279000 -1.765344000

H -4.808482000 -2.771318000 -3.022343000

H -2.159764000 -4.933068000 -0.396332000

H -3.967854000 -4.928879000 -2.108768000

C -3.125947000 1.291928000 -0.232166000

C -3.946757000 1.267232000 0.902881000

C -3.422976000 2.181045000 -1.270902000

C -5.051610000 2.111399000 0.990249000

H -3.722099000 0.587423000 1.729452000

C -4.527124000 3.029570000 -1.177788000

H -2.796362000 2.223977000 -2.164690000

C -5.343336000 2.994759000 -0.049195000

H -5.684881000 2.082242000 1.880306000

H -4.748689000 3.721446000 -1.994339000

H -6.207269000 3.660003000 0.022992000

**Table S7. *cis*-*cis*-Ru(CO)2(dpae)(H)2 (*cis*-*cis*-3)** (-5797.257621)

Ru -0.009971000 -0.447229000 1.549429000

C 1.136038000 -1.173772000 2.859985000

O 1.797494000 -1.671598000 3.654935000

C -0.331375000 1.240971000 2.424563000

O -0.573589000 2.207862000 2.996397000

As 1.615059000 -0.043617000 -0.271986000

As -1.679941000 -0.179902000 -0.223771000

C -0.729201000 0.189472000 -1.921140000

C 0.638959000 -0.469481000 -1.934107000

H -0.639026000 1.285179000 -1.992642000

H -1.352111000 -0.146199000 -2.764033000

H 1.228217000 -0.143263000 -2.805530000

H 0.548976000 -1.567233000 -1.963822000

C -2.972098000 1.274560000 -0.172777000

C -4.339614000 1.045392000 0.009191000

C -2.501137000 2.592218000 -0.230136000

C -5.223846000 2.119573000 0.113614000

H -4.721978000 0.023672000 0.071312000

C -3.387218000 3.662827000 -0.132896000

H -1.431309000 2.793812000 -0.341298000

C -4.751388000 3.428207000 0.037991000

H -6.290369000 1.928904000 0.257100000

H -3.007939000 4.686456000 -0.182373000

H -5.445854000 4.267921000 0.119496000

C -2.785514000 -1.708177000 -0.682224000

C -3.602491000 -1.687721000 -1.820515000

C -2.755356000 -2.848343000 0.124446000

C -4.374914000 -2.799669000 -2.149263000

H -3.649421000 -0.796115000 -2.452743000

C -3.533067000 -3.959256000 -0.205869000

H -2.110064000 -2.859843000 1.007094000

C -4.340160000 -3.937305000 -1.341445000

H -5.008710000 -2.777302000 -3.039379000

H -3.503605000 -4.847735000 0.429659000

H -4.946499000 -4.809129000 -1.599933000

C 2.319185000 1.725790000 -0.722825000

C 3.280422000 1.898863000 -1.726164000

C 1.831848000 2.844105000 -0.041346000

C 3.733447000 3.175926000 -2.051414000

H 3.691071000 1.031041000 -2.250662000

C 2.286349000 4.123256000 -0.367767000

H 1.100353000 2.712132000 0.760437000

C 3.235128000 4.290098000 -1.374276000

H 4.485666000 3.302269000 -2.834307000

H 1.901404000 4.990590000 0.174426000

H 3.594925000 5.290365000 -1.628020000

C 3.222202000 -1.124195000 -0.426229000

C 4.085129000 -1.165531000 0.675398000

C 3.545388000 -1.855133000 -1.574413000

C 5.256959000 -1.917002000 0.625440000

H 3.837714000 -0.612144000 1.585546000

C 4.717197000 -2.612015000 -1.620359000

H 2.885229000 -1.845968000 -2.444718000

C 5.574929000 -2.642187000 -0.522941000

H 5.921629000 -1.942241000 1.492396000

H 4.958167000 -3.182311000 -2.521048000

H 6.491377000 -3.236224000 -0.559967000

H 0.057794000 -1.983587000 0.922162000

H -1.221835000 -1.067806000 2.420170000

**Table S8. *trans*-*cis*-Ru(CO)2(dpae)(H)2 (*trans*-*cis*-3)** (-5797.253131)

Ru 0.006444000 -0.299627000 1.630192000

C 0.197499000 -2.202574000 1.701435000

O 0.310316000 -3.328588000 1.887281000

C -0.212338000 1.425359000 2.425843000

O -0.354600000 2.387456000 3.035684000

As 1.664781000 -0.000425000 -0.183050000

As -1.646323000 -0.071937000 -0.202645000

C -0.647760000 0.309843000 -1.873896000

C 0.714372000 -0.361919000 -1.879846000

H -0.543923000 1.406304000 -1.908537000

H -1.250802000 0.014778000 -2.745751000

H 1.320954000 -0.015261000 -2.731348000

H 0.619802000 -1.457916000 -1.951666000

C -2.925013000 1.398295000 -0.219642000

C -4.306734000 1.192364000 -0.271036000

C -2.431152000 2.704989000 -0.118631000

C -5.180290000 2.280155000 -0.235704000

H -4.708457000 0.178472000 -0.338091000

C -3.304899000 3.789526000 -0.091438000

H -1.353599000 2.883842000 -0.052015000

C -4.682603000 3.578646000 -0.150122000

H -6.258899000 2.107915000 -0.274334000

H -2.907188000 4.804522000 -0.015277000

H -5.368770000 4.428672000 -0.122771000

C -2.771757000 -1.585621000 -0.685758000

C -3.366090000 -1.709188000 -1.948087000

C -2.997790000 -2.575024000 0.276107000

C -4.164298000 -2.812495000 -2.244935000

H -3.218867000 -0.937650000 -2.708867000

C -3.800645000 -3.676846000 -0.020674000

H -2.540319000 -2.478975000 1.264347000

C -4.381157000 -3.798408000 -1.281588000

H -4.621479000 -2.901823000 -3.233651000

H -3.968897000 -4.444570000 0.738474000

H -5.006294000 -4.663657000 -1.515972000

C 2.499038000 1.720845000 -0.586159000

C 3.413614000 1.859172000 -1.637423000

C 2.169803000 2.838975000 0.184122000

C 3.976139000 3.101685000 -1.921611000

H 3.705735000 0.989887000 -2.233286000

C 2.734555000 4.083662000 -0.100544000

H 1.476533000 2.736497000 1.022143000

C 3.635136000 4.216866000 -1.154756000

H 4.690380000 3.199020000 -2.743192000

H 2.471623000 4.950227000 0.511184000

H 4.079526000 5.190243000 -1.376976000

C 3.186751000 -1.205419000 -0.295319000

C 3.842805000 -1.527997000 0.898232000

C 3.638237000 -1.763172000 -1.497123000

C 4.944178000 -2.381914000 0.887383000

H 3.475925000 -1.116826000 1.843365000

C 4.736737000 -2.623110000 -1.504441000

H 3.132657000 -1.539858000 -2.439905000

C 5.393150000 -2.930011000 -0.313728000

H 5.448810000 -2.627300000 1.825076000

H 5.078858000 -3.057589000 -2.447185000

H 6.252771000 -3.604709000 -0.321070000

H 1.136592000 -0.410606000 2.790327000

H -1.137990000 -0.613139000 2.736759000

**Table S9. SP4-Ru(CO)(PPh3)(dpae) (SP4-2’)** (-6718.386136)

Ru -0.379142000 0.529840000 -0.408770000

C -0.892367000 1.443253000 -1.914768000

O -1.191436000 1.855186000 -2.963183000

As -2.627432000 -0.203010000 0.021139000

As 0.153837000 -1.803119000 0.088809000

C -1.499362000 -2.765310000 0.649238000

C -2.710303000 -2.181864000 -0.048611000

H -1.591169000 -2.643974000 1.739885000

H -1.370414000 -3.837573000 0.435844000

H -3.657034000 -2.536762000 0.387464000

H -2.720151000 -2.437115000 -1.120459000

C 1.452165000 -2.602626000 1.324317000

C 2.780008000 -2.794964000 0.919474000

C 1.112641000 -2.860045000 2.659323000

C 3.738106000 -3.251618000 1.823765000

H 3.075114000 -2.584723000 -0.112246000

C 2.071594000 -3.318986000 3.562431000

H 0.090835000 -2.699035000 3.012736000

C 3.387301000 -3.518179000 3.146626000

H 4.768308000 -3.395251000 1.488184000

H 1.786063000 -3.523122000 4.597769000

H 4.139017000 -3.877255000 3.853957000

C 0.542867000 -2.815169000 -1.542686000

C 0.907590000 -4.166090000 -1.511031000

C 0.376101000 -2.176728000 -2.774905000

C 1.110484000 -4.865582000 -2.700227000

H 1.043602000 -4.677327000 -0.553549000

C 0.576573000 -2.878983000 -3.964316000

H 0.083167000 -1.119603000 -2.776264000

C 0.945923000 -4.222926000 -3.928093000

H 1.399030000 -5.919527000 -2.667960000

H 0.443530000 -2.371293000 -4.923321000

H 1.105392000 -4.773444000 -4.858895000

C -3.159370000 0.137270000 1.864430000

C -2.387120000 1.041627000 2.602995000

C -4.228024000 -0.519343000 2.486804000

C -2.678476000 1.286266000 3.945077000

H -1.549274000 1.552296000 2.114567000

C -4.520289000 -0.271669000 3.827762000

H -4.844956000 -1.226552000 1.925059000

C -3.745489000 0.630586000 4.557776000

H -2.064662000 1.990892000 4.511621000

H -5.357431000 -0.787030000 4.305747000

H -3.975547000 0.821584000 5.609126000

C -4.197361000 0.269570000 -1.024388000

C -4.166009000 0.003870000 -2.399062000

C -5.319108000 0.895699000 -0.472751000

C -5.252760000 0.336503000 -3.204624000

H -3.279349000 -0.451199000 -2.850691000

C -6.403262000 1.233864000 -1.283632000

H -5.349970000 1.127008000 0.594789000

C -6.374620000 0.950696000 -2.647752000

H -5.217635000 0.125005000 -4.276190000

H -7.275185000 1.724651000 -0.843563000

H -7.224503000 1.216963000 -3.281118000

P 1.704402000 1.517102000 -0.253602000

C 3.256665000 0.579614000 -0.578134000

C 4.355308000 0.572333000 0.289034000

C 3.327199000 -0.152263000 -1.771813000

C 5.500993000 -0.157347000 -0.031337000

H 4.316593000 1.135902000 1.224386000

C 4.475493000 -0.871463000 -2.095584000

H 2.466770000 -0.164641000 -2.446173000

C 5.565154000 -0.877860000 -1.223108000

H 6.349983000 -0.159617000 0.657124000

H 4.514414000 -1.436868000 -3.029962000

H 6.464539000 -1.446630000 -1.472770000

C 2.048621000 3.114968000 -1.111775000

C 0.986553000 4.008066000 -1.304472000

C 3.327972000 3.478210000 -1.550833000

C 1.200580000 5.243168000 -1.912356000

H -0.016829000 3.720547000 -0.977803000

C 3.537891000 4.710226000 -2.169878000

H 4.168662000 2.794336000 -1.414801000

C 2.476926000 5.596059000 -2.349687000

H 0.360787000 5.927492000 -2.055989000

H 4.539979000 4.977437000 -2.514916000

H 2.643502000 6.560011000 -2.837207000

C 1.821637000 1.979317000 1.528962000

C 1.868120000 3.310022000 1.964659000

C 1.782732000 0.954100000 2.488941000

C 1.866228000 3.608489000 3.327239000

H 1.905857000 4.121565000 1.234959000

C 1.787006000 1.256333000 3.848955000

H 1.758347000 -0.090428000 2.170366000

C 1.823745000 2.584961000 4.272737000

H 1.901823000 4.652161000 3.649954000

H 1.762189000 0.443803000 4.579429000

H 1.825415000 2.822257000 5.339704000

**Table S10. ax-Ru(CO)(PPh3)(dpae)(H)2 (7a)** (-6719.606311)

Ru 0.370838000 -0.489581000 -0.301999000

C 0.624291000 -0.345926000 -2.185415000

O 0.799727000 -0.298111000 -3.326841000

As -0.092885000 1.785110000 0.498845000

As 2.654566000 0.002039000 0.276270000

C 2.786420000 1.908864000 0.795175000

C 1.522364000 2.338366000 1.514471000

H 2.925090000 2.476542000 -0.138843000

H 3.684247000 2.062154000 1.413544000

H 1.488064000 3.427665000 1.669717000

H 1.453129000 1.855679000 2.501537000

C 4.072680000 -0.147150000 -1.051054000

C 5.030443000 -1.164607000 -0.988347000

C 4.079646000 0.728564000 -2.143790000

C 5.990285000 -1.291770000 -1.992544000

H 5.030773000 -1.865581000 -0.150035000

C 5.043730000 0.604379000 -3.142284000

H 3.320783000 1.511808000 -2.230198000

C 6.002651000 -0.405508000 -3.067854000

H 6.733023000 -2.091374000 -1.932221000

H 5.039582000 1.296502000 -3.988005000

H 6.755894000 -0.505164000 -3.853331000

C 3.458976000 -0.885452000 1.810875000

C 4.711668000 -0.488001000 2.296530000

C 2.773854000 -1.925150000 2.444869000

C 5.267574000 -1.118944000 3.407491000

H 5.267970000 0.312435000 1.799887000

C 3.335214000 -2.559024000 3.554874000

H 1.792983000 -2.223843000 2.063611000

C 4.578664000 -2.156248000 4.038074000

H 6.244574000 -0.801805000 3.781131000

H 2.793486000 -3.372452000 4.044165000

H 5.015750000 -2.652327000 4.908498000

C -0.287896000 3.359995000 -0.649905000

C -0.479091000 4.644982000 -0.124704000

C -0.166794000 3.202210000 -2.033373000

C -0.552272000 5.749513000 -0.971296000

H -0.580299000 4.787377000 0.955195000

C -0.238061000 4.309084000 -2.881841000

H -0.008470000 2.203883000 -2.450721000

C -0.432346000 5.582950000 -2.351987000

H -0.703786000 6.747167000 -0.550946000

H -0.141030000 4.171635000 -3.961804000

H -0.490081000 6.450063000 -3.014847000

C -1.468826000 2.115264000 1.843384000

C -2.670050000 2.755010000 1.519234000

C -1.293783000 1.620798000 3.142402000

C -3.667888000 2.913826000 2.481091000

H -2.836960000 3.128531000 0.506051000

C -2.289043000 1.786600000 4.104547000

H -0.377991000 1.086083000 3.409211000

C -3.478603000 2.436601000 3.776565000

H -4.602124000 3.412235000 2.210550000

H -2.133621000 1.402872000 5.116267000

H -4.259860000 2.565110000 4.529891000

H 0.226507000 -0.792530000 1.330879000

H 0.838026000 -2.041276000 -0.318450000

P -1.752606000 -1.416758000 -0.470700000

C -2.295703000 -2.472141000 0.942692000

C -2.734251000 -3.789854000 0.776473000

C -2.259868000 -1.929056000 2.234541000

C -3.123341000 -4.550980000 1.880748000

H -2.769422000 -4.233592000 -0.220507000

C -2.666162000 -2.682744000 3.331647000

H -1.905748000 -0.905951000 2.379110000

C -3.094257000 -4.000243000 3.159024000

H -3.452693000 -5.582827000 1.734452000

H -2.639687000 -2.239548000 4.330499000

H -3.401916000 -4.596334000 4.021991000

C -2.020635000 -2.539491000 -1.914195000

C -0.950667000 -3.307239000 -2.390408000

C -3.275067000 -2.673763000 -2.525016000

C -1.132285000 -4.194450000 -3.450104000

H 0.031291000 -3.192661000 -1.924491000

C -3.452998000 -3.556917000 -3.588861000

H -4.121688000 -2.081748000 -2.170058000

C -2.382673000 -4.320412000 -4.053219000

H -0.285929000 -4.783747000 -3.811628000

H -4.435820000 -3.646099000 -4.058735000

H -2.522655000 -5.009752000 -4.889820000

C -3.176836000 -0.253232000 -0.667360000

C -3.062243000 0.743422000 -1.647146000

C -4.353060000 -0.326333000 0.086252000

C -4.102249000 1.640517000 -1.874397000

H -2.144499000 0.813854000 -2.236732000

C -5.390894000 0.581890000 -0.133340000

H -4.463042000 -1.095691000 0.853517000

C -5.270887000 1.563543000 -1.114143000

H -3.995969000 2.408007000 -2.645282000

H -6.300915000 0.515748000 0.468480000

H -6.086432000 2.270370000 -1.287404000

**Table S11. ax-Ru(CO)(PPh3)(dpae)(H)2 (7b)** (-6719.60045)

Ru 0.087177000 0.390753000 -1.202725000

C 1.052334000 -0.106807000 -2.719285000

O 1.607218000 -0.327253000 -3.705915000

As 1.897771000 0.971645000 0.371755000

As -1.329602000 1.716078000 0.308047000

C -0.293653000 2.149871000 1.933607000

C 1.169386000 2.363850000 1.588312000

H -0.427849000 1.288283000 2.607861000

H -0.718332000 3.037986000 2.427842000

H 1.800771000 2.422641000 2.488667000

H 1.304102000 3.304082000 1.030288000

C -3.036357000 1.137341000 1.056480000

C -3.917784000 0.461156000 0.204941000

C -3.411456000 1.364824000 2.386416000

C -5.155110000 0.022862000 0.673698000

H -3.624840000 0.260196000 -0.828972000

C -4.649705000 0.923175000 2.854430000

H -2.739566000 1.884817000 3.073885000

C -5.522828000 0.252440000 1.999144000

H -5.828285000 -0.511480000 -0.000962000

H -4.932655000 1.105206000 3.894515000

H -6.490814000 -0.095492000 2.368343000

C -1.866289000 3.493046000 -0.311293000

C -2.577385000 4.354018000 0.534030000

C -1.558080000 3.909815000 -1.607895000

C -2.956726000 5.620218000 0.093903000

H -2.855723000 4.035902000 1.542667000

C -1.944172000 5.176367000 -2.049887000

H -1.009965000 3.231151000 -2.267075000

C -2.639149000 6.034115000 -1.200353000

H -3.509077000 6.284889000 0.763072000

H -1.698867000 5.491324000 -3.067344000

H -2.939762000 7.026117000 -1.547081000

C 2.807535000 -0.224115000 1.625933000

C 3.929656000 -0.946058000 1.197880000

C 2.329530000 -0.428857000 2.924279000

C 4.565125000 -1.843630000 2.053973000

H 4.327418000 -0.792099000 0.190212000

C 2.966423000 -1.326215000 3.781660000

H 1.448307000 0.108688000 3.282600000

C 4.085963000 -2.034372000 3.349984000

H 5.444170000 -2.393316000 1.707623000

H 2.579337000 -1.473431000 4.792892000

H 4.586010000 -2.735622000 4.022669000

C 3.450649000 1.951268000 -0.296489000

C 3.495875000 2.338718000 -1.638485000

C 4.499770000 2.317169000 0.557412000

C 4.575078000 3.080197000 -2.122063000

H 2.676884000 2.060879000 -2.305905000

C 5.573961000 3.061725000 0.074070000

