Intramolecular proton transfer boosts water oxidation catalyzed by a Ru complex

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Outline

Materials

All materials were provided by Sigma-Aldrich unless indicated. [2,2':6',2''-terpyridine]-6,6''-dicarboxylic acid (H_2tda)[1], [2,2'-bipyridine]-6,6'-dicarboxylic acid (H_2bda)[2] and RubdaPic$_2$[2] (where Pic is Picoline) and $RuCl_2DMSO_4$[3] were synthesized and purified according to the literature. High-purity deionized water was obtained by passing distilled water through a nanopure Milli-Q water purification system.

Synthesis of [Ru^{II}(tda-κ-N^{3}O)Py$_2$], **1***:* $RuCl_2dmso_4$ (150 mg, 0.31 mmol), 2',2'':6',2''-terpyridine-6',6''-dicarboxylic acid (H_2tda) (99 mg, 0.31 mmol) and Et_3N (0.3 mL) were degassed in dry MeOH (6 mL), refluxed for 6 hours and cooled down to RT. A brown solid appeared in the reaction mixture and was filtered, washed with MeOH and Ether. The solid was suspended in water (5mL) and pyridine (15 mL) and refluxed overnight. The resulting red-wine solution was cooled to RT and washed with DCM (3x100mL). The watery solution was evaporated and the red solid was dissolved with MeOH and precipitated with Ether. (95 mg, 0.16 mmol, 51 % yield). ^{1}H-NMR (500Hz, [d4] Methanol) δ: 7.09 (4H, t, J=7.5 Hz), 7.58 (2H, tt, J=1.4 and 7.5 Hz), 8.03 (3H, t, J=7.9 Hz), 8.05 (2H, t, J=8.1 Hz), 8.12 (4H, dd, J=1.4 and 7.5), 8.15 (2H, d, 7.9 Hz), 8.49 (2H, d, 7.9 Hz), 8.61 (2H, d, J=8.1 Hz). ^{13}C-NMR (500Hz, [d4] Methanol) δ: 125.2, 125.4, 126.1, 128.1, 133.8, 138.0, 138.1, 153.6, 158.4, 159.6, 163.8, 172.4. UV-vis [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 236 (21700), 282 (24800), 327 (30700) and 530 (3700). ESI$^+$-HRMS m/z: calc. for RutdaPy$_2$-Na$^+$ ($C_{27}H_{19}N_5NaO_4Ru^+$): 602.03727, found m/z: 602.03678 (0.7 ppm). *Anal.* Calc. *for* ***1****·3.5 H_2O*: C, 50.54%; H, 4.08 %; N, 10.92 %. Found: C, 50.46 %; H, 3.78 %; N, 10.87%.

*Synthesis of [Ru^{III}(tda-κ-N^{3}O)Py$_2$] [PF$_6$], (**2**)(PF$_6$):* A solution of Ceric Ammonium Nitrate (CAN) (1.82 mM, 1.05 eq, 2mL) was added drop wise to a solution of **1** in triflic acid (1.72 mM, 25 mL) and the mixture was stirred for 15 minutes. A green powder was obtained when a saturated solution of KPF_6 was added. The suspension was centrifuged for 10 minutes, the solid filtrated and washed with water, methanol and ether (12 mg, 39%). UV-vis [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 279 (25800, 322 (13200) and 441 (1300). *Anal. Calc. for (**2**)(PF$_6$)·0.5 H_2O* : C, 44.27%; H, 2.75 %; N, 9.56 %. Found: C, 44.23 %; H, 2.50 %; N, 9.39%.

*Synthesis of [Ru^{IV}(tda-κ-N^{3}O^2)Py$_2$] [PF$_6$], (**3**)(PF$_6$)$_2$.* A solution of CAN (3.64 mM, 2.1 eq, 2mL) was added drop wise to a solution of **1** in triflic acid (1.72 mM, 25 mL) and the mixture was stirred for 15 minutes. A brown powder was obtained when a saturated solution of KPF_6 was added. The suspension was centrifuged for 10 minutes, the solid filtrated and washed with cold water and ether (12 mg, 32%). ^{1}H-NMR (500 Hz, D_2O) δ: 7.24 (4H, t, J=7.0 Hz), 7.70 (6H, m), 8.20 (2H, d, J=7.8 Hz), 8.62 (2H, t, J=7.8 Hz), 8.93 (2H, d, J=7.8 Hz), 8.98 (1H, d, J=7.9 Hz), 9.08 (2H, d, J=7.9 Hz). ^{13}C-NMR (500Hz, D_2O) δ: 127.3, 123.0, 131.0, 132.2, 141.5, 147.3, 147.6, 150.3, 152.5, 157.8, 157.9, 168.0. UV-vis [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 280 (23600) and 347 (6800).

Preparation of 0.1 M ionic strenght phospahte solutions.

a) pH = 2.0 buffered solution: Powders of H_3PO_4 (10.5 g, 0.1073 M) and NaH_2PO4 (11.83 g, 0.0986 M) were dissolved with deionised water up to 1 L solution.

b) pH = 7.0 buffered solution: Powders of NaH_2PO4 (2.31 g, 0.0193 M) and Na_2HPO_4 (3.77g, 0.0266 M) were with deionised water up to 1 L solution.

c) pH = 12.0 buffered solution: Powders of Na_2HPO_4 (10.293g, 0.0073 M) and Na_3PO_4 (2.06g, 0.0126 M) were dissolved with deionised water up to 1 L solution.

Solutions at pHs between 2.0 and 12.0 were prepared by mixing the above solutions. The pH of all solutions were measured by a pHmeter. All solutions contained a ionic strengh equal to 0.1 M.

Preparation of the ***3^{2+}/4*** *mixtures.*

Bulk electrolysis at E_{app} = 1.25 V (see electrochemical methods for more details) was applied to a phosphate buffer solution of **1** at pH = 7.0 or 10.5 for a given period of time. The final pH was adjusted by further addition of a phosphate buffer solution till the desired pH, monitored by a pH meter. This ensures that all solutions end up with a 0.1 M ionic strength.

The ratio of the **3^{2+}/4** species depends on the initial pH and concentration of **1**, as well as on the duration of the bulk electrolysis, see table S1 for details.

In the case of deuterated solvents for ^{1}H NMR experiments, the same procedure was followed.

Methods

General instrumentation

Electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI) mass spectrometry (MS) experiments were performed on a Waters Micromass LCT Premier equipment and a Bruker Daltonics Autoflex equipped with a nitrogen laser (337 nm), respectively. UV−Vis spectroscopy was performed on a Cary 50 Bio (Varian) UV−Vis spectrophotometer with 1 cm quartz cells unless indicated. A 400 MHz Bruker Avance II spectrometer and a Bruker Avance 500 MHz were used to carry out NMR spectroscopy. FT-IR measurements were carried out on a Bruker Optics FTIR Alpha spectrometer equipped with a DTGS detector, and a KBr beamsplitter at 4 cm^{-1} resolution. The EPR experiments were carried out at 4 K on frozen solutions by using a X-band spectrometer (Bruker ELEXYS E580). The pH of the solutions was determined by a pHmeter (CRISON, Basic 20^{+}) calibrated before measurements through a standard solutions at pH= 4.01, 7.00 and 9.21. Oxygen evolution was analysed with a gas phase Clark type oxygen electrode (Unisense Ox-N needle microsensor) and calibrate by the addition of small quantities of oxygen (99%).

Electrochemical methods

General considerations

All electrochemical experiments were performed in an IJ-Cambria HI-730 bipotentiostat, using a three-electrode cell. $E_{1/2}$ values reported in this work were estimated from CV experiments as the average of the oxidative and reductive peak potentials ($\frac{Ep,a + Ep,c}{2}$) or from DPV. The Reference Electrode (RE) was Hg/Hg_2SO_4 (K_2SO_4 saturated) unless indicated and potentials were converted to NHE by adding 0.65 V.

Cells: A 20 mL vial was used as an electrochemical cell for CV measurements. A Teflon-made with holes for the three electrodes was used as a lid to ensure a reproducible distance between the electrodes. A two compartments cell (25 mL per compartment) with a separation grid was used for Bulk Electrolysis Experiments.

Cyclic voltammetry (CV) and Differential Pulse Voltammetry

Glassy carbon disk (ϕ = 0.3 cm, S = 0.07 cm^2), Pt disk and Hg/Hg_2SO_4 (K_2SO_4 saturated) were used as Working Electrode (WE), Counter Electrode (CE) and Reference Electrode (RE) respectively, unless explicitly mentioned. Glassy carbon electrodes were polished successively with 1.0, 0.3, and 0.05 µm alumina (Al_2O_3), sonicated with MeCN for 15 minutes and washed with acetone. CVs and DPVs were iR compensated by the potentiostat in all the measurements unless indicated. Cyclic Voltammograms (CV) were recorded at 100 $mV \cdot s^{-1}$ scan rate, unless explicitly expressed. The DPV parameters were ΔE = 4 mV, Amplitude = 0mV, Pulse width = 5 s, Sampling width = 0.0167 s, Pulse period = 5 s unless explicated.

Bulk electrolysis

A Pt grid was used as a WE, another Pt grid as a CE and a Hg/Hg_2SO_4 (K_2SO_4 saturated) as a RE. iR compensation by the potentiostat was not applied in this technique. For the bulk electrolysis experiment described in Figure S22, a glassy carbon rod (S = 8.2 cm^2) was used as a working electrode and Ag/AgCl (sat. KCl) as a RE.

CV-monitored Bulk electrolysis in a bipotentiostat

A glassy carbon and a Pt grid were used as working electrodes, another Pt grid as a counter electrode and Hg/Hg_2SO_4 as a Reference electrode. The glassy carbon electrode was used to perform the consecutive CVs and the Pt grid was used to apply a continuous potential through a coulometry technique. The counter electrode was placed in one compartment provided with a magnetic stirrer and the other 3 electrodes were placed in the other compartment also provided with a magnetic stirrer. To be able to simultaneously stir the solution and to perform the CV, the magnetic stirrer power was set at low frequency (100-200 rpm). In addition, the reference electrode was placed between the glassy carbon working electrode and the magnetic stirrer.

Foot of the wave analysis

The analysis was performed by following the procedure of Savéant *et al* in the literature. [4] The expression (equation S1) was deduced for a general scheme where a single chemical step, which is the rate determining step, and a single electron transfer, which is fast, are responsible for the rate of the reaction. Where R is the gas constant, T is the temperature, k_{obs} is a pseudoconstant (s^{-1}), E^0 and are the potentials of the chemical step prior to the electron transfer.

$$\frac{i}{i_p} = \frac{8.97\sqrt{\left(\frac{R\cdot T}{F\cdot \nu}\right)\cdot k_{obs}}}{1+\exp\left(\frac{F(E^0-E)}{RT}\right)} \quad \text{(S1)}$$

$$TON = \frac{k_{obs}t}{1+\exp\left[\frac{F}{R\cdot T}(E^0-E)\right]} \quad \text{(S2)}$$

The intensity of the anodic wave of the Ru^{III}-OH_2/Ru^{II}-OH was used as i_p as an approximation. E^0 was extracted from DPV of the same solution.

The value of k_{obs} is equivalent to TOF_{MAX} (s^{-1}) in the used electrocatalytic scheme. TOF_{MAX} is the maximum Turn Over Frequency (s^{-1}) that a molecule can catalyze the water oxidation reaction when E_{app} tends to infinite potential. [4]

The Turn Over Number (TON) of **4** in the bulk electrolysis experiments were calculated according to formula S2.[4]

Single Crystal XRD Methods

X-ray Crystal Structure Determination

Crystals of **1** were obtained by slow diffusion of ether to a methanol solution (0.2 mM). Crystals of (**2**)(PF_6) (1 mM) were obtained from a pH=7 phosphate buffer solution saturated with KPF_6**.** Crystals of (**3**)$(PF_6)_2$ were obtained from a pH=1 solution (1mM, 0.1 M triflic acid) saturated with KPF_6. The measured crystals were prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation.

Data collection

Crystal structure determinations for **1,** (**2**)(PF_6) and (**3**)$(PF_6)_2$ were carried out using a Bruker-Nonius diffractometer equipped with an APPEX 2 4K CCD area detector, a FR591 rotating anode with MoK_α radiation, Montel mirrors as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus (T = -173 $^\circ$C). Full-sphere data collection was used with ω and φ scans. *Programs used:* Data collection APEX-2[5], data reduction Bruker Saint[6] V/.60A and absorption correction SADABS[7].

Structure Solution and Refinement

Crystal structure solution was achieved using direct methods as implemented in SHELXTL[8] and visualized using the program XP. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F^2 using all measured intensities was carried out using the program SHELXTL. All non hydrogen atoms were refined including anisotropic displacement parameters.

Comments to the structures

1: The asymmetric unit contains two independent molecules of the metal complex, two methanol molecules and one molecule of water. The independent molecules of the metal complex are distributed in three positions with the ratio 1:0.5:0.5. The two half molecules of the metal complex are located on a twofold rotation axes and have *C*2 symmetry. The carboxylate rests of the two half molecules are disordered in two positions (ratio 50:50). The water molecule is disordered in two positions with a ratio of 58:38. One of the methanol molecules is disordered in two positions with a ratio of 52:48. (**2**)(PF_6): The asymmetric unit contains two independent molecules of the metal complex and two PF_6 anions. In one of molecules of the metal complex one of the pyridine rings is disordered in two positions (ratio 60:40). The asymmetric unit contains four half PF_6 anions which have *C*i symmetry and are located on center of inversions. The half PF_6 anions are shared with neighboring molecules. (**3**)$(PF_6)_2$: The asymmetric unit contains two independent molecules of the metal complex and four PF_6 anions. One of the PF_6 anions is disordered in two orientations (ratio 77:23).

Computational Methods

Density functional theory

Geometry optimizations were performed at M06-L[9] and M11-L[10] levels of density functional theory using the Stuttgart [8s7p6d2f | 6s5p3d2f] ECP28MWB contracted pseudopotential basis set[11] on Ru and the 6-31G(d) basis set[12] on all other atoms. Non-analytical integral evaluations

made use of a pruned grid having 99 radial shells and 590 angular points per shell and an automatically generated density-fitting basis set was used within the resolution-of-the-identity approximation to speed the evaluation of Coulomb integrals as implemented in Gaussian 09 software package.[13] The nature of all stationary points was verified by analytic computation of vibrational frequencies, which were also used for the computation of zero-point vibrational energies, molecular partition functions (with all frequencies below 50 cm^{-1} replaced by 50 cm^{-1} when computing free energies), and for determining the reactants and products associated with each transition-state structure (by following the normal modes associated with imaginary frequencies). Partition functions were used in the computation of 298 K thermal contributions to free energy employing the usual ideal-gas, rigid-rotator, harmonic oscillator approximation.[14] Free energy contributions were added to single-point M06-L and M11-L electronic energies computed with the SDD basis set on ruthenium and the 6-311+G(2df,p) basis set on all other atoms to arrive at final, composite free energies.

Solvation and standard reduction potentials

Solvation effects associated with water as solvent were accounted for using the SMD continuum solvation model.[15] A 1 M standard state was used for all species in aqueous solution except for water itself, for which a 55.6 M standard state was employed. Thus, for all molecules but water, the free energy in aqueous solution is computed as the 1 atm gas-phase free energy, plus an adjustment for the 1 atm to 1 M standard-state concentration change of *RT* ln (24.5), or 1.9 kcal/mol, plus the 1 M to 1 M transfer (solvation) free energy computed from the SMD model. In the case of water, the 1 atm gas-phase free energy is adjusted by the sum of a 1 atm to 55.6 M standard-state concentration change, or 4.3 kcal/mol, and the experimental 1 M to 1 M solvation free energy, –6.3 kcal/mol. The 1 M to 1 M solvation free energy of the proton was taken from experiment as –265.9 kcal/mol.[16-19]

Standard reduction potentials were calculated for various possible redox couples to assess the energetic accessibility of different intermediates at various oxidation states. For a redox reaction of the form

$$O_{(\mathrm{aq})} + n\,e^{-}_{(\mathrm{g})} \rightarrow R_{(\mathrm{aq})} \tag{S3}$$

where *O* and *R* denote the oxidized and reduced states of the redox couple, respectively, and *n* is the number of electrons involved in redox reaction, the reduction potential $E^{\mathrm{o}}_{O|R}$ relative to NHE was computed as

$$E^{\mathrm{o}}_{O|R} = -\frac{\Delta G^{\mathrm{o}}_{O|R} - \Delta G^{\mathrm{o}}_{\mathrm{NHE}}}{nF} \tag{S4}$$

where $\Delta G^{\mathrm{o}}_{O|R}$ is the free energy change associated with eq. 1 (using Boltzmann statistics for the electron), $\Delta G^{\mathrm{o}}_{\mathrm{NHE}}$ is the free energy change associated with

$$\mathrm{H}^{+}_{(aq)} + e^{-}_{(g)} \rightarrow \frac{1}{2}\mathrm{H}_{2(g)} \tag{S5}$$

which is –4.28 eV with Boltzmann statistics for the electron,[18,20,21] and *F* is the Faraday constant.

*Non-single-determinantal state energies***.** Several possible intermediates in the water oxidation mechanism have electronic structures that are not well described by a single determinant. In such instances, standard Kohn-Sham DFT is not directly applicable,[14,22-24] and we adopt the Yamaguchi broken-spin-symmetry (BS) procedure[25,26] to compute the energy of the spin-purified low-spin (LS) state as

$$^{\mathrm{LS}}E = \frac{^{\mathrm{BS}}E\left(\left\langle {}^{\mathrm{HS}}\right| S^2 \left| {}^{\mathrm{LS}}\right\rangle S^2 \right\rangle - {}^{\mathrm{HS}}E\left(\left\langle {}^{\mathrm{BS}}\right| S^2 \left| {}^{\mathrm{LS}}\right\rangle S^2 \right\rangle\right)}{\left\langle {}^{\mathrm{HS}}\right| S^2 \left| {}^{\mathrm{BS}}\right\rangle S^2 \rangle} \tag{S6}$$

where HS refers to the single-determinantal high-spin coupled state that is related to the low-spin state by spin flip(s) and < S^2 > is the expectation value of the total spin operator applied to the appropriate determinant. This broken-symmetry DFT approach has routinely proven effective for the prediction of state-energy splittings in metal coordination compounds.[23,27-30]

Characterization of complexes 1, 2^+ and 3^{2+}

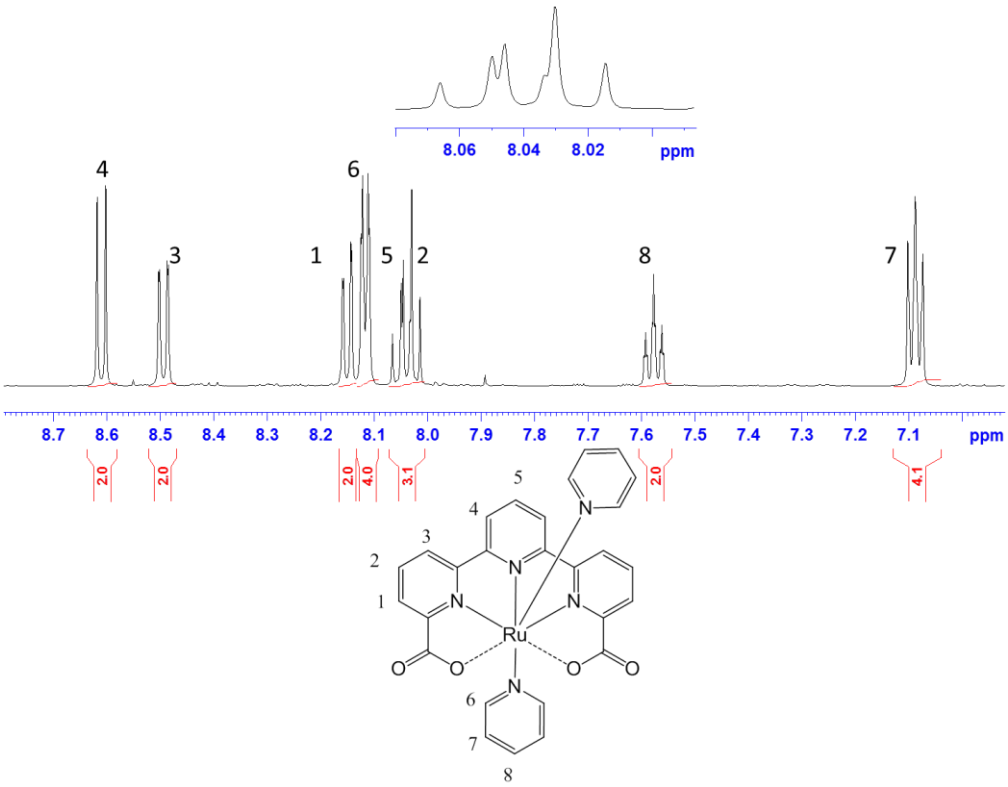


Figure S1: ^{1}H NMR of **1** in [d4]-methanol. T=298K.

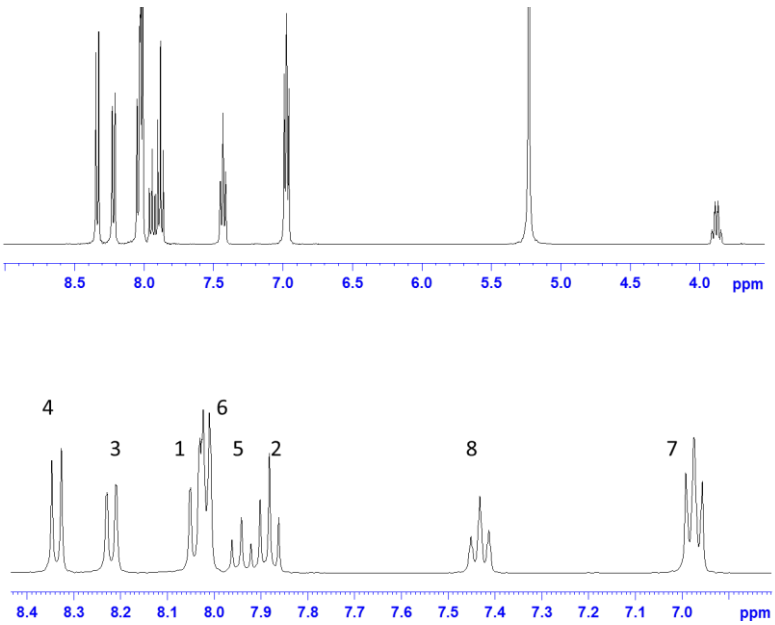


Figure S2: ^{1}H NMR of **1** [d3]-trifluoroehtanol. T=298K.

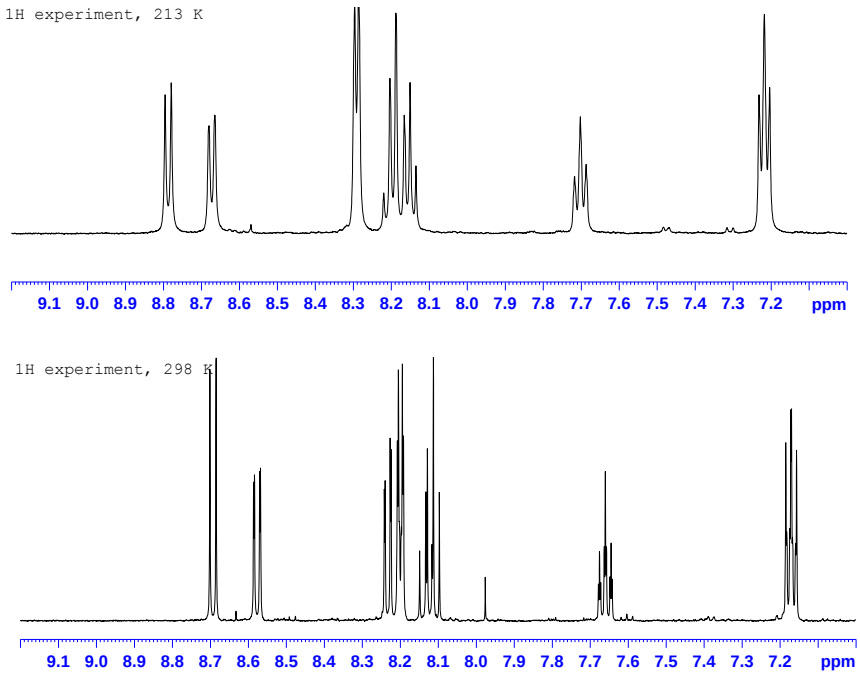


Figure S3: ^{1}H NMR of **1** in [d4]-methanol at 213K and 298K.

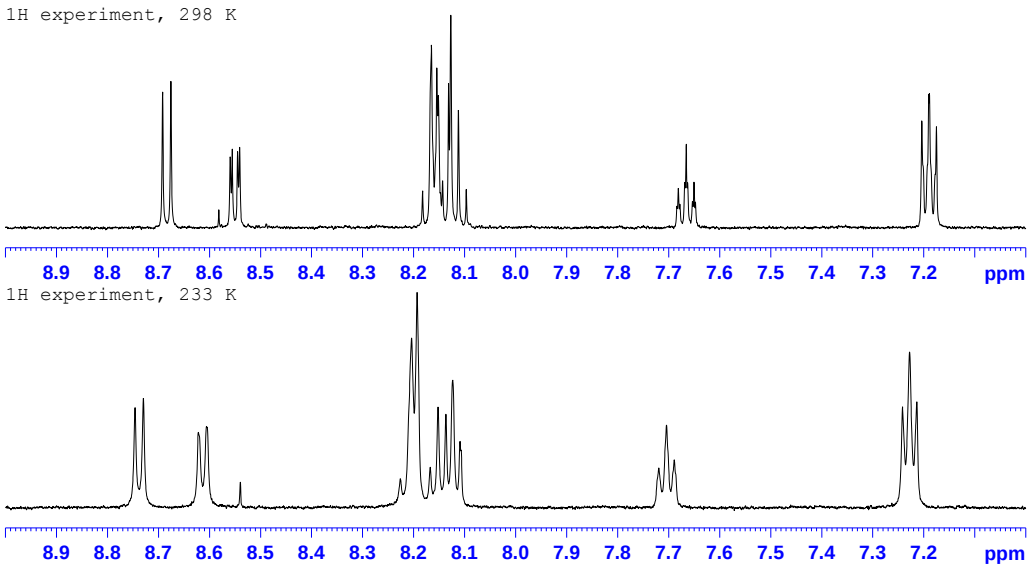


Figure S4: ^{1}H NMR of **1** in [d4]-methanol/ D_2O mixture (4:1) at 298K and 233K.

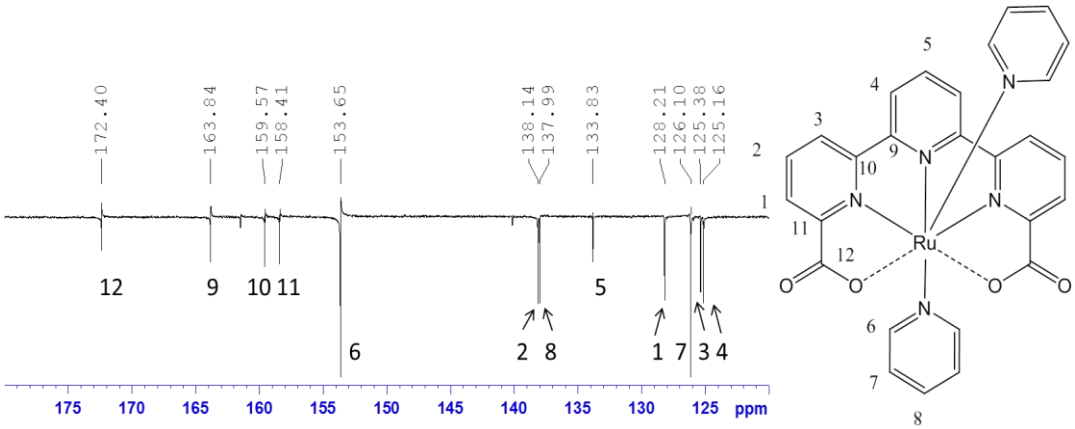


Figure S5: ^{13}C-{H}-NMR (DEPT45) of **1** in [d4]-methanol, T=298K.

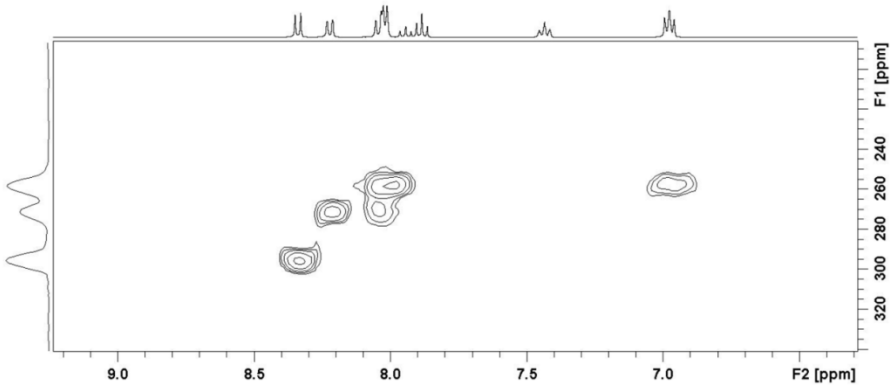


Figure S6: ^{1}H-^{15}N-HMBC of **1** in [d4]-trifluoroethanol, T=298K.

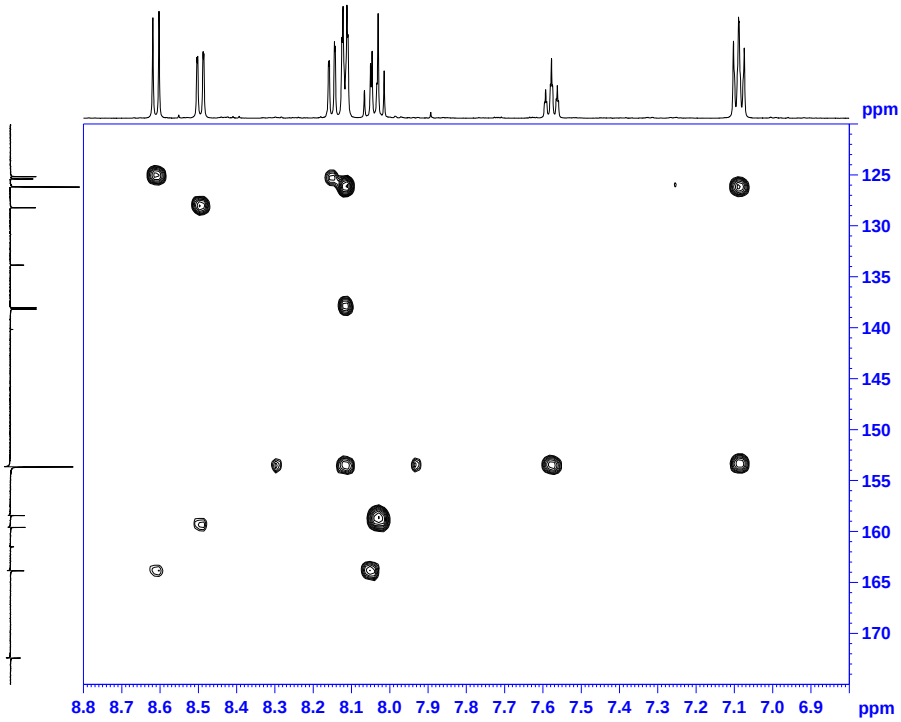


Figure S7: ^{1}H-^{13}C-HMBC NMR of **1** in [d4]-methanol, T=298K.