H 4.486092000 2.012251000 1.607582000

C 5.613930000 3.443243000 -1.267656000

H 4.601197000 3.373078000 -3.174655000

H 6.386402000 3.343482000 0.748924000

H 6.458982000 4.023581000 -1.646818000

H 0.376227000 1.882924000 -1.779888000

H -1.183130000 0.471136000 -2.202159000

P -0.495175000 -1.863506000 -0.611397000

C -2.186703000 -2.439233000 -1.096648000

C -2.693234000 -2.017803000 -2.333694000

C -2.958740000 -3.302820000 -0.310122000

C -3.942061000 -2.450751000 -2.774083000

H -2.101172000 -1.329531000 -2.942635000

C -4.215328000 -3.725463000 -0.746324000

H -2.580185000 -3.648994000 0.654037000

C -4.710020000 -3.302156000 -1.978398000

H -4.320097000 -2.115086000 -3.743172000

H -4.808593000 -4.393561000 -0.116658000

H -5.693102000 -3.636173000 -2.320250000

C 0.558403000 -3.144251000 -1.431167000

C 1.944706000 -2.942336000 -1.459230000

C 0.036051000 -4.308887000 -2.005883000

C 2.790318000 -3.884699000 -2.039115000

H 2.359180000 -2.032254000 -1.019464000

C 0.882537000 -5.246317000 -2.598666000

H -1.041133000 -4.487301000 -1.996689000

C 2.260182000 -5.038847000 -2.615401000

H 3.869087000 -3.710167000 -2.050290000

H 0.457855000 -6.145703000 -3.051826000

H 2.921015000 -5.773649000 -3.082112000

C -0.412500000 -2.419905000 1.153736000

C -1.207663000 -1.754337000 2.098363000

C 0.413996000 -3.460885000 1.590987000

C -1.186606000 -2.126601000 3.440072000

H -1.874449000 -0.950882000 1.777995000

C 0.445246000 -3.824364000 2.938464000

H 1.041037000 -3.997903000 0.876982000

C -0.355020000 -3.163326000 3.866488000

H -1.829538000 -1.604834000 4.154002000

H 1.101958000 -4.636619000 3.259916000

H -0.334869000 -3.456220000 4.919374000

**Table S12. Ru(CO)2(dpae)(C2H2Ph2) (8\_*trans*)** (-6336.308398)

Ru -0.101348000 -0.180516000 1.038264000

As 1.026819000 1.099093000 -0.829882000

As -2.097156000 0.151805000 -0.372700000

C -1.486951000 0.637496000 -2.178398000

H -1.122580000 -0.306519000 -2.614156000

H -2.326599000 0.982371000 -2.801125000

C -0.384383000 1.678833000 -2.083838000

H -0.772158000 2.626649000 -1.676457000

H 0.066094000 1.892446000 -3.065199000

C -0.052713000 1.391564000 2.119256000

O -0.052104000 2.274345000 2.859206000

C 0.778987000 -2.149653000 0.544531000

C 1.683293000 -1.391651000 1.372561000

H 0.191526000 -2.917415000 1.064485000

H 2.529290000 -0.935589000 0.842900000

C 2.039145000 -1.715330000 2.775608000

C 3.003707000 -0.936512000 3.438876000

C 1.481860000 -2.791507000 3.484686000

C 3.377482000 -1.201781000 4.751869000

H 3.463847000 -0.099293000 2.904831000

C 1.849820000 -3.056375000 4.802165000

H 0.750931000 -3.440920000 2.997515000

C 2.796975000 -2.263327000 5.447623000

H 4.129842000 -0.574771000 5.237998000

H 1.394835000 -3.900507000 5.327286000

H 3.085879000 -2.473885000 6.480097000

C 1.137608000 -2.633440000 -0.818479000

C 0.145456000 -2.973636000 -1.754374000

C 2.471938000 -2.891523000 -1.171066000

C 0.469030000 -3.548088000 -2.981071000

H -0.903065000 -2.796563000 -1.502430000

C 2.799664000 -3.462735000 -2.399793000

H 3.264565000 -2.668959000 -0.453173000

C 1.801585000 -3.797908000 -3.312363000

H -0.328818000 -3.811781000 -3.681088000

H 3.848419000 -3.656582000 -2.639380000

H 2.057865000 -4.255452000 -4.271265000

C -1.081983000 -1.046473000 2.382339000

O -1.716630000 -1.555445000 3.195712000

C 2.392055000 0.414223000 -2.045821000

C 3.737482000 0.481126000 -1.665609000

C 2.060778000 -0.115492000 -3.295922000

C 4.735926000 0.034017000 -2.528602000

H 4.016818000 0.904951000 -0.697166000

C 3.062254000 -0.554408000 -4.160548000

H 1.017819000 -0.202534000 -3.608654000

C 4.400533000 -0.478576000 -3.781027000

H 5.783207000 0.096225000 -2.222523000

H 2.789812000 -0.967273000 -5.134647000

H 5.183933000 -0.822423000 -4.460892000

C 1.896066000 2.782963000 -0.380408000

C 1.954583000 3.837408000 -1.299811000

C 2.525329000 2.921881000 0.860499000

C 2.618350000 5.018278000 -0.973888000

H 1.488734000 3.742570000 -2.283813000

C 3.198450000 4.101390000 1.180960000

H 2.484322000 2.106667000 1.587631000

C 3.241812000 5.151757000 0.267021000

H 2.652645000 5.837896000 -1.696003000

H 3.683368000 4.199542000 2.155182000

H 3.762814000 6.078206000 0.520796000

C -3.277173000 1.642163000 0.082192000

C -3.579601000 1.836691000 1.435018000

C -3.824774000 2.512645000 -0.866948000

C -4.427084000 2.869720000 1.829699000

H -3.140538000 1.179812000 2.191046000

C -4.665218000 3.553705000 -0.470178000

H -3.599654000 2.394638000 -1.930014000

C -4.970910000 3.731414000 0.877540000

H -4.655650000 3.007134000 2.889321000

H -5.081784000 4.229717000 -1.221258000

H -5.628962000 4.546852000 1.187497000

C -3.410864000 -1.243367000 -0.739194000

C -4.517082000 -1.008021000 -1.564179000

C -3.245989000 -2.502147000 -0.155017000

C -5.434745000 -2.026204000 -1.813776000

H -4.677467000 -0.021292000 -2.007139000

C -4.169227000 -3.519408000 -0.400943000

H -2.387885000 -2.686395000 0.496518000

C -5.261397000 -3.283269000 -1.232823000

H -6.294740000 -1.835638000 -2.460774000

H -4.032050000 -4.499432000 0.062383000

H -5.984771000 -4.079245000 -1.426305000

**Table S13. Ru(CO)2(dpae)(C2H2Ph2) (8-*cis*)** (-6336.309008)

Ru 0.101727000 0.165740000 -0.772095000

As 1.220351000 -1.437881000 0.798543000

As -1.947952000 -0.791079000 0.237821000

C -1.448302000 -1.756832000 1.882974000

H -1.342993000 -0.962075000 2.637888000

H -2.272935000 -2.403571000 2.219754000

C -0.158064000 -2.535951000 1.691959000

H -0.317258000 -3.403364000 1.030999000

H 0.242680000 -2.909303000 2.647202000

C 0.404053000 -0.996613000 -2.247963000

O 0.585354000 -1.635891000 -3.190584000

C 0.888556000 1.851086000 0.467533000

C 1.785300000 1.498585000 -0.617284000

H 1.186010000 1.444101000 1.438926000

H 2.656506000 0.921683000 -0.270808000

C 2.231140000 2.434356000 -1.699862000

C 2.101830000 2.145750000 -3.063688000

C 2.889270000 3.623957000 -1.342591000

C 2.601540000 3.012424000 -4.036680000

H 1.598154000 1.223608000 -3.360671000

C 3.384290000 4.494025000 -2.310161000

H 3.002567000 3.868114000 -0.282968000

C 3.241609000 4.192453000 -3.665127000

H 2.483910000 2.761743000 -5.094273000

H 3.884489000 5.416710000 -2.003850000

H 3.627492000 4.875214000 -4.426396000

C 0.158902000 3.123975000 0.665913000

C -0.180685000 3.485964000 1.984802000

C -0.216755000 4.018111000 -0.355327000

C -0.870491000 4.660308000 2.273135000

H 0.110249000 2.819432000 2.802503000

C -0.904523000 5.194438000 -0.068013000

H 0.030798000 3.797843000 -1.393493000

C -1.241385000 5.526200000 1.244613000

H -1.113862000 4.903233000 3.311211000

H -1.180337000 5.862910000 -0.887913000

H -1.779698000 6.451845000 1.462786000

C -0.914573000 1.315673000 -1.856333000

O -1.585674000 1.955895000 -2.536276000

C 2.257224000 -0.755588000 2.303715000

C 3.636693000 -0.564547000 2.166796000

C 1.635495000 -0.395213000 3.505344000

C 4.381079000 -0.025795000 3.215761000

H 4.142037000 -0.849542000 1.240152000

C 2.382719000 0.137412000 4.555036000

H 0.558088000 -0.524773000 3.635293000

C 3.756830000 0.324880000 4.411431000

H 5.457759000 0.117395000 3.096160000

H 1.886015000 0.409741000 5.489570000

H 4.341398000 0.745832000 5.232960000

C 2.464839000 -2.767341000 0.122467000

C 2.710483000 -3.960331000 0.813424000

C 3.158943000 -2.502677000 -1.062186000

C 3.628897000 -4.881876000 0.315069000

H 2.190175000 -4.177135000 1.750023000

C 4.085046000 -3.423480000 -1.553835000

H 2.972250000 -1.573106000 -1.606535000

C 4.317422000 -4.614049000 -0.868767000

H 3.810863000 -5.813635000 0.856430000

H 4.621389000 -3.208252000 -2.481068000

H 5.038051000 -5.337862000 -1.257365000

C -2.877773000 -2.159748000 -0.798498000

C -3.078894000 -1.909178000 -2.161319000

C -3.341175000 -3.362889000 -0.255035000

C -3.743492000 -2.836096000 -2.961173000

H -2.705059000 -0.982340000 -2.605326000

C -3.997229000 -4.296414000 -1.059196000

H -3.196647000 -3.590002000 0.804111000

C -4.202402000 -4.033178000 -2.411798000

H -3.895324000 -2.624859000 -4.022429000

H -4.349452000 -5.234628000 -0.622955000

H -4.716231000 -4.764215000 -3.040785000

C -3.436564000 0.291439000 0.868976000

C -4.708700000 -0.246115000 1.097378000

C -3.202228000 1.648500000 1.108356000

C -5.732168000 0.569076000 1.577518000

H -4.908648000 -1.300501000 0.887817000

C -4.229449000 2.460487000 1.590429000

H -2.214677000 2.076604000 0.915328000

C -5.492819000 1.921581000 1.826025000

H -6.725203000 0.146981000 1.752171000

H -4.032666000 3.519828000 1.772143000

H -6.299413000 2.558836000 2.197547000

**Table S14. Ru(CO)2(dpae)( CHPhCH2Ph)(H) (9a)** (-6337.492248)

Ru -0.330730000 0.197660000 1.410282000

As -0.209372000 1.879522000 -0.482150000

As -1.594991000 -1.150732000 -0.280192000

C -1.352114000 -0.320907000 -2.041771000

H -0.371895000 -0.674719000 -2.396368000

H -2.110750000 -0.687709000 -2.750035000

C -1.401737000 1.195105000 -1.910056000

H -2.408391000 1.533124000 -1.615876000

H -1.158529000 1.693304000 -2.860891000

C -1.989751000 0.856354000 2.084562000

O -2.932813000 1.239178000 2.618056000

C 1.704797000 -0.770512000 1.070551000

C 2.872265000 0.233138000 0.939078000

H 1.849939000 -1.295602000 2.026039000

H 2.834076000 0.753702000 -0.028546000

C 4.231173000 -0.406407000 1.100743000

C 5.065146000 -0.654429000 0.004236000

C 4.684897000 -0.788691000 2.371160000

C 6.307690000 -1.266836000 0.167518000

H 4.732193000 -0.361699000 -0.995122000

C 5.925024000 -1.399738000 2.540619000

H 4.052984000 -0.595995000 3.243918000

C 6.742525000 -1.643572000 1.436559000

H 6.940331000 -1.451047000 -0.704947000

H 6.258783000 -1.684058000 3.542255000

H 7.716237000 -2.122789000 1.566767000

C 1.781649000 -1.818866000 0.003736000

C 1.826645000 -3.183636000 0.333998000

C 1.907260000 -1.497509000 -1.360182000

C 1.975606000 -4.171285000 -0.636940000

H 1.759872000 -3.469877000 1.387588000

C 2.054160000 -2.479649000 -2.337570000

H 1.921784000 -0.446231000 -1.657815000

C 2.086791000 -3.828258000 -1.983134000

H 2.011008000 -5.221717000 -0.336298000

H 2.161766000 -2.187299000 -3.386596000

H 2.209038000 -4.601293000 -2.745615000

C 0.595912000 1.038981000 2.812938000

O 1.131677000 1.512820000 3.711454000

C 1.364155000 2.437351000 -1.498987000

C 2.249679000 3.341826000 -0.898722000

C 1.650295000 1.955399000 -2.779883000

C 3.399507000 3.753399000 -1.567175000

H 2.040978000 3.731456000 0.101864000

C 2.804963000 2.367142000 -3.448515000

H 0.977706000 1.249841000 -3.273964000

C 3.681302000 3.264817000 -2.843574000

H 4.082412000 4.457963000 -1.086370000

H 3.017523000 1.981758000 -4.448819000

H 4.585970000 3.585131000 -3.365811000

C -0.980557000 3.647938000 -0.192611000

C -1.214223000 4.512326000 -1.270267000

C -1.296236000 4.067432000 1.101898000

C -1.774686000 5.768846000 -1.053956000

H -0.946987000 4.210946000 -2.287083000

C -1.850345000 5.330353000 1.318256000

H -1.107435000 3.405004000 1.949700000

C -2.094610000 6.179029000 0.241435000

H -1.957363000 6.435192000 -1.900761000

H -2.092315000 5.647946000 2.335359000

H -2.531504000 7.166417000 0.410209000

C -3.538028000 -1.083301000 -0.055619000

C -4.067696000 -1.494657000 1.173221000

C -4.412771000 -0.685036000 -1.070747000

C -5.444784000 -1.512979000 1.380177000

H -3.398250000 -1.799344000 1.982572000

C -5.792322000 -0.695126000 -0.860057000

H -4.033273000 -0.363733000 -2.043462000

C -6.310982000 -1.111112000 0.363818000

H -5.842799000 -1.837270000 2.344736000

H -6.463895000 -0.377353000 -1.661595000

H -7.391284000 -1.120138000 0.527528000

C -1.438809000 -3.062402000 -0.566471000

C -1.521047000 -3.636668000 -1.836976000

C -1.358895000 -3.886163000 0.560811000

C -1.532265000 -5.024444000 -1.976577000

H -1.578079000 -3.011254000 -2.730717000

C -1.382012000 -5.271430000 0.418741000

H -1.265704000 -3.440765000 1.555502000

C -1.469826000 -5.842582000 -0.850551000

H -1.592559000 -5.466994000 -2.973987000

H -1.321856000 -5.908577000 1.304544000

H -1.484744000 -6.929566000 -0.962502000

H -0.494463000 -1.060762000 2.399401000

H 2.778186000 1.021452000 1.701731000

**Table S15. Ru(CO)2(dpae)(CHPhCH2Ph)(H) (9b)** (-6337.497843)

Ru 0.234157000 -0.594998000 -0.635532000

As -0.154888000 1.138819000 1.137778000

As 2.592209000 -0.307357000 -0.000114000

C 2.597315000 0.345052000 1.860676000

H 2.344090000 -0.548793000 2.453658000

H 3.610388000 0.651201000 2.166245000

C 1.585937000 1.460731000 2.062577000

H 1.951212000 2.405392000 1.630593000

H 1.384252000 1.643525000 3.129363000

C 0.333283000 0.449776000 -2.238085000

O 0.365371000 0.967285000 -3.261975000

C -1.884956000 -0.900833000 -1.274140000

C -2.764472000 0.351154000 -1.117670000

H -1.791537000 -1.093818000 -2.353612000

H -2.931683000 0.576380000 -0.052338000

C -4.098181000 0.246796000 -1.820165000

C -5.283876000 -0.015339000 -1.124011000

C -4.172340000 0.396403000 -3.212100000

C -6.502433000 -0.126790000 -1.793175000

H -5.250802000 -0.136605000 -0.038289000

C -5.386325000 0.286373000 -3.885913000

H -3.258169000 0.608453000 -3.775644000

C -6.558805000 0.022503000 -3.177357000

H -7.414690000 -0.333496000 -1.227279000

H -5.418883000 0.410818000 -4.971638000

H -7.512964000 -0.064460000 -3.703278000

C -2.493328000 -2.136532000 -0.680224000

C -2.446368000 -3.351440000 -1.384457000

C -3.111484000 -2.153273000 0.582077000

C -2.974359000 -4.525552000 -0.854371000

H -1.977272000 -3.367132000 -2.372878000

C -3.644414000 -3.325097000 1.114861000

H -3.160640000 -1.235878000 1.174397000

C -3.579521000 -4.521613000 0.402232000

H -2.919186000 -5.452241000 -1.432407000

H -4.114074000 -3.300788000 2.102174000

H -3.997592000 -5.440620000 0.820392000

C 0.072604000 -2.084887000 0.580103000

O 0.031832000 -3.018689000 1.240239000

C -1.313535000 0.682187000 2.635924000

C -2.610179000 1.198846000 2.745204000

C -0.881930000 -0.272442000 3.564543000

C -3.454423000 0.773004000 3.770975000

H -2.968218000 1.943096000 2.029226000

C -1.726079000 -0.695442000 4.589836000

H 0.119523000 -0.705363000 3.489755000

C -3.014731000 -0.173603000 4.695029000

H -4.463817000 1.185250000 3.845491000

H -1.375754000 -1.442457000 5.306202000

H -3.677900000 -0.507470000 5.496672000

C -0.637063000 2.999208000 0.811170000

C -0.882961000 3.884038000 1.869776000

C -0.656751000 3.480765000 -0.500502000

C -1.150463000 5.227538000 1.614079000

H -0.874057000 3.524066000 2.902194000

C -0.924565000 4.826505000 -0.754765000

H -0.457696000 2.802453000 -1.332878000

C -1.173515000 5.700133000 0.301330000

H -1.343713000 5.909710000 2.445857000

H -0.940656000 5.189592000 -1.785142000

H -1.387304000 6.753231000 0.102585000

C 3.697228000 0.987926000 -0.944866000

C 3.824467000 0.836357000 -2.331617000

C 4.351165000 2.050200000 -0.312602000

C 4.600314000 1.726348000 -3.070223000

H 3.311357000 0.015387000 -2.840975000

C 5.122577000 2.945563000 -1.055586000

H 4.267429000 2.193957000 0.767496000

C 5.250042000 2.784079000 -2.433357000

H 4.693552000 1.595663000 -4.151089000

H 5.626396000 3.773917000 -0.551162000

H 5.854285000 3.485480000 -3.013798000

C 3.814015000 -1.817456000 0.111029000

C 5.129097000 -1.651565000 0.562829000

C 3.367870000 -3.087213000 -0.265045000

C 5.980805000 -2.749981000 0.654216000

H 5.499765000 -0.658577000 0.833488000

C 4.224568000 -4.185374000 -0.175023000

H 2.348047000 -3.214408000 -0.637700000

C 5.528131000 -4.018405000 0.287219000

H 7.005948000 -2.615113000 1.008326000

H 3.868465000 -5.175232000 -0.470572000

H 6.198540000 -4.878658000 0.357284000

H 0.559587000 -1.777845000 -1.689152000

H -2.232520000 1.222379000 -1.529746000

**Table S16. Ru(CO)2(dpae)(PhCH=CPh-CPh=CHPh) (10)** (-6875.327414)

Ru -0.976374000 -0.872787000 0.195345000

As -2.554246000 0.902332000 -0.597582000

As 0.084183000 -0.393951000 -2.093306000

C -1.284011000 0.603495000 -3.144453000

H -0.904487000 1.634821000 -3.201257000

H -1.283855000 0.200349000 -4.167935000

C -2.669195000 0.576800000 -2.533849000

H -3.141637000 -0.412682000 -2.631958000

H -3.335192000 1.311108000 -3.012520000

C -1.834166000 -2.327057000 -0.663215000

O -2.361430000 -3.273106000 -1.058863000

C 0.776804000 -0.497987000 1.627269000

C 0.698504000 -1.860264000 1.112455000

H 1.436269000 -2.028186000 0.322238000

H 1.030767000 2.090614000 1.703060000

C 0.492539000 -3.137234000 1.848314000

C 1.143095000 -4.280796000 1.347170000

C -0.287149000 -3.304909000 3.006914000

C 1.012990000 -5.528201000 1.952764000

H 1.779741000 -4.179787000 0.462782000

C -0.413978000 -4.550099000 3.617371000

H -0.804656000 -2.454901000 3.449266000

C 0.229127000 -5.672202000 3.095422000

H 1.533688000 -6.391776000 1.530264000

H -1.029110000 -4.641668000 4.516428000

H 0.121899000 -6.647279000 3.576853000

C 0.411830000 -0.169952000 3.063762000

C 1.202591000 -0.681254000 4.107969000

C -0.621768000 0.704387000 3.421363000

C 0.957136000 -0.354383000 5.438194000

H 2.025234000 -1.359525000 3.874005000

C -0.869373000 1.045942000 4.751769000

H -1.253086000 1.118185000 2.632601000

C -0.082843000 0.514654000 5.769375000

H 1.586114000 -0.781788000 6.223454000

H -1.689567000 1.728355000 4.989386000

H -0.276328000 0.774456000 6.813057000

C 1.999168000 0.312615000 1.237887000

C 2.000126000 1.657054000 1.437760000

C 3.091797000 2.638808000 1.442993000

C 2.803453000 3.971711000 1.095489000

C 4.402116000 2.349055000 1.867340000

C 3.781876000 4.962190000 1.128120000

H 1.785210000 4.228585000 0.789070000

C 5.378662000 3.338923000 1.905419000

H 4.650026000 1.335986000 2.187480000

C 5.079941000 4.649303000 1.528238000

H 3.526698000 5.987351000 0.846200000

H 6.386180000 3.085395000 2.245459000

H 5.850620000 5.423335000 1.561448000

C 3.234864000 -0.398880000 0.792731000

C 3.695281000 -1.556454000 1.444787000

C 4.004689000 0.094584000 -0.271825000

C 4.880024000 -2.180567000 1.062461000

H 3.118728000 -1.979924000 2.268151000

C 5.185407000 -0.532342000 -0.662027000

H 3.673801000 0.993347000 -0.791144000

C 5.632630000 -1.671927000 0.004369000

H 5.213797000 -3.073924000 1.596418000

H 5.759284000 -0.121879000 -1.496694000

H 6.559884000 -2.163693000 -0.300547000

C -2.131250000 -1.146540000 1.646733000

O -2.941267000 -1.316435000 2.443364000

C -4.421102000 0.735545000 -0.070190000

C -5.110895000 1.778273000 0.556396000

C -5.070747000 -0.487763000 -0.279554000

C -6.436281000 1.603419000 0.955339000

H -4.615628000 2.735366000 0.736766000

C -6.396965000 -0.655634000 0.112394000

H -4.540871000 -1.326132000 -0.740465000

C -7.082683000 0.389837000 0.730583000

H -6.965104000 2.424076000 1.446567000

H -6.893709000 -1.613777000 -0.058563000

H -8.120882000 0.254830000 1.043542000

C -2.309808000 2.841028000 -0.533440000

C -2.989276000 3.711203000 -1.396182000

C -1.432361000 3.371754000 0.416223000

C -2.787246000 5.087598000 -1.309836000

H -3.693413000 3.320862000 -2.135880000

C -1.240795000 4.751211000 0.512722000

H -0.893189000 2.694789000 1.084193000

C -1.914860000 5.609584000 -0.353578000

H -3.319545000 5.757904000 -1.989460000

H -0.562274000 5.153495000 1.269222000

H -1.763214000 6.689548000 -0.283452000

C 1.588331000 0.760480000 -2.554261000

C 1.570188000 2.072008000 -2.063923000

C 2.644937000 0.346111000 -3.369508000

C 2.585994000 2.963600000 -2.403648000

H 0.764483000 2.400660000 -1.400468000

C 3.658937000 1.242271000 -3.710558000

H 2.686384000 -0.679985000 -3.740561000

C 3.630698000 2.550611000 -3.231355000

H 2.570118000 3.980344000 -2.005686000

H 4.479207000 0.910006000 -4.351971000

H 4.428335000 3.249566000 -3.494261000

C 0.430980000 -1.948816000 -3.216195000

C 0.652898000 -3.186937000 -2.605691000

C 0.472353000 -1.861521000 -4.614136000

C 0.909412000 -4.320302000 -3.377567000

H 0.611420000 -3.271491000 -1.517282000

C 0.723920000 -2.995074000 -5.384706000

H 0.320368000 -0.902231000 -5.116220000

C 0.942968000 -4.226683000 -4.766956000

H 1.075823000 -5.281544000 -2.885601000

H 0.750258000 -2.915050000 -6.474343000

H 1.138453000 -5.115351000 -5.372169000

**Table S17 Compound 1 Molfile**

RuC29As2H24O3 - Chemcraft

59 63 0 0 0 0 0 0 0 0 1 V2000

0.0335 -0.3748 1.4585 Ru 0 0 0 0 0 0 0 0 0 0 0 0

-0.4179 -2.2337 1.5861 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6937 -3.3406 1.7508 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.8341 0.9372 2.5465 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.3800 1.6649 3.2561 O 0 0 0 0 0 0 0 0 0 0 0 0

1.4300 -0.5393 2.7296 C 0 0 0 0 0 0 0 0 0 0 0 0

2.2846 -0.6328 3.4906 O 0 0 0 0 0 0 0 0 0 0 0 0

1.6617 -0.0047 -0.3529 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.6106 0.0086 -0.3569 As 0 0 0 0 0 0 0 0 0 0 0 0

-0.6260 0.4226 -2.0189 C 0 0 0 0 0 0 0 0 0 0 0 0

0.7165 -0.2776 -2.0654 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4981 1.5167 -1.9935 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2548 0.1978 -2.8935 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3395 0.0906 -2.8949 H 0 0 0 0 0 0 0 0 0 0 0 0

0.6076 -1.3674 -2.1825 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.8243 1.5287 -0.2929 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1762 1.4189 -0.6306 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3061 2.7716 0.0893 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.9997 2.5445 -0.5899 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.5935 0.4526 -0.9242 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.1302 3.8943 0.1212 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.2535 2.8613 0.3743 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.4789 3.7818 -0.2166 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.0567 2.4505 -0.8514 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7180 4.8605 0.4222 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.1267 4.6613 -0.1833 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.8185 -1.4439 -0.8219 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.0430 -1.8689 -2.1351 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4897 -2.0831 0.2281 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9246 -2.9190 -2.3942 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.5336 -1.3882 -2.9733 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.3777 -3.1242 -0.0337 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.3095 -1.7698 1.2605 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.5945 -3.5458 -1.3453 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.0875 -3.2473 -3.4238 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.8949 -3.6151 0.7942 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.2843 -4.3683 -1.5498 H 0 0 0 0 0 0 0 0 0 0 0 0

2.4585 1.7566 -0.6363 C 0 0 0 0 0 0 0 0 0 0 0 0

3.1487 2.0986 -1.8067 C 0 0 0 0 0 0 0 0 0 0 0 0

2.2929 2.7163 0.3659 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6654 3.3833 -1.9671 C 0 0 0 0 0 0 0 0 0 0 0 0

3.2953 1.3601 -2.6003 H 0 0 0 0 0 0 0 0 0 0 0 0

2.8163 4.0002 0.2075 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7379 2.4457 1.2708 H 0 0 0 0 0 0 0 0 0 0 0 0

3.5012 4.3347 -0.9591 C 0 0 0 0 0 0 0 0 0 0 0 0

4.2010 3.6433 -2.8838 H 0 0 0 0 0 0 0 0 0 0 0 0

2.6848 4.7420 0.9993 H 0 0 0 0 0 0 0 0 0 0 0 0

3.9084 5.3409 -1.0865 H 0 0 0 0 0 0 0 0 0 0 0 0

3.1796 -1.2087 -0.5586 C 0 0 0 0 0 0 0 0 0 0 0 0

4.5051 -0.7722 -0.6400 C 0 0 0 0 0 0 0 0 0 0 0 0

2.9078 -2.5827 -0.5627 C 0 0 0 0 0 0 0 0 0 0 0 0

5.5427 -1.7000 -0.7455 C 0 0 0 0 0 0 0 0 0 0 0 0

4.7368 0.2951 -0.6154 H 0 0 0 0 0 0 0 0 0 0 0 0

3.9443 -3.5054 -0.6806 C 0 0 0 0 0 0 0 0 0 0 0 0

1.8777 -2.9356 -0.4508 H 0 0 0 0 0 0 0 0 0 0 0 0

5.2650 -3.0650 -0.7732 C 0 0 0 0 0 0 0 0 0 0 0 0

6.5764 -1.3496 -0.8033 H 0 0 0 0 0 0 0 0 0 0 0 0

3.7200 -4.5750 -0.6865 H 0 0 0 0 0 0 0 0 0 0 0 0

6.0795 -3.7887 -0.8560 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 8 1 0 0 0 0

1 9 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 7 3 0 0 0 0

8 11 1 0 0 0 0

8 38 1 0 0 0 0

8 49 1 0 0 0 0

9 10 1 0 0 0 0

9 16 1 0 0 0 0

9 27 1 0 0 0 0

10 11 1 0 0 0 0

10 12 1 0 0 0 0

10 13 1 0 0 0 0

11 14 1 0 0 0 0

11 15 1 0 0 0 0

16 17 2 0 0 0 0

16 18 1 0 0 0 0

17 19 1 0 0 0 0

17 20 1 0 0 0 0

18 21 2 0 0 0 0

18 22 1 0 0 0 0

19 23 2 0 0 0 0

19 24 1 0 0 0 0

21 23 1 0 0 0 0

21 25 1 0 0 0 0

23 26 1 0 0 0 0

27 28 2 0 0 0 0

27 29 1 0 0 0 0

28 30 1 0 0 0 0

28 31 1 0 0 0 0

29 32 2 0 0 0 0

29 33 1 0 0 0 0

30 34 2 0 0 0 0

30 35 1 0 0 0 0

32 34 1 0 0 0 0

32 36 1 0 0 0 0

34 37 1 0 0 0 0

38 39 2 0 0 0 0

38 40 1 0 0 0 0

39 41 1 0 0 0 0

39 42 1 0 0 0 0

40 43 2 0 0 0 0

40 44 1 0 0 0 0

41 45 2 0 0 0 0

41 46 1 0 0 0 0

43 45 1 0 0 0 0

43 47 1 0 0 0 0

45 48 1 0 0 0 0

49 50 2 0 0 0 0

49 51 1 0 0 0 0

50 52 1 0 0 0 0

50 53 1 0 0 0 0

51 54 2 0 0 0 0

51 55 1 0 0 0 0

52 56 2 0 0 0 0

52 57 1 0 0 0 0

54 56 1 0 0 0 0

54 58 1 0 0 0 0

56 59 1 0 0 0 0

M END

**Table S18 Compound trans-cis-3 Molfile**

RuC28As2H26O2 - Chemcraft

59 63 0 0 0 0 0 0 0 0 1 V2000

0.0064 -0.2996 1.6302 Ru 0 0 0 0 0 0 0 0 0 0 0 0

0.1975 -2.2026 1.7014 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3103 -3.3286 1.8873 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.2123 1.4254 2.4258 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.3546 2.3875 3.0357 O 0 0 0 0 0 0 0 0 0 0 0 0

1.6648 -0.0004 -0.1831 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.6463 -0.0719 -0.2026 As 0 0 0 0 0 0 0 0 0 0 0 0

-0.6478 0.3098 -1.8739 C 0 0 0 0 0 0 0 0 0 0 0 0

0.7144 -0.3619 -1.8798 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5439 1.4063 -1.9085 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2508 0.0148 -2.7458 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3210 -0.0153 -2.7313 H 0 0 0 0 0 0 0 0 0 0 0 0

0.6198 -1.4579 -1.9517 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9250 1.3983 -0.2196 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3067 1.1924 -0.2710 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.4312 2.7050 -0.1186 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.1803 2.2802 -0.2357 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7085 0.1785 -0.3381 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.3049 3.7895 -0.0914 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.3536 2.8838 -0.0520 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.6826 3.5786 -0.1501 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.2589 2.1079 -0.2743 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9072 4.8045 -0.0153 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.3688 4.4287 -0.1228 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7718 -1.5856 -0.6858 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.3661 -1.7092 -1.9481 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9978 -2.5750 0.2761 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1643 -2.8125 -2.2449 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2189 -0.9377 -2.7089 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.8006 -3.6768 -0.0207 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.5403 -2.4790 1.2643 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.3812 -3.7984 -1.2816 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.6215 -2.9018 -3.2337 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.9689 -4.4446 0.7385 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.0063 -4.6637 -1.5160 H 0 0 0 0 0 0 0 0 0 0 0 0

2.4990 1.7208 -0.5862 C 0 0 0 0 0 0 0 0 0 0 0 0

3.4136 1.8592 -1.6374 C 0 0 0 0 0 0 0 0 0 0 0 0

2.1698 2.8390 0.1841 C 0 0 0 0 0 0 0 0 0 0 0 0

3.9761 3.1017 -1.9216 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7057 0.9899 -2.2333 H 0 0 0 0 0 0 0 0 0 0 0 0

2.7346 4.0837 -0.1005 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4765 2.7365 1.0221 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6351 4.2169 -1.1548 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6904 3.1990 -2.7432 H 0 0 0 0 0 0 0 0 0 0 0 0

2.4716 4.9502 0.5112 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0795 5.1902 -1.3770 H 0 0 0 0 0 0 0 0 0 0 0 0

3.1868 -1.2054 -0.2953 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8428 -1.5280 0.8982 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6382 -1.7632 -1.4971 C 0 0 0 0 0 0 0 0 0 0 0 0

4.9442 -2.3819 0.8874 C 0 0 0 0 0 0 0 0 0 0 0 0

3.4759 -1.1168 1.8434 H 0 0 0 0 0 0 0 0 0 0 0 0

4.7367 -2.6231 -1.5044 C 0 0 0 0 0 0 0 0 0 0 0 0

3.1327 -1.5399 -2.4399 H 0 0 0 0 0 0 0 0 0 0 0 0

5.3932 -2.9300 -0.3137 C 0 0 0 0 0 0 0 0 0 0 0 0

5.4488 -2.6273 1.8251 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0789 -3.0576 -2.4472 H 0 0 0 0 0 0 0 0 0 0 0 0

6.2528 -3.6047 -0.3211 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1366 -0.4106 2.7903 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.1380 -0.6131 2.7368 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

1 58 1 0 0 0 0

1 59 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

M END

**Table S19 Compound SP4-2’ Molfile**

RuC45As2PH39O - Chemcraft

89 96 0 0 0 0 0 0 0 0 1 V2000

-0.3791 0.5298 -0.4088 Ru 0 0 0 0 0 0 0 0 0 0 0 0

-0.8924 1.4433 -1.9148 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1914 1.8552 -2.9632 O 0 0 0 0 0 0 0 0 0 0 0 0

-2.6274 -0.2030 0.0211 As 0 0 0 0 0 0 0 0 0 0 0 0

0.1538 -1.8031 0.0888 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.4994 -2.7653 0.6492 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7103 -2.1819 -0.0486 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.5912 -2.6440 1.7399 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.3704 -3.8376 0.4358 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.6570 -2.5368 0.3875 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7202 -2.4371 -1.1205 H 0 0 0 0 0 0 0 0 0 0 0 0

1.4522 -2.6026 1.3243 C 0 0 0 0 0 0 0 0 0 0 0 0

2.7800 -2.7950 0.9195 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1126 -2.8600 2.6593 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7381 -3.2516 1.8238 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0751 -2.5847 -0.1122 H 0 0 0 0 0 0 0 0 0 0 0 0

2.0716 -3.3190 3.5624 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0908 -2.6990 3.0127 H 0 0 0 0 0 0 0 0 0 0 0 0