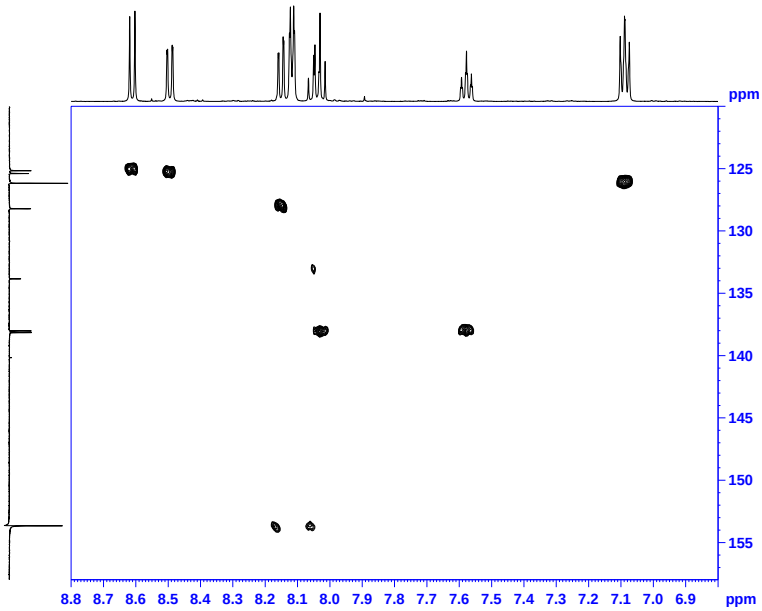


Figure S8: ^{1}H-^{13}C-HQSC NMR of **1** in [d4]-methanol, T=298K.

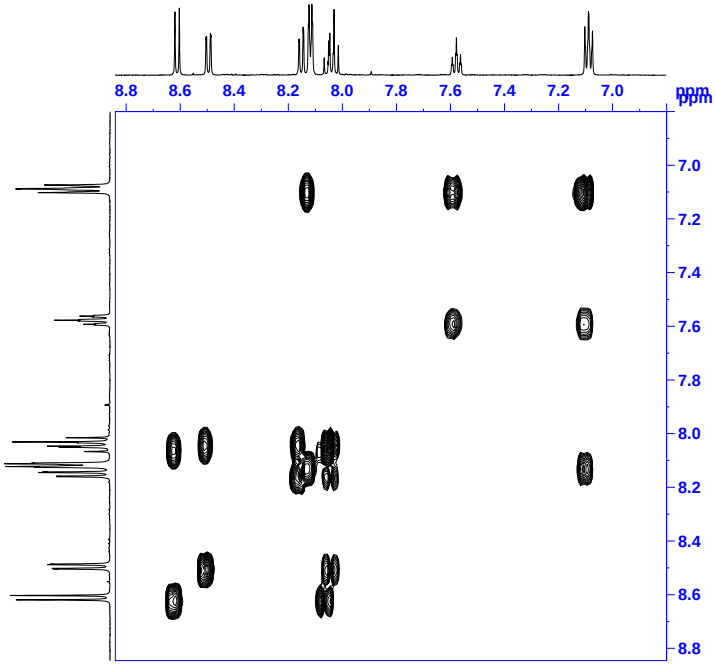


Figure S9: ^{1}H-^{1}H-COSY NMR of **1** in [d4]-methanol, T=298K.

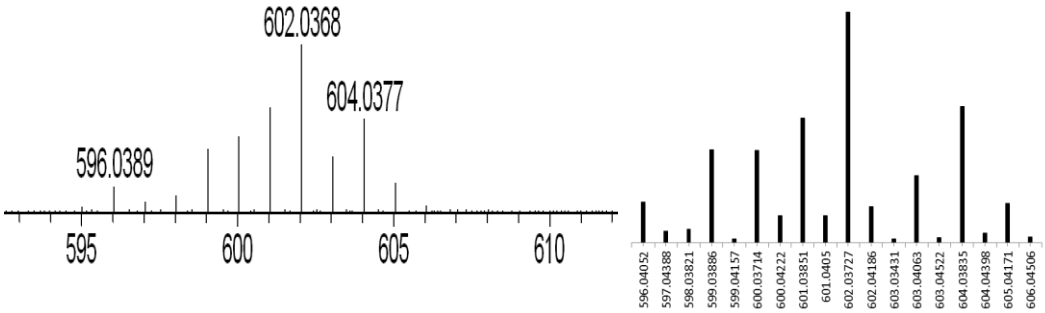


Figure S10: HR-MS for **1**-Na^+ ($C_{27}H_{19}N_5NaO_4Ru^+$) (0.7 ppm error) (left) and simulated (right).

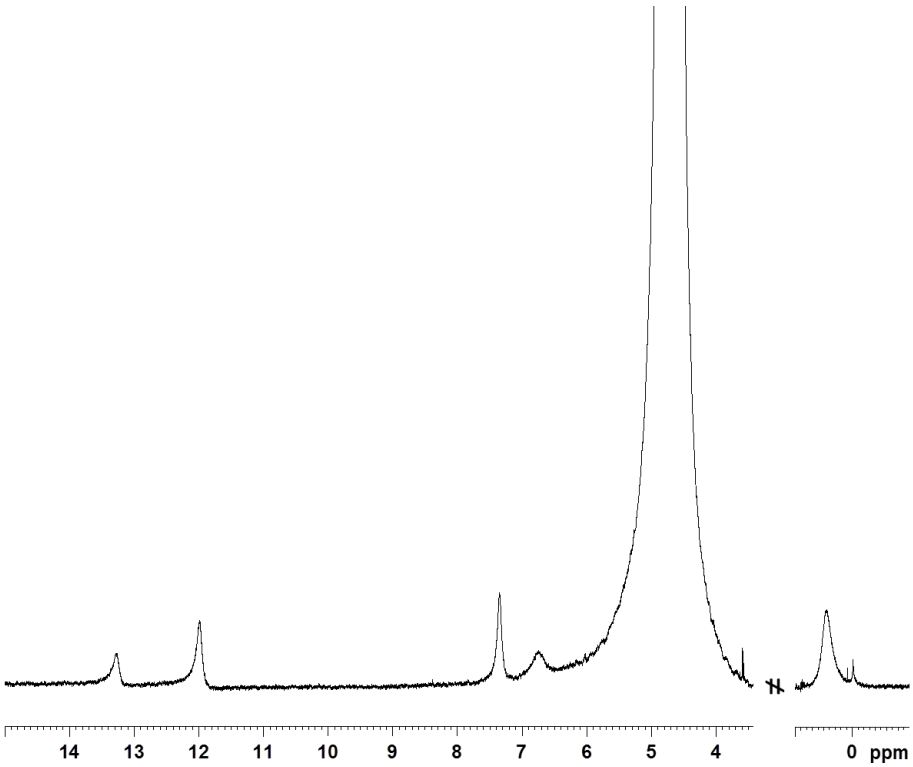


Figure S11: ^{1}H NMR of **2**$^+$ in pD = 7 phosphate buffered solution.

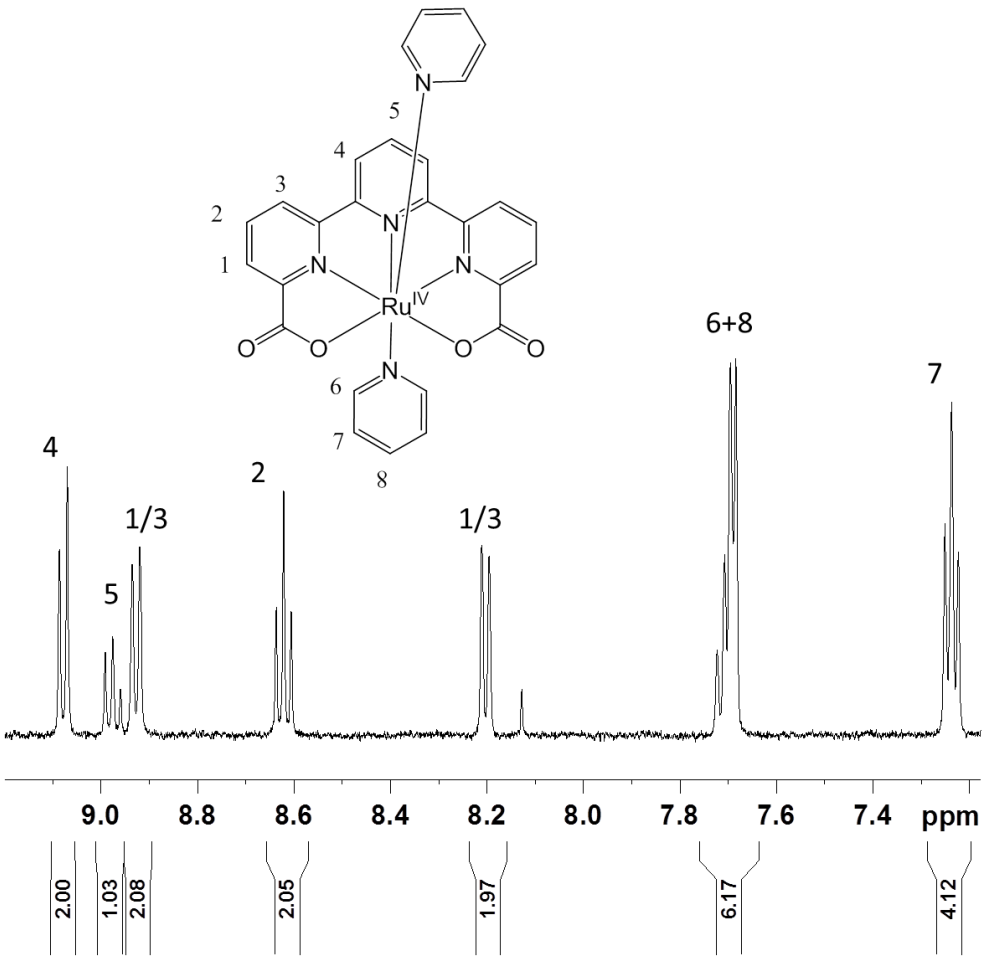


Figure S12: ^{1}H NMR of **3**$^{2+}$ in D_2O (0.1M [d1]-triflic acid).

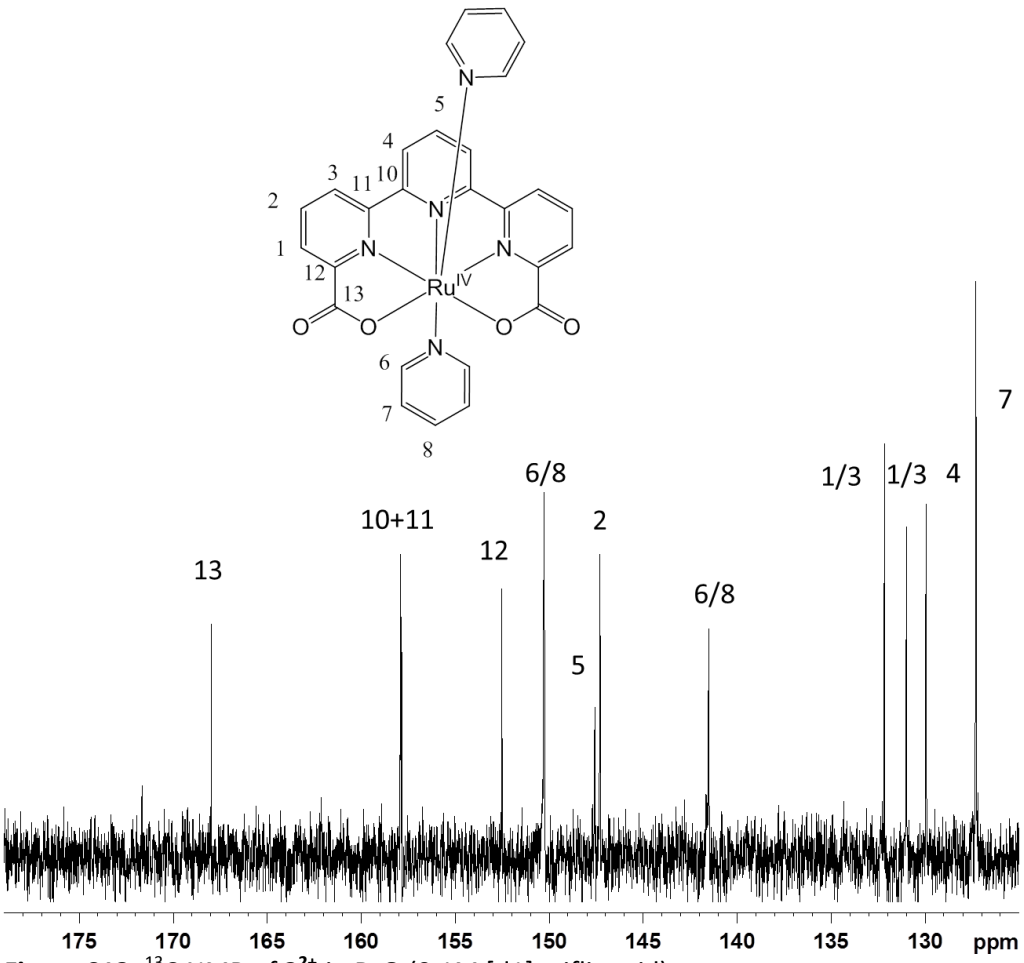


Figure S13: ^{13}C NMR of $\mathbf{3}^{2+}$ in D_2O (0.1M [d1]-triflic acid).

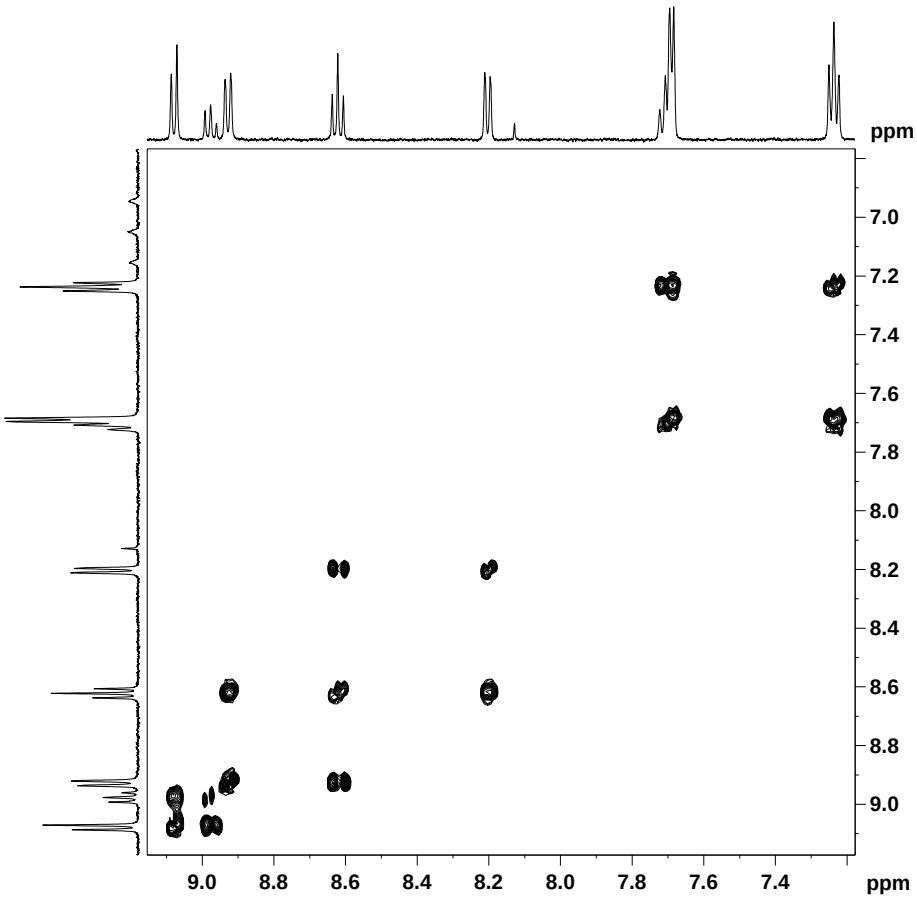


Figure S14: ^{1}H-^{1}H-COSY NMR of **3**$^{2+}$in D_2O (0.1M [d1]-triflic acid).

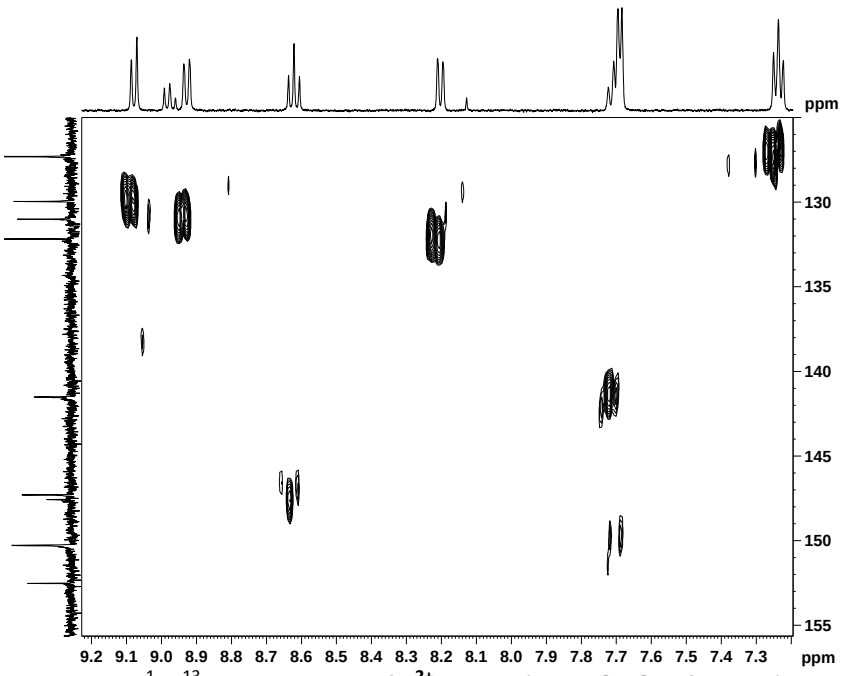


Figure S15: ^{1}H-^{13}H-HSQC NMR of **3**$^{2+}$ in D_2O (0.1M [d1]-triflic acid).

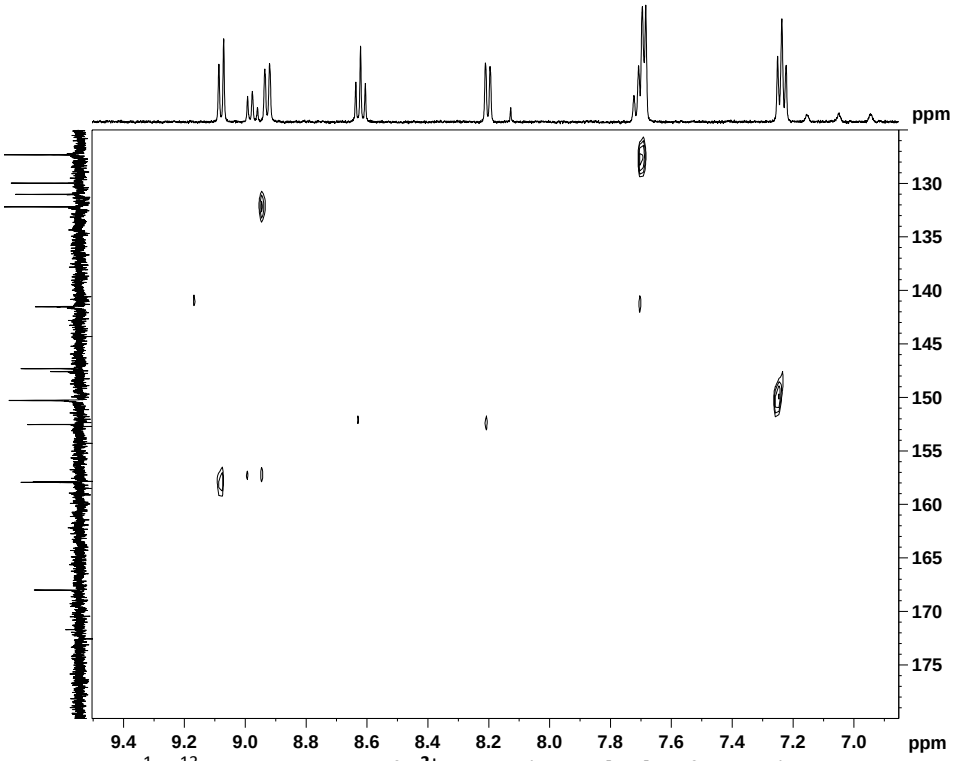


Figure S16: ^{1}H-^{13}H-HMBC NMR of **3**$^{2+}$ in D_2O (0.1M [d1]-triflic acid).

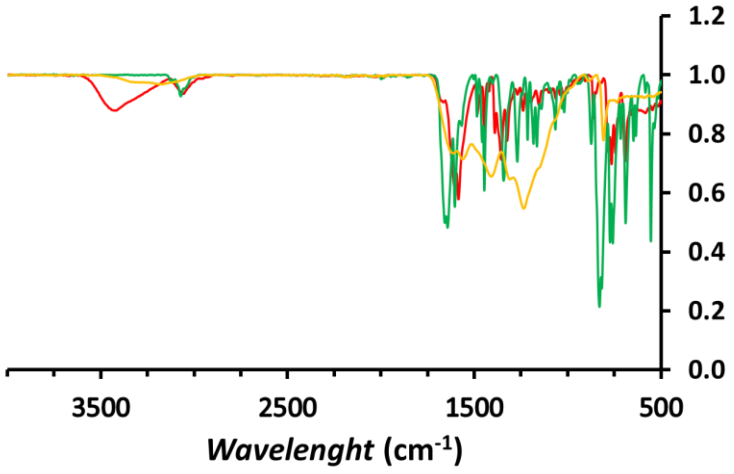


Figure S17: IR of **1** (red line), **2**$^{+}$(green line) and **3**$^{2+}$ (orange line).

Table S1: Experimental conditions to generate different rations of $\mathbf{3^{2+}}$/**4** after applying a bulk electrolysis at E_{app} = 1.25 V to a solution of **1**.

[1] (mM)	Initial pH[a]	I (M)	Time (h)	Ratio 3^{2+} / 4[a]
1.7	7	0.1	12	2:1
1.7	10.5	0.1	1.5	2:1
7	10.5	0.1	1.5	5:1

a) The ratio was estimated from the charge (Q) under the III/II cathodic waves of the "Ru-non aqua" and "Ru-aqua" species, the estimation has a 10% error.

Redox properties of Ru-non aqua and Ru-aqua complexes

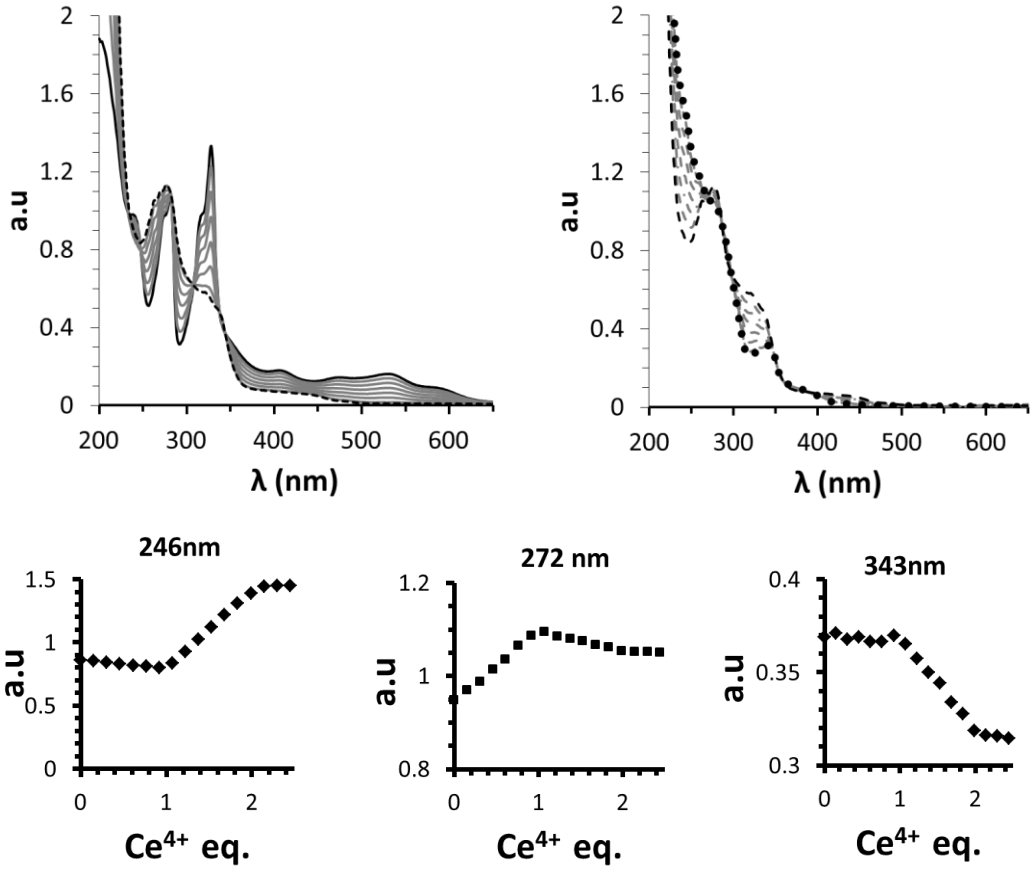


Figure S18: Spectrophotometric redox titration of **1** at pH = 1.0 by CAN (10 μL, 1.66 mM).Top left: UV-vis spectra of **1** (solid black line) and successive additions of 0.152 eq of Ce^{4+} (grey solid lines) up to aprox. 1 equivalent of Cerium (dashed black line).
Top Right: UV-vis spectra of one-electron oxidized **1** (dashed black line), and successive additions of 0.152 eq. of Ce^{4+} (dashed grey lines) up to 2 equivalents of Ce^{4+} (pointed black line). Bottom: plot of absorbance against equivalents of CAN at selected wavelengths (246 nm, 272 nm and 343 nm).

pH dependency of Ru-aqua species

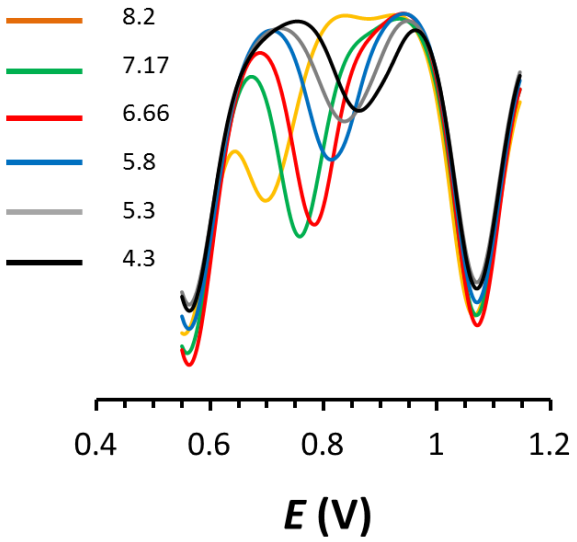


Figure S19: DPV of $\mathbf{3}^{2+}$/**4** mixture at the pHs indicated in the legend. The conditions for the generation of the $\mathbf{3}^{2+}$/**4** mixture were E_{app} = 1.25 V, initial pH=10.5, initial [**1**] = 1.7 mM. Buffered solutions at pH=2 and pH=12 were used to ajust the pH.

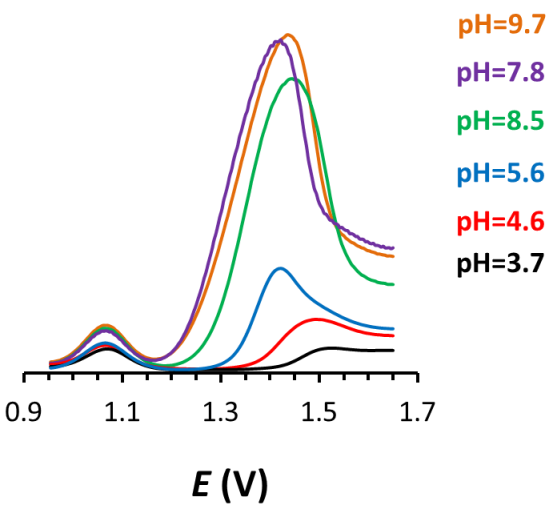


Figure S20: DPV of $\mathbf{3}^{2+}$/**4** mixture at the pHs indicated in the legend. The conditions for the generation of the $\mathbf{3}^{2+}$/**4** mixture were E_{app} = 1.25 V, initial pH=10.5, initial [**1**] = 1.7 mM. Buffered solutions at pH=2 and pH=12 were used to ajust the pH.

Recovery of 1 upon reduction

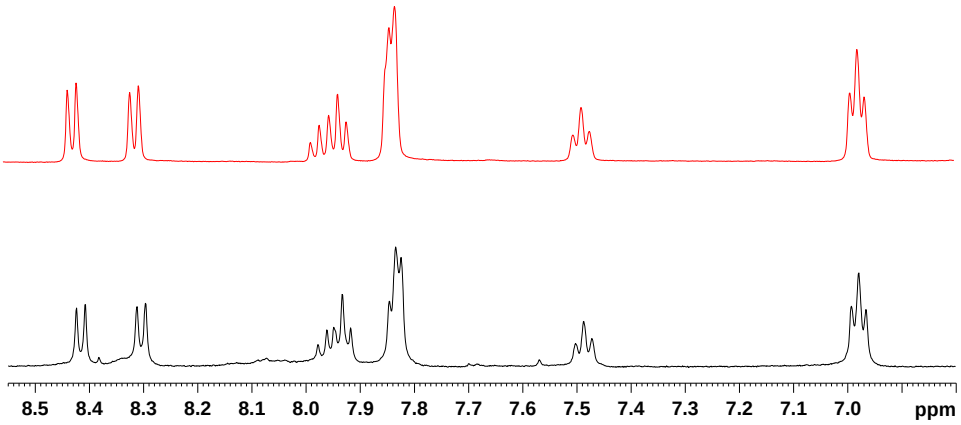


Figure S21. ^{1}H-NMR spectrum of **1** at pD = 7.0 phosphate buffer, obtained from chemical reduction with ascorbic acid of: top, $\mathbf{3}^{2+}$; bottom, from a mixture of $\mathbf{3}^{2+}$/**4** (2/1)**.**

Faradaic efficiency of the electrocatalysis by 4.