3.3873 -3.5182 3.1466 C 0 0 0 0 0 0 0 0 0 0 0 0

4.7683 -3.3953 1.4882 H 0 0 0 0 0 0 0 0 0 0 0 0

1.7861 -3.5231 4.5978 H 0 0 0 0 0 0 0 0 0 0 0 0

4.1390 -3.8773 3.8540 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5429 -2.8152 -1.5427 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9076 -4.1661 -1.5110 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3761 -2.1767 -2.7749 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1105 -4.8656 -2.7002 C 0 0 0 0 0 0 0 0 0 0 0 0

1.0436 -4.6773 -0.5535 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5766 -2.8790 -3.9643 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0832 -1.1196 -2.7763 H 0 0 0 0 0 0 0 0 0 0 0 0

0.9459 -4.2229 -3.9281 C 0 0 0 0 0 0 0 0 0 0 0 0

1.3990 -5.9195 -2.6680 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4435 -2.3713 -4.9233 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1054 -4.7734 -4.8589 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.1594 0.1373 1.8644 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3871 1.0416 2.6030 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.2280 -0.5193 2.4868 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6785 1.2863 3.9451 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.5493 1.5523 2.1146 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.5203 -0.2717 3.8278 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.8450 -1.2266 1.9251 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.7455 0.6306 4.5578 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.0647 1.9909 4.5116 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.3574 -0.7870 4.3057 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.9755 0.8216 5.6091 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.1974 0.2696 -1.0244 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1660 0.0039 -2.3991 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.3191 0.8957 -0.4728 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2528 0.3365 -3.2046 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2793 -0.4512 -2.8507 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.4033 1.2339 -1.2836 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.3500 1.1270 0.5948 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.3746 0.9507 -2.6478 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2176 0.1250 -4.2762 H 0 0 0 0 0 0 0 0 0 0 0 0

-7.2752 1.7247 -0.8436 H 0 0 0 0 0 0 0 0 0 0 0 0

-7.2245 1.2170 -3.2811 H 0 0 0 0 0 0 0 0 0 0 0 0

1.7044 1.5171 -0.2536 P 0 0 0 0 0 0 0 0 0 0 0 0

3.2567 0.5796 -0.5781 C 0 0 0 0 0 0 0 0 0 0 0 0

4.3553 0.5723 0.2890 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3272 -0.1523 -1.7718 C 0 0 0 0 0 0 0 0 0 0 0 0

5.5010 -0.1573 -0.0313 C 0 0 0 0 0 0 0 0 0 0 0 0

4.3166 1.1359 1.2244 H 0 0 0 0 0 0 0 0 0 0 0 0

4.4755 -0.8715 -2.0956 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4668 -0.1646 -2.4462 H 0 0 0 0 0 0 0 0 0 0 0 0

5.5652 -0.8779 -1.2231 C 0 0 0 0 0 0 0 0 0 0 0 0

6.3500 -0.1596 0.6571 H 0 0 0 0 0 0 0 0 0 0 0 0

4.5144 -1.4369 -3.0300 H 0 0 0 0 0 0 0 0 0 0 0 0

6.4645 -1.4466 -1.4728 H 0 0 0 0 0 0 0 0 0 0 0 0

2.0486 3.1150 -1.1118 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9866 4.0081 -1.3045 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3280 3.4782 -1.5508 C 0 0 0 0 0 0 0 0 0 0 0 0

1.2006 5.2432 -1.9124 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.0168 3.7205 -0.9778 H 0 0 0 0 0 0 0 0 0 0 0 0

3.5379 4.7102 -2.1699 C 0 0 0 0 0 0 0 0 0 0 0 0

4.1687 2.7943 -1.4148 H 0 0 0 0 0 0 0 0 0 0 0 0

2.4769 5.5961 -2.3497 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3608 5.9275 -2.0560 H 0 0 0 0 0 0 0 0 0 0 0 0

4.5400 4.9774 -2.5149 H 0 0 0 0 0 0 0 0 0 0 0 0

2.6435 6.5600 -2.8372 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8216 1.9793 1.5290 C 0 0 0 0 0 0 0 0 0 0 0 0

1.8681 3.3100 1.9647 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7827 0.9541 2.4889 C 0 0 0 0 0 0 0 0 0 0 0 0

1.8662 3.6085 3.3272 C 0 0 0 0 0 0 0 0 0 0 0 0

1.9059 4.1216 1.2350 H 0 0 0 0 0 0 0 0 0 0 0 0

1.7870 1.2563 3.8490 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7583 -0.0904 2.1704 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8237 2.5850 4.2727 C 0 0 0 0 0 0 0 0 0 0 0 0

1.9018 4.6522 3.6500 H 0 0 0 0 0 0 0 0 0 0 0 0

1.7622 0.4438 4.5794 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8254 2.8223 5.3397 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 5 1 0 0 0 0

1 56 1 0 0 0 0

2 3 3 0 0 0 0

4 7 1 0 0 0 0

4 34 1 0 0 0 0

4 45 1 0 0 0 0

5 6 1 0 0 0 0

5 12 1 0 0 0 0

5 23 1 0 0 0 0

6 7 1 0 0 0 0

6 8 1 0 0 0 0

6 9 1 0 0 0 0

7 10 1 0 0 0 0

7 11 1 0 0 0 0

12 13 2 0 0 0 0

12 14 1 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

14 17 2 0 0 0 0

14 18 1 0 0 0 0

15 19 2 0 0 0 0

15 20 1 0 0 0 0

17 19 1 0 0 0 0

17 21 1 0 0 0 0

19 22 1 0 0 0 0

23 24 2 0 0 0 0

23 25 1 0 0 0 0

24 26 1 0 0 0 0

24 27 1 0 0 0 0

25 28 2 0 0 0 0

25 29 1 0 0 0 0

26 30 2 0 0 0 0

26 31 1 0 0 0 0

28 30 1 0 0 0 0

28 32 1 0 0 0 0

30 33 1 0 0 0 0

34 35 2 0 0 0 0

34 36 1 0 0 0 0

35 37 1 0 0 0 0

35 38 1 0 0 0 0

36 39 2 0 0 0 0

36 40 1 0 0 0 0

37 41 2 0 0 0 0

37 42 1 0 0 0 0

39 41 1 0 0 0 0

39 43 1 0 0 0 0

41 44 1 0 0 0 0

45 46 2 0 0 0 0

45 47 1 0 0 0 0

46 48 1 0 0 0 0

46 49 1 0 0 0 0

47 50 2 0 0 0 0

47 51 1 0 0 0 0

48 52 2 0 0 0 0

48 53 1 0 0 0 0

50 52 1 0 0 0 0

50 54 1 0 0 0 0

52 55 1 0 0 0 0

56 57 1 0 0 0 0

56 68 1 0 0 0 0

56 79 1 0 0 0 0

57 58 2 0 0 0 0

57 59 1 0 0 0 0

58 60 1 0 0 0 0

58 61 1 0 0 0 0

59 62 2 0 0 0 0

59 63 1 0 0 0 0

60 64 2 0 0 0 0

60 65 1 0 0 0 0

62 64 1 0 0 0 0

62 66 1 0 0 0 0

64 67 1 0 0 0 0

68 69 2 0 0 0 0

68 70 1 0 0 0 0

69 71 1 0 0 0 0

69 72 1 0 0 0 0

70 73 2 0 0 0 0

70 74 1 0 0 0 0

71 75 2 0 0 0 0

71 76 1 0 0 0 0

73 75 1 0 0 0 0

73 77 1 0 0 0 0

75 78 1 0 0 0 0

79 80 2 0 0 0 0

79 81 1 0 0 0 0

80 82 1 0 0 0 0

80 83 1 0 0 0 0

81 84 2 0 0 0 0

81 85 1 0 0 0 0

82 86 2 0 0 0 0

82 87 1 0 0 0 0

84 86 1 0 0 0 0

84 88 1 0 0 0 0

86 89 1 0 0 0 0

M END

**Table S20 Compound TP-1’ Molfile**

RuC28As2H24O2 - Chemcraft

57 61 0 0 0 0 0 0 0 0 1 V2000

-0.0665 -0.4618 1.5218 Ru 0 0 0 0 0 0 0 0 0 0 0 0

-0.4756 -2.3180 1.4983 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.7465 -3.4405 1.5880 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.8610 0.9147 2.5755 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.3886 1.6464 3.3015 O 0 0 0 0 0 0 0 0 0 0 0 0

1.8109 -0.0945 -0.0558 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.5234 -0.0516 -0.2564 As 0 0 0 0 0 0 0 0 0 0 0 0

-0.4097 0.2680 -1.8632 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9338 -0.4346 -1.7994 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.2786 1.3614 -1.8892 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.9789 -0.0035 -2.7651 H 0 0 0 0 0 0 0 0 0 0 0 0

1.5926 -0.1007 -2.6159 H 0 0 0 0 0 0 0 0 0 0 0 0

0.8282 -1.5279 -1.8773 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.5999 1.5694 -0.2436 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9764 1.5437 -0.4836 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.9643 2.7909 0.0092 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7090 2.7314 -0.4747 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.4838 0.5956 -0.6771 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6984 3.9744 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8909 2.8185 0.2202 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.0723 3.9462 -0.2302 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.7857 2.7034 -0.6594 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.1950 4.9236 0.2099 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.6484 4.8748 -0.2228 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.8336 -1.3975 -0.7616 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1518 -1.6805 -2.0941 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5061 -2.0720 0.2637 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1238 -2.6340 -2.3965 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6503 -1.1590 -2.9125 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.4834 -3.0176 -0.0413 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2534 -1.8594 1.3063 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7907 -3.3026 -1.3711 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3608 -2.8535 -3.4405 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.0009 -3.5402 0.7668 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.5513 -4.0502 -1.6098 H 0 0 0 0 0 0 0 0 0 0 0 0

2.5944 1.6663 -0.4044 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3561 1.9560 -1.5443 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3301 2.6852 0.5155 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8442 3.2445 -1.7564 C 0 0 0 0 0 0 0 0 0 0 0 0

3.5805 1.1714 -2.2731 H 0 0 0 0 0 0 0 0 0 0 0 0

2.8227 3.9744 0.3058 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7215 2.4580 1.3981 H 0 0 0 0 0 0 0 0 0 0 0 0

3.5787 4.2550 -0.8307 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4362 3.4617 -2.6493 H 0 0 0 0 0 0 0 0 0 0 0 0

2.6119 4.7622 1.0337 H 0 0 0 0 0 0 0 0 0 0 0 0

3.9628 5.2644 -0.9985 H 0 0 0 0 0 0 0 0 0 0 0 0

3.3565 -1.2799 -0.1960 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6805 -0.8291 -0.1984 C 0 0 0 0 0 0 0 0 0 0 0 0

3.1045 -2.6583 -0.2082 C 0 0 0 0 0 0 0 0 0 0 0 0

5.7342 -1.7438 -0.2384 C 0 0 0 0 0 0 0 0 0 0 0 0

4.8979 0.2411 -0.1654 H 0 0 0 0 0 0 0 0 0 0 0 0

4.1576 -3.5686 -0.2606 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0743 -3.0252 -0.1562 H 0 0 0 0 0 0 0 0 0 0 0 0

5.4761 -3.1127 -0.2772 C 0 0 0 0 0 0 0 0 0 0 0 0

6.7650 -1.3803 -0.2379 H 0 0 0 0 0 0 0 0 0 0 0 0

3.9468 -4.6409 -0.2761 H 0 0 0 0 0 0 0 0 0 0 0 0

6.3030 -3.8263 -0.3099 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

M END

**Table S21 Compound SP-1’ Molfile**

RuC28As2H24O2 - Chemcraft

57 61 0 0 0 0 0 0 0 0 1 V2000

0.0287 -0.2611 1.5658 Ru 0 0 0 0 0 0 0 0 0 0 0 0

1.3254 -1.0274 2.6714 C 0 0 0 0 0 0 0 0 0 0 0 0

2.1150 -1.5703 3.3153 O 0 0 0 0 0 0 0 0 0 0 0 0

-1.3097 -0.6579 2.8108 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.1504 -0.8965 3.5663 O 0 0 0 0 0 0 0 0 0 0 0 0

-1.6041 0.0794 -0.2732 As 0 0 0 0 0 0 0 0 0 0 0 0

1.6642 0.1457 -0.2555 As 0 0 0 0 0 0 0 0 0 0 0 0

0.7086 -0.0506 -1.9715 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6408 0.6413 -1.9061 C 0 0 0 0 0 0 0 0 0 0 0 0

0.5964 -1.1367 -2.1203 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3299 0.3299 -2.7968 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2566 0.4137 -2.7903 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.5184 1.7350 -1.8426 H 0 0 0 0 0 0 0 0 0 0 0 0

3.1955 -1.0166 -0.5321 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4518 -0.5527 -0.9321 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0037 -2.3844 -0.3029 C 0 0 0 0 0 0 0 0 0 0 0 0

5.5011 -1.4532 -1.1176 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6214 0.5151 -1.0904 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0523 -3.2812 -0.4966 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0305 -2.7440 0.0467 H 0 0 0 0 0 0 0 0 0 0 0 0

5.3022 -2.8165 -0.9055 C 0 0 0 0 0 0 0 0 0 0 0 0

6.4826 -1.0840 -1.4257 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8952 -4.3471 -0.3144 H 0 0 0 0 0 0 0 0 0 0 0 0

6.1270 -3.5188 -1.0494 H 0 0 0 0 0 0 0 0 0 0 0 0

2.3952 1.9430 -0.3794 C 0 0 0 0 0 0 0 0 0 0 0 0

2.8526 2.5067 -1.5770 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4345 2.7034 0.7958 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3500 3.8092 -1.5956 C 0 0 0 0 0 0 0 0 0 0 0 0

2.8281 1.9324 -2.5071 H 0 0 0 0 0 0 0 0 0 0 0 0

2.9344 4.0052 0.7750 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0613 2.2686 1.7288 H 0 0 0 0 0 0 0 0 0 0 0 0

3.3928 4.5584 -0.4196 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7056 4.2415 -2.5343 H 0 0 0 0 0 0 0 0 0 0 0 0

2.9608 4.5906 1.6972 H 0 0 0 0 0 0 0 0 0 0 0 0

3.7822 5.5794 -0.4366 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.4396 -1.5714 -0.8849 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4627 -1.5705 -1.8399 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.9756 -2.7834 -0.3651 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.0070 -2.7759 -2.2792 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8497 -0.6264 -2.2347 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.5232 -3.9881 -0.8081 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1875 -2.7630 0.3971 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.5362 -3.9853 -1.7653 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.8085 -2.7713 -3.0223 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.1598 -4.9331 -0.3963 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.9679 -4.9289 -2.1088 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.1259 1.2919 -0.2322 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9468 1.2672 0.9029 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4230 2.1810 -1.2709 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.0516 2.1114 0.9902 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.7221 0.5874 1.7295 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.5271 3.0296 -1.1778 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7964 2.2240 -2.1647 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.3433 2.9948 -0.0492 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.6849 2.0822 1.8803 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7487 3.7214 -1.9943 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.2073 3.6600 0.0230 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

M END

**Table S22 Compound Eq 2 Molfile**

RuC46As2PH39O2 - Chemcraft

91 98 0 0 0 0 0 0 0 0 1 V2000

0.2421 0.0947 -1.0850 Ru 0 0 0 0 0 0 0 0 0 0 0 0

0.0242 1.3138 -2.5004 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.1142 2.0611 -3.3758 O 0 0 0 0 0 0 0 0 0 0 0 0

0.8106 -1.1964 -2.3271 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1878 -1.9753 -3.0896 O 0 0 0 0 0 0 0 0 0 0 0 0

2.0262 -0.6195 0.4458 As 0 0 0 0 0 0 0 0 0 0 0 0

0.1779 2.0280 0.4573 As 0 0 0 0 0 0 0 0 0 0 0 0

0.9693 1.4890 2.1812 C 0 0 0 0 0 0 0 0 0 0 0 0

2.2257 0.6753 1.9411 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1956 0.9063 2.7060 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1902 2.3896 2.7757 H 0 0 0 0 0 0 0 0 0 0 0 0

2.5426 0.1280 2.8420 H 0 0 0 0 0 0 0 0 0 0 0 0

3.0599 1.3261 1.6365 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.4485 2.9563 0.9942 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.4301 3.1570 0.0170 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.6802 3.4070 2.3000 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6243 3.7997 0.3389 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.2670 2.7924 -1.0006 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.8777 4.0475 2.6206 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.9306 3.2583 3.0812 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.8503 4.2443 1.6410 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3854 3.9407 -0.4322 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0510 4.3937 3.6428 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7894 4.7422 1.8951 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3243 3.5496 0.0074 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1490 4.8076 0.5954 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3778 3.3514 -0.8891 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0246 5.8499 0.2949 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3176 4.9843 1.2830 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2557 4.3946 -1.1845 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4965 2.3714 -1.3622 H 0 0 0 0 0 0 0 0 0 0 0 0

3.0808 5.6442 -0.5930 C 0 0 0 0 0 0 0 0 0 0 0 0

1.8771 6.8310 0.7538 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0769 4.2282 -1.8862 H 0 0 0 0 0 0 0 0 0 0 0 0

3.7649 6.4633 -0.8288 H 0 0 0 0 0 0 0 0 0 0 0 0

1.9975 -2.3369 1.3846 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6411 -3.4574 0.8437 C 0 0 0 0 0 0 0 0 0 0 0 0

1.2293 -2.4887 2.5446 C 0 0 0 0 0 0 0 0 0 0 0 0

2.5311 -4.7022 1.4635 C 0 0 0 0 0 0 0 0 0 0 0 0

3.2398 -3.3593 -0.0662 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1265 -3.7324 3.1669 C 0 0 0 0 0 0 0 0 0 0 0 0

0.6881 -1.6371 2.9671 H 0 0 0 0 0 0 0 0 0 0 0 0

1.7777 -4.8417 2.6288 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0419 -5.5677 1.0335 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5249 -3.8333 4.0736 H 0 0 0 0 0 0 0 0 0 0 0 0

1.6948 -5.8167 3.1154 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8711 -0.6418 -0.2078 C 0 0 0 0 0 0 0 0 0 0 0 0

4.1330 -0.2264 -1.5150 C 0 0 0 0 0 0 0 0 0 0 0 0

4.9368 -1.0105 0.6235 C 0 0 0 0 0 0 0 0 0 0 0 0

5.4447 -0.1808 -1.9904 C 0 0 0 0 0 0 0 0 0 0 0 0

3.2945 0.0646 -2.1567 H 0 0 0 0 0 0 0 0 0 0 0 0

6.2465 -0.9582 0.1502 C 0 0 0 0 0 0 0 0 0 0 0 0

4.7459 -1.3499 1.6458 H 0 0 0 0 0 0 0 0 0 0 0 0

6.5016 -0.5441 -1.1583 C 0 0 0 0 0 0 0 0 0 0 0 0

5.6389 0.1393 -3.0173 H 0 0 0 0 0 0 0 0 0 0 0 0

7.0732 -1.2450 0.8052 H 0 0 0 0 0 0 0 0 0 0 0 0

7.5291 -0.5078 -1.5292 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.7659 -1.0428 -0.4664 P 0 0 0 0 0 0 0 0 0 0 0 0

-3.3476 -0.2717 -1.0482 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.5534 -0.3815 -0.3429 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.3445 0.4138 -2.2699 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.7222 0.1940 -0.8417 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.5843 -0.9188 0.6073 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.5153 0.9760 -2.7755 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.4071 0.5139 -2.8224 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.7077 0.8737 -2.0586 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.6518 0.1057 -0.2736 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.4913 1.5033 -3.7326 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.6250 1.3220 -2.4490 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.8942 -2.7321 -1.2056 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8321 -3.6274 -1.0081 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9946 -3.1520 -1.9620 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8774 -4.9131 -1.5403 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0415 -3.3159 -0.4295 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0298 -4.4351 -2.5097 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8326 -2.4735 -2.1325 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.9756 -5.3203 -2.2981 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.0411 -5.5956 -1.3695 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.8927 -4.7421 -3.1063 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.0056 -6.3246 -2.7279 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.1925 -1.3959 1.3042 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3247 -2.6848 1.8334 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3641 -0.3010 2.1654 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6039 -2.8714 3.1892 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.2113 -3.5564 1.1865 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6517 -0.4866 3.5145 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.2950 0.7139 1.7675 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7652 -1.7774 4.0356 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7019 -3.8872 3.5813 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7943 0.3839 4.1604 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9887 -1.9271 5.0949 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

1 58 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

58 59 1 0 0 0 0

58 70 1 0 0 0 0

58 81 1 0 0 0 0

59 60 2 0 0 0 0

59 61 1 0 0 0 0

60 62 1 0 0 0 0

60 63 1 0 0 0 0

61 64 2 0 0 0 0

61 65 1 0 0 0 0

62 66 2 0 0 0 0

62 67 1 0 0 0 0

64 66 1 0 0 0 0

64 68 1 0 0 0 0

66 69 1 0 0 0 0

70 71 2 0 0 0 0

70 72 1 0 0 0 0

71 73 1 0 0 0 0

71 74 1 0 0 0 0

72 75 2 0 0 0 0

72 76 1 0 0 0 0

73 77 2 0 0 0 0

73 78 1 0 0 0 0

75 77 1 0 0 0 0

75 79 1 0 0 0 0

77 80 1 0 0 0 0

81 82 2 0 0 0 0

81 83 1 0 0 0 0

82 84 1 0 0 0 0

82 85 1 0 0 0 0

83 86 2 0 0 0 0

83 87 1 0 0 0 0

84 88 2 0 0 0 0

84 89 1 0 0 0 0

86 88 1 0 0 0 0

86 90 1 0 0 0 0

88 91 1 0 0 0 0

M END

**Table S23 Compound Cis-Cis-3 Molfile**

RuC28As2H26O2 - Chemcraft

59 63 0 0 0 0 0 0 0 0 1 V2000

-0.0100 -0.4472 1.5494 Ru 0 0 0 0 0 0 0 0 0 0 0 0

1.1360 -1.1738 2.8600 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7975 -1.6716 3.6549 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.3314 1.2410 2.4246 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5736 2.2079 2.9964 O 0 0 0 0 0 0 0 0 0 0 0 0

1.6151 -0.0436 -0.2720 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.6799 -0.1799 -0.2238 As 0 0 0 0 0 0 0 0 0 0 0 0

-0.7292 0.1895 -1.9211 C 0 0 0 0 0 0 0 0 0 0 0 0

0.6390 -0.4695 -1.9341 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6390 1.2852 -1.9926 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.3521 -0.1462 -2.7640 H 0 0 0 0 0 0 0 0 0 0 0 0

1.2282 -0.1433 -2.8055 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5490 -1.5672 -1.9638 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9721 1.2746 -0.1728 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3396 1.0454 0.0092 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.5011 2.5922 -0.2301 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2238 2.1196 0.1136 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7220 0.0237 0.0713 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.3872 3.6628 -0.1329 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.4313 2.7938 -0.3413 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7514 3.4282 0.0380 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.2904 1.9289 0.2571 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0079 4.6865 -0.1824 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.4459 4.2679 0.1195 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7855 -1.7082 -0.6822 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6025 -1.6877 -1.8205 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7554 -2.8483 0.1244 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3749 -2.7997 -2.1493 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6494 -0.7961 -2.4527 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.5331 -3.9593 -0.2059 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.1101 -2.8598 1.0071 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.3402 -3.9373 -1.3414 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.0087 -2.7773 -3.0394 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.5036 -4.8477 0.4297 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.9465 -4.8091 -1.5999 H 0 0 0 0 0 0 0 0 0 0 0 0

2.3192 1.7258 -0.7228 C 0 0 0 0 0 0 0 0 0 0 0 0

3.2804 1.8989 -1.7262 C 0 0 0 0 0 0 0 0 0 0 0 0

1.8318 2.8441 -0.0413 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7334 3.1759 -2.0514 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6911 1.0310 -2.2507 H 0 0 0 0 0 0 0 0 0 0 0 0

2.2863 4.1233 -0.3678 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1004 2.7121 0.7604 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2351 4.2901 -1.3743 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4857 3.3023 -2.8343 H 0 0 0 0 0 0 0 0 0 0 0 0

1.9014 4.9906 0.1744 H 0 0 0 0 0 0 0 0 0 0 0 0

3.5949 5.2904 -1.6280 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2222 -1.1242 -0.4262 C 0 0 0 0 0 0 0 0 0 0 0 0

4.0851 -1.1655 0.6754 C 0 0 0 0 0 0 0 0 0 0 0 0

3.5454 -1.8551 -1.5744 C 0 0 0 0 0 0 0 0 0 0 0 0

5.2570 -1.9170 0.6254 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8377 -0.6121 1.5855 H 0 0 0 0 0 0 0 0 0 0 0 0

4.7172 -2.6120 -1.6204 C 0 0 0 0 0 0 0 0 0 0 0 0

2.8852 -1.8460 -2.4447 H 0 0 0 0 0 0 0 0 0 0 0 0

5.5749 -2.6422 -0.5229 C 0 0 0 0 0 0 0 0 0 0 0 0

5.9216 -1.9422 1.4924 H 0 0 0 0 0 0 0 0 0 0 0 0

4.9582 -3.1823 -2.5210 H 0 0 0 0 0 0 0 0 0 0 0 0

6.4914 -3.2362 -0.5600 H 0 0 0 0 0 0 0 0 0 0 0 0

0.0578 -1.9836 0.9222 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2218 -1.0678 2.4202 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

1 58 1 0 0 0 0

1 59 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

M END

**Table S24 Compound 10 Molfile**

RuC56As2H46O2 - Chemcraft

107114 0 0 0 0 0 0 0 0 1 V2000

-0.9764 -0.8728 0.1953 Ru 0 0 0 0 0 0 0 0 0 0 0 0

-2.5542 0.9023 -0.5976 As 0 0 0 0 0 0 0 0 0 0 0 0

0.0842 -0.3940 -2.0933 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.2840 0.6035 -3.1445 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.9045 1.6348 -3.2013 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2839 0.2003 -4.1679 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6692 0.5768 -2.5338 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1416 -0.4127 -2.6320 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.3352 1.3111 -3.0125 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.8342 -2.3271 -0.6632 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3614 -3.2731 -1.0589 O 0 0 0 0 0 0 0 0 0 0 0 0

0.7768 -0.4980 1.6273 C 0 0 0 0 0 0 0 0 0 0 0 0

0.6985 -1.8603 1.1125 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4363 -2.0282 0.3222 H 0 0 0 0 0 0 0 0 0 0 0 0

1.0308 2.0906 1.7031 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4925 -3.1372 1.8483 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1431 -4.2808 1.3472 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.2871 -3.3049 3.0069 C 0 0 0 0 0 0 0 0 0 0 0 0

1.0130 -5.5282 1.9528 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7797 -4.1798 0.4628 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.4140 -4.5501 3.6174 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8047 -2.4549 3.4493 H 0 0 0 0 0 0 0 0 0 0 0 0

0.2291 -5.6722 3.0954 C 0 0 0 0 0 0 0 0 0 0 0 0

1.5337 -6.3918 1.5303 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.0291 -4.6417 4.5164 H 0 0 0 0 0 0 0 0 0 0 0 0

0.1219 -6.6473 3.5769 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4118 -0.1700 3.0638 C 0 0 0 0 0 0 0 0 0 0 0 0

1.2026 -0.6813 4.1080 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6218 0.7044 3.4214 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9571 -0.3544 5.4382 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0252 -1.3595 3.8740 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.8694 1.0459 4.7518 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.2531 1.1182 2.6326 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.0828 0.5147 5.7694 C 0 0 0 0 0 0 0 0 0 0 0 0

1.5861 -0.7818 6.2235 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.6896 1.7284 4.9894 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.2763 0.7745 6.8131 H 0 0 0 0 0 0 0 0 0 0 0 0

1.9992 0.3126 1.2379 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0001 1.6571 1.4378 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0918 2.6388 1.4430 C 0 0 0 0 0 0 0 0 0 0 0 0

2.8035 3.9717 1.0955 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4021 2.3491 1.8673 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7819 4.9622 1.1281 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7852 4.2286 0.7891 H 0 0 0 0 0 0 0 0 0 0 0 0

5.3787 3.3389 1.9054 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6500 1.3360 2.1875 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0799 4.6493 1.5282 C 0 0 0 0 0 0 0 0 0 0 0 0

3.5267 5.9874 0.8462 H 0 0 0 0 0 0 0 0 0 0 0 0

6.3862 3.0854 2.2455 H 0 0 0 0 0 0 0 0 0 0 0 0

5.8506 5.4233 1.5614 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2349 -0.3989 0.7927 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6953 -1.5565 1.4448 C 0 0 0 0 0 0 0 0 0 0 0 0

4.0047 0.0946 -0.2718 C 0 0 0 0 0 0 0 0 0 0 0 0

4.8800 -2.1806 1.0625 C 0 0 0 0 0 0 0 0 0 0 0 0

3.1187 -1.9799 2.2682 H 0 0 0 0 0 0 0 0 0 0 0 0

5.1854 -0.5323 -0.6620 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6738 0.9933 -0.7911 H 0 0 0 0 0 0 0 0 0 0 0 0

5.6326 -1.6719 0.0044 C 0 0 0 0 0 0 0 0 0 0 0 0

5.2138 -3.0739 1.5964 H 0 0 0 0 0 0 0 0 0 0 0 0

5.7593 -0.1219 -1.4967 H 0 0 0 0 0 0 0 0 0 0 0 0

6.5599 -2.1637 -0.3005 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.1313 -1.1465 1.6467 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9413 -1.3164 2.4434 O 0 0 0 0 0 0 0 0 0 0 0 0

-4.4211 0.7355 -0.0702 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.1109 1.7783 0.5564 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.0707 -0.4878 -0.2796 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.4363 1.6034 0.9553 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.6156 2.7354 0.7368 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.3970 -0.6556 0.1124 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.5409 -1.3261 -0.7405 H 0 0 0 0 0 0 0 0 0 0 0 0

-7.0827 0.3898 0.7306 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.9651 2.4241 1.4466 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.8937 -1.6138 -0.0586 H 0 0 0 0 0 0 0 0 0 0 0 0

-8.1209 0.2548 1.0435 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.3098 2.8410 -0.5334 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9893 3.7112 -1.3962 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.4324 3.3718 0.4162 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7872 5.0876 -1.3098 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6934 3.3209 -2.1359 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2408 4.7512 0.5127 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8932 2.6948 1.0842 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.9149 5.6096 -0.3536 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.3195 5.7579 -1.9895 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.5623 5.1535 1.2692 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.7632 6.6895 -0.2835 H 0 0 0 0 0 0 0 0 0 0 0 0

1.5883 0.7605 -2.5543 C 0 0 0 0 0 0 0 0 0 0 0 0

1.5702 2.0720 -2.0639 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6449 0.3461 -3.3695 C 0 0 0 0 0 0 0 0 0 0 0 0

2.5860 2.9636 -2.4036 C 0 0 0 0 0 0 0 0 0 0 0 0

0.7645 2.4007 -1.4005 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6589 1.2423 -3.7106 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6864 -0.6800 -3.7406 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6307 2.5506 -3.2314 C 0 0 0 0 0 0 0 0 0 0 0 0

2.5701 3.9803 -2.0057 H 0 0 0 0 0 0 0 0 0 0 0 0

4.4792 0.9100 -4.3520 H 0 0 0 0 0 0 0 0 0 0 0 0

4.4283 3.2496 -3.4943 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4310 -1.9488 -3.2162 C 0 0 0 0 0 0 0 0 0 0 0 0

0.6529 -3.1869 -2.6057 C 0 0 0 0 0 0 0 0 0 0 0 0

0.4724 -1.8615 -4.6141 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9094 -4.3203 -3.3776 C 0 0 0 0 0 0 0 0 0 0 0 0

0.6114 -3.2715 -1.5173 H 0 0 0 0 0 0 0 0 0 0 0 0

0.7239 -2.9951 -5.3847 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3204 -0.9022 -5.1162 H 0 0 0 0 0 0 0 0 0 0 0 0

0.9430 -4.2267 -4.7670 C 0 0 0 0 0 0 0 0 0 0 0 0

1.0758 -5.2815 -2.8856 H 0 0 0 0 0 0 0 0 0 0 0 0

0.7503 -2.9151 -6.4743 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1385 -5.1154 -5.3722 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

3 4 1 0 0 0 0

4 5 1 0 0 0 0

4 6 1 0 0 0 0

4 7 1 0 0 0 0

2 7 1 0 0 0 0

7 8 1 0 0 0 0

7 9 1 0 0 0 0

1 10 1 0 0 0 0

10 11 3 0 0 0 0

1 13 1 0 0 0 0

12 13 1 0 0 0 0

13 14 1 0 0 0 0

13 16 1 0 0 0 0

16 17 2 0 0 0 0

16 18 1 0 0 0 0

17 19 1 0 0 0 0

17 20 1 0 0 0 0

18 21 2 0 0 0 0

18 22 1 0 0 0 0

19 23 2 0 0 0 0

21 23 1 0 0 0 0

19 24 1 0 0 0 0

21 25 1 0 0 0 0

23 26 1 0 0 0 0

12 27 2 0 0 0 0

27 28 1 0 0 0 0

27 29 1 0 0 0 0

28 30 2 0 0 0 0

28 31 1 0 0 0 0

29 32 2 0 0 0 0

29 33 1 0 0 0 0

30 34 1 0 0 0 0

32 34 1 0 0 0 0

30 35 1 0 0 0 0

32 36 1 0 0 0 0

34 37 1 0 0 0 0

12 38 1 0 0 0 0

15 39 1 0 0 0 0

38 39 2 0 0 0 0

39 40 1 0 0 0 0

40 41 2 0 0 0 0

40 42 1 0 0 0 0

41 43 1 0 0 0 0

41 44 1 0 0 0 0

42 45 2 0 0 0 0

42 46 1 0 0 0 0

45 47 1 0 0 0 0

43 47 2 0 0 0 0

43 48 1 0 0 0 0

45 49 1 0 0 0 0

47 50 1 0 0 0 0

38 51 1 0 0 0 0

51 52 2 0 0 0 0

51 53 1 0 0 0 0

52 54 1 0 0 0 0

52 55 1 0 0 0 0

53 56 2 0 0 0 0

53 57 1 0 0 0 0

56 58 1 0 0 0 0

54 58 2 0 0 0 0

54 59 1 0 0 0 0

56 60 1 0 0 0 0

58 61 1 0 0 0 0

1 62 1 0 0 0 0

62 63 3 0 0 0 0

2 64 1 0 0 0 0

64 65 2 0 0 0 0

64 66 1 0 0 0 0

65 67 1 0 0 0 0

65 68 1 0 0 0 0

66 69 2 0 0 0 0

66 70 1 0 0 0 0

69 71 1 0 0 0 0

67 71 2 0 0 0 0

67 72 1 0 0 0 0

69 73 1 0 0 0 0

71 74 1 0 0 0 0

2 75 1 0 0 0 0

75 76 2 0 0 0 0

75 77 1 0 0 0 0

76 78 1 0 0 0 0

76 79 1 0 0 0 0

77 80 2 0 0 0 0

77 81 1 0 0 0 0

78 82 2 0 0 0 0

80 82 1 0 0 0 0

78 83 1 0 0 0 0

80 84 1 0 0 0 0

82 85 1 0 0 0 0

3 86 1 0 0 0 0

86 87 2 0 0 0 0

86 88 1 0 0 0 0

87 89 1 0 0 0 0

87 90 1 0 0 0 0

88 91 2 0 0 0 0

88 92 1 0 0 0 0

91 93 1 0 0 0 0

89 93 2 0 0 0 0

89 94 1 0 0 0 0

91 95 1 0 0 0 0

93 96 1 0 0 0 0

3 97 1 0 0 0 0

97 98 2 0 0 0 0

97 99 1 0 0 0 0

98100 1 0 0 0 0

98101 1 0 0 0 0

99102 2 0 0 0 0

99103 1 0 0 0 0

102104 1 0 0 0 0

100104 2 0 0 0 0

100105 1 0 0 0 0

102106 1 0 0 0 0

104107 1 0 0 0 0

M END

**Table S25 Compound 9a Molfile**

RuC42As2H38O2 - Chemcraft

85 91 0 0 0 0 0 0 0 0 1 V2000

0.2342 -0.5950 -0.6355 Ru 0 0 0 0 0 0 0 0 0 0 0 0

-0.1549 1.1388 1.1378 As 0 0 0 0 0 0 0 0 0 0 0 0

2.5922 -0.3074 -0.0001 As 0 0 0 0 0 0 0 0 0 0 0 0

2.5973 0.3451 1.8607 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3441 -0.5488 2.4537 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6104 0.6512 2.1662 H 0 0 0 0 0 0 0 0 0 0 0 0

1.5859 1.4607 2.0626 C 0 0 0 0 0 0 0 0 0 0 0 0

1.9512 2.4054 1.6306 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3843 1.6435 3.1294 H 0 0 0 0 0 0 0 0 0 0 0 0