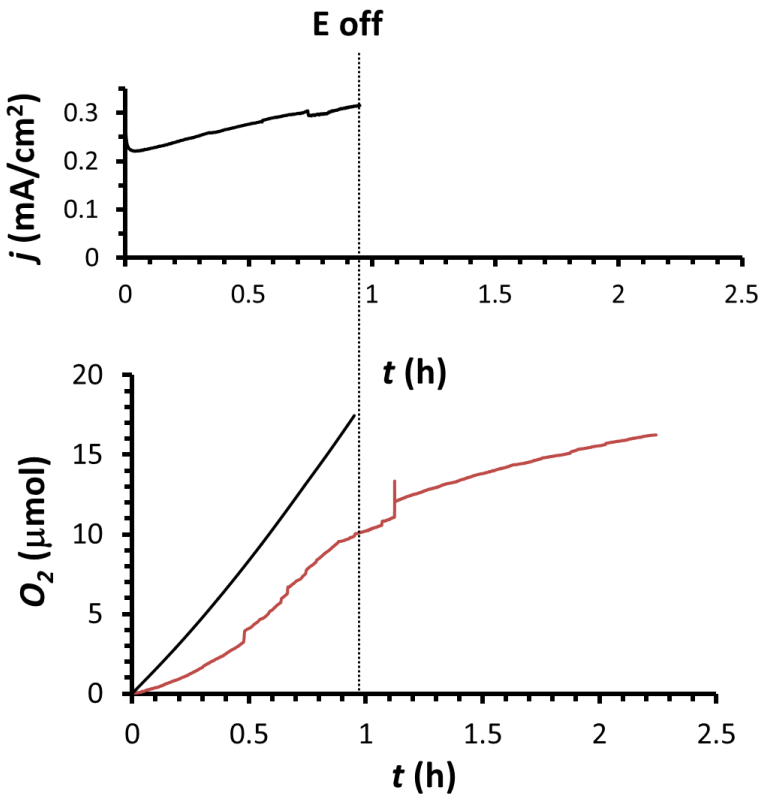


Figure S22: Bulk electrolysis for a mixture of $\mathbf{3}^{2+}$ (0.3 mM) and **4** (0.1 mM) at pH = 7.0 (3 mL) at E_{app} = 1.5 V (vs. NHE). A glassy carbon rod (S = 8.2 cm^2) was used as working, a Pt grid as counter electrode and Ag/AgCl (sat KCl) as a reference electrode.

Top, current density over time. Bottom, oxygen evolution *vs.* time monitored with a Clark electrode (red line) and the theoretical amount of oxygen obtained assuming 100 % Faradaic efficiency from the measured current density on the top (black solid line).
The E_{app} was stopped at 1 h, but oxygen evolution continued till approx. 2.2 h, due to a large number of bubbles trapped in the working electrode. The Faradaic efficiency turned out to be 92%.
A blank experiment with a bare glassy carbon rod showed no O_2 formation under the same conditions.
It is interesting to observe that the current density in the top figures increases with time due to the increasing [**4**] during the experiment.

The TON of **4** for the 1 hour experiment is 27 000 000 using equation S2.

Electrocatalytic behavior of [Ru(bda)(pic)$_2$] and 4 at pH = 7.0.

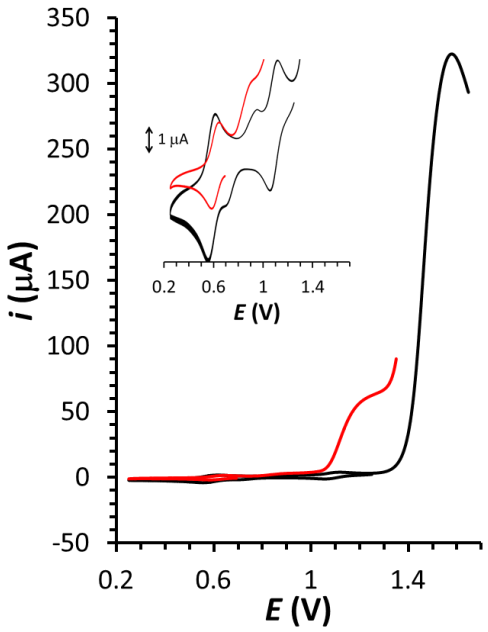


Figure S23: Comparison of the electrocatalytic response of [Ru(bda)(pic)$_2$] and **4** catalyst at pH=7 by cyclic voltammetry. CV of [Ru(bda)(pic)$_2$] (red solid line, 0.28 mM) and mixture of **3**$^{2+}$ /**4** (black line, 0.3 mM and 0.15 mM respectively) at pH = 7 buffered phosphate solution (I = 0.1M). The inset shows an enlargement of the CV in the 0.2-1.4 V region.

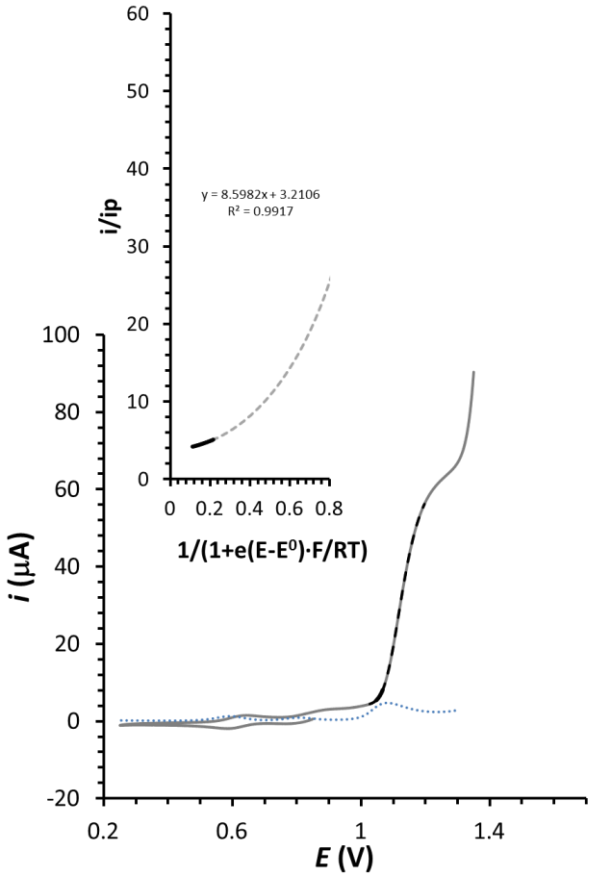
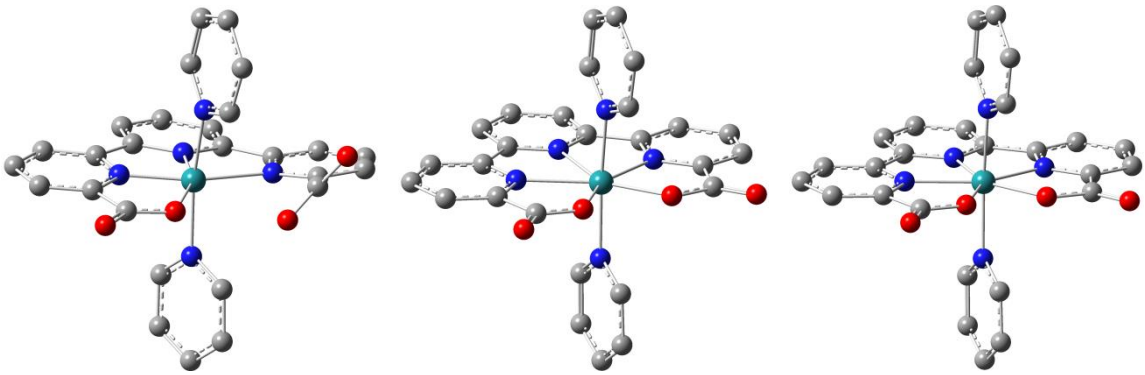


Figure S24: CV and DPV (grey solid line and blue dotted line respectively) of [Ru(bda)(pic)$_2$] (0.28 mM at pH = 7.0) and FOWA plot (inset). The points from the catalytic wave used for FOWA are plotted as a dashed black line and the fitting points at the foot of the wave are represented as a black solid line. A TOF_{MAX} of 5 s^{-1} assuming a first order kinetics.

Computational results

The "Ru non-aqua" species and optimized structures for **1**, **2**$^{+}$ and **3**$^{2+}$ (Figure S25). Complexes **1** and **3**$^{2+}$ have closed-shell singlets in their ground electronic states while the ground state of **2**$^{+}$ is a doublet, in agreement with EPR data. The calculated oxidation potentials for III/II and IV/III couples are 0.15 V and 0.84 V, respectively, at M11-L level of theory and 0.01 V and 0.47 V at the M06-L level. The corresponding experimental measurements are 0.52 V and 1.10 V, which indicate that the potential for III/II couple is significantly underestimated by the calculations. Following this observation and noting that **1** has a dangling carboxylate group that coordinates at oxidation state III, we performed calculations including explicit H_2O molecules with hydrogen bonding interactions to the carboxylate groups. This led to calculated potentials of 0.41 V and 0.85 V for III/II and IV/III couples, respectively at the M11-L level of theory, in fair agreement with experimental observations. This finding, one more time shows the importance of explicitly including H_2O molecules in modeling of reactions, especially for the cases where hydrogen bonding could impact the relative energetics of the species involved.



[Ru^{II}(tda-κ-N^{3}O)Py$_2$] **[Ru^{III}(tda-κ-N^{2}O^{2})Py$_2$]$^{+}$** **[Ru^{IV}(tda-κ-N^{3}O^{2})Py$_2$]$^{2+}$**

Figure S25. The optimized structures of [Ru^{II}(tda-κ-N^{3}O)Py$_2$], [Ru^{III}(tda-κ-N^{2}O^{2})Py$_2$]$^{+}$ and [Ru^{IV}(tda-κ-N^{3}O^{2})Py$_2$]$^{2+}$ at M11-L level of theory. Color code: Ruthenium teal, carbon gray, oxygen red, nitrogen blue, hydrogen atoms were omitted for clarity.

Table S2. Selected geometrical features for $[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]$, $[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$ and $[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ for calculated structures at M11-L and M06-L (in parenthesis) level of theories. The X-ray data are also presented for comparison.

	$[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]$		**$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$**		**$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$**	
r (Å)	**M11-L (M06-L)**	**X-ray**	**M11-L (M06-L)**	**X-ray**	**M11-L (M06-L)**	**X-ray**
$Ru–N_1$ (tda)	1.92 (1.95)	1.96	2.19 (2.24)	2.16	2.09 (2.13)	2.10 / 2.11
$Ru–N_2$ (tda)	1.93 (1.94)	1.92	2.46 (2.50)	2.38	2.09 (2.13)	2.12 / 2.11
$Ru–N_3$ (tda)	2.19 (2.21)	2.14	2.19 (2.24)	2.22	2.09 (2.13)	2.13 / 2.11
$Ru–N_4$ (py)	2.05 (2.10)	-	2.06 (2.11)	-	2.08 (2.13)	-
$Ru–N_5$ (py)	2.04 (2.09)	-	2.06 (2.11)	-	2.08 (2.13)	-
$Ru–O_1$ (tda)	2.09 (2.18)	2.20	1.95 (2.01)	2.04	1.96 (2.03)	2.02 / 2.03
$Ru–O_2$ (tda)	2.99 (3.22)	-	1.95 (2.01)	2.04	1.96 (2.03)	2.02 / 2.02

The presence of possible different binding modes at oxidation states II-IV for the "Ru-aqua" coupled with different hydrogen bonding capabilities of each of the isomers have brought a complex picture in terms of calculated redox potentials (Scheme S1-S2.) The possible competition between thermodynamically and kinetically favored species towards the PCET reactions further complicates the comparison between the calculated redox potentials and those obtained from Pourbaix diagrams as recently shown for a Co-based hydrogen evolution catalyst.[31] Noting these points, we tentatively assigned the first PCET step to oxidation of $[Ru^{II}(H_2O)(tda\text{-}\kappa\text{-}N^3)(py)_2]$ to $[Ru^{III}(OH)(tda\text{-}\kappa\text{-}N^3)(py)_2]$ ($E_{1/2}{}^2$ = 0.70 V calc obs 0.70), which could isomerize to $[Ru^{III}(OH)(tda\text{-}\kappa\text{-}N^2O)(py)_2]$. The second PCET step results in generation of $[Ru^{IV}(O)(tda\text{-}\kappa\text{-}N^2O)(py)_2]$ from $[Ru^{III}(OH)(tda\text{-}\kappa\text{-}N^3)(py)_2]$ ($E_{1/2}{}^3$ = 1.18 V calc obs 0.87 V), which will be in equilibrium with $[Ru^{IV}(O)(tda\text{-}\kappa\text{-}N^3O)(py)_2]$. The dynamic nature of the catalyst requires further work to gain more insight on the equilibrium of different binding modes and interaction with solvent molecules.

Table S3. Absolute and relative free energies at pH 0.0 and 7.0 for computed species at M06-L level of theory. The structures are grouped in an order following the water oxidation pathway and in each group a relative zero free energy species is chosen.

Complex	**Absolute Free Energy (G) (a.u.)**	**Relative Free Energy (ΔG) (kcal/mol)**	
		pH 0.0	**pH 7.0**
$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^+$ (closed-shell singlet)	**-1710.5191**	**0.0**	**0.0**
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]$ (closed-shell singlet)	-1710.0557	20.5	11.0
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]$ (closed-shell singlet)	-1710.0774	6.9	-2.6
$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (closed-shell singlet)	-1786.9496	7.0	7.0
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]$ (closed-shell singlet)	-1786.5106	12.2	2.7
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]$ (closed-shell singlet)	-1786.0363	39.6	20.6
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$ (doublet)	**-1709.9200**	**0.0**	**0.0**
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^{2+}$ (doublet)	-1786.7664	16.3	25.9
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH)]^+$ (doublet)	-1786.3274	21.5	21.5
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^+$ (doublet)	-1786.3412	12.9	12.9
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (doublet)	-1786.3320	18.6	18.6
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]$ (doublet)	-1785.8836	29.7	20.2
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH)]$ (doublet)	-1785.8783	33.1	23.5
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^-$ (doublet)	-1785.4154	53.2	34.2
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^-$ (quartet)	-1785.3893	69.6	50.6
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ (closed-shell singlet)	**-1709.7460**	**0.0**	**0.0**
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ (closed-shell singlet)	-1786.1512	22.9	22.9
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^{2+}$ (closed-shell singlet)	-1786.1408	29.4	22.9

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(O)]^+$ (triplet)	-1785.7169	25.2	15.7
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3)Py_2(O)]^+$ (broken-symmetry singlet)	-1785.6854	44.9	35.4
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3)Py_2(O)]^+$ (triplet)	-1785.7062	31.9	22.4
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^+$ (closed-shell singlet)	-1785.7179	24.6	15.0
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]$ (triplet)	-1785.2720	34.1	15.1
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]$ (broken-symmetry singlet)	-1785.2633	39.6	20.5
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]$ (triplet)	-1785.2761	31.5	12.5
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{3+}$ (doublet)	**-1709.4987**	**0.0**	**0.0**
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^+$ (doublet)	-1785.0764	1.7	-17.4
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]^+$ (doublet)	-1785.0780	0.6	-18.4
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O)Py_2(O)]^+$ (doublet)	-1785.0839	-3.1	-22.1
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]^+$ WNA TS (doublet)	-1861.4989	13.7	-5.3
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (doublet)	**-1861.4997**	**0.0**	**0.0**
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (quartet)	-1861.4631	23.0	23.0
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 2 (doublet)	-1861.4915	5.1	5.1
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 2 (quartet)	-1861.4528	29.4	29.4
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]$ (doublet)	-1861.0422	16.8	7.3
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]$ (quartet)	-1861.0008	42.8	33.3
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]$ (doublet)	-1861.0515	11.0	1.4
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (closed-shell singlet)	**-1861.3061**	**0.0**	**0.0**

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (triplet)	-1861.2993	4.3	4.3
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^{+}$ (broken-symmetry singlet)	-1860.8904	-9.4	-19.0
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^{+}$ (triplet)	-1860.8846	-5.8	-15.3
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{+}$ (triplet)	-1860.8629	7.8	-1.7
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OO)]$ (triplet)	-1860.4184	16.5	-2.6
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^{+}$ (doublet)	**-1860.2320**	**0.0**	**0.0**
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^{+}$ (quartet)	-1860.2340	-1.2	-1.2

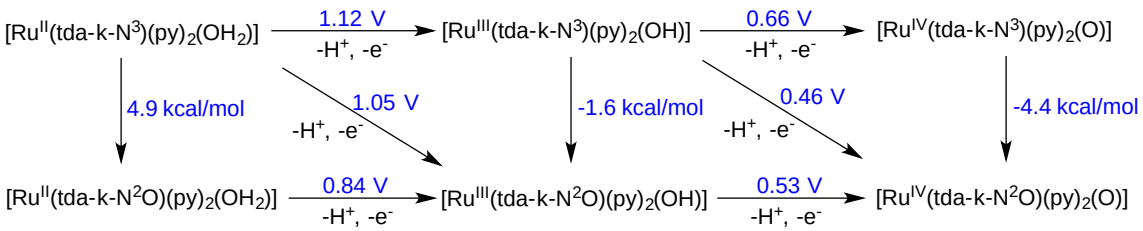
Table S4. Absolute and relative free energies at pH 0.0 and 7.0 for computed species at M11-L level of theory. The structures are grouped in an order following the water oxidation pathway and in each group a relative zero free energy species is chosen.

Complex	**Absolute Free Energy (G) (a.u.)**	**Relative Free Energy (ΔG) (kcal/mol)**	
		pH 0.0	**pH 7.0**
$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^+$ (closed-shell singlet)	**-1710.4742**	**0.0**	**0.0**
$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^+\bullet H_2O$ (closed-shell singlet)	-1786.9080	-0.9	-0.9
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]$ (closed-shell singlet)	-1710.0281	9.7	0.1
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]\bullet H_2O$ (closed-shell singlet)	-1786.4595	10.3	0.8
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3O)Py_2]\bullet(H_2O)_2$ (closed-shell singlet)	-1862.8921	10.2	0.7
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]$ (closed-shell singlet)	-1710.0191	15.3	5.8
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]\bullet H_2O$ (closed-shell singlet)	-1786.4507	15.8	6.3
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]\bullet(H_2O)_2$ (closed-shell singlet)	-1786.4482	17.4	7.8
$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (closed-shell singlet)	-1786.8916	9.4	9.4
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]$ (closed-shell singlet)	-1786.4536	14.0	4.5
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]\bullet H_2O$ Conformer 1 (closed-shell singlet)	-1862.8794	18.2	8.6
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]\bullet H_2O$ Conformer 2 (closed-shell singlet)	-1862.8852	14.5	5.0
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH_2)]$ (closed-shell singlet)	-1786.4457	18.9	9.4
$[Ru^{II}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH_2)]\bullet H_2O$ (closed-shell singlet)	-1862.8747	21.1	11.6
$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]^-$ (closed-shell singlet)	-1785.9755	43.7	24.7
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^{2+}$ (doublet)	**-1710.2897**	**0.0**	**0.0**
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$ (doublet)	-1709.8658	-4.3	-13.8
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+\bullet H_2O$ (doublet)	-1786.2931	-1.1	-10.6
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+\bullet(H_2O)_2$ (doublet)	-1862.7203	2.2	-7.3

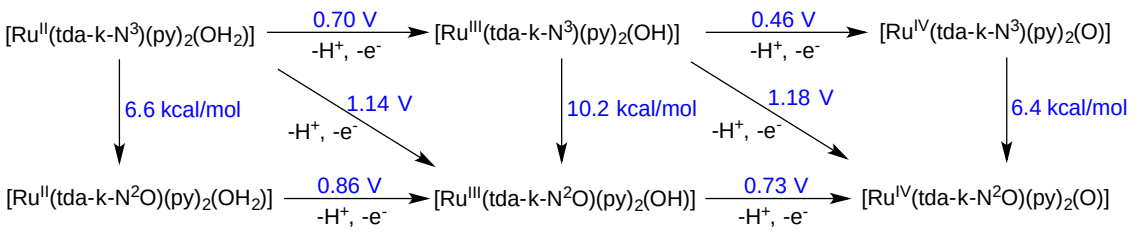
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^{2+}$ (doublet)	-1786.6881	21.3	21.3
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH)]^{+}$ (doublet)	-1786.2515	25.0	15.5
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^{+}$ (doublet)	-1786.2521	24.7	15.2
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]$ (doublet)	-1785.8098	31.9	12.9
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]\bullet(H_2O)$ (doublet)	-1862.2567	22.8	3.8
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH)]$ (doublet)	-1785.8122	30.4	11.3
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH)]\bullet(H_2O)$ (doublet)	-1862.2404	33.0	14.0
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^{-}$ (doublet)	-1785.3380	57.7	29.1
$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^{-}$ (quartet)	-1785.3071	77.1	48.5
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ (closed-shell singlet)	**-1709.6782**	**0.0**	**0.0**
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}\bullet H_2O$ (closed-shell singlet)	-1786.1045	3.8	3.8
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}\bullet(H_2O)_2$ (closed-shell singlet)	-1862.5320	6.9	6.9
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 1 (closed-shell singlet)	-1786.0733	23.4	23.4
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^{2+}$ Conformer 1 (triplet)	-1786.0566	33.9	33.9
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 2 (closed-shell singlet)	-1786.0640	29.2	29.2
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^{2+}$ Conformer 2 (triplet)	-1786.0564	34.0	34.0
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(O)]^{+}$ (triplet)	-1785.6350	28.2	18.6
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{+}$ (closed-shell singlet)	-1785.6397	25.2	15.7
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{+}\bullet H_2O$ (closed-shell singlet)	-1862.0664	28.8	19.3
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]$ (broken-symmetry singlet)	-1785.1761	45.9	26.8
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]$ (triplet)	-1785.1900	37.1	18.1
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]\bullet H_2O$ (triplet)	-1861.6107	44.5	25.5

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(O)]$ (triplet)	-1785.1805	43.1	24.1
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]$ (triplet)	-1785.1829	41.6	22.5
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]\bullet H_2O$ (triplet)	-1861.6208	38.1	19.1
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OO)]$ (triplet)	-1860.3144	15.9	-3.1
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{3+}$ (doublet)	**-1709.4171**	**0.0**	**0.0**
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ (doublet)	-1785.3974	13.4	3.9
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O)Py_2(O)]^{+}$ (doublet)	-1784.9846	2.2	-16.9
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^{+}$ (doublet)	-1784.9629	15.8	-3.2
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(O)]^{+}$ WNA TS (doublet)	-1861.3859	21.7	2.6
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{+}$ Conformer 1 (doublet)	**-1861.4114**	**0.0**	**0.0**
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{+}$ Conformer 1 (quartet)	-1861.3624	30.8	30.8
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{+}$ Conformer 2 (doublet)	-1861.4032	5.2	5.2
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{+}$ Conformer 2 (quartet)	-1861.3541	35.9	35.9
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]$ (doublet)	-1860.9532	17.2	7.7
$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]$ (quartet)	-1860.9089	45.0	35.5
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]$ (doublet)	-1860.9618	11.8	2.3
$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]$ (quartet)	-1860.8902	56.7	47.2
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (closed-shell singlet)	**-1861.2013**	**0.0**	**0.0**
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (triplet)	-1861.1947	4.1	4.1
$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^{+}$ (triplet)	-1860.7845	-8.7	-18.3

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ (triplet)	-1860.7540	10.4	0.9
$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OO)]$ (triplet)	-1860.3144	15.9	-3.1
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (doublet)	**-1860.1154**	**0.0**	**0.0**
$[Ru^{V}(tda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (quartet)	-1860.1163	-0.5	-0.5
$[Ru^{V}(tda\text{-}\kappa\text{-}N^3O)Py_2(OO)]^+$ (doublet)	-1860.1212	-3.6	-3.6



Scheme S1. Calculated free energy changes (in units of kcal/mol) and redox potentials (in units of volts) for relevant species at oxidation states of II, III and IV for Ru center.



Scheme S2. Calculated free energy changes (in units of kcal/mol) and redox potentials (in units of volts) for relevant species including one explicit H_2O molecule hydrogen bonded to complex at oxidation states of II, III and IV for Ru center.

Cartesian Coordinates and Electronic Energies of Optimized Structures at M06-L Level

[Ru^{II}(Htda-κ-N^3O)Py_2] (Closed-shell singlet)

E = -1710.34867958 a.u.

6	-2.174487	0.310147	1.618137
6	-3.446789	0.413928	2.185872
6	-4.563421	0.534141	1.373232
6	-4.380206	0.555587	-0.002915
6	-3.087403	0.483520	-0.516338
1	-3.558548	0.386071	3.266873
1	-5.558438	0.603707	1.805361
1	-5.209595	0.629670	-0.700803
6	-0.971641	0.133247	2.438701
6	-0.898087	0.099177	3.831564
6	0.338862	-0.072998	4.447910
1	-1.794490	0.209490	4.436844
6	1.396423	-0.192686	2.289053
6	1.491053	-0.224813	3.675514
1	0.405846	-0.095605	5.532072
1	2.458161	-0.372431	4.151102
6	2.474890	-0.390036	1.316014
6	3.826626	-0.642101	1.551313
6	2.837318	-0.551509	-1.035744
6	4.679380	-0.847439	0.466781
1	4.210578	-0.680516	2.568560
6	4.187620	-0.806920	-0.840628
1	5.733751	-1.043408	0.645952
1	4.820909	-0.965850	-1.710312
7	0.162755	0.001800	1.699582
7	2.038933	-0.348088	0.023121
7	-1.986916	0.353260	0.258268
6	-2.958360	0.527817	-2.004317
8	-3.875688	0.261861	-2.748304
6	2.113620	-0.465413	-2.369346
8	2.751865	-0.633214	-3.396910
8	0.833201	-0.198735	-2.278331
44	0.145328	0.011930	-0.234796
6	-0.115325	-2.931947	0.612437
6	-0.445166	-4.273024	0.487720
6	-0.994644	-4.725497	-0.707819
6	-1.185191	-3.811084	-1.739273
6	-0.827611	-2.485561	-1.545141
1	0.318716	-2.541942	1.531452
1	-0.267673	-4.947732	1.321033
1	-1.263301	-5.771539	-0.835088
1	-1.600801	-4.115073	-2.696146
1	-0.917845	-1.738230	-2.329473
6	0.471084	2.921988	0.703288

6	0.680429	4.289388	0.615175
6	0.944283	4.854664	-0.628392
6	0.984253	4.017213	-1.737826
6	0.763469	2.657473	-1.575215
1	0.261108	2.450911	1.660877
1	0.637008	4.895572	1.516275
1	1.114557	5.924054	-0.729338
1	1.187135	4.405232	-2.732507
1	0.781808	1.961549	-2.409521
7	0.507834	2.103062	-0.369635
7	-0.304538	-2.040757	-0.381822
8	-1.735762	0.905303	-2.407223
1	-1.714598	0.850918	-3.381184

$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (Closed-shell singlet)

E = -1786.76226689 a.u.

6	-2.251661	0.861339	1.442887
6	-3.508208	1.143755	1.964139
6	-4.646897	0.822484	1.231146
6	-4.485418	0.207254	0.004456
6	-3.201168	-0.009269	-0.509930
1	-3.599901	1.593027	2.949278
1	-5.636873	1.028820	1.631048
1	-5.332514	-0.124617	-0.590121
6	-1.026882	1.101482	2.202625
6	-0.940813	1.688790	3.463058
6	0.302216	1.853580	4.067022
1	-1.840553	2.021376	3.973216
6	1.335998	0.865367	2.137512
6	1.451214	1.445350	3.399867
1	0.374181	2.306860	5.051834
1	2.426994	1.580372	3.858757
6	2.439444	0.417852	1.291807
6	3.778152	0.603237	1.643591
6	3.075826	-0.609512	-0.700117
6	4.783975	0.224493	0.770163
1	4.024454	1.066677	2.595248
6	4.422303	-0.392461	-0.422670
1	5.828946	0.390477	1.018252
1	5.167958	-0.738323	-1.132744
7	0.107920	0.690008	1.570749
7	2.074191	-0.166509	0.100460
7	-2.089542	0.317724	0.187200
6	-3.083038	-0.697126	-1.860337
8	-2.449636	-0.068386	-2.761727
8	-3.622424	-1.810280	-1.900979
6	2.727209	-1.512878	-1.834328

8	1.909949	-2.407701	-1.758085
44	-0.012176	-0.042159	-0.215936
6	0.517647	-2.524739	1.456530
6	0.436005	-3.838666	1.886513
6	-0.474130	-4.695815	1.274302
6	-1.275043	-4.189024	0.258057
6	-1.139861	-2.859791	-0.116630
1	1.220416	-1.830144	1.911597
1	1.082980	-4.179058	2.690831
1	-0.558680	-5.733722	1.587881
1	-2.013029	-4.803518	-0.250463
1	-1.777213	-2.442395	-0.893131
6	1.126559	2.787437	-0.681901
6	1.235724	4.059256	-1.221390
6	0.310528	4.468680	-2.176919
6	-0.691019	3.579033	-2.546356
6	-0.744214	2.321588	-1.960189
1	1.840020	2.441705	0.062073
1	2.040738	4.712074	-0.893964
1	0.371841	5.459406	-2.621733
1	-1.439877	3.843930	-3.288121
1	-1.512626	1.591885	-2.231437
7	0.158315	1.918084	-1.037731
7	-0.250286	-2.028129	0.464599
8	-0.027034	-0.687065	-2.307324
1	-0.946830	-0.525035	-2.695753
1	0.170993	-1.632802	-2.403683
8	3.503009	-1.284373	-2.900687
1	3.282533	-1.957936	-3.571662

[Ru^{II}(tda-κ-N^3O)Py_2] (Closed-shell singlet)

E = -1709.91086603 a.u.