0.3333 0.4498 -2.2381 C 0 0 0 0 0 0 0 0 0 0 0 0

0.3654 0.9673 -3.2620 O 0 0 0 0 0 0 0 0 0 0 0 0

-1.8850 -0.9008 -1.2741 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7645 0.3512 -1.1177 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.7915 -1.0938 -2.3536 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9317 0.5764 -0.0523 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.0982 0.2468 -1.8202 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2839 -0.0153 -1.1240 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1723 0.3964 -3.2121 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.5024 -0.1268 -1.7932 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2508 -0.1366 -0.0383 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.3863 0.2864 -3.8859 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2582 0.6085 -3.7756 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.5588 0.0225 -3.1774 C 0 0 0 0 0 0 0 0 0 0 0 0

-7.4147 -0.3335 -1.2273 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.4189 0.4108 -4.9716 H 0 0 0 0 0 0 0 0 0 0 0 0

-7.5130 -0.0645 -3.7033 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.4933 -2.1365 -0.6802 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.4464 -3.3514 -1.3845 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1115 -2.1533 0.5821 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9744 -4.5256 -0.8544 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.9773 -3.3671 -2.3729 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.6444 -3.3251 1.1149 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1606 -1.2359 1.1744 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.5795 -4.5216 0.4022 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9192 -5.4522 -1.4324 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.1141 -3.3008 2.1022 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.9976 -5.4406 0.8204 H 0 0 0 0 0 0 0 0 0 0 0 0

0.0726 -2.0849 0.5801 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0318 -3.0187 1.2402 O 0 0 0 0 0 0 0 0 0 0 0 0

-1.3135 0.6822 2.6359 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6102 1.1988 2.7452 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8819 -0.2724 3.5645 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4544 0.7730 3.7710 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9682 1.9431 2.0292 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.7261 -0.6954 4.5898 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1195 -0.7054 3.4898 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0147 -0.1736 4.6950 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.4638 1.1852 3.8455 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.3758 -1.4425 5.3062 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.6779 -0.5075 5.4967 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.6371 2.9992 0.8112 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8830 3.8840 1.8698 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6568 3.4808 -0.5005 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1505 5.2275 1.6141 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8741 3.5241 2.9022 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.9246 4.8265 -0.7548 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4577 2.8025 -1.3329 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.1735 5.7001 0.3013 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.3437 5.9097 2.4459 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.9407 5.1896 -1.7851 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.3873 6.7532 0.1026 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6972 0.9879 -0.9449 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8245 0.8364 -2.3316 C 0 0 0 0 0 0 0 0 0 0 0 0

4.3512 2.0502 -0.3126 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6003 1.7263 -3.0702 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3114 0.0154 -2.8410 H 0 0 0 0 0 0 0 0 0 0 0 0

5.1226 2.9456 -1.0556 C 0 0 0 0 0 0 0 0 0 0 0 0

4.2674 2.1940 0.7675 H 0 0 0 0 0 0 0 0 0 0 0 0

5.2500 2.7841 -2.4334 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6936 1.5957 -4.1511 H 0 0 0 0 0 0 0 0 0 0 0 0

5.6264 3.7739 -0.5512 H 0 0 0 0 0 0 0 0 0 0 0 0

5.8543 3.4855 -3.0138 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8140 -1.8175 0.1110 C 0 0 0 0 0 0 0 0 0 0 0 0

5.1291 -1.6516 0.5628 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3679 -3.0872 -0.2650 C 0 0 0 0 0 0 0 0 0 0 0 0

5.9808 -2.7500 0.6542 C 0 0 0 0 0 0 0 0 0 0 0 0

5.4998 -0.6586 0.8335 H 0 0 0 0 0 0 0 0 0 0 0 0

4.2246 -4.1854 -0.1750 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3480 -3.2144 -0.6377 H 0 0 0 0 0 0 0 0 0 0 0 0

5.5281 -4.0184 0.2872 C 0 0 0 0 0 0 0 0 0 0 0 0

7.0059 -2.6151 1.0083 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8685 -5.1752 -0.4706 H 0 0 0 0 0 0 0 0 0 0 0 0

6.1985 -4.8787 0.3573 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5596 -1.7778 -1.6892 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.2325 1.2224 -1.5297 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 3 1 0 0 0 0

1 10 1 0 0 0 0

1 12 1 0 0 0 0

1 38 1 0 0 0 0

1 84 1 0 0 0 0

2 7 1 0 0 0 0

2 40 1 0 0 0 0

2 51 1 0 0 0 0

3 4 1 0 0 0 0

3 62 1 0 0 0 0

3 73 1 0 0 0 0

4 5 1 0 0 0 0

4 6 1 0 0 0 0

4 7 1 0 0 0 0

7 8 1 0 0 0 0

7 9 1 0 0 0 0

10 11 3 0 0 0 0

12 13 1 0 0 0 0

12 14 1 0 0 0 0

12 27 1 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

13 85 1 0 0 0 0

16 17 2 0 0 0 0

16 18 1 0 0 0 0

17 19 1 0 0 0 0

17 20 1 0 0 0 0

18 21 2 0 0 0 0

18 22 1 0 0 0 0

19 23 2 0 0 0 0

19 24 1 0 0 0 0

21 23 1 0 0 0 0

21 25 1 0 0 0 0

23 26 1 0 0 0 0

27 28 2 0 0 0 0

27 29 1 0 0 0 0

28 30 1 0 0 0 0

28 31 1 0 0 0 0

29 32 2 0 0 0 0

29 33 1 0 0 0 0

30 34 2 0 0 0 0

30 35 1 0 0 0 0

32 34 1 0 0 0 0

32 36 1 0 0 0 0

34 37 1 0 0 0 0

38 39 3 0 0 0 0

40 41 2 0 0 0 0

40 42 1 0 0 0 0

41 43 1 0 0 0 0

41 44 1 0 0 0 0

42 45 2 0 0 0 0

42 46 1 0 0 0 0

43 47 2 0 0 0 0

43 48 1 0 0 0 0

45 47 1 0 0 0 0

45 49 1 0 0 0 0

47 50 1 0 0 0 0

51 52 2 0 0 0 0

51 53 1 0 0 0 0

52 54 1 0 0 0 0

52 55 1 0 0 0 0

53 56 2 0 0 0 0

53 57 1 0 0 0 0

54 58 2 0 0 0 0

54 59 1 0 0 0 0

56 58 1 0 0 0 0

56 60 1 0 0 0 0

58 61 1 0 0 0 0

62 63 2 0 0 0 0

62 64 1 0 0 0 0

63 65 1 0 0 0 0

63 66 1 0 0 0 0

64 67 2 0 0 0 0

64 68 1 0 0 0 0

65 69 2 0 0 0 0

65 70 1 0 0 0 0

67 69 1 0 0 0 0

67 71 1 0 0 0 0

69 72 1 0 0 0 0

73 74 2 0 0 0 0

73 75 1 0 0 0 0

74 76 1 0 0 0 0

74 77 1 0 0 0 0

75 78 2 0 0 0 0

75 79 1 0 0 0 0

76 80 2 0 0 0 0

76 81 1 0 0 0 0

78 80 1 0 0 0 0

78 82 1 0 0 0 0

80 83 1 0 0 0 0

M END

**Table S26 Compound 8-trans Molfile**

RuC42As2H36O2 - Chemcraft

83 89 0 0 0 0 0 0 0 0 1 V2000

-0.1013 -0.1805 1.0383 Ru 0 0 0 0 0 0 0 0 0 0 0 0

1.0268 1.0991 -0.8299 As 0 0 0 0 0 0 0 0 0 0 0 0

-2.0972 0.1518 -0.3727 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.4870 0.6375 -2.1784 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1226 -0.3065 -2.6142 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.3266 0.9824 -2.8011 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.3844 1.6788 -2.0838 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.7722 2.6266 -1.6765 H 0 0 0 0 0 0 0 0 0 0 0 0

0.0661 1.8924 -3.0652 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.0527 1.3916 2.1193 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.0521 2.2743 2.8592 O 0 0 0 0 0 0 0 0 0 0 0 0

0.7790 -2.1497 0.5445 C 0 0 0 0 0 0 0 0 0 0 0 0

1.6833 -1.3917 1.3726 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1915 -2.9174 1.0645 H 0 0 0 0 0 0 0 0 0 0 0 0

2.5293 -0.9356 0.8429 H 0 0 0 0 0 0 0 0 0 0 0 0

2.0391 -1.7153 2.7756 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0037 -0.9365 3.4389 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4819 -2.7915 3.4847 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3775 -1.2018 4.7519 C 0 0 0 0 0 0 0 0 0 0 0 0

3.4638 -0.0993 2.9048 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8498 -3.0564 4.8022 C 0 0 0 0 0 0 0 0 0 0 0 0

0.7509 -3.4409 2.9975 H 0 0 0 0 0 0 0 0 0 0 0 0

2.7970 -2.2633 5.4476 C 0 0 0 0 0 0 0 0 0 0 0 0

4.1298 -0.5748 5.2380 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3948 -3.9005 5.3273 H 0 0 0 0 0 0 0 0 0 0 0 0

3.0859 -2.4739 6.4801 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1376 -2.6334 -0.8185 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1455 -2.9736 -1.7544 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4719 -2.8915 -1.1711 C 0 0 0 0 0 0 0 0 0 0 0 0

0.4690 -3.5481 -2.9811 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.9031 -2.7966 -1.5024 H 0 0 0 0 0 0 0 0 0 0 0 0

2.7997 -3.4627 -2.3998 C 0 0 0 0 0 0 0 0 0 0 0 0

3.2646 -2.6690 -0.4532 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8016 -3.7979 -3.3124 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.3288 -3.8118 -3.6811 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8484 -3.6566 -2.6394 H 0 0 0 0 0 0 0 0 0 0 0 0

2.0579 -4.2555 -4.2713 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.0820 -1.0465 2.3823 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.7166 -1.5554 3.1957 O 0 0 0 0 0 0 0 0 0 0 0 0

2.3921 0.4142 -2.0458 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7375 0.4811 -1.6656 C 0 0 0 0 0 0 0 0 0 0 0 0

2.0608 -0.1155 -3.2959 C 0 0 0 0 0 0 0 0 0 0 0 0

4.7359 0.0340 -2.5286 C 0 0 0 0 0 0 0 0 0 0 0 0

4.0168 0.9050 -0.6972 H 0 0 0 0 0 0 0 0 0 0 0 0

3.0623 -0.5544 -4.1605 C 0 0 0 0 0 0 0 0 0 0 0 0

1.0178 -0.2025 -3.6087 H 0 0 0 0 0 0 0 0 0 0 0 0

4.4005 -0.4786 -3.7810 C 0 0 0 0 0 0 0 0 0 0 0 0

5.7832 0.0962 -2.2225 H 0 0 0 0 0 0 0 0 0 0 0 0

2.7898 -0.9673 -5.1346 H 0 0 0 0 0 0 0 0 0 0 0 0

5.1839 -0.8224 -4.4609 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8961 2.7830 -0.3804 C 0 0 0 0 0 0 0 0 0 0 0 0

1.9546 3.8374 -1.2998 C 0 0 0 0 0 0 0 0 0 0 0 0

2.5253 2.9219 0.8605 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6184 5.0183 -0.9739 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4887 3.7426 -2.2838 H 0 0 0 0 0 0 0 0 0 0 0 0

3.1985 4.1014 1.1810 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4843 2.1067 1.5876 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2418 5.1518 0.2670 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6526 5.8379 -1.6960 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6834 4.1995 2.1552 H 0 0 0 0 0 0 0 0 0 0 0 0

3.7628 6.0782 0.5208 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.2772 1.6422 0.0822 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5796 1.8367 1.4350 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8248 2.5126 -0.8669 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.4271 2.8697 1.8297 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1405 1.1798 2.1910 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.6652 3.5537 -0.4702 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5997 2.3946 -1.9300 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.9709 3.7314 0.8775 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.6556 3.0071 2.8893 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.0818 4.2297 -1.2213 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.6290 4.5469 1.1875 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4109 -1.2434 -0.7392 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.5171 -1.0080 -1.5642 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2460 -2.5021 -0.1550 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.4347 -2.0262 -1.8138 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.6775 -0.0213 -2.0071 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.1692 -3.5194 -0.4009 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.3879 -2.6864 0.4965 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.2614 -3.2833 -1.2328 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.2947 -1.8356 -2.4608 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.0321 -4.4994 0.0624 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.9848 -4.0792 -1.4263 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 3 1 0 0 0 0

1 10 1 0 0 0 0

1 13 1 0 0 0 0

1 38 1 0 0 0 0

2 7 1 0 0 0 0

2 40 1 0 0 0 0

2 51 1 0 0 0 0

3 4 1 0 0 0 0

3 62 1 0 0 0 0

3 73 1 0 0 0 0

4 5 1 0 0 0 0

4 6 1 0 0 0 0

4 7 1 0 0 0 0

7 8 1 0 0 0 0

7 9 1 0 0 0 0

10 11 3 0 0 0 0

12 13 1 0 0 0 0

12 14 1 0 0 0 0

12 27 2 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

16 17 2 0 0 0 0

16 18 1 0 0 0 0

17 19 1 0 0 0 0

17 20 1 0 0 0 0

18 21 2 0 0 0 0

18 22 1 0 0 0 0

19 23 2 0 0 0 0

19 24 1 0 0 0 0

21 23 1 0 0 0 0

21 25 1 0 0 0 0

23 26 1 0 0 0 0

27 28 1 0 0 0 0

27 29 1 0 0 0 0

28 30 2 0 0 0 0

28 31 1 0 0 0 0

29 32 2 0 0 0 0

29 33 1 0 0 0 0

30 34 1 0 0 0 0

30 35 1 0 0 0 0

32 34 1 0 0 0 0

32 36 1 0 0 0 0

34 37 1 0 0 0 0

38 39 3 0 0 0 0

40 41 2 0 0 0 0

40 42 1 0 0 0 0

41 43 1 0 0 0 0

41 44 1 0 0 0 0

42 45 2 0 0 0 0

42 46 1 0 0 0 0

43 47 2 0 0 0 0

43 48 1 0 0 0 0

45 47 1 0 0 0 0

45 49 1 0 0 0 0

47 50 1 0 0 0 0

51 52 2 0 0 0 0

51 53 1 0 0 0 0

52 54 1 0 0 0 0

52 55 1 0 0 0 0

53 56 2 0 0 0 0

53 57 1 0 0 0 0

54 58 2 0 0 0 0

54 59 1 0 0 0 0

56 58 1 0 0 0 0

56 60 1 0 0 0 0

58 61 1 0 0 0 0

62 63 2 0 0 0 0

62 64 1 0 0 0 0

63 65 1 0 0 0 0

63 66 1 0 0 0 0

64 67 2 0 0 0 0

64 68 1 0 0 0 0

65 69 2 0 0 0 0

65 70 1 0 0 0 0

67 69 1 0 0 0 0

67 71 1 0 0 0 0

69 72 1 0 0 0 0

73 74 2 0 0 0 0

73 75 1 0 0 0 0

74 76 1 0 0 0 0

74 77 1 0 0 0 0

75 78 2 0 0 0 0

75 79 1 0 0 0 0

76 80 2 0 0 0 0

76 81 1 0 0 0 0

78 80 1 0 0 0 0

78 82 1 0 0 0 0

80 83 1 0 0 0 0

M END

**Table S27 Compound AX-2 Molfile**

RuC46As2PH39O2 - Chemcraft

91 98 0 0 0 0 0 0 0 0 1 V2000

0.3494 -0.6030 -0.1578 Ru 0 0 0 0 0 0 0 0 0 0 0 0

0.4483 -1.8874 1.2404 C 0 0 0 0 0 0 0 0 0 0 0 0

0.5279 -2.7307 2.0296 O 0 0 0 0 0 0 0 0 0 0 0 0

0.7249 -0.9341 -1.9868 C 0 0 0 0 0 0 0 0 0 0 0 0

0.9692 -1.2448 -3.0778 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.1128 1.6885 0.6566 As 0 0 0 0 0 0 0 0 0 0 0 0

2.6708 0.0349 0.2777 As 0 0 0 0 0 0 0 0 0 0 0 0

2.7274 1.9081 0.9068 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4809 2.2590 1.6920 C 0 0 0 0 0 0 0 0 0 0 0 0

2.7907 2.5050 -0.0174 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6577 2.0878 1.4670 H 0 0 0 0 0 0 0 0 0 0 0 0

1.4112 3.3394 1.8934 H 0 0 0 0 0 0 0 0 0 0 0 0

1.4547 1.7223 2.6531 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0270 0.1332 -1.1230 C 0 0 0 0 0 0 0 0 0 0 0 0

5.3490 -0.2684 -0.9049 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6704 0.6666 -2.3664 C 0 0 0 0 0 0 0 0 0 0 0 0

6.2990 -0.1376 -1.9183 C 0 0 0 0 0 0 0 0 0 0 0 0

5.6438 -0.6882 0.0598 H 0 0 0 0 0 0 0 0 0 0 0 0

4.6222 0.8008 -3.3752 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6386 0.9725 -2.5542 H 0 0 0 0 0 0 0 0 0 0 0 0

5.9384 0.3971 -3.1536 C 0 0 0 0 0 0 0 0 0 0 0 0

7.3285 -0.4574 -1.7381 H 0 0 0 0 0 0 0 0 0 0 0 0

4.3300 1.2150 -4.3433 H 0 0 0 0 0 0 0 0 0 0 0 0

6.6833 0.4960 -3.9472 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6310 -0.9667 1.6435 C 0 0 0 0 0 0 0 0 0 0 0 0

4.1743 -0.3774 2.7887 C 0 0 0 0 0 0 0 0 0 0 0 0

3.7553 -2.3501 1.4634 C 0 0 0 0 0 0 0 0 0 0 0 0

4.8372 -1.1584 3.7370 C 0 0 0 0 0 0 0 0 0 0 0 0

4.0865 0.6984 2.9576 H 0 0 0 0 0 0 0 0 0 0 0 0

4.4269 -3.1264 2.4043 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3119 -2.8251 0.5833 H 0 0 0 0 0 0 0 0 0 0 0 0

4.9684 -2.5318 3.5443 C 0 0 0 0 0 0 0 0 0 0 0 0

5.2536 -0.6872 4.6309 H 0 0 0 0 0 0 0 0 0 0 0 0

4.5178 -4.2045 2.2516 H 0 0 0 0 0 0 0 0 0 0 0 0

5.4884 -3.1422 4.2868 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.1637 3.2122 -0.5874 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4731 4.5140 -0.1740 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1942 2.9885 -1.9185 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4259 5.5704 -1.0827 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.7618 4.7079 0.8631 H 0 0 0 0 0 0 0 0 0 0 0 0