6	1.879972	-1.434941	-1.388918
6	3.022610	-2.087280	-1.841669
6	4.191658	-2.019896	-1.086653
6	4.192616	-1.256526	0.067256
6	3.005935	-0.660889	0.512553
1	3.005293	-2.625539	-2.786814
1	5.093350	-2.526385	-1.426539
1	5.092147	-1.080359	0.651352
6	0.649196	-1.365136	-2.179111
6	0.416941	-1.931832	-3.431363
6	-0.808040	-1.732508	-4.065795
1	1.190491	-2.524917	-3.913859
6	-1.557600	-0.434845	-2.184398
6	-1.801550	-0.981528	-3.440549
1	-0.990010	-2.168204	-5.044938

1	-2.766969	-0.829485	-3.919103
6	-2.492769	0.318590	-1.351848
6	-3.804918	0.697448	-1.641478
6	-2.669996	1.301634	0.813879
6	-4.541788	1.390068	-0.683123
1	-4.244112	0.452196	-2.606840
6	-3.974475	1.694663	0.558769
1	-5.563595	1.689551	-0.906075
1	-4.514677	2.227786	1.337984
7	-0.329170	-0.627262	-1.581160
7	-1.971517	0.645337	-0.129223
7	1.856180	-0.781821	-0.178996
6	3.030780	0.238402	1.745402
8	2.077540	0.127603	2.549525
8	4.011021	1.011201	1.728472
6	-1.889130	1.521333	2.101809
8	-2.450874	2.115851	3.016110
8	-0.683829	1.035988	2.091922
44	-0.137304	0.093800	0.208804
6	-1.685262	-2.516429	0.654129
6	-2.086693	-3.651033	1.341893
6	-1.485935	-3.941796	2.563609
6	-0.503447	-3.082980	3.045862
6	-0.144937	-1.962236	2.308608
1	-2.132202	-2.242557	-0.301675
1	-2.861484	-4.288591	0.923055
1	-1.782020	-4.822930	3.129638
1	-0.008602	-3.267370	3.995980
1	0.629249	-1.247593	2.616352
6	0.597794	2.502066	-1.548186
6	1.211056	3.703660	-1.863621
6	1.935380	4.368219	-0.876454
6	2.006174	3.805798	0.392390
6	1.355833	2.605876	0.646118
1	0.033033	1.937153	-2.288962
1	1.124837	4.103006	-2.871280
1	2.439998	5.306538	-1.098001
1	2.572557	4.271756	1.193832
1	1.376275	2.119543	1.621723
7	0.666509	1.956764	-0.317977
7	-0.733354	-1.687781	1.122201

[Ru^{II}(tda-κ-N^2O^2)Py_2] (Closed-shell singlet)

E = -1709.92048460 a.u.

6	2.292677	-1.020217	1.455616
6	3.608270	-1.192683	1.888552
6	4.643198	-0.548664	1.224936

6	4.324883	0.247761	0.132466
6	2.993914	0.383450	-0.248553
1	3.803715	-1.819418	2.757134
1	5.673424	-0.665756	1.555376
1	5.065692	0.782880	-0.456106
6	1.156811	-1.724411	2.055581
6	1.206945	-2.964748	2.699334
6	0.000890	-3.568581	3.053700
1	2.155495	-3.464965	2.888345
6	-1.156054	-1.725185	2.055346
6	-1.205498	-2.965556	2.699079
1	0.001162	-4.534931	3.553926
1	-2.153754	-3.466409	2.887887
6	-2.292269	-1.021713	1.455189
6	-3.607814	-1.194967	1.887956
6	-2.994113	0.381581	-0.249028
6	-4.643037	-0.551527	1.224232
1	-3.802998	-1.821828	2.756504
6	-4.325052	0.245113	0.131826
1	-5.673234	-0.669221	1.554548
1	-5.066099	0.779820	-0.456822
7	0.000195	-1.104180	1.810217
7	-1.971661	-0.224266	0.394962
7	1.971733	-0.222980	0.395325
6	2.657463	1.231071	-1.448915
8	1.395045	1.290305	-1.742408
8	3.563637	1.784415	-2.064386
6	-2.658015	1.229381	-1.449361
8	-3.564438	1.782165	-2.064968
8	-1.395595	1.289334	-1.742702
44	-0.000088	0.412340	-0.540784
6	-0.001057	2.165887	1.952460
6	-0.001576	3.342478	2.685118
6	-0.001854	4.561745	2.011204
6	-0.001599	4.550064	0.620157
6	-0.001082	3.335172	-0.050245
1	-0.000806	1.179891	2.415491
1	-0.001754	3.296864	3.771767
1	-0.002259	5.501140	2.560532
1	-0.001797	5.473707	0.046727
1	-0.000854	3.262980	-1.135036
6	0.001206	-2.494118	-1.450995
6	0.001712	-3.549768	-2.348574
6	0.001597	-3.276023	-3.714787
6	0.000971	-1.946202	-4.123287
6	0.000490	-0.939292	-3.168605
1	0.001274	-2.655041	-0.373256
1	0.002191	-4.571178	-1.975275
1	0.001985	-4.083688	-4.443881
1	0.000853	-1.679037	-5.177153

1	-0.000021	0.116650	-3.426175
7	0.000604	-1.203269	-1.843349
7	-0.000811	2.152485	0.603310

[Ru^{II}(tda-κ-N^3)Py_2(OH_2)] (Closed-shell singlet)

E = -1786.33637334 a.u.

6	-2.090423	0.055187	1.850030
6	-3.248270	0.262886	2.590917
6	-4.360785	0.835732	1.982963
6	-4.282764	1.158188	0.641528
6	-3.083400	0.979631	-0.059910
1	-3.282200	-0.029869	3.637085
1	-5.275036	1.001398	2.549336
1	-5.136675	1.550591	0.094992
6	-0.919800	-0.611895	2.417684
6	-0.841294	-1.188867	3.682123
6	0.323659	-1.843892	4.074548
1	-1.693648	-1.144335	4.354915
6	1.302870	-1.315771	1.942433
6	1.400826	-1.910883	3.198680
1	0.386886	-2.303829	5.057353
1	2.316711	-2.419816	3.489337
6	2.356567	-1.233437	0.937740
6	3.647972	-1.707220	1.144999
6	2.979800	-0.247297	-1.097746
6	4.629149	-1.446978	0.191429
1	3.889608	-2.248010	2.056868
6	4.298938	-0.675876	-0.909979
1	5.644434	-1.811613	0.335175
1	5.046025	-0.383407	-1.644042
7	0.148952	-0.682061	1.570224
7	2.004664	-0.571881	-0.218614
7	-1.988106	0.450289	0.533077
6	-3.078891	1.323476	-1.544799
8	-2.336198	2.272481	-1.914712
8	-3.846630	0.599166	-2.201307
6	2.605156	0.690140	-2.226808
8	2.929538	1.866295	-1.993874
8	1.998909	0.167820	-3.199985
44	-0.024705	0.029521	-0.218801
6	-0.011892	-2.997329	-0.719964
6	-0.409434	-4.219172	-1.239778
6	-1.542348	-4.273611	-2.045751
6	-2.232210	-3.092564	-2.292158
6	-1.776624	-1.905563	-1.736247
1	0.877682	-2.918615	-0.100181
1	0.173712	-5.109411	-1.017377

1	-1.877081	-5.216886	-2.472700
1	-3.124435	-3.069061	-2.912300
1	-2.300666	-0.970944	-1.918619
6	1.726033	2.137254	1.109596
6	2.259176	3.385576	1.381761
6	1.659115	4.510505	0.826736
6	0.528099	4.332562	0.040098
6	0.039444	3.052702	-0.181845
1	2.182637	1.237427	1.514488
1	3.144438	3.463009	2.007828
1	2.065547	5.503785	1.006446
1	0.013672	5.175618	-0.413987
1	-0.858273	2.872715	-0.780358
7	0.638528	1.957797	0.333087
7	-0.675805	-1.848833	-0.956839
8	-0.348396	0.605817	-2.255660
1	-0.916900	1.393477	-2.428349
1	0.463147	0.578153	-2.840583

$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]^-$ (Closed-shell singlet)

E = -1785.76679452 a.u.

6	-2.130292	-0.320217	1.778480
6	-3.337712	-0.314958	2.472030
6	-4.479371	0.187060	1.856413
6	-4.376026	0.662876	0.563919
6	-3.143722	0.650738	-0.112094
1	-3.377986	-0.698030	3.489025
1	-5.431218	0.200344	2.387220
1	-5.238788	1.060811	0.033361
6	-0.906147	-0.848530	2.374887
6	-0.802825	-1.471612	3.611765
6	0.431616	-1.965056	4.047522
1	-1.685761	-1.592417	4.236134
6	1.425986	-1.187892	1.995397
6	1.548792	-1.821306	3.230485
1	0.513798	-2.462804	5.011136
1	2.516576	-2.204250	3.550705
6	2.486648	-0.914007	1.045491
6	3.831681	-1.171660	1.321490
6	3.050649	0.100447	-0.998571
6	4.806835	-0.754420	0.427120
1	4.102248	-1.664574	2.253374
6	4.407519	-0.074027	-0.715278
1	5.861161	-0.934135	0.636376
1	5.123485	0.336645	-1.423462
7	0.202947	-0.714833	1.574101
7	2.086272	-0.324406	-0.143153

7	-2.028493	0.170678	0.490259
6	-3.182136	1.197235	-1.540956
8	-3.030707	2.433265	-1.617129
8	-3.509836	0.339493	-2.389183
6	2.673588	0.775444	-2.308533
8	3.140629	1.924619	-2.428570
8	1.997469	0.061209	-3.089927
44	-0.012178	0.031070	-0.219377
6	0.314351	-2.955167	-0.757088
6	0.083653	-4.186931	-1.350366
6	-0.943121	-4.301220	-2.283421
6	-1.697183	-3.170656	-2.577523
6	-1.413027	-1.964631	-1.949100
1	1.114595	-2.817319	-0.032177
1	0.711205	-5.035406	-1.085731
1	-1.148251	-5.253859	-2.770490
1	-2.513253	-3.201651	-3.295782
1	-1.979437	-1.051973	-2.156880
6	1.217447	2.360243	1.305127
6	1.502220	3.674533	1.639820
6	0.865799	4.697196	0.941453
6	-0.030796	4.354331	-0.063585
6	-0.266859	3.016685	-0.354647
1	1.693495	1.526072	1.819324
1	2.218898	3.883831	2.431120
1	1.069005	5.740936	1.178175
1	-0.559622	5.111859	-0.636965
1	-0.960017	2.693008	-1.132054
7	0.351925	2.029491	0.328244
7	-0.413200	-1.860975	-1.044940
8	-0.449740	0.718197	-2.007329
1	0.301620	0.554912	-2.615708

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^{2+}$ (Doublet)

E = -1786.42836026 a.u.

6	2.283780	-0.814684	1.418017
6	3.545508	-1.056861	1.941740
6	4.679675	-0.601097	1.269384
6	4.506150	0.109253	0.099248
6	3.217133	0.288281	-0.423933
1	3.650952	-1.582482	2.886478
1	5.671532	-0.781085	1.676206
1	5.343126	0.541222	-0.443122
6	1.064398	-1.208528	2.124614
6	1.004699	-1.906761	3.331475
6	-0.233652	-2.204614	3.888330
1	1.914493	-2.218600	3.835755

6	-1.309632	-1.127882	2.032823
6	-1.403033	-1.819864	3.238311
1	-0.289016	-2.743493	4.830595
1	-2.369343	-2.060526	3.671544
6	-2.435561	-0.678533	1.210248
6	-3.758054	-0.970493	1.552919
6	-3.143917	0.484731	-0.679359
6	-4.791238	-0.565160	0.725042
1	-3.973042	-1.528158	2.459941
6	-4.475379	0.175620	-0.407629
1	-5.823968	-0.805984	0.963804
1	-5.247194	0.544406	-1.076597
7	-0.088995	-0.831664	1.517038
7	-2.116352	0.029523	0.079743
7	2.112472	-0.166443	0.212441
6	3.070223	1.070805	-1.708059
8	2.519297	0.516056	-2.693744
8	3.517899	2.226990	-1.599534
6	-2.859621	1.481640	-1.758566
8	-1.974119	2.312007	-1.687949
44	0.027914	0.052480	-0.239053
6	-0.677687	2.355491	1.628291
6	-0.700944	3.641587	2.138694
6	0.072330	4.626415	1.526927
6	0.845646	4.276630	0.425210
6	0.820110	2.967717	-0.030103
1	-1.268330	1.562339	2.080606
1	-1.318257	3.863511	3.004884
1	0.072916	5.645626	1.906089
1	1.474067	5.000411	-0.086344
1	1.424807	2.670549	-0.881762
6	-0.840939	-2.848943	-0.858094
6	-0.827557	-4.086369	-1.478591
6	0.136262	-4.342623	-2.451453
6	1.051270	-3.341836	-2.761444
6	0.978666	-2.123529	-2.102495
1	-1.584008	-2.618635	-0.098900
1	-1.566693	-4.833423	-1.202678
1	0.168335	-5.303529	-2.959831
1	1.819757	-3.489171	-3.515328
1	1.670786	-1.309739	-2.328986
7	0.043449	-1.872807	-1.157004
7	0.069135	2.010844	0.556672
8	0.053285	0.768037	-2.231118
1	0.975255	0.759752	-2.649554
1	-0.360903	1.641093	-2.361553
8	-3.750863	1.395546	-2.741009
1	-3.587255	2.119173	-3.377587

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH)]^+$ (Doublet)

E = -1786.12129656 a.u.

6	2.267615	-0.650921	1.496035
6	3.534899	-0.756058	2.050075
6	4.628603	-0.216421	1.372562
6	4.414285	0.420590	0.166291
6	3.127251	0.464166	-0.389088
1	3.668668	-1.236489	3.015609
1	5.625332	-0.280072	1.802901
1	5.218717	0.907070	-0.379352
6	1.065759	-1.148159	2.169195
6	1.017424	-1.863628	3.365073
6	-0.214534	-2.283424	3.859902
1	1.930820	-2.101143	3.903454
6	-1.297598	-1.264490	1.978540
6	-1.384589	-1.989716	3.165889
1	-0.261817	-2.844472	4.789526
1	-2.347102	-2.317386	3.549487
6	-2.417651	-0.835947	1.136897
6	-3.749721	-1.141510	1.411133
6	-3.053108	0.405740	-0.742529
6	-4.746178	-0.702642	0.550582
1	-4.000488	-1.728800	2.290579
6	-4.392581	0.088223	-0.536875
1	-5.786634	-0.957353	0.735618
1	-5.140616	0.480414	-1.221100
7	-0.086771	-0.864263	1.514604
7	-2.070554	-0.093783	0.035380
7	2.070880	-0.062786	0.266661
6	2.906203	1.162372	-1.723225
8	2.484997	0.436665	-2.662186
8	3.176967	2.371710	-1.676575
6	-2.695289	1.470824	-1.740200
8	-2.315604	2.559330	-1.381586
44	0.015772	0.052187	-0.276146
6	-0.693115	2.287217	1.670624
6	-0.806068	3.570742	2.176180
6	-0.233710	4.624500	1.467907
6	0.428257	4.344253	0.279971
6	0.494321	3.034154	-0.173620
1	-1.128048	1.436358	2.192045
1	-1.337063	3.735208	3.110016
1	-0.304807	5.644428	1.839138
1	0.897554	5.126121	-0.310423
1	0.991229	2.781073	-1.104649
6	-0.755327	-2.861212	-0.977833
6	-0.657330	-4.122429	-1.542950
6	0.435513	-4.414279	-2.353982

6	1.383411	-3.420958	-2.565138
6	1.224307	-2.178615	-1.964308
1	-1.605636	-2.603633	-0.351623
1	-1.434951	-4.857075	-1.351140
1	0.538648	-5.393729	-2.815824
1	2.249467	-3.589069	-3.199779
1	1.925788	-1.355896	-2.140379
7	0.165574	-1.895503	-1.172876
7	-0.056504	2.015137	0.514580
8	-0.059625	0.866967	-2.008847
1	0.650993	0.533142	-2.608407
8	-2.970650	1.097849	-2.992134
1	-2.717390	1.839041	-3.575741

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^+$ Conformer 1 (Doublet)

E = -1786.14403548 a.u.

6	2.229239	-1.589964	0.889005
6	3.097621	-2.682726	0.781002
6	4.319245	-2.501852	0.141348
6	4.633296	-1.243675	-0.353344
6	3.674419	-0.231163	-0.263505
1	2.820887	-3.655613	1.183180
1	5.019438	-3.328842	0.045861
1	5.593450	-1.023752	-0.813260
6	0.996355	-1.674047	1.697634
6	0.993877	-2.458202	2.855472
6	-0.104049	-2.455723	3.701514
1	1.884016	-3.029017	3.105541
6	-1.152296	-0.898292	2.204500
6	-1.183334	-1.648753	3.377818
1	-0.109006	-3.053332	4.609553
1	-2.054621	-1.604053	4.025210
6	-2.268977	-0.053230	1.790995
6	-3.434059	0.214482	2.514127
6	-3.057932	1.259198	0.004067
6	-4.411855	1.035374	1.960677
1	-3.577074	-0.210744	3.504190
6	-4.229128	1.559355	0.681070
1	-5.316462	1.254432	2.522224
1	-4.967316	2.186970	0.187400
7	-0.079232	-0.919777	1.352621
7	-2.104348	0.490152	0.565487
7	2.492561	-0.394308	0.343429
6	4.020266	1.133701	-0.799612
8	3.037595	1.806839	-1.390456
8	5.143502	1.566996	-0.671544
6	-2.751158	1.669674	-1.406398

8	-3.497764	2.386441	-2.042424
8	-1.637822	1.122803	-1.867677
44	-0.441698	0.172278	-0.534585
6	0.887318	2.207234	1.315063
6	1.464986	3.405473	1.699944
6	1.457664	4.476545	0.810591
6	0.866141	4.303745	-0.434370
6	0.308797	3.074468	-0.754151
1	0.893586	1.336726	1.965525
1	1.922285	3.488007	2.682203
1	1.913590	5.425605	1.082527
1	0.843698	5.103770	-1.168849
1	-0.146203	2.883617	-1.722703
6	-2.385053	-1.864558	-1.714521
6	-2.813343	-3.049645	-2.294183
6	-1.889681	-4.066208	-2.515065
6	-0.563726	-3.855346	-2.146730
6	-0.209607	-2.645383	-1.569940
1	-3.068286	-1.036356	-1.543200
1	-3.857089	-3.161285	-2.574691
1	-2.196130	-5.004183	-2.972197
1	0.196309	-4.614984	-2.308935
1	0.816443	-2.419133	-1.282635
7	-1.104877	-1.660615	-1.349543
7	0.315223	2.035781	0.106825
8	0.993487	0.162113	-1.884382
1	2.253606	1.210922	-1.560482
1	0.652169	-0.072036	-2.762615

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^+$ Conformer 2 (Doublet)

E = -1786.13635785 a.u.

6	2.188193	-1.607469	0.930712
6	2.881206	-2.794429	0.653201
6	4.080413	-2.720228	-0.041543
6	4.550585	-1.469892	-0.431585
6	3.775687	-0.348467	-0.129769
1	2.471223	-3.756361	0.956678
1	4.635484	-3.622604	-0.287637
1	5.471001	-1.377638	-1.006506
6	0.943053	-1.630611	1.732095
6	0.907345	-2.422586	2.880466
6	-0.194219	-2.380299	3.724046
1	1.773361	-3.033079	3.124745
6	-1.182590	-0.788387	2.215283
6	-1.240450	-1.536702	3.390579
1	-0.228591	-2.980788	4.629416
1	-2.118896	-1.468146	4.026464

6	-2.285437	0.069254	1.788320
6	-3.427102	0.403078	2.522056
6	-3.064259	1.334716	-0.037675
6	-4.391680	1.225417	1.947599
1	-3.560778	0.032420	3.535361
6	-4.214114	1.696234	0.645596
1	-5.279787	1.494161	2.514012
1	-4.939051	2.332576	0.143450
7	-0.099932	-0.837651	1.370727
7	-2.131175	0.551018	0.536484
7	2.620612	-0.406558	0.541838
6	4.121685	1.008579	-0.667385
8	5.418708	1.357778	-0.668157
8	3.279756	1.745840	-1.128515
6	-2.735887	1.716289	-1.454293
8	-3.479585	2.425856	-2.105291
8	-1.608785	1.183758	-1.887165
44	-0.464288	0.169516	-0.542939
6	0.869230	2.276649	1.227053
6	1.461827	3.483894	1.557431
6	1.556070	4.478859	0.588038
6	1.049975	4.221453	-0.679665
6	0.466989	2.989818	-0.939182
1	0.794291	1.463958	1.944809
1	1.845822	3.634376	2.563013
1	2.020431	5.435126	0.817989
1	1.106336	4.959714	-1.474633
1	0.056127	2.740818	-1.914471
6	-2.518866	-1.822521	-1.596353
6	-3.013932	-2.987315	-2.162733
6	-2.132374	-4.023250	-2.453596
6	-0.781508	-3.846385	-2.170824
6	-0.359577	-2.652676	-1.605212
1	-3.171142	-0.981808	-1.372497
1	-4.075590	-3.067583	-2.379717
1	-2.490321	-4.946995	-2.902439
1	-0.051442	-4.619251	-2.396655
1	0.688749	-2.441197	-1.406890
7	-1.214193	-1.653489	-1.310212
7	0.370183	2.026191	0.000671
8	1.034864	-0.154149	-1.711197
1	5.949144	0.709573	-0.175981
1	1.692573	0.566635	-1.619119

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (Doublet)

E = -1861.27654796 a.u.

6	2.066191	-1.678824	1.025307

6	2.632663	-2.903835	0.662457
6	3.806969	-2.904622	-0.086107
6	4.375521	-1.688369	-0.437414
6	3.751232	-0.518484	-0.005105
1	2.147799	-3.836968	0.947030
1	4.266034	-3.842741	-0.390648
1	5.286181	-1.613094	-1.026221
6	0.820025	-1.629415	1.822856
6	0.723102	-2.379589	2.996235
6	-0.398738	-2.262033	3.805073
1	1.556620	-3.017396	3.281065
6	-1.287506	-0.689071	2.218414
6	-1.405120	-1.390150	3.415977
1	-0.480670	-2.827013	4.730092
1	-2.294362	-1.264636	4.028088
6	-2.333784	0.208479	1.724794
6	-3.485277	0.622326	2.398376
6	-2.958232	1.477134	-0.164937
6	-4.372583	1.486913	1.761815
1	-3.686651	0.282484	3.411323
6	-4.112516	1.922499	0.461693
1	-5.268366	1.817411	2.281837
1	-4.776104	2.591903	-0.080621
7	-0.184170	-0.816026	1.409774
7	-2.106307	0.654191	0.471389
7	2.624087	-0.501365	0.714927
6	4.333889	0.813685	-0.381573
8	5.270480	0.917606	-1.137399
8	3.731581	1.864694	0.191816
6	-2.545130	1.801808	-1.579711
8	-3.215825	2.549111	-2.266361
8	-1.447331	1.178741	-1.961267
44	-0.446460	0.118529	-0.529495
6	0.689344	2.291573	1.296632
6	1.204182	3.523068	1.669068
6	1.464826	4.471511	0.682978
6	1.191324	4.145704	-0.639403
6	0.674675	2.893022	-0.939822
1	0.485603	1.516827	2.032513
1	1.401429	3.726521	2.718294
1	1.876299	5.443771	0.943396
1	1.377854	4.848874	-1.446183
1	0.445218	2.592925	-1.956979
6	-2.625796	-1.706721	-1.643198
6	-3.217222	-2.860045	-2.136664
6	-2.474312	-4.035047	-2.180524
6	-1.157961	-4.007340	-1.729388
6	-0.636042	-2.816494	-1.248612
1	-3.165266	-0.763564	-1.615707
1	-4.243880	-2.824483	-2.490642

1	-2.910057	-4.953445	-2.567031
1	-0.532285	-4.895629	-1.755376
1	0.396190	-2.734429	-0.911729
7	-1.355821	-1.678294	-1.196251
7	0.430908	1.968315	0.011342
8	0.992405	-0.480629	-1.676779
8	1.952116	0.519760	-2.047360
1	2.982273	1.507390	0.713018
1	2.309725	0.121942	-2.862488

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (Quartet)

E = -1861.22767364 a.u.

6	2.203614	-1.533922	1.170703
6	3.014867	-2.620448	0.824736
6	4.196552	-2.387749	0.127836
6	4.540997	-1.079940	-0.185646
6	3.686229	-0.057320	0.222918
1	2.706464	-3.634738	1.072904
1	4.837590	-3.217359	-0.162863
1	5.451425	-0.823185	-0.721148
6	0.920523	-1.749974	1.875424
6	0.789303	-2.736042	2.858009
6	-0.432686	-2.892197	3.500188
1	1.646452	-3.345223	3.135997
6	-1.299276	-1.114572	2.144218
6	-1.495609	-2.073161	3.141661
1	-0.556694	-3.646446	4.273750
1	-2.468174	-2.195445	3.611643
6	-2.380402	-0.238134	1.663060
6	-3.548085	0.012891	2.387295
6	-3.150156	1.102535	-0.089663
6	-4.528855	0.838091	1.847835
1	-3.677352	-0.418797	3.376683
6	-4.331225	1.386297	0.585795
1	-5.436585	1.046952	2.409407
1	-5.057186	2.029732	0.095051
7	-0.109443	-0.956251	1.530766
7	-2.192423	0.321135	0.445212
7	2.534991	-0.266270	0.874807
6	4.058825	1.369024	-0.066140
8	4.992295	1.663759	-0.773652
8	3.287103	2.277996	0.547919
6	-2.886148	1.631472	-1.484941
8	-3.681264	2.414569	-1.979967
8	-1.802572	1.159436	-2.032697
44	-0.363932	0.173790	-0.723558
6	0.200163	2.385838	1.336505

6	0.453474	3.655104	1.830483
6	0.628125	4.704148	0.930317
6	0.541866	4.441280	-0.431772
6	0.300095	3.142550	-0.856163
1	0.062922	1.526375	1.991348
1	0.511993	3.813855	2.903924
1	0.828173	5.711427	1.288179
1	0.666340	5.228576	-1.169681
1	0.229009	2.880720	-1.907702
6	-2.113512	-2.138480	-1.738519
6	-2.451259	-3.385711	-2.241129
6	-1.446696	-4.329822	-2.432622
6	-0.133752	-3.984027	-2.126541
6	0.131100	-2.711780	-1.642500
1	-2.858482	-1.360797	-1.586141
1	-3.487684	-3.603675	-2.483481
1	-1.682673	-5.316582	-2.824638
1	0.684551	-4.683800	-2.274137
1	1.142450	-2.371475	-1.426584
7	-0.843629	-1.804731	-1.438630
7	0.137677	2.127935	0.014266
8	1.130892	-0.042843	-1.917360
8	2.059024	1.064212	-1.953300
1	2.590212	1.776642	1.019689
1	2.497810	0.891004	-2.806211

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 2 (Doublet)

E = -1861.26564125 a.u.

6	2.036814	-1.786402	0.814305
6	2.616532	-2.998166	0.417862
6	3.831393	-2.967174	-0.254253
6	4.445263	-1.738188	-0.469196
6	3.787016	-0.584015	-0.038800
1	2.110783	-3.942133	0.616230
1	4.295014	-3.886558	-0.604435
1	5.388511	-1.680066	-1.010487
6	0.797847	-1.766757	1.628744
6	0.712314	-2.607987	2.739006
6	-0.360586	-2.498786	3.613801
1	1.520792	-3.309463	2.931541
6	-1.230028	-0.751411	2.208599
6	-1.327444	-1.539676	3.353109
1	-0.431513	-3.135816	4.491626
1	-2.175852	-1.413614	4.020732
6	-2.252083	0.229184	1.839441
6	-3.332517	0.664744	2.610166
6	-2.934552	1.617337	0.056549

6	-4.212803	1.603390	2.076881
1	-3.483363	0.284438	3.617630
6	-4.019750	2.086441	0.781530
1	-5.052439	1.952755	2.672729
1	-4.685361	2.809866	0.316609
7	-0.179325	-0.873719	1.330457
7	-2.083220	0.728490	0.596976
7	2.598098	-0.597480	0.573449
6	4.345203	0.789408	-0.281775
8	3.639502	1.746206	-0.513048
8	5.680596	0.918667	-0.246245
6	-2.605413	1.975355	-1.372232
8	-3.282019	2.784708	-1.979348
8	-1.576404	1.309319	-1.856516
44	-0.521420	0.155534	-0.529209
6	0.984760	2.174290	1.211482
6	1.609394	3.360649	1.558506
6	1.761899	4.351578	0.593878
6	1.277982	4.112820	-0.686850
6	0.654293	2.905412	-0.962366
1	0.868504	1.362507	1.924753
1	1.977703	3.495011	2.572120
1	2.255339	5.290153	0.835554
1	1.378235	4.849947	-1.478559
1	0.253264	2.673743	-1.945648
6	-2.855516	-1.526893	-1.549767
6	-3.529526	-2.629382	-2.053169
6	-2.841397	-3.827692	-2.211728
6	-1.495149	-3.873238	-1.862589
6	-0.889680	-2.729986	-1.364784
1	-3.350501	-0.566124	-1.435503
1	-4.576934	-2.536104	-2.326682
1	-3.342326	-4.706994	-2.610055
1	-0.910040	-4.781018	-1.983802
1	0.169141	-2.700661	-1.114529
7	-1.555841	-1.570142	-1.200331
7	0.504288	1.941496	-0.026460
8	0.829244	-0.499938	-1.750101
8	1.919458	0.296832	-2.173559
1	6.100620	0.096419	0.055546
1	2.116306	0.884243	-1.406358

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 2 (Quartet)

E = -1861.21714671 a.u.

6	2.223889	-1.401589	1.136796
6	3.106565	-2.441032	0.811392
6	4.304698	-2.131538	0.183645

6	4.602798	-0.795034	-0.060596
6	3.655058	0.170865	0.286769
1	2.842167	-3.475367	1.022861
1	4.998855	-2.916868	-0.106648
1	5.532469	-0.515919	-0.554766
6	0.951878	-1.682645	1.842613
6	0.872552	-2.687467	2.809881
6	-0.328813	-2.884866	3.481675
1	1.751490	-3.277915	3.059030
6	-1.278415	-1.125192	2.156312
6	-1.422426	-2.096571	3.152592
1	-0.412479	-3.650944	4.248987
1	-2.383428	-2.254865	3.636008
6	-2.417900	-0.340687	1.654685
6	-3.595306	-0.137422	2.377332
6	-3.308673	0.791442	-0.179388
6	-4.649997	0.551686	1.788508
1	-3.675767	-0.500190	3.399396
6	-4.509851	1.012558	0.484546
1	-5.569567	0.722868	2.343474
1	-5.295205	1.544808	-0.046236
7	-0.105346	-0.913304	1.528410
7	-2.282759	0.137637	0.396137
7	2.474604	-0.118135	0.847036
6	3.910684	1.627617	0.028284
8	3.058788	2.403983	-0.345275
8	5.168646	2.053678	0.222905
6	-3.087339	1.272474	-1.595838
8	-3.982591	1.872454	-2.167536
8	-1.906435	0.991567	-2.076207
44	-0.415291	0.186262	-0.766403
6	0.339169	2.343567	1.363660
6	0.532129	3.604210	1.907979
6	0.287406	4.723371	1.118723
6	-0.142821	4.538143	-0.191041
6	-0.307534	3.247630	-0.672484
1	0.540190	1.434181	1.924954
1	0.875692	3.699431	2.934694
1	0.432529	5.724991	1.517568
1	-0.348021	5.380737	-0.845585
1	-0.622139	3.044756	-1.693161
6	-1.350887	-2.788716	-0.854188
6	-1.495457	-4.091541	-1.302787
6	-0.706717	-4.527050	-2.364619
6	0.196889	-3.636236	-2.933621
6	0.284610	-2.345684	-2.430010
1	-1.956690	-2.402803	-0.036929
1	-2.222855	-4.746567	-0.830803
1	-0.802041	-5.541485	-2.745847
1	0.826582	-3.926682	-3.770335

1	0.963095	-1.602153	-2.843446
7	-0.474924	-1.922332	-1.400381
7	-0.069216	2.164809	0.094969
8	1.073197	0.285498	-1.967750
8	1.377930	1.607442	-2.425821
1	5.711683	1.357547	0.628658
1	1.976335	1.927470	-1.710804

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] Conformer 1 (Doublet)

E = -1860.84444692 a.u.