0.2459 4.0456 -2.8287 C 0 0 0 0 0 0 0 0 0 0 0 0

0.4285 1.9650 -2.2325 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.0665 5.3381 -2.4114 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.6719 6.5827 -0.7515 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5288 3.8568 -3.8677 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.0306 6.1681 -3.1217 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.5463 2.2084 1.8783 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7821 2.6245 1.3658 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.4030 2.0640 3.2643 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8461 2.9004 2.2234 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9208 2.7332 0.2864 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.4678 2.3442 4.1208 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4569 1.7213 3.6909 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.6924 2.7633 3.6024 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.8040 3.2215 1.8064 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.3374 2.2335 5.2005 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.5273 2.9805 4.2733 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.8640 -1.2911 -0.5284 P 0 0 0 0 0 0 0 0 0 0 0 0

-3.0580 -0.0173 -1.1271 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3642 0.0886 -0.6341 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6343 0.8699 -2.1251 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.2271 1.0675 -1.1287 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7099 -0.5932 0.1457 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4973 1.8449 -2.6198 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.6127 0.7972 -2.5048 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7965 1.9478 -2.1201 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.2429 1.1418 -0.7320 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.1479 2.5344 -3.3921 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.4724 2.7164 -2.5035 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.0608 -2.6210 -1.7904 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1144 -3.6536 -1.8238 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1364 -2.6532 -2.6859 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.2499 -4.7043 -2.7277 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.2591 -3.6147 -1.1436 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.2632 -3.7011 -3.5978 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8810 -1.8541 -2.6765 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.3230 -4.7295 -3.6186 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5039 -5.5026 -2.7441 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.1028 -3.7104 -4.2974 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.4222 -5.5489 -4.3350 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.7575 -2.0037 0.9193 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5034 -3.1855 0.8400 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6945 -1.3211 2.1413 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1738 -3.6727 1.9628 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5596 -3.7365 -0.1011 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.3742 -1.8026 3.2566 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.1040 -0.4059 2.2203 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.1138 -2.9823 3.1713 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7448 -4.6017 1.8888 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.3168 -1.2539 4.1998 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.6389 -3.3665 4.0494 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 6 1 0 0 0 0

1 7 1 0 0 0 0

1 58 1 0 0 0 0

2 3 3 0 0 0 0

4 5 3 0 0 0 0

6 9 1 0 0 0 0

6 36 1 0 0 0 0

6 47 1 0 0 0 0

7 8 1 0 0 0 0

7 14 1 0 0 0 0

7 25 1 0 0 0 0

8 9 1 0 0 0 0

8 10 1 0 0 0 0

8 11 1 0 0 0 0

9 12 1 0 0 0 0

9 13 1 0 0 0 0

14 15 2 0 0 0 0

14 16 1 0 0 0 0

15 17 1 0 0 0 0

15 18 1 0 0 0 0

16 19 2 0 0 0 0

16 20 1 0 0 0 0

17 21 2 0 0 0 0

17 22 1 0 0 0 0

19 21 1 0 0 0 0

19 23 1 0 0 0 0

21 24 1 0 0 0 0

25 26 2 0 0 0 0

25 27 1 0 0 0 0

26 28 1 0 0 0 0

26 29 1 0 0 0 0

27 30 2 0 0 0 0

27 31 1 0 0 0 0

28 32 2 0 0 0 0

28 33 1 0 0 0 0

30 32 1 0 0 0 0

30 34 1 0 0 0 0

32 35 1 0 0 0 0

36 37 2 0 0 0 0

36 38 1 0 0 0 0

37 39 1 0 0 0 0

37 40 1 0 0 0 0

38 41 2 0 0 0 0

38 42 1 0 0 0 0

39 43 2 0 0 0 0

39 44 1 0 0 0 0

41 43 1 0 0 0 0

41 45 1 0 0 0 0

43 46 1 0 0 0 0

47 48 2 0 0 0 0

47 49 1 0 0 0 0

48 50 1 0 0 0 0

48 51 1 0 0 0 0

49 52 2 0 0 0 0

49 53 1 0 0 0 0

50 54 2 0 0 0 0

50 55 1 0 0 0 0

52 54 1 0 0 0 0

52 56 1 0 0 0 0

54 57 1 0 0 0 0

58 59 1 0 0 0 0

58 70 1 0 0 0 0

58 81 1 0 0 0 0

59 60 2 0 0 0 0

59 61 1 0 0 0 0

60 62 1 0 0 0 0

60 63 1 0 0 0 0

61 64 2 0 0 0 0

61 65 1 0 0 0 0

62 66 2 0 0 0 0

62 67 1 0 0 0 0

64 66 1 0 0 0 0

64 68 1 0 0 0 0

66 69 1 0 0 0 0

70 71 2 0 0 0 0

70 72 1 0 0 0 0

71 73 1 0 0 0 0

71 74 1 0 0 0 0

72 75 2 0 0 0 0

72 76 1 0 0 0 0

73 77 2 0 0 0 0

73 78 1 0 0 0 0

75 77 1 0 0 0 0

75 79 1 0 0 0 0

77 80 1 0 0 0 0

81 82 2 0 0 0 0

81 83 1 0 0 0 0

82 84 1 0 0 0 0

82 85 1 0 0 0 0

83 86 2 0 0 0 0

83 87 1 0 0 0 0

84 88 2 0 0 0 0

84 89 1 0 0 0 0

86 88 1 0 0 0 0

86 90 1 0 0 0 0

88 91 1 0 0 0 0

M END

**Table S28 Compound 7b Molfile**

RuC45As2PH41O - Chemcraft

91 98 0 0 0 0 0 0 0 0 1 V2000

0.0872 0.3908 -1.2027 Ru 0 0 0 0 0 0 0 0 0 0 0 0

1.0523 -0.1068 -2.7193 C 0 0 0 0 0 0 0 0 0 0 0 0

1.6072 -0.3273 -3.7059 O 0 0 0 0 0 0 0 0 0 0 0 0

1.8978 0.9716 0.3718 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.3296 1.7161 0.3080 As 0 0 0 0 0 0 0 0 0 0 0 0

-0.2937 2.1499 1.9336 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1694 2.3638 1.5883 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4278 1.2883 2.6079 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.7183 3.0380 2.4278 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8008 2.4226 2.4887 H 0 0 0 0 0 0 0 0 0 0 0 0

1.3041 3.3041 1.0303 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0364 1.1373 1.0565 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9178 0.4612 0.2049 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4115 1.3648 2.3864 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.1551 0.0229 0.6737 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6248 0.2602 -0.8290 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.6497 0.9232 2.8544 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7396 1.8848 3.0739 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.5228 0.2524 1.9991 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.8283 -0.5115 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.9327 1.1052 3.8945 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.4908 -0.0955 2.3683 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.8663 3.4930 -0.3113 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.5774 4.3540 0.5340 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.5581 3.9098 -1.6079 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9567 5.6202 0.0939 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.8557 4.0359 1.5427 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.9442 5.1764 -2.0499 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.0100 3.2312 -2.2671 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6391 6.0341 -1.2004 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.5091 6.2849 0.7631 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.6989 5.4913 -3.0673 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.9398 7.0261 -1.5471 H 0 0 0 0 0 0 0 0 0 0 0 0

2.8075 -0.2241 1.6259 C 0 0 0 0 0 0 0 0 0 0 0 0

3.9297 -0.9461 1.1979 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3295 -0.4289 2.9243 C 0 0 0 0 0 0 0 0 0 0 0 0

4.5651 -1.8436 2.0540 C 0 0 0 0 0 0 0 0 0 0 0 0

4.3274 -0.7921 0.1902 H 0 0 0 0 0 0 0 0 0 0 0 0

2.9664 -1.3262 3.7817 C 0 0 0 0 0 0 0 0 0 0 0 0

1.4483 0.1087 3.2826 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0860 -2.0344 3.3500 C 0 0 0 0 0 0 0 0 0 0 0 0

5.4442 -2.3933 1.7076 H 0 0 0 0 0 0 0 0 0 0 0 0

2.5793 -1.4734 4.7929 H 0 0 0 0 0 0 0 0 0 0 0 0

4.5860 -2.7356 4.0227 H 0 0 0 0 0 0 0 0 0 0 0 0

3.4506 1.9513 -0.2965 C 0 0 0 0 0 0 0 0 0 0 0 0

3.4959 2.3387 -1.6385 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4998 2.3172 0.5574 C 0 0 0 0 0 0 0 0 0 0 0 0

4.5751 3.0802 -2.1221 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6769 2.0609 -2.3059 H 0 0 0 0 0 0 0 0 0 0 0 0

5.5740 3.0617 0.0741 C 0 0 0 0 0 0 0 0 0 0 0 0

4.4861 2.0123 1.6076 H 0 0 0 0 0 0 0 0 0 0 0 0

5.6139 3.4432 -1.2677 C 0 0 0 0 0 0 0 0 0 0 0 0

4.6012 3.3731 -3.1747 H 0 0 0 0 0 0 0 0 0 0 0 0

6.3864 3.3435 0.7489 H 0 0 0 0 0 0 0 0 0 0 0 0

6.4590 4.0236 -1.6468 H 0 0 0 0 0 0 0 0 0 0 0 0

0.3762 1.8829 -1.7799 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.1831 0.4711 -2.2022 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.4952 -1.8635 -0.6114 P 0 0 0 0 0 0 0 0 0 0 0 0

-2.1867 -2.4392 -1.0966 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6932 -2.0178 -2.3337 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.9587 -3.3028 -0.3101 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9421 -2.4508 -2.7741 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.1012 -1.3295 -2.9426 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.2153 -3.7255 -0.7463 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.5802 -3.6490 0.6540 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7100 -3.3022 -1.9784 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3201 -2.1151 -3.7432 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.8086 -4.3936 -0.1167 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.6931 -3.6362 -2.3203 H 0 0 0 0 0 0 0 0 0 0 0 0

0.5584 -3.1443 -1.4312 C 0 0 0 0 0 0 0 0 0 0 0 0

1.9447 -2.9423 -1.4592 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0361 -4.3089 -2.0059 C 0 0 0 0 0 0 0 0 0 0 0 0

2.7903 -3.8847 -2.0391 C 0 0 0 0 0 0 0 0 0 0 0 0

2.3592 -2.0323 -1.0195 H 0 0 0 0 0 0 0 0 0 0 0 0

0.8825 -5.2463 -2.5987 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.0411 -4.4873 -1.9967 H 0 0 0 0 0 0 0 0 0 0 0 0

2.2602 -5.0388 -2.6154 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8691 -3.7102 -2.0503 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4579 -6.1457 -3.0518 H 0 0 0 0 0 0 0 0 0 0 0 0

2.9210 -5.7736 -3.0821 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.4125 -2.4199 1.1537 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.2077 -1.7543 2.0984 C 0 0 0 0 0 0 0 0 0 0 0 0

0.4140 -3.4609 1.5910 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1866 -2.1266 3.4401 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.8744 -0.9509 1.7780 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4452 -3.8244 2.9385 C 0 0 0 0 0 0 0 0 0 0 0 0

1.0410 -3.9979 0.8770 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.3550 -3.1633 3.8665 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.8295 -1.6048 4.1540 H 0 0 0 0 0 0 0 0 0 0 0 0

1.1020 -4.6366 3.2599 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.3349 -3.4562 4.9194 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 5 1 0 0 0 0

1 56 1 0 0 0 0

1 57 1 0 0 0 0

1 58 1 0 0 0 0

2 3 3 0 0 0 0

4 7 1 0 0 0 0

4 34 1 0 0 0 0

4 45 1 0 0 0 0

5 6 1 0 0 0 0

5 12 1 0 0 0 0

5 23 1 0 0 0 0

6 7 1 0 0 0 0

6 8 1 0 0 0 0

6 9 1 0 0 0 0

7 10 1 0 0 0 0

7 11 1 0 0 0 0

12 13 2 0 0 0 0

12 14 1 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

14 17 2 0 0 0 0

14 18 1 0 0 0 0

15 19 2 0 0 0 0

15 20 1 0 0 0 0

17 19 1 0 0 0 0

17 21 1 0 0 0 0

19 22 1 0 0 0 0

23 24 2 0 0 0 0

23 25 1 0 0 0 0

24 26 1 0 0 0 0

24 27 1 0 0 0 0

25 28 2 0 0 0 0

25 29 1 0 0 0 0

26 30 2 0 0 0 0

26 31 1 0 0 0 0

28 30 1 0 0 0 0

28 32 1 0 0 0 0

30 33 1 0 0 0 0

34 35 2 0 0 0 0

34 36 1 0 0 0 0

35 37 1 0 0 0 0

35 38 1 0 0 0 0

36 39 2 0 0 0 0

36 40 1 0 0 0 0

37 41 2 0 0 0 0

37 42 1 0 0 0 0

39 41 1 0 0 0 0

39 43 1 0 0 0 0

41 44 1 0 0 0 0

45 46 2 0 0 0 0

45 47 1 0 0 0 0

46 48 1 0 0 0 0

46 49 1 0 0 0 0

47 50 2 0 0 0 0

47 51 1 0 0 0 0

48 52 2 0 0 0 0

48 53 1 0 0 0 0

50 52 1 0 0 0 0

50 54 1 0 0 0 0

52 55 1 0 0 0 0

58 59 1 0 0 0 0

58 70 1 0 0 0 0

58 81 1 0 0 0 0

59 60 2 0 0 0 0

59 61 1 0 0 0 0

60 62 1 0 0 0 0

60 63 1 0 0 0 0

61 64 2 0 0 0 0

61 65 1 0 0 0 0

62 66 2 0 0 0 0

62 67 1 0 0 0 0

64 66 1 0 0 0 0

64 68 1 0 0 0 0

66 69 1 0 0 0 0

70 71 2 0 0 0 0

70 72 1 0 0 0 0

71 73 1 0 0 0 0

71 74 1 0 0 0 0

72 75 2 0 0 0 0

72 76 1 0 0 0 0

73 77 2 0 0 0 0

73 78 1 0 0 0 0

75 77 1 0 0 0 0

75 79 1 0 0 0 0

77 80 1 0 0 0 0

81 82 2 0 0 0 0

81 83 1 0 0 0 0

82 84 1 0 0 0 0

82 85 1 0 0 0 0

83 86 2 0 0 0 0

83 87 1 0 0 0 0

84 88 2 0 0 0 0

84 89 1 0 0 0 0

86 88 1 0 0 0 0

86 90 1 0 0 0 0

88 91 1 0 0 0 0

M END

**Table S29 Compound 7a Molfile**

RuC45As2PH41O - Chemcraft

91 98 0 0 0 0 0 0 0 0 1 V2000

0.3708 -0.4896 -0.3020 Ru 0 0 0 0 0 0 0 0 0 0 0 0

0.6243 -0.3459 -2.1854 C 0 0 0 0 0 0 0 0 0 0 0 0

0.7997 -0.2981 -3.3268 O 0 0 0 0 0 0 0 0 0 0 0 0

-0.0929 1.7851 0.4988 As 0 0 0 0 0 0 0 0 0 0 0 0

2.6546 0.0020 0.2763 As 0 0 0 0 0 0 0 0 0 0 0 0

2.7864 1.9089 0.7952 C 0 0 0 0 0 0 0 0 0 0 0 0

1.5224 2.3384 1.5145 C 0 0 0 0 0 0 0 0 0 0 0 0

2.9251 2.4765 -0.1388 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6842 2.0622 1.4135 H 0 0 0 0 0 0 0 0 0 0 0 0

1.4881 3.4277 1.6697 H 0 0 0 0 0 0 0 0 0 0 0 0

1.4531 1.8557 2.5015 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0727 -0.1472 -1.0511 C 0 0 0 0 0 0 0 0 0 0 0 0

5.0304 -1.1646 -0.9883 C 0 0 0 0 0 0 0 0 0 0 0 0

4.0796 0.7286 -2.1438 C 0 0 0 0 0 0 0 0 0 0 0 0

5.9903 -1.2918 -1.9925 C 0 0 0 0 0 0 0 0 0 0 0 0

5.0308 -1.8656 -0.1500 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0437 0.6044 -3.1423 C 0 0 0 0 0 0 0 0 0 0 0 0

3.3208 1.5118 -2.2302 H 0 0 0 0 0 0 0 0 0 0 0 0

6.0027 -0.4055 -3.0679 C 0 0 0 0 0 0 0 0 0 0 0 0

6.7330 -2.0914 -1.9322 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0396 1.2965 -3.9880 H 0 0 0 0 0 0 0 0 0 0 0 0

6.7559 -0.5052 -3.8533 H 0 0 0 0 0 0 0 0 0 0 0 0

3.4590 -0.8855 1.8109 C 0 0 0 0 0 0 0 0 0 0 0 0

4.7117 -0.4880 2.2965 C 0 0 0 0 0 0 0 0 0 0 0 0

2.7739 -1.9252 2.4449 C 0 0 0 0 0 0 0 0 0 0 0 0

5.2676 -1.1189 3.4075 C 0 0 0 0 0 0 0 0 0 0 0 0

5.2680 0.3124 1.7999 H 0 0 0 0 0 0 0 0 0 0 0 0

3.3352 -2.5590 3.5549 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7930 -2.2238 2.0636 H 0 0 0 0 0 0 0 0 0 0 0 0

4.5787 -2.1562 4.0381 C 0 0 0 0 0 0 0 0 0 0 0 0

6.2446 -0.8018 3.7811 H 0 0 0 0 0 0 0 0 0 0 0 0

2.7935 -3.3725 4.0442 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0158 -2.6523 4.9085 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.2879 3.3600 -0.6499 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.4791 4.6450 -0.1247 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.1668 3.2022 -2.0334 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5523 5.7495 -0.9713 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.5803 4.7874 0.9552 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.2381 4.3091 -2.8818 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.0085 2.2039 -2.4507 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.4323 5.5830 -2.3520 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.7038 6.7472 -0.5509 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.1410 4.1716 -3.9618 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.4901 6.4501 -3.0148 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.4688 2.1153 1.8434 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.6700 2.7550 1.5192 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.2938 1.6208 3.1424 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.6679 2.9138 2.4811 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.8370 3.1285 0.5061 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.2890 1.7866 4.1045 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.3780 1.0861 3.4092 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4786 2.4366 3.7766 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.6021 3.4122 2.2106 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.1336 1.4029 5.1163 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.2599 2.5651 4.5299 H 0 0 0 0 0 0 0 0 0 0 0 0