6	2.084623	-1.740114	0.798312
6	2.693597	-2.946408	0.435406
6	3.932378	-2.906478	-0.196962
6	4.523325	-1.673165	-0.425473
6	3.814326	-0.521997	-0.073444
1	2.198568	-3.894612	0.643772
1	4.430558	-3.827388	-0.494801
1	5.506220	-1.573244	-0.878735
6	0.850285	-1.741398	1.615716
6	0.786620	-2.584549	2.726418
6	-0.290584	-2.511524	3.600557
1	1.617090	-3.260763	2.916437
6	-1.213378	-0.791132	2.191819
6	-1.286344	-1.584454	3.334984
1	-0.342974	-3.150529	4.478756
1	-2.142656	-1.484418	3.997962
6	-2.266709	0.154027	1.829827
6	-3.369666	0.545030	2.594018
6	-2.975871	1.550118	0.052515
6	-4.273733	1.462055	2.064555
1	-3.518500	0.144749	3.595013
6	-4.081431	1.967793	0.774635
1	-5.130500	1.777009	2.655979
1	-4.768056	2.671172	0.309018
7	-0.153751	-0.877430	1.307168
7	-2.098923	0.677433	0.592219
7	2.620092	-0.542441	0.527468
6	4.443297	0.825083	-0.303761
8	5.633915	0.991170	-0.131639
8	3.610704	1.792972	-0.668698
6	-2.661895	1.931608	-1.378465
8	-3.399416	2.717070	-1.962161
8	-1.613614	1.330705	-1.880387
44	-0.531618	0.169409	-0.503176
6	0.896464	2.207981	1.258719
6	1.532566	3.392804	1.593034
6	1.728059	4.354927	0.607409

6	1.278540	4.087120	-0.680129
6	0.653225	2.877447	-0.945325
1	0.741946	1.417416	1.989079
1	1.879502	3.545072	2.611880
1	2.232330	5.291113	0.837330
1	1.417608	4.799656	-1.488727
1	0.289728	2.613130	-1.933670
6	-2.777617	-1.602107	-1.550525
6	-3.396458	-2.729513	-2.069652
6	-2.643935	-3.882744	-2.268365
6	-1.290883	-3.856265	-1.943558
6	-0.741595	-2.691648	-1.428858
1	-3.322327	-0.673035	-1.398881
1	-4.453059	-2.691015	-2.322069
1	-3.101186	-4.781692	-2.676588
1	-0.655907	-4.726036	-2.093473
1	0.317881	-2.602238	-1.195299
7	-1.471492	-1.576441	-1.223837
7	0.455342	1.946146	0.013195
8	0.907832	-0.407133	-1.766181
8	1.896996	0.404881	-2.116781
1	2.761462	1.368474	-1.000424

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] Conformer 1 (Quartet)

E = -1860.81408827 a.u.

6	2.079268	-1.704480	0.945232
6	2.598325	-2.936551	0.529462
6	3.763576	-2.963367	-0.231233
6	4.385998	-1.763852	-0.546896
6	3.809575	-0.586863	-0.073461
1	2.074985	-3.854383	0.794544
1	4.174872	-3.910601	-0.575720
1	5.293162	-1.706054	-1.142435
6	0.846671	-1.643935	1.763462
6	0.784475	-2.392537	2.928102
6	-0.343234	-2.268839	3.770922
1	1.632682	-3.014082	3.204058
6	-1.279175	-0.687666	2.192050
6	-1.348439	-1.410667	3.402603
1	-0.404302	-2.830857	4.699840
1	-2.227461	-1.288122	4.033074
6	-2.304524	0.185354	1.734014
6	-3.499582	0.570764	2.389553
6	-2.951971	1.543418	-0.137963
6	-4.378920	1.439982	1.778780
1	-3.716424	0.182261	3.382884
6	-4.115193	1.948456	0.485483

1	-5.288055	1.732880	2.300415
1	-4.785095	2.625621	-0.036296
7	-0.155339	-0.825466	1.350860
7	-2.095152	0.706808	0.476058
7	2.687245	-0.545486	0.653378
6	4.452068	0.734075	-0.374691
8	5.474249	0.840422	-1.013024
8	3.802970	1.786498	0.146980
6	-2.538388	1.908416	-1.545411
8	-3.203153	2.693367	-2.205591
8	-1.459298	1.282271	-1.963360
44	-0.491478	0.137001	-0.519713
6	0.650381	2.259501	1.342784
6	1.234823	3.460894	1.710822
6	1.635594	4.351757	0.717367
6	1.430132	4.003440	-0.611371
6	0.835100	2.785206	-0.909785
1	0.326171	1.525489	2.077563
1	1.374714	3.686938	2.764879
1	2.103934	5.298325	0.978006
1	1.729511	4.660903	-1.422884
1	0.636589	2.470320	-1.930271
6	-2.724859	-1.571733	-1.647874
6	-3.362285	-2.707988	-2.121616
6	-2.672586	-3.916241	-2.145223
6	-1.357291	-3.936049	-1.688256
6	-0.786599	-2.762716	-1.223662
1	-3.223061	-0.606280	-1.628566
1	-4.387996	-2.633974	-2.473556
1	-3.147266	-4.821923	-2.516232
1	-0.770183	-4.851118	-1.690784
1	0.241408	-2.724054	-0.865738
7	-1.453392	-1.589025	-1.198069
7	0.454489	1.919362	0.051689
8	1.093067	-0.288774	-1.665703
8	2.023593	0.351540	-2.252341
1	3.012823	1.418040	0.602343

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] Conformer 2 (Doublet)

E = -1860.84072986 a.u.

6	2.093451	-1.624767	0.998862
6	2.637050	-2.858428	0.626123
6	3.809105	-2.877512	-0.125266
6	4.404987	-1.672790	-0.464300
6	3.795855	-0.493341	-0.035025
1	2.128996	-3.781633	0.903047
1	4.245104	-3.823193	-0.442518

1	5.317241	-1.609237	-1.051111
6	0.858729	-1.570405	1.815552
6	0.799070	-2.298479	3.002404
6	-0.317808	-2.199478	3.825816
1	1.652515	-2.912518	3.282166
6	-1.276603	-0.687728	2.212059
6	-1.352442	-1.369272	3.426421
1	-0.372712	-2.748220	4.762892
1	-2.240349	-1.255889	4.044287
6	-2.356088	0.165486	1.724571
6	-3.534443	0.525234	2.385939
6	-3.002617	1.446543	-0.164071
6	-4.440567	1.369938	1.751633
1	-3.742342	0.154678	3.387967
6	-4.176759	1.835650	0.458029
1	-5.355874	1.659379	2.262989
1	-4.860754	2.483657	-0.085508
7	-0.172501	-0.796212	1.381936
7	-2.126796	0.642202	0.476364
7	2.672903	-0.458622	0.690068
6	4.426674	0.825795	-0.369819
8	5.510440	0.913125	-0.902512
8	3.713973	1.893230	0.011124
6	-2.604385	1.781682	-1.587784
8	-3.331861	2.511477	-2.251315
8	-1.501971	1.206044	-1.993501
44	-0.488362	0.132467	-0.499579
6	0.578934	2.377611	1.270931
6	1.119492	3.614499	1.586169
6	1.477179	4.475834	0.551289
6	1.278088	4.058741	-0.758883
6	0.743173	2.800737	-1.003417
1	0.288689	1.668535	2.044185
1	1.260698	3.888480	2.628654
1	1.908176	5.451434	0.765671
1	1.544377	4.692319	-1.600527
1	0.581194	2.418014	-2.004701
6	-2.625003	-1.750755	-1.581288
6	-3.185806	-2.917062	-2.080377
6	-2.390173	-4.051939	-2.201730
6	-1.053538	-3.967638	-1.823166
6	-0.563132	-2.766708	-1.333110
1	-3.206292	-0.836159	-1.487519
1	-4.231565	-2.922841	-2.377082
1	-2.801462	-4.980768	-2.591601
1	-0.385585	-4.821076	-1.912297
1	0.482937	-2.632377	-1.063651
7	-1.335462	-1.668980	-1.201633
7	0.395827	1.964625	-0.000354
8	1.085127	-0.479871	-1.607477

8	1.964829	0.421393	-1.993487
1	2.858284	1.545909	0.343431

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] Conformer 2 (Quartet)

E = -1860.81414102 a.u.

6	2.129542	-1.751370	0.811344
6	2.609671	-2.964476	0.300793
6	3.780601	-2.975020	-0.448159
6	4.449189	-1.776833	-0.662193
6	3.912307	-0.622881	-0.096208
1	2.050953	-3.880752	0.487198
1	4.160622	-3.905985	-0.864911
1	5.365353	-1.705818	-1.242336
6	0.896295	-1.715330	1.628566
6	0.832806	-2.538753	2.738777
6	-0.268376	-2.440443	3.620149
1	1.671391	-3.196708	2.953950
6	-1.172205	-0.707694	2.188941
6	-1.241004	-1.512850	3.344438
1	-0.330489	-3.069541	4.504676
1	-2.099396	-1.400880	4.004547
6	-2.165357	0.246115	1.836885
6	-3.266877	0.685557	2.609993
6	-2.872204	1.702435	0.079761
6	-4.138491	1.628472	2.107840
1	-3.411423	0.284385	3.611224
6	-3.949597	2.158009	0.812745
1	-4.975337	1.964011	2.717266
1	-4.613910	2.891645	0.364955
7	-0.090097	-0.837692	1.292703
7	-2.017891	0.790095	0.581745
7	2.783966	-0.596593	0.623209
6	4.613023	0.690632	-0.271829
8	5.634801	0.816274	-0.908044
8	4.010195	1.716179	0.350005
6	-2.560563	2.096466	-1.338674
8	-3.223515	2.945909	-1.917804
8	-1.567170	1.418773	-1.864702
44	-0.504125	0.151415	-0.555681
6	0.815107	2.247801	1.201043
6	1.459270	3.435178	1.512098
6	1.890470	4.262606	0.477857
6	1.654734	3.867900	-0.833405
6	0.994157	2.671142	-1.073541
1	0.463556	1.560242	1.967909
1	1.621505	3.699346	2.554093
1	2.404856	5.196483	0.693190

1	1.974388	4.477090	-1.674432
1	0.758358	2.322375	-2.076200
6	-2.885930	-1.390730	-1.602039
6	-3.637464	-2.478674	-2.018372
6	-3.070815	-3.749176	-1.987694
6	-1.759357	-3.878083	-1.539366
6	-1.069817	-2.746325	-1.135298
1	-3.280309	-0.378986	-1.630561
1	-4.654237	-2.319500	-2.368030
1	-3.636850	-4.619853	-2.311659
1	-1.265989	-4.846146	-1.501832
1	-0.039015	-2.792615	-0.788731
7	-1.617790	-1.513465	-1.159976
7	0.584732	1.866696	-0.072143
8	1.104119	-0.687212	-1.549151
8	0.720698	-0.073234	-2.632403
1	3.209317	1.340102	0.780957

$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$ (Doublet)

E = -1709.74511300 a.u.

6	-2.327941	-0.093967	1.699914
6	-3.652409	-0.114520	2.139842
6	-4.686804	-0.058055	1.213131
6	-4.368951	0.017188	-0.137214
6	-3.029589	0.033265	-0.506647
1	-3.870813	-0.173702	3.203309
1	-5.722520	-0.072976	1.543946
1	-5.116120	0.064194	-0.925789
6	-1.163257	-0.148215	2.584709
6	-1.202972	-0.236568	3.978831
6	0.000009	-0.280445	4.675073
1	-2.149119	-0.271588	4.512766
6	1.163285	-0.147266	2.584780
6	1.202991	-0.235497	3.978911
1	0.000004	-0.350038	5.760213
1	2.149134	-0.269651	4.512912
6	2.327992	-0.092263	1.700078
6	3.652434	-0.112161	2.140119
6	3.029710	0.035700	-0.506379
6	4.686867	-0.054951	1.213492
1	3.870794	-0.171391	3.203591
6	4.369059	0.020370	-0.136862
1	5.722569	-0.069352	1.544376
1	5.116250	0.067940	-0.925381
7	0.000019	-0.105979	1.920621
7	2.024966	-0.018335	0.382991
7	-2.024872	-0.020053	0.382816

6	-2.611162	0.110786	-1.940253
8	-1.308926	0.112875	-2.098774
8	-3.428397	0.164006	-2.839864
6	2.611339	0.113041	-1.940001
8	3.428622	0.167067	-2.839541
8	1.309140	0.114007	-2.098652
44	-0.000004	0.030871	-0.577407
6	0.000553	-2.944836	0.202967
6	0.001119	-4.316061	0.003945
6	0.002103	-4.808432	-1.298705
6	0.002471	-3.902172	-2.352997
6	0.001873	-2.541223	-2.080044
1	-0.000241	-2.512846	1.201537
1	0.000770	-4.983128	0.861931
1	0.002547	-5.879701	-1.486460
1	0.003206	-4.235638	-3.387117
1	0.002138	-1.790236	-2.865506
6	-0.001326	2.906098	0.519068
6	-0.002019	4.290782	0.466839
6	-0.002396	4.918678	-0.776216
6	-0.002067	4.129738	-1.921017
6	-0.001378	2.747592	-1.794298
1	-0.000993	2.369789	1.465846
1	-0.002248	4.862911	1.390886
1	-0.002934	6.003845	-0.848860
1	-0.002340	4.571477	-2.913687
1	-0.001096	2.083143	-2.654366
7	-0.001000	2.139308	-0.589209
7	0.000954	-2.064178	-0.817217

[Ru^{III}(tda-κ-N^2O)Py_2(OH)] (Doublet)

E = -1785.69907506 a.u.

6	2.420767	0.740871	1.048120
6	3.666411	1.331385	1.199418
6	3.846605	2.649415	0.776782
6	2.740414	3.350947	0.342899
6	1.504143	2.700057	0.181555
1	4.480212	0.781960	1.666633
1	4.820108	3.128867	0.859850
1	2.788537	4.417019	0.134710
6	2.075387	-0.550957	1.651964
6	2.903661	-1.304914	2.492733
6	2.376260	-2.434639	3.108606
1	3.930639	-1.004806	2.686564
6	0.305332	-2.018299	1.992192
6	1.053969	-2.800685	2.873543
1	2.997246	-3.030262	3.774664

1	0.627129	-3.685748	3.341071
6	-1.054268	-2.313134	1.524074
6	-1.936931	-3.229035	2.098080
6	-2.508287	-1.929269	-0.237710
6	-3.159904	-3.464968	1.475507
1	-1.672421	-3.744298	3.019808
6	-3.444994	-2.823040	0.274482
1	-3.869510	-4.164400	1.913378
1	-4.353505	-3.002130	-0.295439
7	0.815804	-0.927203	1.412119
7	-1.366120	-1.647074	0.396123
7	1.382835	1.375479	0.421483
6	0.273452	3.604645	0.001620
8	-0.351575	3.675324	-1.078275
8	0.105007	4.197574	1.085122
6	-2.623441	-1.313980	-1.604343
8	-3.626029	-1.509812	-2.281830
8	-1.556690	-0.670132	-1.977701
44	-0.173781	0.139519	-0.667117
6	-1.778709	1.658767	1.384786
6	-2.786135	2.461248	1.893862
6	-3.756210	2.954971	1.028253
6	-3.678455	2.625574	-0.320336
6	-2.639170	1.823092	-0.762767
1	-0.982235	1.259577	2.010710
1	-2.788113	2.709314	2.951745
1	-4.553441	3.596487	1.397969
1	-4.404762	2.996795	-1.038182
1	-2.516401	1.548154	-1.807572
6	1.201311	-2.396832	-1.605338
6	2.168214	-3.207228	-2.180052
6	3.318146	-2.619842	-2.700687
6	3.445191	-1.236408	-2.633950
6	2.432882	-0.488799	-2.048431
1	0.278021	-2.801731	-1.195806
1	2.011319	-4.282153	-2.222793
1	4.095320	-3.229272	-3.157585
1	4.317102	-0.728712	-3.039013
1	2.452027	0.597833	-2.002614
7	1.328159	-1.058821	-1.528657
7	-1.703191	1.337930	0.078861
8	0.256569	1.316288	-2.093392
1	-0.025417	2.248897	-1.865012

[Ru^{III}(tda-κ-N^2O)Py_2(OOH)] (Doublet)

E = -1860.83641010 a.u.

6	2.030798	-1.869100	0.765652

6	2.709578	-3.049782	0.456736
6	3.967048	-2.946327	-0.138371
6	4.496696	-1.686303	-0.364393
6	3.717241	-0.555395	-0.081686
1	2.265928	-4.022322	0.669769
1	4.524964	-3.843827	-0.401883
1	5.496241	-1.536550	-0.765580
6	0.780803	-1.884847	1.552414
6	0.649613	-2.790373	2.610561
6	-0.433263	-2.711350	3.472695
1	1.442654	-3.515980	2.773749
6	-1.233112	-0.858306	2.169470
6	-1.372440	-1.712874	3.260689
1	-0.532288	-3.399369	4.309100
1	-2.229360	-1.605389	3.920987
6	-2.232228	0.159733	1.848410
6	-3.310274	0.570034	2.636581
6	-2.897980	1.638625	0.132435
6	-4.180972	1.541230	2.149838
1	-3.463658	0.142095	3.624812
6	-3.980914	2.078379	0.876411
1	-5.017405	1.871533	2.761464
1	-4.640117	2.824182	0.438451
7	-0.173743	-0.950404	1.298786
7	-2.048208	0.719195	0.631536
7	2.498714	-0.649221	0.465065
6	4.261044	0.841934	-0.345754
8	5.459281	1.001266	-0.083530
8	3.409536	1.678543	-0.790351
6	-2.585206	2.053344	-1.284366
8	-3.292443	2.876409	-1.848156
8	-1.559514	1.426059	-1.805818
44	-0.491134	0.205090	-0.512398
6	1.127249	2.044411	1.286161
6	1.831742	3.169942	1.677005
6	1.968396	4.225411	0.782338
6	1.390122	4.109437	-0.474071
6	0.695706	2.953933	-0.797012
1	1.028426	1.178734	1.934587
1	2.286286	3.199677	2.663751
1	2.533392	5.114133	1.055179
1	1.486806	4.894412	-1.218968
1	0.241913	2.805893	-1.772782
6	-2.807081	-1.477700	-1.579992
6	-3.461666	-2.572692	-2.124195
6	-2.743223	-3.740973	-2.357808
6	-1.388619	-3.763276	-2.040773
6	-0.802943	-2.628919	-1.498940
1	-3.323337	-0.536751	-1.403397
1	-4.517769	-2.497114	-2.369778

1	-3.228365	-4.614649	-2.787929
1	-0.779851	-4.646270	-2.217834
1	0.259367	-2.580936	-1.264988
7	-1.499837	-1.499951	-1.261461
7	0.553431	1.934205	0.073294
8	0.810797	-0.339606	-1.849594
8	1.795996	0.492294	-2.351952
1	2.297652	0.958901	-1.558731

$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (Doublet)

E = -1786.10708492 a.u.

6	-2.104415	0.060335	1.844194
6	-3.267844	0.263366	2.570887
6	-4.369886	0.865588	1.962713
6	-4.277535	1.220063	0.632899
6	-3.069380	1.036275	-0.056463
1	-3.324173	-0.054245	3.608294
1	-5.286490	1.028379	2.524526
1	-5.118738	1.644728	0.091191
6	-0.941188	-0.625259	2.413987
6	-0.868460	-1.198915	3.682157
6	0.293600	-1.859893	4.069332
1	-1.714740	-1.144925	4.360744
6	1.275926	-1.343885	1.941079
6	1.374016	-1.938774	3.197801
1	0.354523	-2.317151	5.053383
1	2.284507	-2.452094	3.494670
6	2.325429	-1.269968	0.927654
6	3.603322	-1.777218	1.111695
6	2.959637	-0.263568	-1.098328
6	4.583241	-1.532802	0.148567
1	3.842532	-2.338592	2.011064
6	4.267333	-0.739766	-0.938410
1	5.587346	-1.930353	0.276184
1	5.013064	-0.467694	-1.681030
7	0.128805	-0.708612	1.581893
7	1.984070	-0.574170	-0.214807
7	-1.989771	0.480315	0.535972
6	-3.020263	1.381366	-1.529174
8	-2.281201	2.322156	-1.906301
8	-3.747492	0.626675	-2.204292
6	2.591716	0.700269	-2.197662
8	2.844392	1.883180	-1.900524
8	2.041730	0.226093	-3.221412
44	-0.028562	0.034651	-0.226019
6	-0.077623	-3.010640	-0.681307
6	-0.490315	-4.224494	-1.203274

6	-1.584082	-4.251237	-2.065115
6	-2.219834	-3.053442	-2.368611
6	-1.746339	-1.872284	-1.816284
1	0.777927	-2.954695	-0.013862
1	0.046661	-5.131365	-0.938990
1	-1.928984	-5.189468	-2.493808
1	-3.076636	-3.012834	-3.035366
1	-2.216562	-0.922108	-2.050809
6	1.731311	2.093957	1.172210
6	2.284451	3.327295	1.465067
6	1.736071	4.466729	0.883977
6	0.634554	4.321395	0.049668
6	0.126900	3.054886	-0.197885
1	2.142300	1.184296	1.602055
1	3.141820	3.384809	2.129897
1	2.161273	5.448376	1.080021
1	0.163408	5.177841	-0.424472
1	-0.746954	2.902469	-0.832956
7	0.671646	1.946171	0.348143
7	-0.688674	-1.844383	-0.976359
8	-0.317918	0.632221	-2.262193
1	-0.886855	1.417927	-2.448072
1	0.480814	0.607924	-2.862168

[Ru^{III}(tda-κ-N^3)Py_2(OH)] (Doublet)

E = -1785.68500419 a.u.

6	-2.149490	0.086073	1.781433
6	-3.274718	0.403928	2.528001
6	-4.143157	1.393556	2.066778
6	-3.859151	2.019932	0.871260
6	-2.700342	1.688694	0.146769
1	-3.470685	-0.114800	3.462822
1	-5.028926	1.657151	2.641521
1	-4.512277	2.786394	0.460575
6	-1.214106	-0.966343	2.176700
6	-1.371538	-1.853334	3.238956
6	-0.421340	-2.852618	3.440210
1	-2.237084	-1.780397	3.892138
6	0.798374	-2.047482	1.533534
6	0.665375	-2.961078	2.580294
1	-0.535938	-3.553238	4.263712
1	1.406677	-3.742740	2.725432
6	1.886743	-1.991780	0.563307
6	2.958449	-2.873727	0.567838
6	2.953321	-0.596724	-0.995348
6	4.037657	-2.639357	-0.282665
1	2.963256	-3.718562	1.252486

6	4.061794	-1.457109	-0.998440
1	4.876248	-3.331639	-0.313523
1	4.942249	-1.139006	-1.549514
7	-0.128926	-1.067259	1.365681
7	1.826767	-0.938306	-0.330914
7	-1.857042	0.738533	0.605463
6	-2.449355	2.422036	-1.165914
8	-1.735130	3.436542	-1.059278
8	-3.074164	1.925730	-2.125998
6	3.180185	0.827892	-1.536358
8	4.182389	1.284793	-0.953077
8	2.432084	1.337623	-2.395468
44	-0.045117	0.071008	-0.296343
6	-0.923343	-2.770809	-1.211942
6	-1.650859	-3.718714	-1.914767
6	-2.687820	-3.292346	-2.739614
6	-2.946713	-1.930382	-2.826453
6	-2.174660	-1.033793	-2.097697
1	-0.095380	-3.067544	-0.571848
1	-1.396231	-4.771148	-1.817143
1	-3.276918	-4.010905	-3.306449
1	-3.740849	-1.539289	-3.457119
1	-2.350753	0.044089	-2.156199
6	1.891816	1.501472	1.547520
6	2.695464	2.510619	2.046634
6	2.643257	3.766110	1.448733
6	1.773958	3.959617	0.384236
6	0.989285	2.905693	-0.064146
1	1.914641	0.498647	1.970549
1	3.364565	2.301566	2.877084
1	3.274878	4.576537	1.806742
1	1.692379	4.919699	-0.117477
1	0.266632	3.025595	-0.868033
7	1.048462	1.686747	0.511118
7	-1.175561	-1.451892	-1.291576
8	-0.090334	0.867050	-2.020814
1	0.799528	1.246423	-2.271139

$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^-$ (Doublet)

E = -1785.12632969 a.u.

6	-2.246910	-0.675903	1.526155
6	-3.532904	-0.859308	2.036516
6	-4.626429	-0.386031	1.323756
6	-4.409450	0.270090	0.122116
6	-3.107021	0.464004	-0.355626
1	-3.664950	-1.371920	2.986774
1	-5.636012	-0.530539	1.708248

1	-5.233742	0.653033	-0.475718
6	-1.052384	-1.149626	2.201469
6	-1.004303	-1.876756	3.383869
6	0.228788	-2.280950	3.904575
1	-1.926672	-2.138777	3.899213
6	1.328311	-1.232948	2.030711
6	1.399143	-1.963514	3.211278
1	0.274690	-2.850734	4.829814
1	2.365502	-2.292073	3.590068
6	2.438913	-0.845791	1.180574
6	3.768498	-1.154291	1.478564
6	3.089808	0.271909	-0.795827
6	4.769983	-0.784614	0.591603
1	4.002271	-1.687021	2.397917
6	4.421930	-0.086403	-0.555110
1	5.809390	-1.038577	0.800164
1	5.158813	0.216388	-1.295321
7	0.110129	-0.811321	1.546827
7	2.103993	-0.147266	0.036388
7	-2.042446	-0.016315	0.330364
6	-2.921041	1.240622	-1.654238
8	-2.695859	2.454608	-1.480165
8	-3.109005	0.556074	-2.684992
6	2.817485	1.220747	-1.962025
8	2.401738	2.337661	-1.576751
8	3.159211	0.784618	-3.076301
44	0.005118	0.101212	-0.250131
6	0.493011	-2.889912	-0.857572
6	0.360780	-4.098612	-1.525258
6	-0.531318	-4.181768	-2.590656
6	-1.255777	-3.048033	-2.939663
6	-1.072434	-1.866336	-2.231673
1	1.184988	-2.775700	-0.024650
1	0.958034	-4.952542	-1.213302
1	-0.657243	-5.115522	-3.137330
1	-1.968621	-3.059174	-3.760738
1	-1.624287	-0.951821	-2.471596
6	0.317275	2.357925	1.776830
6	0.389268	3.653809	2.261739
6	0.244464	4.710485	1.365399
6	0.039043	4.421592	0.024234
6	-0.012783	3.097991	-0.396085
1	0.421053	1.495070	2.432799
1	0.555628	3.822438	3.323558
1	0.292757	5.742165	1.712867
1	-0.079405	5.209104	-0.715179
1	-0.162434	2.801479	-1.429095
7	0.118328	2.081887	0.475918
7	-0.203793	-1.793545	-1.199838
8	-0.118848	0.767919	-1.908578

[Ru^{III}(tda-κ-N^3)Py_2(O)]$^-$ (Quartet)

E = -1785.10652356 a.u.

6	-2.220361	-0.629346	1.531604
6	-3.522127	-0.784034	2.042154
6	-4.603386	-0.275210	1.349075
6	-4.388826	0.396252	0.144811
6	-3.086205	0.555587	-0.341029
1	-3.661782	-1.305467	2.987348
1	-5.611909	-0.399068	1.744438
1	-5.209455	0.807598	-0.437848
6	-1.051373	-1.122176	2.194032
6	-0.991767	-1.858922	3.388733
6	0.228234	-2.296253	3.876625
1	-1.908342	-2.097891	3.926620
6	1.335867	-1.278814	2.001455
6	1.424425	-2.021915	3.168009
1	0.267589	-2.870266	4.800746
1	2.379488	-2.394819	3.528902
6	2.454366	-0.909442	1.125790
6	3.773217	-1.250007	1.411804
6	3.113578	0.204596	-0.844273
6	4.781143	-0.897480	0.518946
1	3.999919	-1.791870	2.327149
6	4.441190	-0.185671	-0.618894
1	5.815289	-1.177124	0.719475
1	5.177017	0.104747	-1.365119
7	0.142909	-0.821542	1.559194
7	2.128052	-0.195711	-0.006839
7	-2.027221	0.047557	0.323073
6	-2.875584	1.319247	-1.643365
8	-2.578768	2.521341	-1.489971
8	-3.090714	0.636286	-2.672004
6	2.844665	1.160268	-2.004423
8	2.405473	2.268747	-1.621370
8	3.200996	0.730720	-3.117121
44	0.001509	0.129001	-0.296078
6	0.398534	-2.889802	-0.856323
6	0.185840	-4.112722	-1.474346
6	-0.775055	-4.200305	-2.477904
6	-1.483591	-3.054228	-2.819377
6	-1.221001	-1.858783	-2.162006
1	1.144328	-2.774687	-0.072269
1	0.772889	-4.976226	-1.169850
1	-0.964334	-5.146039	-2.984030
1	-2.245801	-3.065591	-3.594723
1	-1.764125	-0.935883	-2.399796

6	0.378446	2.297298	1.810574
6	0.476683	3.574407	2.338832
6	0.346746	4.664665	1.482243
6	0.125795	4.427700	0.133204
6	0.045504	3.121322	-0.332453
1	0.466368	1.410688	2.435300
1	0.650025	3.701965	3.405102
1	0.416034	5.682144	1.865555
1	0.013784	5.242241	-0.577176
1	-0.125902	2.878065	-1.374432
7	0.168295	2.071050	0.501023
7	-0.286543	-1.782193	-1.188556
8	-0.107697	0.795392	-1.938814

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 1 (Closed-shell singlet)

E = -1785.81557413 a.u.

6	-0.197504	-2.524474	1.046200
6	-0.114205	-3.899478	1.220449
6	0.983067	-4.574977	0.694678
6	1.994917	-3.838103	0.098152
6	1.846364	-2.457784	-0.079803
1	-0.885893	-4.432471	1.769835
1	1.072179	-5.653272	0.800815
1	2.922116	-4.309586	-0.218856
6	-1.150711	-1.652613	1.709060
6	-1.984558	-2.028670	2.761556
6	-2.666529	-1.053027	3.477875
1	-2.059497	-3.075051	3.044741
6	-1.670518	0.609257	2.063078
6	-2.481148	0.284094	3.147397
1	-3.310929	-1.330430	4.308054
1	-2.966529	1.072050	3.717320
6	-1.413907	1.939491	1.554714
6	-1.815223	3.157987	2.102958
6	-0.533513	3.032084	-0.311142
6	-1.517106	4.339659	1.430318
1	-2.359038	3.179028	3.044307
6	-0.885865	4.277355	0.189187
1	-1.809967	5.297008	1.854296
1	-0.685394	5.157562	-0.418122
7	-1.044491	-0.352971	1.336097
7	-0.740800	1.904888	0.382769
7	0.726263	-1.827252	0.323963
6	3.112892	-1.705946	-0.467611
8	3.320071	-1.332426	-1.714488
8	3.925275	-1.585308	0.419242
6	-0.063841	2.765147	-1.700317

8	0.242355	3.619827	-2.495907
8	-0.129772	1.463951	-1.965509
44	-0.024129	0.093635	-0.471407
6	2.212656	0.883701	1.434953
6	3.419916	1.409177	1.859555
6	4.285567	1.957972	0.915655
6	3.903655	1.968443	-0.421529
6	2.677076	1.429057	-0.779509
1	1.514268	0.420502	2.129848
1	3.680659	1.370817	2.913414
1	5.246634	2.365904	1.219390
1	4.546994	2.380343	-1.193795
1	2.340805	1.399784	-1.812955
6	-2.905076	0.167531	-1.480305
6	-4.084923	-0.257807	-2.071190
6	-4.187343	-1.578664	-2.498927
6	-3.097785	-2.427121	-2.322253
6	-1.947814	-1.931863	-1.725478
1	-2.771708	1.196703	-1.154760
1	-4.902698	0.445308	-2.202860
1	-5.097705	-1.937852	-2.973060
1	-3.126196	-3.461218	-2.654699
1	-1.056037	-2.542967	-1.601459
7	-1.852088	-0.654504	-1.302790
7	1.844879	0.887591	0.135489
8	0.789731	-0.825041	-2.002763
1	2.447942	-1.301098	-2.179707
1	0.292784	-0.535833	-2.789476

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 2 (Closed-shell singlet)

E = -1785.80528270 a.u.

6	2.358996	-0.961028	1.050751
6	3.586008	-1.634438	1.025184
6	4.685224	-0.991581	0.478231
6	4.538831	0.325680	0.049551
6	3.276191	0.918871	0.081543
1	3.668164	-2.649553	1.406509
1	5.648025	-1.492399	0.412634
1	5.394295	0.876106	-0.339004
6	1.181433	-1.474144	1.757648
6	1.302904	-2.303575	2.870955
6	0.186665	-2.588091	3.648573
1	2.283162	-2.676762	3.155410
6	-1.109921	-1.234481	2.150251
6	-1.029511	-2.023911	3.296428
1	0.270963	-3.222543	4.527113
1	-1.922303	-2.209187	3.887745

6	-2.339709	-0.683545	1.615828
6	-3.605162	-0.691112	2.204549
6	-3.213438	0.242509	-0.333107
6	-4.689380	-0.183742	1.493014
1	-3.743508	-1.094660	3.204677
6	-4.498995	0.272334	0.190003
1	-5.679051	-0.173477	1.942909
1	-5.312978	0.630862	-0.436093
7	-0.020009	-0.970982	1.379042
7	-2.164391	-0.185890	0.375579
7	2.182776	0.262542	0.520288
6	3.107505	2.356316	-0.336406
8	4.091677	3.188512	-0.003388
8	2.143901	2.771984	-0.945856
6	-2.843369	0.552348	-1.739896
8	-3.601545	0.989974	-2.571940
8	-1.582835	0.203801	-1.984116
44	-0.221053	0.050617	-0.529011
6	-0.301149	2.508652	1.262975
6	-0.430339	3.842652	1.611666
6	-0.794524	4.765123	0.632543
6	-1.015620	4.314612	-0.663954
6	-0.864621	2.964570	-0.945222
1	-0.005775	1.751957	1.987722
1	-0.245899	4.149799	2.637560
1	-0.900034	5.819108	0.878366
1	-1.295466	4.995467	-1.462847
1	-1.007816	2.569869	-1.949620
6	-0.913558	-2.823721	-1.258327
6	-0.813240	-4.074805	-1.845521
6	0.360990	-4.413026	-2.512678
6	1.391499	-3.480084	-2.565706
6	1.218746	-2.244679	-1.958235
1	-1.820756	-2.510344	-0.745809
1	-1.651784	-4.763318	-1.788884
1	0.465255	-5.383148	-2.992811
1	2.319547	-3.692205	-3.089491
1	1.974436	-1.465461	-2.013359
7	0.084943	-1.920215	-1.307089
7	-0.513484	2.072771	0.004906
8	0.934098	0.558860	-1.891769
1	4.754446	2.776384	0.576561
1	1.267469	1.477504	-1.719166

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(O)]^+$ (Broken-symmetry singlet)

E = -1785.50565404 a.u.

6	2.283419	-1.510875	0.932442

6	3.109729	-2.633581	0.799211
6	4.343278	-2.483118	0.173324
6	4.705297	-1.229426	-0.301634
6	3.784062	-0.186775	-0.185573
1	2.790570	-3.606551	1.168849
1	5.010854	-3.334596	0.061028
1	5.665609	-1.040735	-0.775186
6	1.033314	-1.582162	1.721650
6	1.038994	-2.353991	2.888112
6	-0.062794	-2.372382	3.728002
1	1.943041	-2.898200	3.147166
6	-1.139700	-0.856488	2.206534
6	-1.158584	-1.597749	3.386104
1	-0.059575	-2.962586	4.640882
1	-2.039847	-1.574490	4.020760
6	-2.289388	-0.057441	1.786760
6	-3.440958	0.214777	2.531098
6	-3.140271	1.171954	-0.021291
6	-4.448631	0.991153	1.965441
1	-3.551895	-0.164074	3.543799
6	-4.304903	1.477125	0.664912
1	-5.345177	1.213046	2.539021
1	-5.064484	2.079292	0.172258
7	-0.058091	-0.853494	1.361245
7	-2.168197	0.433826	0.539587
7	2.604729	-0.313076	0.432785
6	4.115847	1.160923	-0.762376
8	3.076073	1.832325	-1.268554
8	5.245813	1.589318	-0.760568
6	-2.832110	1.573764	-1.432380
8	-3.594170	2.249204	-2.093519
8	-1.679325	1.089106	-1.868597
44	-0.420855	0.158888	-0.589266
6	0.775272	2.311639	1.241431
6	1.301959	3.542887	1.594503
6	1.300628	4.572046	0.656952
6	0.767034	4.328285	-0.602713
6	0.254735	3.071502	-0.887971
1	0.781891	1.469833	1.928591
1	1.718015	3.682433	2.588490
1	1.718589	5.545283	0.903490
1	0.755159	5.094169	-1.372881
1	-0.159736	2.824701	-1.862280
6	-2.356239	-1.995082	-1.591265
6	-2.773010	-3.194082	-2.149474
6	-1.818156	-4.147374	-2.488338
6	-0.476188	-3.859206	-2.259605
6	-0.133853	-2.637618	-1.699815
1	-3.067012	-1.214856	-1.329932
1	-3.831835	-3.363935	-2.323990

1	-2.114554	-5.094755	-2.932659
1	0.306807	-4.565219	-2.522874
1	0.900434	-2.341118	-1.538005
7	-1.059751	-1.719785	-1.360722
7	0.253884	2.075424	0.022066
8	0.980672	0.034409	-1.649718
1	2.287534	1.233889	-1.330152

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(O)]^+$ (Triplet)

E = -1785.51136537 a.u.

6	2.317773	1.624650	-0.840962
6	3.147320	2.740946	-0.674370
6	4.375436	2.573952	-0.042793
6	4.730146	1.309074	0.406597
6	3.804774	0.273693	0.262306
1	2.836106	3.723586	-1.024289
1	5.044434	3.420858	0.092760
1	5.686775	1.106361	0.881759
6	1.074585	1.717482	-1.638775
6	1.063985	2.560430	-2.757843
6	-0.036149	2.594766	-3.596711
1	1.949871	3.147936	-2.982877
6	-1.068145	0.955501	-2.174957
6	-1.109451	1.765544	-3.307300
1	-0.050507	3.238160	-4.472931
1	-1.985433	1.754544	-3.949561
6	-2.203565	0.085547	-1.830245
6	-3.318932	-0.187990	-2.627308
6	-3.067917	-1.278392	-0.117107
6	-4.312280	-1.033086	-2.135498
1	-3.415475	0.237406	-3.622691
6	-4.198254	-1.587554	-0.860519
1	-5.179721	-1.255660	-2.752578
1	-4.951653	-2.243639	-0.431607
7	0.007729	0.940462	-1.325567
7	-2.115731	-0.476366	-0.614109
7	2.629502	0.415655	-0.359911
6	4.129892	-1.085966	0.812534
8	3.085027	-1.764251	1.303453
8	5.256412	-1.522379	0.807294
6	-2.798557	-1.747056	1.291934
8	-3.579873	-2.487059	1.858105
8	-1.692745	-1.261440	1.825457
44	-0.441197	-0.201498	0.612312
6	0.923727	-2.207699	-1.264409
6	1.513910	-3.396498	-1.660450
6	1.501277	-4.480200	-0.786994

6	0.892211	-4.333218	0.453738
6	0.317582	-3.115397	0.784565
1	0.939291	-1.323016	-1.894706
1	1.987736	-3.460614	-2.636115
1	1.968783	-5.421403	-1.066919
1	0.869436	-5.144808	1.175286
1	-0.157004	-2.941253	1.747209
6	-2.556142	1.765215	1.653167
6	-3.068945	2.922066	2.220998
6	-2.199264	3.959784	2.538654
6	-0.841640	3.797043	2.278158
6	-0.401543	2.613507	1.706905
1	-3.197333	0.920684	1.413875
1	-4.134456	2.992686	2.421134
1	-2.571263	4.875530	2.992265
1	-0.121157	4.571969	2.525375
1	0.651625	2.417997	1.514665
7	-1.245793	1.611646	1.389840
7	0.328626	-2.066188	-0.063942
8	0.936207	-0.014803	1.708110
1	2.301068	-1.165277	1.364823

[Ru^{IV}(Htda-κ-N^2O)Py_2(OOH)]$^{2+}$ (Closed-shell singlet)

E = -1860.93460608 a.u.

6	2.004723	-1.676275	1.084399
6	2.651457	-2.889793	0.832588
6	3.859796	-2.872859	0.139129
6	4.378601	-1.651109	-0.270289
6	3.676501	-0.489381	0.054172
1	2.208854	-3.830467	1.157289
1	4.384106	-3.800830	-0.077330
1	5.311888	-1.567959	-0.822178
6	0.732091	-1.635610	1.833435
6	0.590380	-2.403125	2.993857
6	-0.554350	-2.302105	3.769419
1	1.417422	-3.039509	3.299070
6	-1.392694	-0.699607	2.191557
6	-1.551308	-1.422869	3.368530
1	-0.661883	-2.884911	4.680756
1	-2.460147	-1.310545	3.953317
6	-2.403853	0.209668	1.667428
6	-3.565082	0.645028	2.310004
6	-2.936004	1.503195	-0.210247
6	-4.412197	1.539164	1.660384
1	-3.802048	0.298764	3.312792
6	-4.097446	1.982934	0.375873
1	-5.315636	1.886743	2.155514

1	-4.723392	2.677922	-0.179234
7	-0.266024	-0.808024	1.422409
7	-2.122148	0.650593	0.425341
7	2.509988	-0.488571	0.714775
6	4.203001	0.842165	-0.402190
8	5.011413	0.933010	-1.291872
8	3.679485	1.904005	0.228985
6	-2.460523	1.829013	-1.589391
8	-3.006423	2.596367	-2.339643
8	-1.366224	1.118760	-1.887761
44	-0.360245	0.089461	-0.544270
6	0.692410	2.262110	1.342072
6	1.163126	3.499483	1.750340
6	1.407353	4.481458	0.791823
6	1.162388	4.182790	-0.542976
6	0.687114	2.923508	-0.881525
1	0.506732	1.464778	2.057434
1	1.338028	3.683480	2.807078
1	1.783914	5.459027	1.083046
1	1.338808	4.911054	-1.329501
1	0.483117	2.653798	-1.912802
6	-2.524214	-1.748816	-1.688125
6	-3.105741	-2.898938	-2.199367
6	-2.360183	-4.073069	-2.240483
6	-1.051418	-4.050946	-1.765882
6	-0.536714	-2.863995	-1.268832
1	-3.067153	-0.808092	-1.662354
1	-4.126459	-2.861952	-2.569687
1	-2.788527	-4.987849	-2.643131
1	-0.426709	-4.939686	-1.787838
1	0.489285	-2.794319	-0.909432
7	-1.259162	-1.725911	-1.223310
7	0.460166	1.967492	0.043493
8	0.963104	-0.393627	-1.743904
8	1.942945	0.545642	-2.086649
1	3.042888	1.571454	0.890874
1	2.320295	0.148377	-2.902221

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (Triplet)

E = -1860.92904388 a.u.

6	2.025906	-1.740754	1.058002
6	2.691191	-2.938058	0.774122
6	3.891704	-2.886620	0.070020
6	4.389741	-1.647554	-0.314202
6	3.672067	-0.505939	0.045005
1	2.264034	-3.892902	1.077065
1	4.426925	-3.801259	-0.174526

1	5.320381	-1.536446	-0.865820
6	0.750924	-1.733034	1.800257
6	0.593402	-2.532365	2.937001
6	-0.558501	-2.429682	3.701775
1	1.405616	-3.190437	3.236241
6	-1.364940	-0.774245	2.158928
6	-1.539963	-1.522396	3.317530
1	-0.684284	-3.031366	4.598609
1	-2.445919	-1.409783	3.906876
6	-2.377229	0.165949	1.665797
6	-3.555121	0.569019	2.303339
6	-2.907036	1.521857	-0.193583
6	-4.399285	1.476155	1.665995
1	-3.812803	0.187085	3.287944
6	-4.082856	1.963275	0.394975
1	-5.312883	1.797793	2.159933
1	-4.723402	2.659786	-0.141253
7	-0.230568	-0.889787	1.392467
7	-2.095269	0.668818	0.450664
7	2.513081	-0.538525	0.712055
6	4.182432	0.848438	-0.361522
8	5.016661	0.984043	-1.221685
8	3.621493	1.877740	0.289771
6	-2.420406	1.863639	-1.570868
8	-2.947156	2.671002	-2.290711
8	-1.333285	1.139291	-1.945293
44	-0.412807	0.150098	-0.538190
6	0.609091	2.283347	1.388627
6	1.117064	3.498220	1.816604
6	1.444879	4.467204	0.869184
6	1.248819	4.178670	-0.476194
6	0.743162	2.938945	-0.838975
1	0.348266	1.496921	2.093185
1	1.251570	3.677136	2.879992
1	1.846510	5.429311	1.177895
1	1.487979	4.899819	-1.252577
1	0.578638	2.670184	-1.878039
6	-2.579956	-1.721623	-1.631480
6	-3.146141	-2.873035	-2.154537
6	-2.361358	-4.016307	-2.276601
6	-1.030376	-3.961823	-1.871334
6	-0.528989	-2.774285	-1.362972
1	-3.155095	-0.803693	-1.539853
1	-4.185480	-2.861696	-2.470648
1	-2.777784	-4.931895	-2.689905
1	-0.376793	-4.825338	-1.959076
1	0.512385	-2.673345	-1.063103
7	-1.291588	-1.668432	-1.236935
7	0.430963	1.998111	0.078317
8	1.012874	-0.421491	-1.752988

8	1.942526	0.569012	-2.081566
1	2.975816	1.503827	0.921328
1	2.379248	0.181909	-2.869457

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (Closed-shell singlet)

E = -1860.65212954 a.u.

6	2.091287	-1.714383	0.804154
6	2.737776	-2.922778	0.523229
6	3.988096	-2.887507	-0.087457
6	4.558693	-1.653360	-0.360656
6	3.815355	-0.501360	-0.091479
1	2.270264	-3.871729	0.783239
1	4.514266	-3.809960	-0.322663
1	5.555005	-1.552004	-0.783032
6	0.861499	-1.701445	1.628882
6	0.815065	-2.519861	2.762336
6	-0.249108	-2.436338	3.646691
1	1.654083	-3.180961	2.962613
6	-1.196421	-0.749168	2.224935
6	-1.255992	-1.520028	3.381718
1	-0.283169	-3.058035	4.537715
1	-2.101626	-1.413063	4.055774
6	-2.251632	0.193723	1.855730
6	-3.322033	0.620931	2.645208
6	-2.998580	1.530616	0.073497
6	-4.236272	1.528143	2.115087
1	-3.437377	0.260754	3.664505
6	-4.080336	1.992353	0.808884
1	-5.069657	1.870980	2.723378
1	-4.768081	2.696242	0.346390
7	-0.153391	-0.846991	1.337852
7	-2.121146	0.664567	0.601357
7	2.597450	-0.518597	0.466380
6	4.444149	0.839695	-0.358568
8	5.640249	0.990404	-0.277315
8	3.597652	1.833083	-0.647672
6	-2.689632	1.891307	-1.352749
8	-3.382490	2.665904	-1.980639
8	-1.628982	1.256628	-1.822216
44	-0.501471	0.134869	-0.559002
6	0.915421	2.208723	1.202968
6	1.520124	3.408370	1.542179
6	1.661793	4.392734	0.569542
6	1.188996	4.135240	-0.712364
6	0.592717	2.912734	-0.982286
1	0.810998	1.401921	1.923389
1	1.886009	3.555032	2.554672

1	2.142519	5.339379	0.804317
1	1.285761	4.865316	-1.510861
1	0.214813	2.663429	-1.969594
6	-2.765324	-1.644485	-1.590212
6	-3.394768	-2.774795	-2.089262
6	-2.665245	-3.951908	-2.220417
6	-1.324578	-3.950729	-1.847454
6	-0.764288	-2.781285	-1.357146
1	-3.292507	-0.698975	-1.494287
1	-4.440179	-2.719952	-2.380085
1	-3.130922	-4.852189	-2.614473
1	-0.709400	-4.841375	-1.943054
1	0.287210	-2.723703	-1.079428
7	-1.470101	-1.641308	-1.222221
7	0.453238	1.955927	-0.038070
8	0.798457	-0.364951	-1.799624
8	1.828886	0.335363	-2.125059
1	2.723611	1.437180	-0.869277

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (Broken-symmetry singlet)

E = -1860.65291038 a.u.

6	2.003405	-1.723271	0.983322
6	2.517305	-2.956798	0.574325
6	3.697806	-2.979870	-0.165576
6	4.330120	-1.779114	-0.453344
6	3.752616	-0.599710	0.017319
1	1.991425	-3.878583	0.821040
1	4.113377	-3.924231	-0.510056
1	5.250283	-1.720655	-1.028687
6	0.766129	-1.640737	1.791950
6	0.653061	-2.397273	2.959589
6	-0.446898	-2.233573	3.790350
1	1.461021	-3.075026	3.224487
6	-1.289179	-0.605956	2.235350
6	-1.416244	-1.308729	3.430402
1	-0.538680	-2.803658	4.711308
1	-2.286533	-1.144785	4.060411
6	-2.297849	0.343416	1.762199
6	-3.395394	0.839922	2.469133
6	-2.903750	1.613844	-0.123647
6	-4.249499	1.746715	1.845434
1	-3.578911	0.533158	3.496033
6	-4.007407	2.143135	0.529618
1	-5.103854	2.142920	2.388797
1	-4.645701	2.844713	-0.002212
7	-0.210301	-0.780566	1.405735
7	-2.086302	0.748111	0.494676

7	2.613285	-0.559834	0.719534
6	4.414057	0.717504	-0.274814
8	5.417843	0.804386	-0.938296
8	3.798488	1.776213	0.274158
6	-2.507353	1.895579	-1.549498
8	-3.146390	2.660878	-2.243183
8	-1.446553	1.208862	-1.935645
44	-0.441308	0.106896	-0.554991
6	0.707535	2.354437	1.175744
6	1.288108	3.577566	1.470845
6	1.707164	4.394746	0.423397
6	1.524136	3.952471	-0.880662
6	0.937984	2.714183	-1.102286
1	0.373853	1.679526	1.961682
1	1.412392	3.876316	2.508294
1	2.172707	5.356693	0.623782
1	1.837291	4.550620	-1.731506
1	0.776422	2.326391	-2.103084
6	-2.738000	-1.631334	-1.589508
6	-3.398410	-2.756471	-2.059547
6	-2.715037	-3.966820	-2.115349
6	-1.387632	-4.002055	-1.699423
6	-0.794842	-2.835010	-1.242721
1	-3.229802	-0.662789	-1.551769
1	-4.431071	-2.672484	-2.386748
1	-3.205362	-4.864503	-2.484704
1	-0.807200	-4.920076	-1.736385
1	0.250019	-2.804711	-0.938034
7	-1.455861	-1.662696	-1.179232
7	0.536699	1.919384	-0.090096
8	0.932887	-0.546607	-1.678083
8	1.980877	0.110945	-2.019182
1	3.014437	1.428769	0.748878

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (Triplet)

E = -1860.64943532 a.u.

6	2.067198	-1.694413	1.003210
6	2.608972	-2.924871	0.621713
6	3.775913	-2.940371	-0.139563
6	4.369196	-1.732668	-0.478483
6	3.770391	-0.556019	-0.029056
1	2.111901	-3.852287	0.904253
1	4.210926	-3.883950	-0.461684
1	5.276493	-1.668015	-1.073518
6	0.834148	-1.629668	1.821841
6	0.755100	-2.364116	3.006410
6	-0.355059	-2.237101	3.830375

1	1.591383	-3.000831	3.285743
6	-1.267109	-0.683533	2.238563
6	-1.367363	-1.369503	3.446183
1	-0.423411	-2.791651	4.762707
1	-2.246282	-1.235211	4.071373
6	-2.313068	0.219241	1.755040
6	-3.456958	0.643020	2.434341
6	-2.938755	1.513980	-0.131614
6	-4.337739	1.522409	1.808583
1	-3.656812	0.297623	3.445692
6	-4.082704	1.964170	0.509110
1	-5.225687	1.860091	2.337265
1	-4.743755	2.642757	-0.025004
7	-0.176838	-0.823124	1.411479
7	-2.094935	0.675283	0.499674
7	2.644176	-0.524790	0.693605
6	4.383240	0.770413	-0.377836
8	5.366200	0.870352	-1.069915
8	3.741163	1.825956	0.149436
6	-2.537748	1.837261	-1.554513
8	-3.216590	2.597829	-2.219181
8	-1.460054	1.199646	-1.959193
44	-0.496253	0.124366	-0.489310
6	0.671996	2.330829	1.280601
6	1.263160	3.543911	1.593014
6	1.633981	4.401360	0.558772
6	1.390665	4.008776	-0.750906
6	0.787638	2.781837	-0.992104
1	0.380446	1.623450	2.054278
1	1.434692	3.804546	2.634037
1	2.108804	5.355482	0.774129
1	1.665368	4.638524	-1.592222
1	0.560168	2.440483	-1.997983
6	-2.677901	-1.642149	-1.682651
6	-3.271135	-2.774944	-2.219504
6	-2.548460	-3.962305	-2.261121
6	-1.250185	-3.969283	-1.758669
6	-0.727144	-2.799552	-1.231361
1	-3.200412	-0.689621	-1.659383
1	-4.283106	-2.712973	-2.610110
1	-2.985048	-4.863913	-2.684212
1	-0.639957	-4.868266	-1.779557
1	0.289784	-2.750434	-0.843294
7	-1.424751	-1.646075	-1.187683
7	0.435961	1.945963	0.007944
8	1.083744	-0.320351	-1.655057
8	1.967028	0.299779	-2.303368
1	2.990812	1.465393	0.667968

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH)]^+$ (Triplet)

E = -1785.80588068 a.u.

6	2.304312	-0.843031	1.254604
6	3.546270	-1.386966	1.552910
6	4.610176	-1.200033	0.675150
6	4.425191	-0.358625	-0.406680
6	3.158533	0.179150	-0.676790
1	3.682126	-1.956005	2.468933
1	5.579869	-1.648982	0.873883
1	5.250370	-0.058414	-1.045419
6	1.176186	-0.907970	2.198227
6	1.225698	-1.317097	3.532837
6	0.064803	-1.236006	4.299229
1	2.148675	-1.675971	3.979807
6	-1.132676	-0.395814	2.403353
6	-1.129137	-0.772916	3.744565
1	0.088725	-1.541575	5.342443
1	-2.032763	-0.730576	4.346752
6	-2.297671	0.009243	1.599113
6	-3.547083	0.297418	2.142157
6	-3.134646	0.292892	-0.570645
6	-4.597453	0.647085	1.300707
1	-3.691497	0.265474	3.219043
6	-4.391392	0.635392	-0.073820
1	-5.570178	0.904612	1.712288
1	-5.193046	0.861621	-0.772108
7	0.011146	-0.461856	1.691738
7	-2.092689	0.041228	0.246376
7	2.085821	-0.148151	0.080686
6	3.180774	1.331914	-1.679408
8	2.164792	1.640579	-2.461385
8	4.202301	1.978902	-1.675731
6	-2.949654	-0.007850	-2.031015
8	-2.481584	-1.056069	-2.406107
44	-0.033267	0.028130	-0.313266
6	0.767916	2.628218	1.118546
6	0.881208	3.990947	1.342753
6	0.217792	4.872093	0.493087
6	-0.540214	4.351148	-0.551386
6	-0.609312	2.976732	-0.716675
1	1.280919	1.906505	1.751306
1	1.491678	4.349652	2.166783
1	0.297462	5.946748	0.638318
1	-1.067041	4.998448	-1.246939
1	-1.162253	2.525440	-1.537807
6	-0.793527	-2.945201	-0.086142
6	-0.919663	-4.269861	-0.471360
6	-0.294842	-4.694850	-1.640287

6	0.437294	-3.771088	-2.379268
6	0.519815	-2.462196	-1.931866
1	-1.283356	-2.572037	0.810918
1	-1.510059	-4.950778	0.135421
1	-0.383921	-5.726259	-1.972887
1	0.934904	-4.050613	-3.303668
1	1.050876	-1.701001	-2.497218
7	-0.082894	-2.049132	-0.798569
7	0.034809	2.120945	0.105624
8	-0.103658	0.402972	-2.046157
1	1.376070	1.045343	-2.399194
8	-3.435141	0.971153	-2.796615
1	-3.363023	0.692735	-3.731337

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3)Py_2(O)]^+$ (Broken-symmetry singlet)

E = -1785.46428878 a.u.

6	-2.285517	0.139015	1.652841
6	-3.459257	0.497052	2.296322
6	-4.224260	1.552066	1.794418
6	-3.789717	2.211183	0.662838
6	-2.586090	1.836408	0.041335
1	-3.775144	-0.039274	3.187054
1	-5.147714	1.842235	2.289918
1	-4.356268	3.029610	0.225532
6	-1.428801	-0.956106	2.094907
6	-1.699489	-1.861870	3.120244
6	-0.787765	-2.880049	3.378709
1	-2.614028	-1.783973	3.701623
6	0.601868	-2.068849	1.598854
6	0.368710	-2.998586	2.611074
1	-0.983950	-3.594310	4.174238
1	1.071374	-3.803792	2.805582
6	1.755860	-2.044192	0.696037
6	2.771911	-2.990422	0.768717
6	2.963694	-0.791363	-0.869946
6	3.892669	-2.860606	-0.040384
1	2.691112	-3.817303	1.468864
6	4.010638	-1.719600	-0.813716
1	4.686736	-3.602301	-0.014864
1	4.919999	-1.494673	-1.362021
7	-0.280446	-1.065781	1.384400
7	1.802280	-1.003132	-0.206115
7	-1.854065	0.817344	0.536287
6	-2.119125	2.562841	-1.206515
8	-1.281873	3.459994	-0.993807
8	-2.663790	2.158884	-2.252844
6	3.366591	0.526636	-1.525531

8	4.480484	0.905282	-1.229806
8	2.613209	1.177009	-2.383705
44	-0.052969	0.122470	-0.295634
6	-1.042816	-2.703219	-1.227647
6	-1.777705	-3.615214	-1.967876
6	-2.724773	-3.139614	-2.870923
6	-2.893043	-1.766118	-2.995256
6	-2.120106	-0.906512	-2.225030
1	-0.286496	-3.041745	-0.523146
1	-1.599938	-4.679362	-1.837837
1	-3.315645	-3.830313	-3.468474
1	-3.614665	-1.340718	-3.687344
1	-2.224344	0.179366	-2.306715
6	1.633732	1.534892	1.813531
6	2.439046	2.499812	2.390908
6	2.683232	3.679147	1.689189
6	2.101542	3.844220	0.440117
6	1.299636	2.837456	-0.081957
1	1.421383	0.596234	2.321768
1	2.870022	2.321954	3.372329
1	3.318327	4.453309	2.113651
1	2.256652	4.745268	-0.146069
1	0.806090	2.932179	-1.043047
7	1.071445	1.693783	0.595686
7	-1.205877	-1.372113	-1.345613
8	0.116992	0.876393	-1.887251
1	1.649597	0.917244	-2.387917

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3)Py_2(O)]^+$ (Triplet)

E = -1785.47447328 a.u.

6	2.325863	0.146497	1.574086
6	3.567495	-0.033894	2.161583
6	4.496091	-0.886600	1.558646
6	4.148086	-1.531076	0.390085
6	2.875325	-1.337257	-0.176413
1	3.810898	0.481270	3.086930
1	5.474715	-1.035068	2.009005
1	4.837594	-2.199284	-0.120032
6	1.297007	1.020816	2.134448
6	1.426423	1.856031	3.245314
6	0.345034	2.647014	3.617653
1	2.355920	1.897365	3.806233
6	-0.924989	1.770864	1.779967
6	-0.839533	2.619292	2.883382
1	0.426695	3.301100	4.482226
1	-1.673844	3.249244	3.177281
6	-2.085897	1.627491	0.887990

6	-3.226231	2.403513	1.065008
6	-3.124791	0.400274	-0.810290
6	-4.329254	2.208248	0.245267
1	-3.251304	3.156721	1.847379
6	-4.290343	1.163314	-0.658650
1	-5.218784	2.823725	0.351519
1	-5.159565	0.881108	-1.243698
7	0.126423	0.988150	1.458074
7	-1.997171	0.685341	-0.115945
7	1.990313	-0.507309	0.410059
6	2.497480	-2.057336	-1.458560
8	1.889874	-3.127654	-1.269659
8	2.871545	-1.473021	-2.494152
6	-3.349795	-0.858442	-1.646064
8	-4.448913	-1.355673	-1.521184
8	-2.453297	-1.358205	-2.466724
44	0.051703	-0.109235	-0.298301
6	0.434395	2.898979	-1.078794
6	0.947977	3.980860	-1.775358
6	1.929562	3.755897	-2.736901
6	2.354158	2.451937	-2.960082
6	1.796505	1.411471	-2.227929
1	-0.342654	3.038947	-0.330645
1	0.574622	4.979813	-1.566489
1	2.350225	4.584180	-3.302798
1	3.114002	2.219267	-3.701193
1	2.107352	0.372899	-2.384156
6	-1.127777	-1.945238	1.845542
6	-1.627044	-3.097815	2.425511
6	-1.667950	-4.267784	1.669609
6	-1.202001	-4.232570	0.362698
6	-0.710388	-3.042959	-0.158937
1	-1.081952	-1.009901	2.399400
1	-1.980211	-3.071294	3.452766
1	-2.057516	-5.189012	2.096770
1	-1.205875	-5.116797	-0.267994
1	-0.306999	-2.977703	-1.164006
7	-0.675282	-1.910453	0.573660
7	0.845826	1.634793	-1.292967
8	-0.003280	-0.844717	-1.908637
1	-1.538881	-0.968879	-2.403418

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ (Closed-shell singlet)

E = -1709.42252083 a.u.