0.2265 -0.7925 1.3309 H 0 0 0 0 0 0 0 0 0 0 0 0

0.8380 -2.0413 -0.3185 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.7526 -1.4168 -0.4707 P 0 0 0 0 0 0 0 0 0 0 0 0

-2.2957 -2.4721 0.9427 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7343 -3.7899 0.7765 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.2599 -1.9291 2.2345 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1233 -4.5510 1.8807 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7694 -4.2336 -0.2205 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6662 -2.6827 3.3316 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.9057 -0.9060 2.3791 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.0943 -4.0002 3.1590 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.4527 -5.5828 1.7345 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.6397 -2.2395 4.3305 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4019 -4.5963 4.0220 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.0206 -2.5395 -1.9142 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.9507 -3.3072 -2.3904 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2751 -2.6738 -2.5250 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1323 -4.1945 -3.4501 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0313 -3.1927 -1.9245 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4530 -3.5569 -3.5889 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1217 -2.0817 -2.1701 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.3827 -4.3204 -4.0532 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.2859 -4.7837 -3.8116 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.4358 -3.6461 -4.0587 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.5227 -5.0098 -4.8898 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.1768 -0.2532 -0.6674 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.0622 0.7434 -1.6471 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.3531 -0.3263 0.0863 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.1022 1.6405 -1.8744 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.1445 0.8139 -2.2367 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.3909 0.5819 -0.1333 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.4630 -1.0957 0.8535 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.2709 1.5635 -1.1141 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.9960 2.4080 -2.6453 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.3009 0.5157 0.4685 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.0864 2.2704 -1.2874 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 4 1 0 0 0 0

1 5 1 0 0 0 0

1 56 1 0 0 0 0

1 57 1 0 0 0 0

1 58 1 0 0 0 0

2 3 3 0 0 0 0

4 7 1 0 0 0 0

4 34 1 0 0 0 0

4 45 1 0 0 0 0

5 6 1 0 0 0 0

5 12 1 0 0 0 0

5 23 1 0 0 0 0

6 7 1 0 0 0 0

6 8 1 0 0 0 0

6 9 1 0 0 0 0

7 10 1 0 0 0 0

7 11 1 0 0 0 0

12 13 2 0 0 0 0

12 14 1 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

14 17 2 0 0 0 0

14 18 1 0 0 0 0

15 19 2 0 0 0 0

15 20 1 0 0 0 0

17 19 1 0 0 0 0

17 21 1 0 0 0 0

19 22 1 0 0 0 0

23 24 2 0 0 0 0

23 25 1 0 0 0 0

24 26 1 0 0 0 0

24 27 1 0 0 0 0

25 28 2 0 0 0 0

25 29 1 0 0 0 0

26 30 2 0 0 0 0

26 31 1 0 0 0 0

28 30 1 0 0 0 0

28 32 1 0 0 0 0

30 33 1 0 0 0 0

34 35 2 0 0 0 0

34 36 1 0 0 0 0

35 37 1 0 0 0 0

35 38 1 0 0 0 0

36 39 2 0 0 0 0

36 40 1 0 0 0 0

37 41 2 0 0 0 0

37 42 1 0 0 0 0

39 41 1 0 0 0 0

39 43 1 0 0 0 0

41 44 1 0 0 0 0

45 46 2 0 0 0 0

45 47 1 0 0 0 0

46 48 1 0 0 0 0

46 49 1 0 0 0 0

47 50 2 0 0 0 0

47 51 1 0 0 0 0

48 52 2 0 0 0 0

48 53 1 0 0 0 0

50 52 1 0 0 0 0

50 54 1 0 0 0 0

52 55 1 0 0 0 0

58 59 1 0 0 0 0

58 70 1 0 0 0 0

58 81 1 0 0 0 0

59 60 2 0 0 0 0

59 61 1 0 0 0 0

60 62 1 0 0 0 0

60 63 1 0 0 0 0

61 64 2 0 0 0 0

61 65 1 0 0 0 0

62 66 2 0 0 0 0

62 67 1 0 0 0 0

64 66 1 0 0 0 0

64 68 1 0 0 0 0

66 69 1 0 0 0 0

70 71 2 0 0 0 0

70 72 1 0 0 0 0

71 73 1 0 0 0 0

71 74 1 0 0 0 0

72 75 2 0 0 0 0

72 76 1 0 0 0 0

73 77 2 0 0 0 0

73 78 1 0 0 0 0

75 77 1 0 0 0 0

75 79 1 0 0 0 0

77 80 1 0 0 0 0

81 82 2 0 0 0 0

81 83 1 0 0 0 0

82 84 1 0 0 0 0

82 85 1 0 0 0 0

83 86 2 0 0 0 0

83 87 1 0 0 0 0

84 88 2 0 0 0 0

84 89 1 0 0 0 0

86 88 1 0 0 0 0

86 90 1 0 0 0 0

88 91 1 0 0 0 0

M END

**Table S30 Compound 8-cis Molfile**

RuC42As2H36O2 - Chemcraft

83 89 0 0 0 0 0 0 0 0 1 V2000

0.1017 0.1657 -0.7721 Ru 0 0 0 0 0 0 0 0 0 0 0 0

1.2204 -1.4379 0.7985 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.9480 -0.7911 0.2378 As 0 0 0 0 0 0 0 0 0 0 0 0

-1.4483 -1.7568 1.8830 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.3430 -0.9621 2.6379 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.2729 -2.4036 2.2198 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.1581 -2.5360 1.6920 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.3173 -3.4034 1.0310 H 0 0 0 0 0 0 0 0 0 0 0 0

0.2427 -2.9093 2.6472 H 0 0 0 0 0 0 0 0 0 0 0 0

0.4041 -0.9966 -2.2480 C 0 0 0 0 0 0 0 0 0 0 0 0

0.5854 -1.6359 -3.1906 O 0 0 0 0 0 0 0 0 0 0 0 0

0.8886 1.8511 0.4675 C 0 0 0 0 0 0 0 0 0 0 0 0

1.7853 1.4986 -0.6173 C 0 0 0 0 0 0 0 0 0 0 0 0

1.1860 1.4441 1.4389 H 0 0 0 0 0 0 0 0 0 0 0 0

2.6565 0.9217 -0.2708 H 0 0 0 0 0 0 0 0 0 0 0 0

2.2311 2.4344 -1.6999 C 0 0 0 0 0 0 0 0 0 0 0 0

2.1018 2.1458 -3.0637 C 0 0 0 0 0 0 0 0 0 0 0 0

2.8893 3.6240 -1.3426 C 0 0 0 0 0 0 0 0 0 0 0 0

2.6015 3.0124 -4.0367 C 0 0 0 0 0 0 0 0 0 0 0 0

1.5982 1.2236 -3.3607 H 0 0 0 0 0 0 0 0 0 0 0 0

3.3843 4.4940 -2.3102 C 0 0 0 0 0 0 0 0 0 0 0 0

3.0026 3.8681 -0.2830 H 0 0 0 0 0 0 0 0 0 0 0 0

3.2416 4.1925 -3.6651 C 0 0 0 0 0 0 0 0 0 0 0 0

2.4839 2.7617 -5.0943 H 0 0 0 0 0 0 0 0 0 0 0 0

3.8845 5.4167 -2.0039 H 0 0 0 0 0 0 0 0 0 0 0 0

3.6275 4.8752 -4.4264 H 0 0 0 0 0 0 0 0 0 0 0 0

0.1589 3.1240 0.6659 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.1807 3.4860 1.9848 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.2168 4.0181 -0.3553 C 0 0 0 0 0 0 0 0 0 0 0 0

-0.8705 4.6603 2.2731 C 0 0 0 0 0 0 0 0 0 0 0 0

0.1102 2.8194 2.8025 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.9045 5.1944 -0.0680 C 0 0 0 0 0 0 0 0 0 0 0 0

0.0308 3.7978 -1.3935 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.2414 5.5262 1.2446 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.1139 4.9032 3.3112 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.1803 5.8629 -0.8879 H 0 0 0 0 0 0 0 0 0 0 0 0

-1.7797 6.4518 1.4628 H 0 0 0 0 0 0 0 0 0 0 0 0

-0.9146 1.3157 -1.8563 C 0 0 0 0 0 0 0 0 0 0 0 0

-1.5857 1.9559 -2.5363 O 0 0 0 0 0 0 0 0 0 0 0 0

2.2572 -0.7556 2.3037 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6367 -0.5645 2.1668 C 0 0 0 0 0 0 0 0 0 0 0 0

1.6355 -0.3952 3.5053 C 0 0 0 0 0 0 0 0 0 0 0 0

4.3811 -0.0258 3.2158 C 0 0 0 0 0 0 0 0 0 0 0 0

4.1420 -0.8495 1.2402 H 0 0 0 0 0 0 0 0 0 0 0 0

2.3827 0.1374 4.5550 C 0 0 0 0 0 0 0 0 0 0 0 0

0.5581 -0.5248 3.6353 H 0 0 0 0 0 0 0 0 0 0 0 0

3.7568 0.3249 4.4114 C 0 0 0 0 0 0 0 0 0 0 0 0

5.4578 0.1174 3.0962 H 0 0 0 0 0 0 0 0 0 0 0 0

1.8860 0.4097 5.4896 H 0 0 0 0 0 0 0 0 0 0 0 0

4.3414 0.7458 5.2330 H 0 0 0 0 0 0 0 0 0 0 0 0

2.4648 -2.7673 0.1225 C 0 0 0 0 0 0 0 0 0 0 0 0

2.7105 -3.9603 0.8134 C 0 0 0 0 0 0 0 0 0 0 0 0

3.1589 -2.5027 -1.0622 C 0 0 0 0 0 0 0 0 0 0 0 0

3.6289 -4.8819 0.3151 C 0 0 0 0 0 0 0 0 0 0 0 0

2.1902 -4.1771 1.7500 H 0 0 0 0 0 0 0 0 0 0 0 0

4.0850 -3.4235 -1.5538 C 0 0 0 0 0 0 0 0 0 0 0 0

2.9723 -1.5731 -1.6065 H 0 0 0 0 0 0 0 0 0 0 0 0

4.3174 -4.6140 -0.8688 C 0 0 0 0 0 0 0 0 0 0 0 0

3.8109 -5.8136 0.8564 H 0 0 0 0 0 0 0 0 0 0 0 0

4.6214 -3.2083 -2.4811 H 0 0 0 0 0 0 0 0 0 0 0 0

5.0381 -5.3379 -1.2574 H 0 0 0 0 0 0 0 0 0 0 0 0

-2.8778 -2.1597 -0.7985 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.0789 -1.9092 -2.1613 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.3412 -3.3629 -0.2550 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.7435 -2.8361 -2.9612 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.7051 -0.9823 -2.6053 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.9972 -4.2964 -1.0592 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.1966 -3.5900 0.8041 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.2024 -4.0332 -2.4118 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.8953 -2.6249 -4.0224 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.3495 -5.2346 -0.6230 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.7162 -4.7642 -3.0408 H 0 0 0 0 0 0 0 0 0 0 0 0

-3.4366 0.2914 0.8690 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.7087 -0.2461 1.0974 C 0 0 0 0 0 0 0 0 0 0 0 0

-3.2022 1.6485 1.1084 C 0 0 0 0 0 0 0 0 0 0 0 0

-5.7322 0.5691 1.5775 C 0 0 0 0 0 0 0 0 0 0 0 0

-4.9086 -1.3005 0.8878 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.2294 2.4605 1.5904 C 0 0 0 0 0 0 0 0 0 0 0 0

-2.2147 2.0766 0.9153 H 0 0 0 0 0 0 0 0 0 0 0 0

-5.4928 1.9216 1.8260 C 0 0 0 0 0 0 0 0 0 0 0 0

-6.7252 0.1470 1.7522 H 0 0 0 0 0 0 0 0 0 0 0 0

-4.0327 3.5198 1.7721 H 0 0 0 0 0 0 0 0 0 0 0 0

-6.2994 2.5588 2.1975 H 0 0 0 0 0 0 0 0 0 0 0 0

1 2 1 0 0 0 0

1 3 1 0 0 0 0

1 10 1 0 0 0 0

1 13 1 0 0 0 0

1 38 1 0 0 0 0

2 7 1 0 0 0 0

2 40 1 0 0 0 0

2 51 1 0 0 0 0

3 4 1 0 0 0 0

3 62 1 0 0 0 0

3 73 1 0 0 0 0

4 5 1 0 0 0 0

4 6 1 0 0 0 0

4 7 1 0 0 0 0

7 8 1 0 0 0 0

7 9 1 0 0 0 0

10 11 3 0 0 0 0

12 13 1 0 0 0 0

12 14 1 0 0 0 0

12 27 2 0 0 0 0

13 15 1 0 0 0 0

13 16 1 0 0 0 0

16 17 2 0 0 0 0

16 18 1 0 0 0 0

17 19 1 0 0 0 0

17 20 1 0 0 0 0

18 21 2 0 0 0 0

18 22 1 0 0 0 0

19 23 2 0 0 0 0

19 24 1 0 0 0 0

21 23 1 0 0 0 0

21 25 1 0 0 0 0

23 26 1 0 0 0 0

27 28 1 0 0 0 0

27 29 1 0 0 0 0

28 30 2 0 0 0 0

28 31 1 0 0 0 0

29 32 2 0 0 0 0

29 33 1 0 0 0 0

30 34 1 0 0 0 0

30 35 1 0 0 0 0

32 34 1 0 0 0 0

32 36 1 0 0 0 0

34 37 1 0 0 0 0

38 39 3 0 0 0 0

40 41 2 0 0 0 0

40 42 1 0 0 0 0

41 43 1 0 0 0 0

41 44 1 0 0 0 0

42 45 2 0 0 0 0

42 46 1 0 0 0 0

43 47 2 0 0 0 0

43 48 1 0 0 0 0

45 47 1 0 0 0 0

45 49 1 0 0 0 0

47 50 1 0 0 0 0

51 52 2 0 0 0 0

51 53 1 0 0 0 0

52 54 1 0 0 0 0

52 55 1 0 0 0 0

53 56 2 0 0 0 0

53 57 1 0 0 0 0

54 58 2 0 0 0 0

54 59 1 0 0 0 0

56 58 1 0 0 0 0

56 60 1 0 0 0 0

58 61 1 0 0 0 0

62 63 2 0 0 0 0

62 64 1 0 0 0 0

63 65 1 0 0 0 0

63 66 1 0 0 0 0

64 67 2 0 0 0 0

64 68 1 0 0 0 0

65 69 2 0 0 0 0

65 70 1 0 0 0 0

67 69 1 0 0 0 0

67 71 1 0 0 0 0

69 72 1 0 0 0 0

73 74 2 0 0 0 0

73 75 1 0 0 0 0

74 76 1 0 0 0 0

74 77 1 0 0 0 0

75 78 2 0 0 0 0

75 79 1 0 0 0 0

76 80 2 0 0 0 0

76 81 1 0 0 0 0

78 80 1 0 0 0 0

78 82 1 0 0 0 0

80 83 1 0 0 0 0

M END

**References**

1. Schott D*, et al.* (2002) Ruthenium dihydride complexes: NMR studies of intramolecular isomerization and fluxionality including the detection of minor isomers by parahydrogen-induced polarization. *Inorg. Chem.* 41(11):2960-2970.

2. Blazina D*, et al.* (2005) Generation and interrogation of a pure nuclear spin state by parahydrogen-enhanced NMR spectroscopy: a defined initial state for quantum computation. *Mag. Res. Chem.* 43(3):200-208.

3. Bodenhausen G, Caravatti P, Deli J, Ernst RR, & Sauter H (1982) Optical Alignment In Magic-Angle Nmr. *J. Mag. Res.* 48(1):143-147.

4. Blazina D*, et al.* (2001) NMR studies of Ru-3(CO)(10)(PMe2Ph)(2) and Ru-3(CO)(10)(PPh3)(2) and their H-2 addition products: Detection of new isomers with complex dynamic behavior. *J. Am. Chem. Soc.* 123(40):9760-9768.

5. Godard C*, et al.* (2002) NMR characterisation of unstable solvent and dihydride complexes generated at low temperature by in-situ UV irradiation. *Chem. Commun. (*23):2836-2837.

6. Pople JA, Headgordon M, Fox DJ, Raghavachari K, & Curtiss LA (1989) Gaussian-1 Theory - A General Procedure For Prediction Of Molecular-Energies. *J. Chem. Phys.* 90(10):5622-5629.

7. Becke AD (1993) Density-Functional Thermochemistry.3. The Role Of Exact Exchange. *J. Chem. Phys.* 98(7):5648-5652.

8. Lee C & Parr RG (1990) Exchange-Correlation Functional For Atoms And Molecules. *Phys. Rev. A* 42(1):193-200.

9. Hay PJ & Wadt WR (1985) Abinitio Effective Core Potentials For Molecular Calculations - Potentials For K To Au Including The Outermost Core Orbitals. *J. Chem. Phys.* 82(1):299-310.

10. Hollwarth A*, et al.* (1993) A Set Of D-Polarization Functions For Pseudo-Potential Basis-Sets Of The Main-Group Elements Al-Bi And F-Type Polarization Functions For Zn, Cd, Hg. *Chem. Phys. Let.* 208(3-4):237-240.

11. Hehre WJ, Ditchfie.R, & Pople JA (1972) Self-Consistent Molecular-Orbital Methods.12. Further Extensions Of Gaussian-Type Basis Sets For Use In Molecular-Orbital Studies Of Organic-Molecules. *J. Chem. Phys* 56(5):2257-&.

12. Harihara.Pc & Pople JA (1973) Influence Of Polarization Functions On Molecular-Orbital Hydrogenation Energies. *Theor. Chim. Acta* 28(3):213-222.

13. Francl MM*, et al.* (1982) Self-Consistent Molecular-Orbital Methods.23. A Polarization-Type Basis Set For 2nd-Row Elements. *J. Chem. Phys.* 77(7):3654-3665.

14. Maseras F & Morokuma K (1995) Imomm - A New Integrated Ab-Initio Plus Molecular Mechanics Geometry Optimization Scheme Of Equilibrium Structures And Transition-States. *J. Comput. Chem.* 16(9):1170-1179.

15. Svensson M*, et al.* (1996) ONIOM: A multilayered integrated MO+MM method for geometry optimizations and single point energy predictions. A test for Diels-Alder reactions and Pt(P(t-Bu)(3))(2)+H-2 oxidative addition. *J. Phys. Chem* 100(50):19357-19363.

16. Dapprich S, Komaromi I, Byun KS, Morokuma K, & Frisch MJ (1999) A new ONIOM implementation in Gaussian98. Part I. The calculation of energies, gradients, vibrational frequencies and electric field derivatives. J. Mol. Struct.: THEOCHEM 461:1-21.