6	-2.341470	-0.009317	1.579634

6	-3.673202	-0.011056	1.994639
6	-4.690603	-0.004467	1.045369
6	-4.352553	0.003579	-0.304045
6	-3.008630	0.004770	-0.648731
1	-3.911269	-0.017431	3.055249
1	-5.731587	-0.005699	1.358789
1	-5.089633	0.008888	-1.104563
6	-1.172588	-0.015315	2.430677
6	-1.195405	-0.025376	3.823444
6	-0.000360	-0.031001	4.530182
1	-2.147916	-0.028989	4.346230
6	1.172149	-0.015630	2.430835
6	1.194786	-0.025954	3.823602
1	-0.000442	-0.039149	5.616986
1	2.147248	-0.029945	4.346482
6	2.341203	-0.009264	1.580077
6	3.672825	-0.011180	1.995410
6	3.008958	0.006322	-0.648139
6	4.690464	-0.003691	1.046413
1	3.910595	-0.018272	3.056086
6	4.352785	0.005282	-0.303079
1	5.731367	-0.004960	1.360104
1	5.090098	0.011314	-1.103372
7	-0.000178	-0.010657	1.735796
7	2.029574	-0.000577	0.262910
7	-2.029487	-0.001334	0.262564
6	-2.491711	0.012341	-2.039420
8	-1.168418	0.010630	-2.052347
8	-3.183364	0.018876	-3.029150
6	2.492378	0.014307	-2.038970
8	3.184196	0.021665	-3.028531
8	1.168999	0.011750	-2.052031
44	0.000089	0.002039	-0.395910
6	-0.000698	-2.960767	0.510862
6	-0.000529	-4.338658	0.370293
6	0.000866	-4.887522	-0.910026
6	0.001903	-4.028461	-2.003204
6	0.001721	-2.656611	-1.792506
1	-0.002124	-2.498580	1.495449
1	-0.001558	-4.967379	1.256549
1	0.001050	-5.965852	-1.050383
1	0.002855	-4.405762	-3.022133
1	0.002514	-1.946555	-2.614581
6	-0.000640	2.954818	0.543532
6	-0.000957	4.334180	0.417801
6	-0.001096	4.896798	-0.856527
6	-0.000920	4.049593	-1.958938
6	-0.000624	2.675584	-1.763055
1	-0.000469	2.482026	1.523109
1	-0.001075	4.953288	1.310806

1	-0.001335	5.976583	-0.985205
1	-0.001026	4.437910	-2.973713
1	-0.000562	1.974342	-2.592690
7	-0.000484	2.130746	-0.525919
7	0.000536	-2.125135	-0.549560

[Ru^{IV}(tda-κ-N^3O)Py_2(OH)]$^+$ (Closed-shell singlet)

E = -1785.50019576 a.u.

6	2.540256	0.146258	1.025837
6	3.898599	0.375524	1.169487
6	4.434511	1.555936	0.649906
6	3.571613	2.490828	0.112605
6	2.208784	2.188706	-0.057734
1	4.525479	-0.338533	1.697875
1	5.499519	1.759860	0.730533
1	3.912575	3.481222	-0.177374
6	1.791623	-0.886293	1.717953
6	2.284314	-1.651915	2.775908
6	1.412722	-2.436495	3.517906
1	3.336152	-1.589670	3.040781
6	-0.371716	-1.681098	2.107806
6	0.060284	-2.428555	3.200525
1	1.779414	-3.027451	4.353254
1	-0.654262	-3.008119	3.778961
6	-1.727890	-1.635374	1.602831
6	-2.866552	-2.174566	2.201558
6	-2.948628	-1.045001	-0.284375
6	-4.084707	-2.100886	1.533881
1	-2.795926	-2.646911	3.178427
6	-4.123660	-1.547583	0.257053
1	-4.984478	-2.502976	1.993178
1	-5.024571	-1.514471	-0.351292
7	0.486746	-0.944671	1.360702
7	-1.793991	-1.039842	0.392399
7	1.730483	0.988768	0.319652
6	1.276116	3.353902	-0.436289
8	0.642922	3.345428	-1.518284
8	1.314708	4.180187	0.485940
6	-2.782892	-0.612847	-1.703361
8	-3.720843	-0.535526	-2.474133
8	-1.520461	-0.426850	-1.995814
44	-0.097235	-0.006170	-0.532777
6	-1.122470	2.172207	1.311342
6	-1.810950	3.304608	1.711159
6	-2.598406	3.976142	0.781105
6	-2.667536	3.487265	-0.518241
6	-1.947169	2.351730	-0.853336

1	-0.473146	1.624763	1.992277
1	-1.706237	3.662016	2.731462
1	-3.138915	4.876557	1.063116
1	-3.253741	3.986793	-1.283957
1	-1.936428	1.952935	-1.864811
6	0.434273	-2.905036	-1.316095
6	1.059547	-3.997251	-1.896791
6	2.293722	-3.814473	-2.513953
6	2.851665	-2.540741	-2.530296
6	2.163660	-1.493358	-1.933879
1	-0.540634	-2.992330	-0.840344
1	0.575239	-4.969570	-1.873164
1	2.806464	-4.650508	-2.984120
1	3.805695	-2.346799	-3.012774
1	2.529366	-0.469846	-1.957027
7	0.976408	-1.674290	-1.327950
7	-1.190830	1.697865	0.051745
8	0.607320	0.838774	-2.022831
1	0.591225	1.863806	-1.942767

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ (Triplet)

E = -1860.61291342 a.u.

6	2.012434	-1.878587	0.788180
6	2.753331	-3.038063	0.543994
6	4.017318	-2.913621	-0.027754
6	4.505009	-1.643310	-0.296314
6	3.671235	-0.544403	-0.069609
1	2.350819	-4.017795	0.796896
1	4.616782	-3.797133	-0.235896
1	5.506294	-1.474524	-0.686014
6	0.762311	-1.910185	1.571776
6	0.636409	-2.800036	2.643416
6	-0.458188	-2.719223	3.490793
1	1.433302	-3.514528	2.832212
6	-1.264252	-0.890177	2.161401
6	-1.407755	-1.733897	3.259727
1	-0.557704	-3.397010	4.334947
1	-2.267391	-1.627647	3.915947
6	-2.255723	0.131590	1.820478
6	-3.362862	0.531820	2.573669
6	-2.861662	1.627439	0.100417
6	-4.210476	1.514021	2.067785
1	-3.560392	0.088036	3.546296
6	-3.968380	2.068513	0.809378
1	-5.068537	1.837021	2.652050
1	-4.615038	2.820143	0.362913
7	-0.196800	-0.989582	1.307557

7	-2.033403	0.708228	0.623471
7	2.443767	-0.654844	0.442284
6	4.152982	0.863863	-0.350581
8	5.363799	1.088090	-0.150134
8	3.313936	1.721639	-0.741545
6	-2.496109	2.031962	-1.303338
8	-3.106829	2.896162	-1.896257
8	-1.498099	1.318112	-1.815379
44	-0.448615	0.197319	-0.511972
6	1.033641	2.098900	1.328594
6	1.681090	3.249135	1.744245
6	1.809718	4.311841	0.854920
6	1.284645	4.177853	-0.423913
6	0.649402	2.997113	-0.775342
1	0.936354	1.231902	1.976770
1	2.088470	3.299368	2.750259
1	2.321883	5.223831	1.152201
1	1.371993	4.970902	-1.160923
1	0.236471	2.840325	-1.768751
6	-2.740076	-1.526596	-1.588403
6	-3.380061	-2.620916	-2.149935
6	-2.647759	-3.778410	-2.393113
6	-1.295143	-3.793995	-2.066966
6	-0.723664	-2.660507	-1.509681
1	-3.269105	-0.594509	-1.405105
1	-4.434764	-2.553038	-2.401646
1	-3.121081	-4.650111	-2.838952
1	-0.678056	-4.668871	-2.252482
1	0.337082	-2.609180	-1.271567
7	-1.433550	-1.542086	-1.265149
7	0.516790	1.969349	0.090167
8	0.827380	-0.340846	-1.909752
8	1.780611	0.509597	-2.407415
1	2.203186	1.018549	-1.619781

[Ru^{IV}(tda-κ-N^2O)Py_2(O)] (Triplet)

E = -1785.05335926 a.u.

6	1.968518	-1.905316	0.797611
6	2.444552	-3.125036	0.315206
6	3.611804	-3.110023	-0.445988
6	4.246520	-1.897541	-0.666032
6	3.705778	-0.725543	-0.118851
1	1.903893	-4.051738	0.511600
1	4.012015	-4.034871	-0.859744
1	5.160093	-1.806463	-1.248456
6	0.742771	-1.825677	1.618406
6	0.571617	-2.657730	2.726636

6	-0.499743	-2.455460	3.587993
1	1.321299	-3.420173	2.925393
6	-1.210249	-0.646869	2.171371
6	-1.381329	-1.419567	3.320059
1	-0.631899	-3.080616	4.468233
1	-2.220141	-1.219022	3.982086
6	-2.143606	0.410616	1.788759
6	-3.205114	0.924027	2.540032
6	-2.698677	1.838369	-0.010626
6	-4.004595	1.922039	1.989998
1	-3.402447	0.557030	3.544948
6	-3.759910	2.384652	0.691518
1	-4.826556	2.333650	2.571471
1	-4.370111	3.146190	0.211987
7	-0.163635	-0.865682	1.308080
7	-1.916056	0.898573	0.549643
7	2.579412	-0.729802	0.601791
6	4.424352	0.599836	-0.355215
8	3.898826	1.636213	0.124613
8	5.489018	0.536092	-1.010280
6	-2.346093	2.146779	-1.448375
8	-2.988432	2.983947	-2.065118
8	-1.368462	1.419743	-1.936710
44	-0.370391	0.170065	-0.613920
6	1.160586	2.128932	1.140490
6	1.842073	3.292253	1.455411
6	2.207986	4.156216	0.431608
6	1.886833	3.815358	-0.876176
6	1.184143	2.646541	-1.116870
1	0.886802	1.401351	1.899909
1	2.110255	3.490579	2.489542
1	2.760378	5.068171	0.647190
1	2.183307	4.439051	-1.714856
1	0.892337	2.338265	-2.116661
6	-2.920686	-1.375293	-1.435099
6	-3.694855	-2.437213	-1.880381
6	-3.079053	-3.657127	-2.139284
6	-1.704873	-3.763345	-1.947575
6	-0.996542	-2.657308	-1.501847
1	-3.358667	-0.398978	-1.239399
1	-4.762104	-2.296459	-2.030127
1	-3.658607	-4.507443	-2.492741
1	-1.175316	-4.691013	-2.149452
1	0.084243	-2.666255	-1.367262
7	-1.595058	-1.478854	-1.240315
7	0.798363	1.829447	-0.118279
8	0.888298	-0.488408	-1.678044

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]^+$ (Closed-shell singlet)

E = -1785.45249459 a.u.

6	-2.124050	0.273238	1.795743
6	-3.213986	0.714516	2.528656
6	-3.962612	1.799766	2.067701
6	-3.604590	2.395529	0.876280
6	-2.484158	1.932270	0.166182
1	-3.481959	0.215120	3.455111
1	-4.815915	2.159568	2.636476
1	-4.158095	3.236907	0.466754
6	-1.306358	-0.873072	2.173979
6	-1.538394	-1.743221	3.237310
6	-0.676283	-2.817088	3.433204
1	-2.387212	-1.595174	3.898318
6	0.602803	-2.113791	1.530656
6	0.399731	-3.014122	2.575223
1	-0.847452	-3.505575	4.256255
1	1.074050	-3.853158	2.720786
6	1.687528	-2.136295	0.559172
6	2.698903	-3.081548	0.545905
6	2.825615	-0.806029	-1.010342
6	3.783924	-2.910494	-0.314895
1	2.658718	-3.929211	1.224370
6	3.877156	-1.735887	-1.033831
1	4.577503	-3.651532	-0.355782
1	4.767614	-1.478912	-1.600013
7	-0.240171	-1.067439	1.360034
7	1.698030	-1.074868	-0.322765
7	-1.757206	0.899199	0.629400
6	-2.134599	2.614797	-1.145180
8	-1.262438	3.498750	-1.100373
8	-2.795983	2.208369	-2.122122
6	3.137648	0.586662	-1.565128
8	4.115427	1.060183	-0.977077
8	2.433468	1.118050	-2.460844
44	-0.059347	0.089489	-0.320211
6	-1.195226	-2.693230	-1.163506
6	-2.000873	-3.588484	-1.847116
6	-2.990330	-3.094379	-2.693329
6	-3.127125	-1.718033	-2.823494
6	-2.281155	-0.878316	-2.113168
1	-0.403352	-3.049896	-0.510301
1	-1.842784	-4.655583	-1.719517
1	-3.635128	-3.772501	-3.246931
1	-3.874697	-1.277469	-3.477208
1	-2.351500	0.202555	-2.216256
6	1.983620	1.289225	1.586067
6	2.895468	2.185522	2.111209
6	3.037541	3.432700	1.508168

6	2.245643	3.734931	0.408784
6	1.343858	2.793643	-0.065144
1	1.855981	0.299588	2.019842
1	3.494198	1.896979	2.970161
1	3.758275	4.152285	1.888153
1	2.318048	4.691170	-0.100968
1	0.696651	3.008893	-0.908223
7	1.210306	1.579850	0.514893
7	-1.329193	-1.357484	-1.283531
8	0.003940	0.815150	-2.003653
1	0.902456	1.216753	-2.260040

[Ru^{IV}(tda-κ-N^3)Py_2(O)] (Broken-symmetry singlet)

E = -1785.04073891 a.u.

6	-2.193362	-0.812257	1.564467
6	-3.459769	-1.114427	2.045250
6	-4.572148	-0.861796	1.242699
6	-4.382312	-0.299351	-0.003569
6	-3.089248	0.010484	-0.457138
1	-3.575320	-1.538959	3.039034
1	-5.571393	-1.100033	1.602011
1	-5.218504	-0.077728	-0.662374
6	-0.973658	-1.009736	2.338252
6	-0.888785	-1.534463	3.626106
6	0.358071	-1.630140	4.238534
1	-1.784006	-1.864051	4.146849
6	1.369387	-0.697469	2.269897
6	1.498287	-1.211252	3.559251
1	0.441182	-2.036030	5.243771
1	2.477139	-1.289566	4.025307
6	2.450908	-0.237183	1.408004
6	3.781762	-0.208652	1.800951
6	3.001747	0.564915	-0.741008
6	4.753295	0.206269	0.889289
1	4.055646	-0.511604	2.808274
6	4.360687	0.568803	-0.383261
1	5.801874	0.229517	1.179645
1	5.080711	0.864442	-1.142384
7	0.145765	-0.598194	1.690116
7	2.069361	0.162784	0.149298
7	-2.017510	-0.268970	0.315802
6	-2.911702	0.680056	-1.812076
8	-2.855051	1.920757	-1.732184
8	-2.895845	-0.119235	-2.771028
6	2.601827	0.990345	-2.144461
8	2.097418	2.129617	-2.209760
8	2.891544	0.125925	-2.991416

44	-0.011615	0.071576	-0.287987
6	1.035559	-2.822916	-0.539277
6	1.167075	-4.091247	-1.081247
6	0.337051	-4.457959	-2.136881
6	-0.593567	-3.538420	-2.604349
6	-0.672616	-2.282010	-2.017294
1	1.675009	-2.486629	0.274928
1	1.918795	-4.769316	-0.685622
1	0.421126	-5.444170	-2.589240
1	-1.260582	-3.773817	-3.429329
1	-1.385198	-1.524850	-2.361001
6	-0.268225	2.568889	1.465582
6	-0.417159	3.906356	1.788868
6	-0.511825	4.836745	0.755900
6	-0.453921	4.385494	-0.554035
6	-0.304206	3.027713	-0.808845
1	-0.193596	1.805220	2.237621
1	-0.459403	4.205570	2.833089
1	-0.631074	5.896184	0.975165
1	-0.527830	5.068550	-1.395287
1	-0.249645	2.622461	-1.812811
7	-0.209485	2.133242	0.192699
7	0.134792	-1.934389	-0.992915
8	-0.175971	0.504613	-1.965473

[Ru^{IV}(tda-κ-N^3)Py_2(O)] (Triplet)

E = -1785.04745186 a.u.

6	-2.245406	-0.576489	1.573037
6	-3.518262	-0.726732	2.105059
6	-4.623715	-0.309252	1.361418
6	-4.416162	0.250099	0.117621
6	-3.111607	0.409119	-0.382226
1	-3.648234	-1.163269	3.091918
1	-5.628563	-0.426578	1.762560
1	-5.244296	0.581809	-0.504373
6	-1.037550	-0.984489	2.295834
6	-0.988731	-1.601528	3.546302
6	0.253114	-1.916567	4.091966
1	-1.901121	-1.838527	4.086779
6	1.329792	-1.014500	2.147059
6	1.424245	-1.629761	3.396189
1	0.307946	-2.398349	5.065594
1	2.391742	-1.888492	3.818149
6	2.441891	-0.653515	1.263974
6	3.769604	-0.850113	1.616316
6	3.061178	0.260986	-0.816393
6	4.774796	-0.504451	0.709985

1	4.018786	-1.269159	2.587955
6	4.414617	0.031325	-0.509055
1	5.820575	-0.662371	0.966623
1	5.154543	0.293541	-1.261508
7	0.113410	-0.701221	1.645425
7	2.094807	-0.102705	0.052093
7	-2.050012	-0.013895	0.334528
6	-2.896963	1.060000	-1.737574
8	-2.609014	2.268889	-1.669859
8	-3.084196	0.278047	-2.693819
6	2.696544	0.928626	-2.129345
8	2.319202	2.111519	-1.997326
8	2.884421	0.192110	-3.114037
44	-0.006600	0.094934	-0.283597
6	0.611132	-2.922223	-0.671546
6	0.528817	-4.180486	-1.246816
6	-0.392176	-4.390820	-2.268762
6	-1.194641	-3.329977	-2.670856
6	-1.061056	-2.094169	-2.051476
1	1.332493	-2.709160	0.115319
1	1.188562	-4.972811	-0.902595
1	-0.475749	-5.365061	-2.746435
1	-1.924545	-3.438486	-3.468582
1	-1.671017	-1.233330	-2.345446
6	0.252498	2.488078	1.604010
6	0.321634	3.812456	1.999948
6	0.223416	4.806289	1.028546
6	0.061660	4.428455	-0.295903
6	0.003443	3.080205	-0.625370
1	0.322996	1.678825	2.328477
1	0.450089	4.052533	3.052371
1	0.273209	5.857603	1.305692
1	-0.020323	5.162582	-1.092067
1	-0.119330	2.735649	-1.645259
7	0.095917	2.122125	0.316896
7	-0.167054	-1.896778	-1.058930
8	-0.140352	0.618170	-1.959789

$[Ru^{V}(Htda\text{-}\kappa\text{-}N^{3}O^{1})Py_{2}(O)]^{2+}$ (Doublet)

E = -1785.17697740 a.u.

6	2.403700	-0.571524	1.363913
6	3.748804	-0.806803	1.660086
6	4.710584	0.026689	1.109011
6	4.297222	1.092229	0.314242
6	2.937606	1.268971	0.056763
1	4.040646	-1.633823	2.301208
1	5.766174	-0.135221	1.313579

1	5.015462	1.812798	-0.072382
6	1.293598	-1.317188	1.952072
6	1.443516	-2.172651	3.044518
6	0.318869	-2.727404	3.639394
1	2.431432	-2.374947	3.447599
6	-1.024040	-1.571177	2.021796
6	-0.932989	-2.409842	3.131031
1	0.416707	-3.388390	4.496890
1	-1.834208	-2.819458	3.579164
6	-2.271565	-1.215433	1.366519
6	-3.558741	-1.496831	1.823052
6	-3.129516	-0.264247	-0.572589
6	-4.655150	-1.121138	1.049063
1	-3.706038	-2.002073	2.774372
6	-4.440616	-0.506073	-0.180198
1	-5.664339	-1.326484	1.398100
1	-5.247044	-0.220196	-0.851999
7	0.075586	-1.037026	1.434225
7	-2.080868	-0.584616	0.189683
7	2.011741	0.420951	0.543081
6	2.482958	2.562559	-0.581241
8	3.102057	2.950844	-1.697097
8	1.688866	3.263985	-0.006254
6	-2.733298	0.275211	-1.903736
8	-3.534321	0.620030	-2.744211
8	-1.426508	0.262372	-2.068593
44	-0.071203	0.135587	-0.519366
6	-0.806415	2.246688	1.552462
6	-1.230222	3.471978	2.036606
6	-1.642676	4.448303	1.132400
6	-1.615880	4.160962	-0.227889
6	-1.180662	2.913277	-0.647677
1	-0.448611	1.460959	2.214818
1	-1.222375	3.657500	3.107016
1	-1.970988	5.423064	1.485259
1	-1.915606	4.894851	-0.970544
1	-1.119423	2.644889	-1.699865
6	-0.372895	-2.678290	-1.688951
6	-0.038622	-3.847563	-2.354758
6	1.280899	-4.046273	-2.749258
6	2.221624	-3.060818	-2.462130
6	1.815473	-1.918569	-1.790613
1	-1.396787	-2.468784	-1.390632
1	-0.811626	-4.579321	-2.572233
1	1.569347	-4.948065	-3.284024
1	3.259224	-3.163349	-2.767693
1	2.507566	-1.107502	-1.573880
7	0.539463	-1.730294	-1.399967
7	-0.790370	1.970671	0.234346
8	0.873223	0.951099	-1.678249

1	3.618621	2.233021	-2.100326

[Ru^{V}(tda-κ-N^3O^2)Py_2]$^{3+}$ (Doublet)

E = -1708.92207119 a.u.

6	-2.346177	-0.003185	1.592454
6	-3.678810	-0.003803	2.009510
6	-4.700773	-0.001576	1.063812
6	-4.371606	0.001208	-0.291411
6	-3.028187	0.001622	-0.638069
1	-3.916772	-0.005987	3.070626
1	-5.741284	-0.002019	1.381649
1	-5.118108	0.003025	-1.084477
6	-1.174014	-0.005105	2.439255
6	-1.196261	-0.008244	3.834611
6	0.000037	-0.009809	4.541529
1	-2.147608	-0.009465	4.360702
6	1.174056	-0.004939	2.439238
6	1.196324	-0.008071	3.834593
1	0.000045	-0.012311	5.629138
1	2.147678	-0.009155	4.360671
6	2.346206	-0.002856	1.592420
6	3.678845	-0.003293	2.009456
6	3.028182	0.002028	-0.638113
6	4.700794	-0.000929	1.063744
1	3.916823	-0.005443	3.070569
6	4.371607	0.001802	-0.291475
1	5.741310	-0.001229	1.381566
1	5.118097	0.003710	-1.084551
7	0.000015	-0.003557	1.749411
7	2.046792	-0.000195	0.269734
7	-2.046783	-0.000481	0.269764
6	-2.510072	0.004249	-2.026721
8	-1.171007	0.003346	-2.033137
8	-3.166813	0.006636	-3.032873
6	2.510047	0.004549	-2.026757
8	3.166769	0.007108	-3.032920
8	1.170979	0.003582	-2.033151
44	0.000000	0.000603	-0.423500
6	0.000246	-2.943965	0.517350
6	0.000348	-4.320907	0.389361
6	0.000380	-4.882559	-0.888277
6	0.000308	-4.032118	-1.996694
6	0.000205	-2.659593	-1.802482
1	0.000217	-2.471957	1.496219
1	0.000400	-4.942680	1.280698
1	0.000459	-5.962750	-1.018979
1	0.000329	-4.423101	-3.011047

1	0.000139	-1.963499	-2.636400
6	-0.000206	2.941803	0.527866
6	-0.000318	4.319202	0.404756
6	-0.000415	4.885378	-0.870881
6	-0.000396	4.038876	-1.982311
6	-0.000279	2.665680	-1.792967
1	-0.000128	2.466314	1.505058
1	-0.000329	4.937798	1.298303
1	-0.000504	5.966027	-0.997736
1	-0.000470	4.433464	-2.995265
1	-0.000255	1.972535	-2.629344
7	-0.000184	2.117997	-0.552776
7	0.000175	-2.116313	-0.560353

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(O)]^{+}$ (Doublet)

E = -1784.84912038 a.u.

6	2.031532	-1.853698	0.846446
6	2.548197	-3.073597	0.399164
6	3.706686	-3.059400	-0.372238
6	4.305091	-1.837334	-0.650328
6	3.722385	-0.678779	-0.135179
1	2.040951	-4.009325	0.633167
1	4.130590	-3.986813	-0.750868
1	5.208707	-1.757224	-1.251310
6	0.802677	-1.787524	1.666108
6	0.659371	-2.605058	2.790125
6	-0.423935	-2.431241	3.638438
1	1.434267	-3.335917	3.009217
6	-1.190230	-0.674558	2.188250
6	-1.344551	-1.434429	3.344672
1	-0.539118	-3.046548	4.527306
1	-2.195394	-1.258209	3.997360
6	-2.158863	0.356741	1.792420
6	-3.217807	0.860793	2.551107
6	-2.748742	1.751984	-0.009762
6	-4.037881	1.841731	1.994617
1	-3.400519	0.507357	3.562818
6	-3.813020	2.297706	0.694796
1	-4.860224	2.246848	2.579753
1	-4.435869	3.051131	0.218786
7	-0.133252	-0.864497	1.338372
7	-1.958383	0.827890	0.550509
7	2.609090	-0.672901	0.600460
6	4.332988	0.652822	-0.420140
8	3.851192	1.712628	0.065910
8	5.343301	0.760135	-1.156702
6	-2.388989	2.060217	-1.443310

8	-3.009433	2.889082	-2.078407
8	-1.400106	1.321785	-1.918146
44	-0.355163	0.143464	-0.626575
6	1.079238	2.187735	1.141659
6	1.716856	3.374507	1.462406
6	2.016237	4.274757	0.445527
6	1.671539	3.948963	-0.860942
6	1.020235	2.750717	-1.109268
1	0.856909	1.436317	1.894710
1	1.991820	3.572285	2.494636
1	2.525902	5.209528	0.666947
1	1.902522	4.610010	-1.691307
1	0.713634	2.455000	-2.108859
6	-2.833995	-1.448963	-1.537353
6	-3.574544	-2.524073	-2.005891
6	-2.940737	-3.747338	-2.195849
6	-1.581820	-3.846467	-1.911851
6	-0.907270	-2.728869	-1.445711
1	-3.285676	-0.469806	-1.400429
1	-4.629351	-2.390306	-2.229271
1	-3.493662	-4.606132	-2.569358
1	-1.039215	-4.776090	-2.060974
1	0.162103	-2.740171	-1.241872
7	-1.522899	-1.545768	-1.252692
7	0.714767	1.888972	-0.118884
8	0.948751	-0.461665	-1.623025

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(O)]^{+}$ (Quartet)

E = -1784.84690574 a.u.

6	2.035847	-1.864237	0.845345
6	2.528491	-3.084484	0.369481
6	3.674633	-3.080660	-0.419296
6	4.291777	-1.865469	-0.689816
6	3.733595	-0.711035	-0.144163
1	2.007782	-4.014529	0.595699
1	4.075164	-4.009748	-0.818258
1	5.187101	-1.794211	-1.304569
6	0.813804	-1.792412	1.677305
6	0.677789	-2.604973	2.804368
6	-0.403796	-2.425393	3.655256
1	1.451259	-3.337349	3.024109
6	-1.174869	-0.675820	2.196397
6	-1.325019	-1.430854	3.357594
1	-0.517347	-3.035952	4.547573
1	-2.174158	-1.252302	4.012002
6	-2.147177	0.354141	1.800743
6	-3.208291	0.854136	2.559383

6	-2.742846	1.750500	-0.003462
6	-4.031882	1.832273	2.002634
1	-3.391151	0.499773	3.570826
6	-3.809329	2.290243	0.702834
1	-4.855939	2.233637	2.587991
1	-4.436058	3.041000	0.227628
7	-0.119237	-0.870171	1.344686
7	-1.949954	0.829077	0.559125
7	2.634124	-0.693453	0.610195
6	4.343760	0.613977	-0.405929
8	3.881482	1.683049	0.089156
8	5.353192	0.782786	-1.132077
6	-2.387424	2.062117	-1.440619
8	-3.021791	2.891405	-2.064116
8	-1.394755	1.339341	-1.926076
44	-0.366747	0.148096	-0.618657
6	1.082920	2.205444	1.133440
6	1.729102	3.391574	1.442042
6	2.036202	4.277921	0.414831
6	1.691303	3.938113	-0.888142
6	1.032838	2.740365	-1.123439
1	0.848347	1.466785	1.895896
1	1.999425	3.602061	2.473091
1	2.549077	5.213329	0.626243
1	1.924369	4.589739	-1.725472
1	0.723248	2.434623	-2.119153
6	-2.859643	-1.436140	-1.495043
6	-3.608258	-2.503823	-1.967785
6	-2.974792	-3.718947	-2.204549
6	-1.607654	-3.816182	-1.962407
6	-0.925314	-2.705999	-1.490053
1	-3.313553	-0.463825	-1.321202
1	-4.669645	-2.370245	-2.157727
1	-3.534048	-4.571896	-2.582023
1	-1.064785	-4.738854	-2.149444
1	0.149822	-2.712482	-1.320551
7	-1.540161	-1.530815	-1.250002
7	0.720093	1.891672	-0.124146
8	0.953034	-0.477354	-1.614694

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(O)]^{+}$ Water Nucleophilic Attack TS (Doublet)

E = -1861.24394914 a.u.

6	1.698423	-2.108745	1.017250
6	2.154520	-3.340032	0.547766
6	3.306495	-3.344601	-0.238448
6	3.926160	-2.138700	-0.533737
6	3.427892	-0.961460	0.040031

1	1.607118	-4.260099	0.750089
1	3.688851	-4.278066	-0.646136
1	4.783305	-2.093544	-1.202061
6	0.423050	-1.960968	1.742728
6	0.092520	-2.805514	2.807729
6	-1.039522	-2.557513	3.566929
1	0.768832	-3.620757	3.053816
6	-1.488383	-0.664248	2.159490
6	-1.823345	-1.452279	3.256278
1	-1.295005	-3.195572	4.409367
1	-2.699679	-1.209855	3.851462
6	-2.277232	0.506872	1.757166
6	-3.334688	1.097662	2.453863
6	-2.487803	2.106383	0.038746
6	-3.953215	2.224806	1.916170
1	-3.667244	0.695320	3.407350
6	-3.534804	2.742136	0.688747
1	-4.770592	2.696521	2.456453
1	-3.998604	3.609707	0.225896
7	-0.393234	-0.935616	1.386268
7	-1.886259	1.039454	0.586921
7	2.348111	-0.953370	0.825840
6	4.017109	0.400441	-0.259676
8	4.486050	1.060060	0.662715
8	3.936501	0.760126	-1.499089
6	-1.961252	2.463067	-1.327781
8	-2.391332	3.412523	-1.946595
8	-1.042596	1.617410	-1.782317
44	-0.333329	0.204750	-0.534030
6	1.324895	1.811456	1.442251
6	2.228527	2.762801	1.873111
6	2.819812	3.606471	0.937060
6	2.449730	3.495348	-0.397199
6	1.516491	2.538440	-0.758493
1	0.884812	1.090760	2.123492
1	2.500312	2.803404	2.923637
1	3.568495	4.332244	1.244123
1	2.893650	4.120146	-1.166136
1	1.182921	2.420027	-1.785206
6	-2.996694	-0.849661	-1.738160
6	-3.901791	-1.749687	-2.280808
6	-3.540676	-3.089041	-2.382352
6	-2.279970	-3.476485	-1.938529
6	-1.428030	-2.519451	-1.408877
1	-3.233073	0.208642	-1.664760
1	-4.867603	-1.393557	-2.628289
1	-4.226442	-3.817102	-2.809472
1	-1.946733	-4.508188	-2.010521
1	-0.419331	-2.764779	-1.081201
7	-1.780426	-1.223501	-1.302677

7	0.969882	1.698527	0.143879
8	0.826961	-0.786959	-1.344647
8	2.214389	-0.337003	-2.820933
1	3.070526	0.164466	-2.173559
1	1.766366	0.378580	-3.303245

[Ru^{V}(tda-κ-N^{3}O)Py_{2}(O)]$^{+}$ (Doublet)

E = -1784.85521341 a.u.

6	2.485317	-0.500776	1.111690
6	3.852700	-0.587172	1.326243
6	4.673967	0.423588	0.825003
6	4.085868	1.513823	0.211696
6	2.700753	1.530048	-0.021664
1	4.272539	-1.414639	1.892482
1	5.750878	0.379096	0.968798
1	4.666637	2.382317	-0.087537
6	1.489082	-1.345397	1.754178
6	1.763405	-2.252166	2.780130
6	0.711368	-2.850747	3.459320
1	2.791476	-2.454147	3.067444
6	-0.806911	-1.641645	2.053746
6	-0.593508	-2.522736	3.111378
1	0.906252	-3.550952	4.267674
1	-1.438203	-2.957207	3.639613
6	-2.107475	-1.262949	1.529618
6	-3.347181	-1.553337	2.098753
6	-3.133509	-0.308170	-0.322364
6	-4.507350	-1.168979	1.432762
1	-3.402208	-2.072315	3.052773
6	-4.401463	-0.552894	0.189831
1	-5.481400	-1.375828	1.869680
1	-5.262225	-0.273754	-0.413365
7	0.219692	-1.081164	1.372862
7	-2.017396	-0.611675	0.349732
7	1.935404	0.493724	0.363789
6	2.091304	2.844804	-0.495488
8	1.528757	2.936171	-1.616453
8	2.266623	3.733833	0.350971
6	-2.868599	0.179678	-1.709446
8	-3.773309	0.507469	-2.456123
8	-1.599170	0.124522	-2.009326
44	-0.074073	0.087125	-0.560316
6	-0.668227	2.304282	1.429289
6	-1.050504	3.555819	1.878085
6	-1.485757	4.496980	0.948196
6	-1.528758	4.147664	-0.395978
6	-1.133640	2.874623	-0.779682

1	-0.295249	1.537308	2.106263
1	-0.985479	3.790176	2.936726
1	-1.777364	5.494227	1.269303
1	-1.848056	4.853554	-1.156984
1	-1.115881	2.554534	-1.817778
6	-0.247468	-2.859850	-1.401465
6	0.101872	-4.053613	-2.013667
6	1.330440	-4.142292	-2.661615
6	2.162314	-3.027563	-2.675536
6	1.742916	-1.865057	-2.044870
1	-1.205411	-2.733773	-0.900868
1	-0.589070	-4.891825	-1.990779
1	1.629270	-5.062919	-3.157567
1	3.123833	-3.044504	-3.181237
1	2.335715	-0.952807	-2.058222
7	0.559445	-1.784355	-1.409913
7	-0.714254	1.968329	0.125176
8	0.756751	0.799273	-1.890679

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3})Py_{2}(O)]^{+}$ (Doublet)

E = -1784.82767502 a.u.

6	-2.307301	-0.400755	1.577477
6	-3.597551	-0.665680	2.009067
6	-4.631522	-0.740001	1.072514
6	-4.353406	-0.510578	-0.261391
6	-3.037234	-0.214733	-0.647379
1	-3.797338	-0.817470	3.066443
1	-5.644826	-0.967138	1.395611
1	-5.125855	-0.546744	-1.025108
6	-1.157344	-0.240624	2.469431
6	-1.181490	-0.258192	3.863962
6	0.001109	-0.010116	4.555445
1	-2.104507	-0.450835	4.403923
6	1.158486	0.230606	2.470014
6	1.183362	0.241368	3.864591
1	0.001378	-0.012808	5.642692
1	2.106689	0.431295	4.404986
6	2.307965	0.395084	1.578195
6	3.598214	0.659485	2.010153
6	3.036827	0.218427	-0.647794
6	4.631544	0.738528	1.073308
1	3.798402	0.807373	3.068008
6	4.352896	0.514072	-0.261354
1	5.644811	0.965439	1.396682
1	5.124890	0.554006	-1.025343
7	0.000412	-0.003426	1.817534
7	2.047597	0.205097	0.244419

7	-2.047497	-0.205789	0.244258
6	-2.756323	0.172700	-2.117175
8	-2.628710	1.399589	-2.232264
8	-2.750194	-0.818296	-2.867448
6	2.755560	-0.164229	-2.118766
8	2.747946	0.828866	-2.866112
8	2.629327	-1.390997	-2.237375
44	0.000016	0.000436	-0.305734
6	0.981488	-2.818418	0.426163
6	1.204106	-4.174902	0.261532
6	0.571570	-4.836322	-0.787185
6	-0.270280	-4.113521	-1.624193
6	-0.450850	-2.756492	-1.401405
1	1.473366	-2.255689	1.217495
1	1.876398	-4.694887	0.938309
1	0.739015	-5.898324	-0.951308
1	-0.781696	-4.582636	-2.459902
1	-1.087522	-2.147932	-2.044799
6	-0.979371	2.817155	0.436913
6	-1.202115	4.174201	0.277145
6	-0.572070	4.838800	-0.771066
6	0.267612	4.118503	-1.612388
6	0.448484	2.760741	-1.394333
1	-1.469292	2.252056	1.227784
1	-1.872616	4.692164	0.957240
1	-0.739724	5.901342	-0.931439
1	0.777137	4.590179	-2.447810
1	1.083734	2.154227	-2.041043
7	-0.169805	2.120134	-0.380817
7	0.169709	-2.118997	-0.387312
8	-0.000902	0.003017	-2.036247

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3})Py_{2}(O)]^{+}$ (Quartet)

E = -1784.82414190 a.u.

6	-2.317887	-0.380687	1.540590
6	-3.606510	-0.629487	1.991552
6	-4.653176	-0.714395	1.073374
6	-4.389636	-0.515801	-0.270243
6	-3.077552	-0.242395	-0.669545
1	-3.794957	-0.760733	3.053724
1	-5.664090	-0.926600	1.413336
1	-5.171664	-0.562824	-1.023242
6	-1.164404	-0.224172	2.437934
6	-1.187299	-0.237611	3.832809
6	0.000521	-0.004093	4.522196
1	-2.110278	-0.417267	4.377347
6	1.164976	0.220095	2.438110

6	1.188186	0.230782	3.833004
1	0.000646	-0.005180	5.609422
1	2.111301	0.409300	4.377684
6	2.318277	0.378290	1.540822
6	3.606927	0.626586	1.991983
6	3.077597	0.243793	-0.669655
6	4.653430	0.713186	1.073778
1	3.795510	0.756161	3.054336
6	4.389705	0.516739	-0.270118
1	5.664359	0.925032	1.413919
1	5.171605	0.565121	-1.023163
7	0.000212	-0.001390	1.793321
7	2.062781	0.211296	0.199429
7	-2.062594	-0.211520	0.199434
6	-2.776990	0.086436	-2.148641
8	-2.636302	1.306617	-2.307667
8	-2.770621	-0.942326	-2.846562
6	2.776900	-0.082593	-2.149281
8	2.770231	0.947289	-2.845516
8	2.636477	-1.302558	-2.310252
44	0.000039	0.000215	-0.289848
6	0.939923	-2.817481	0.505730
6	1.165882	-4.177257	0.372027
6	0.607082	-4.847042	-0.712681
6	-0.163012	-4.126163	-1.617586
6	-0.348883	-2.765499	-1.422274
1	1.373586	-2.251812	1.328665
1	1.781146	-4.694060	1.103485
1	0.775755	-5.912469	-0.851470
1	-0.615246	-4.600716	-2.483826
1	-0.929366	-2.158393	-2.115398
6	-0.939530	2.816648	0.510163
6	-1.165908	4.176538	0.378399
6	-0.608079	4.847869	-0.705856
6	0.161517	4.128355	-1.612265
6	0.347847	2.767480	-1.418876
1	-1.372436	2.249804	1.332690
1	-1.780732	4.692244	1.111002
1	-0.777120	5.913432	-0.843143
1	0.612996	4.604143	-2.478222
1	0.927942	2.161414	-2.113230
7	-0.195986	2.118987	-0.368407
7	0.195866	-2.118508	-0.371351
8	-0.000041	0.001375	-2.053789

Cartesian Coordinates and Electronic Energies of Optimized Structures at M11-L Level

$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^+$ (Closed-shell singlet)

E = -1710.14531118 a.u.

6	-2.108798	0.333492	1.616958
6	-3.371392	0.436570	2.185262
6	-4.481001	0.587197	1.381611
6	-4.291633	0.644890	0.016564
6	-3.002176	0.574998	-0.482491
1	-3.486498	0.379933	3.270478
1	-5.481473	0.654082	1.816882
1	-5.117742	0.747904	-0.691359
6	-0.909990	0.121266	2.431717
6	-0.822431	0.073341	3.815935
6	0.416039	-0.124781	4.401171
1	-1.707573	0.194610	4.445123
6	1.414166	-0.240749	2.234480
6	1.543213	-0.290452	3.610400
1	0.504497	-0.158846	5.489868
1	2.520501	-0.462172	4.069730
6	2.459441	-0.464904	1.230971
6	3.800731	-0.759013	1.424856
6	2.727151	-0.640195	-1.100279
6	4.601536	-0.992904	0.316527
1	4.224868	-0.808138	2.431770
6	4.068776	-0.940019	-0.964314
1	5.660887	-1.224002	0.460338
1	4.667727	-1.123193	-1.860526
7	0.192202	-0.018291	1.684396
7	1.987586	-0.411727	-0.027177
7	-1.914344	0.407111	0.274830
6	-2.864041	0.676959	-1.964209
8	-3.762139	0.433907	-2.708945
6	1.933043	-0.520664	-2.392622
8	2.495329	-0.709266	-3.435932
8	0.697609	-0.200350	-2.219224
44	0.125352	0.014198	-0.231495
6	-0.119295	-2.889704	0.569650
6	-0.487630	-4.212911	0.445805
6	-1.153527	-4.617051	-0.696355
6	-1.413503	-3.672906	-1.672535
6	-1.005655	-2.370865	-1.471755
1	0.412257	-2.538951	1.460951
1	-0.245607	-4.916337	1.246017
1	-1.459851	-5.658776	-0.827640
1	-1.924368	-3.936389	-2.601509
1	-1.143077	-1.597907	-2.234715
6	0.540007	2.843473	0.740016
6	0.809842	4.194483	0.686697
6	1.131425	4.765310	-0.530346
6	1.160002	3.946369	-1.642546
6	0.871758	2.604142	-1.503219
1	0.282138	2.371783	1.693091

1	0.766344	4.787008	1.603722
1	1.353909	5.833286	-0.609787
1	1.405039	4.337197	-2.633056
1	0.869365	1.924608	-2.359312
7	0.566193	2.044931	-0.328988
7	-0.373968	-1.974209	-0.364383
8	-1.665771	1.075896	-2.322670
1	-1.617082	1.041148	-3.288550

$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3O)Py_2]^+ \bullet$ □□□□) (Closed-shell singlet)

E = -1786.56189423 a.u.

6	-1.947564	1.490938	-1.276510
6	-3.164724	1.979318	-1.728247
6	-4.307524	1.220476	-1.577177
6	-4.197434	-0.020698	-0.984933
6	-2.944216	-0.470311	-0.605983
1	-3.222286	2.971535	-2.182798
1	-5.276083	1.601416	-1.912155
1	-5.060041	-0.667958	-0.807093
6	-0.711813	2.277252	-1.341365
6	-0.526118	3.527185	-1.914212
6	0.734105	4.099255	-1.878381
1	-1.351910	4.057922	-2.394528
6	1.560624	2.195309	-0.697775
6	1.785668	3.438164	-1.261328
1	0.899234	5.080141	-2.331134
1	2.777514	3.896380	-1.218466
6	2.509136	1.370420	0.060116
6	3.836416	1.634169	0.364832
6	2.595540	-0.629388	1.297174
6	4.536463	0.731419	1.151474
1	4.328168	2.537753	-0.006596
6	3.918172	-0.415786	1.631327
1	5.584055	0.931154	1.393824
1	4.439492	-1.147842	2.253977
7	0.322019	1.643670	-0.771980
7	1.950421	0.243453	0.537433
7	-1.832736	0.257627	-0.723331
6	-2.840024	-1.831925	0.010609
8	-3.721016	-2.284114	0.678879
6	1.721925	-1.804915	1.687168
8	2.170589	-2.695541	2.359830
8	0.522956	-1.748597	1.222919
44	0.116854	-0.070323	0.053290
6	-0.255991	1.959322	2.258034
6	-0.740655	2.472586	3.442818
6	-1.582055	1.692542	4.214179

6	-1.892413	0.421774	3.766163
6	-1.358389	-0.016335	2.572674
1	0.413672	2.551622	1.624880
1	-0.452193	3.480259	3.751219
1	-1.986489	2.069371	5.157956
1	-2.544785	-0.243483	4.336232
1	-1.544718	-1.028643	2.199998
6	0.902699	-0.488758	-2.832889
6	1.293682	-1.151700	-3.976417
6	1.521591	-2.513575	-3.915587
6	1.337666	-3.147139	-2.702254
6	0.941275	-2.409335	-1.605535
1	0.712460	0.588171	-2.862209
1	1.415033	-0.590802	-4.906282
1	1.833572	-3.072319	-4.802673
1	1.492854	-4.222471	-2.588123
1	0.767376	-2.886225	-0.638332
7	0.725469	-1.091859	-1.655322
7	-0.558092	0.738850	1.817195
8	-1.710187	-2.397129	-0.288658
1	-1.555697	-3.213629	0.251409
8	-0.582407	-4.276139	1.106058
1	0.007377	-3.667060	1.572699
1	-0.863475	-4.922691	1.755372

$[Ru^{II}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (Closed-shell singlet)

E = -1786.53794107 a.u.

6	2.186572	-0.938886	1.388228
6	3.427657	-1.244054	1.912318
6	4.569046	-0.914572	1.205124
6	4.414470	-0.269471	0.003794
6	3.138917	-0.044410	-0.509751
1	3.509457	-1.717669	2.892768
1	5.560018	-1.138443	1.610148
1	5.264491	0.084305	-0.585089
6	0.963612	-1.177264	2.145619
6	0.867067	-1.803841	3.379458
6	-0.372157	-1.943019	3.974852
1	1.755741	-2.191280	3.881410
6	-1.354573	-0.866880	2.091579
6	-1.500127	-1.475273	3.327980
1	-0.460417	-2.429542	4.949410
1	-2.482576	-1.591817	3.790105
6	-2.432182	-0.356325	1.250419
6	-3.770178	-0.505035	1.591547
6	-3.008909	0.714845	-0.694474
6	-4.752102	-0.080163	0.725999

1	-4.041595	-0.981587	2.536049
6	-4.358901	0.544399	-0.441745
1	-5.809912	-0.217274	0.964213
1	-5.086991	0.934165	-1.156644
7	-0.139995	-0.716947	1.539860
7	-2.036969	0.232332	0.091920
7	2.028242	-0.373926	0.159109
6	3.073919	0.653874	-1.867634
8	2.383744	0.090369	-2.738237
8	3.725893	1.677869	-1.913982
6	-2.629058	1.644449	-1.795124
8	-1.783727	2.483849	-1.691958
44	0.001953	0.041746	-0.220990
6	-0.394402	2.443473	1.514862
6	-0.244249	3.724018	1.999997
6	0.681496	4.561553	1.404884
6	1.419746	4.065747	0.348794
6	1.206490	2.768636	-0.071546
1	-1.120422	1.762711	1.969958
1	-0.856772	4.054718	2.842267
1	0.826172	5.584595	1.763738
1	2.175032	4.667105	-0.162271
1	1.801839	2.363117	-0.894687
6	-1.224833	-2.689824	-0.737245
6	-1.368100	-3.945861	-1.286228
6	-0.434909	-4.382317	-2.208115
6	0.602048	-3.530064	-2.531242
6	0.677217	-2.288328	-1.931029
1	-1.960503	-2.328034	-0.014001
1	-2.215012	-4.568611	-0.988137
1	-0.518698	-5.371430	-2.667771
1	1.369892	-3.812189	-3.255630
1	1.481536	-1.582990	-2.180534
7	-0.226559	-1.860326	-1.043037
7	0.311043	1.956954	0.493351
8	0.010260	0.697265	-2.205091
1	0.897806	0.521296	-2.617553
1	-0.158587	1.643366	-2.285194
8	-3.421010	1.503974	-2.830168
1	-3.189474	2.193005	-3.469883

[Ru^{II}(tda-κ-N^2O^2)Py_2]□(Closed-shell singlet)

E = -1709.72515032 a.u.

6	2.258135	1.078994	-1.393931
6	3.563776	1.240817	-1.831966
6	4.578904	0.520842	-1.237002
6	4.241044	-0.326551	-0.202812

6	2.915093	-0.434301	0.178702
1	3.767591	1.919821	-2.665930
1	5.613906	0.622718	-1.577672
1	4.966142	-0.930037	0.349284
6	1.141776	1.847187	-1.940473
6	1.202776	3.125870	-2.484289
6	0.003970	3.751003	-2.787562
1	2.155602	3.643752	-2.631576
6	-1.138271	1.850170	-1.939742
6	-1.196273	3.129006	-2.483525
1	0.005155	4.759802	-3.212297
1	-2.147834	3.649389	-2.630176
6	-2.256271	1.084950	-1.392386
6	-3.561801	1.250246	-1.829463
6	-2.916140	-0.426343	0.180952
6	-4.578425	0.533095	-1.233642
1	-3.764410	1.929727	-2.663332
6	-4.242084	-0.315047	-0.199571
1	-5.613406	0.637747	-1.573528
1	-4.968405	-0.916454	0.353187
7	0.000998	1.223835	-1.741221
7	-1.911629	0.238232	-0.399927
7	1.911951	0.233104	-0.401302
6	2.572579	-1.318953	1.348506
8	1.340004	-1.312795	1.659698
8	3.458378	-1.924516	1.900503
6	-2.575154	-1.311635	1.350720
8	-3.462198	-1.914596	1.903568
8	-1.342332	-1.308763	1.660986
44	-0.000360	-0.409920	0.512574
6	-0.004047	-2.065314	-1.980195
6	-0.006170	-3.216275	-2.739161
6	-0.007741	-4.442672	-2.097207
6	-0.007107	-4.458936	-0.715486
6	-0.004952	-3.262400	-0.026305
1	-0.002728	-1.065319	-2.428773
1	-0.006577	-3.142890	-3.829978
1	-0.009435	-5.375109	-2.670180
1	-0.008277	-5.397706	-0.156040
1	-0.004352	-3.210973	1.067312
6	0.004444	2.414445	1.543758
6	0.006447	3.415550	2.491216
6	0.006627	3.066967	3.830666
6	0.004757	1.723922	4.156301
6	0.002795	0.782445	3.146194
1	0.004216	2.645339	0.471717
1	0.007831	4.460993	2.171987
1	0.008187	3.835166	4.609991
1	0.004784	1.390234	5.197042
1	0.001241	-0.294117	3.342834

7	0.002645	1.118329	1.853661
7	-0.003442	-2.079602	-0.646778

[Ru^{II}(tda-κ-N^2O^2)Py_2] • □□□□) Conformer 1 (Closed-shell singlet)

E = -1786.13272889 a.u.

6	2.334301	1.548674	-0.947360
6	3.650504	1.804660	-1.300925
6	4.624365	0.861984	-1.044993
6	4.235876	-0.303622	-0.419394
6	2.902739	-0.484797	-0.095525
1	3.894555	2.744455	-1.805991
1	5.666035	1.038085	-1.329864
1	4.926157	-1.108479	-0.153850
6	1.262890	2.521821	-1.148385
6	1.390892	3.906794	-1.157458
6	0.226646	4.656921	-1.193985
1	2.368045	4.395578	-1.095374
6	-1.013604	2.633596	-1.144933
6	-1.005311	4.024399	-1.153381
1	0.280305	5.750077	-1.196078
1	-1.929718	4.606442	-1.087592
6	-2.174700	1.770197	-0.940728
6	-3.460755	2.154422	-1.289234
6	-2.936788	-0.198091	-0.087527
6	-4.521460	1.311974	-1.029521
1	-3.612976	3.113713	-1.793656
6	-4.246906	0.113341	-0.405833
1	-5.541922	1.589836	-1.310198
1	-5.011587	-0.620259	-0.137551
7	0.092571	1.925647	-1.202255
7	-1.889663	0.589698	-0.353355
7	1.936910	0.401726	-0.358450
6	2.509575	-1.730753	0.645275
8	1.274858	-1.776511	0.957492
8	3.347859	-2.554455	0.911537
6	-2.665144	-1.477775	0.649763
8	-3.578716	-2.217687	0.914373
8	-1.440348	-1.643077	0.960638
44	-0.021472	-0.451070	0.250126
6	-0.052492	-1.021444	-2.682137
6	-0.092190	-1.783118	-3.830437
6	-0.162070	-3.161052	-3.718937
6	-0.189031	-3.714878	-2.453573
6	-0.145444	-2.884002	-1.351621
1	0.002319	0.072900	-2.704826
1	-0.068141	-1.289563	-4.805660
1	-0.194991	-3.794785	-4.610561

1	-0.243840	-4.795729	-2.302600
1	-0.164202	-3.277792	-0.329235
6	0.090919	1.765538	2.275616
6	0.122440	2.341367	3.527294
6	0.083826	1.520273	4.640722
6	0.015400	0.154831	4.442409
6	-0.012235	-0.343062	3.154408
1	0.119647	2.379635	1.367676
1	0.177033	3.429226	3.619534
1	0.107292	1.942489	5.650095
1	-0.017255	-0.544452	5.281557
1	-0.066326	-1.419455	2.954769
7	0.024864	0.448869	2.078903
7	-0.078151	-1.553938	-1.459404
8	-0.186389	-3.843581	2.296957
1	0.582085	-3.384772	1.940579
1	-0.905034	-3.310790	1.939602

[Ru^{II}(tda-κ-N^2O^2)Py_2] • □□□□) Conformer 2 (Closed-shell singlet)

E = -1786.12652972 a.u.

6	0.091715	2.624682	-1.248500
6	0.670104	3.809663	-1.679360
6	1.946793	4.134987	-1.271587
6	2.594653	3.254391	-0.430123
6	1.947652	2.095318	-0.039744
1	0.114895	4.458055	-2.364337
1	2.426876	5.058030	-1.610544
1	3.603851	3.419961	-0.044604
6	-1.268247	2.229662	-1.610421
6	-2.329389	3.077945	-1.906913
6	-3.582176	2.505993	-2.060989
1	-2.198335	4.162242	-1.977327
6	-2.619749	0.394168	-1.559146
6	-3.752268	1.146941	-1.852714
1	-4.447021	3.136733	-2.289414
1	-4.750213	0.698444	-1.879998
6	-2.587927	-1.006086	-1.143298
6	-3.560562	-1.919358	-1.520438
6	-1.537258	-2.572968	0.136882
6	-3.502241	-3.215163	-1.051180
1	-4.348849	-1.604503	-2.211385
6	-2.471213	-3.538635	-0.194617
1	-4.251029	-3.955249	-1.349833
1	-2.340319	-4.527239	0.253021
7	-1.419065	0.927518	-1.505384
7	-1.556126	-1.319670	-0.331062
7	0.717919	1.751123	-0.435258

6	2.633935	1.166309	0.918087
8	1.919627	0.203136	1.320293
8	3.778676	1.398653	1.250246
6	-0.459680	-2.924586	1.128657
8	-0.433047	-4.038317	1.590310
8	0.319049	-1.958947	1.408942
44	0.218334	-0.259191	0.402179
6	1.114011	-1.040152	-2.346717
6	1.915985	-1.629409	-3.299732
6	3.027063	-2.348646	-2.889333
6	3.282172	-2.448315	-1.536085
6	2.421298	-1.840930	-0.642383
1	0.229479	-0.447738	-2.607418
1	1.667859	-1.516431	-4.358569
1	3.687654	-2.822151	-3.622812
1	4.150255	-2.981910	-1.142132
1	2.584882	-1.892338	0.437304
6	-1.839337	1.319665	1.930790
6	-2.475129	1.824368	3.044814
6	-1.988778	1.494876	4.297930
6	-0.882563	0.669880	4.372882
6	-0.304001	0.206293	3.208014
1	-2.192000	1.555355	0.919614
1	-3.347623	2.471215	2.921239
1	-2.468372	1.877323	5.204103
1	-0.455720	0.375079	5.334868
1	0.569238	-0.453489	3.206790
7	-0.771840	0.524701	1.998258
7	1.355999	-1.140959	-1.038278
8	5.034494	-1.167290	0.979049
1	4.536818	-0.482385	1.443529
1	5.473210	-0.646856	0.304706

[Ru^{II}(tda-κ-N^3O)Py_2] (Closed-shell singlet)

E = -1709.70945223 a.u.

6	-2.071319	-0.672338	1.630376
6	-3.286340	-0.964526	2.228100
6	-4.456470	-0.740628	1.529648
6	-4.363172	-0.200775	0.268794
6	-3.113185	0.054562	-0.289935
1	-3.318570	-1.364228	3.244769
1	-5.425669	-0.973274	1.983227
1	-5.227924	0.059133	-0.346449
6	-0.811754	-0.848931	2.351100
6	-0.649209	-1.299437	3.654325
6	0.622690	-1.389056	4.190453
1	-1.513817	-1.580062	4.260413

6	1.519800	-0.602712	2.125070
6	1.720246	-1.040344	3.421454
1	0.760888	-1.739098	5.216869
1	2.732811	-1.116369	3.827426
6	2.549120	-0.238494	1.156287
6	3.925961	-0.209719	1.327625
6	2.783342	0.426512	-1.085777
6	4.728005	0.148807	0.256687
1	4.372773	-0.463836	2.293432
6	4.157172	0.470380	-0.968038
1	5.814522	0.176652	0.383668
1	4.748614	0.758788	-1.841407
7	0.259140	-0.506507	1.620182
7	2.034392	0.084825	-0.045833
7	-1.977489	-0.196681	0.362357
6	-3.080785	0.678924	-1.700215
8	-1.982139	0.637078	-2.260102
8	-4.158747	1.137271	-2.045560
6	1.953097	0.734046	-2.325163
8	2.541575	1.048418	-3.328868
8	0.696105	0.614784	-2.145183
44	0.122976	0.058286	-0.216384
6	0.705067	-2.905579	-0.388405
6	0.697753	-4.158365	-0.963795
6	0.058801	-4.325384	-2.179189
6	-0.542792	-3.227047	-2.763387
6	-0.492359	-2.001318	-2.127736
1	1.203495	-2.730438	0.572636
1	1.194440	-4.989643	-0.456999
1	0.034154	-5.305291	-2.666208
1	-1.057399	-3.303034	-3.724374
1	-0.952050	-1.084874	-2.530656
6	0.437097	2.653354	1.295332
6	0.356954	4.013698	1.502576
6	-0.195619	4.804043	0.510649
6	-0.638959	4.193005	-0.646369
6	-0.520455	2.823158	-0.784238
1	0.863426	1.992081	2.058863
1	0.726999	4.440899	2.438086
1	-0.278443	5.887531	0.641679
1	-1.085661	4.767803	-1.461058
1	-0.858175	2.274650	-1.675885
7	0.007676	2.063688	0.181967
7	0.122586	-1.849236	-0.949646

[Ru^{II}(tda-κ-N^3O)Py_2] • □□□□) (Closed-shell singlet)

E = -1786.12190394 a.u.

6	0.925371	-2.292309	-1.183868
6	1.710368	-3.356501	-1.592859
6	3.009622	-3.458231	-1.133509
6	3.486741	-2.461124	-0.316337
6	2.636715	-1.440768	0.101659
1	1.310722	-4.099790	-2.287267
1	3.644336	-4.293964	-1.444848
1	4.523337	-2.416605	0.025940
6	-0.416126	-2.080462	-1.725766
6	-1.084919	-2.864831	-2.655405
6	-2.343997	-2.483141	-3.084119
1	-0.628817	-3.774811	-3.052942
6	-2.240247	-0.587227	-1.639799
6	-2.931409	-1.336663	-2.573962
1	-2.877801	-3.090296	-3.819973
1	-3.931626	-1.032599	-2.895095
6	-2.715260	0.602959	-0.936622
6	-3.917298	1.279200	-1.088276
6	-2.064303	2.080864	0.774523
6	-4.174213	2.377282	-0.283153
1	-4.650517	0.954293	-1.832552
6	-3.244333	2.787347	0.663785
1	-5.117971	2.918962	-0.398489
1	-3.408270	3.645327	1.321684
7	-0.995026	-0.970017	-1.246921
7	-1.837537	1.038885	-0.012693
7	1.364536	-1.365406	-0.290775
6	3.226246	-0.344119	0.989069
8	2.475214	0.160530	1.821964
8	4.400214	-0.102479	0.710850
6	-0.916338	2.337826	1.744216
8	-1.032524	3.250580	2.521231
8	0.058850	1.522205	1.619426
44	-0.175127	0.091002	0.127806
6	-2.023290	-1.796691	1.605995
6	-2.465798	-2.547845	2.674057
6	-1.694033	-2.587973	3.821168
6	-0.512189	-1.872040	3.844252
6	-0.134732	-1.140716	2.734462
1	-2.610019	-1.735289	0.681618
1	-3.411967	-3.089869	2.599137
1	-2.015455	-3.171023	4.689883
1	0.132714	-1.865386	4.726428
1	0.794525	-0.552898	2.680704
6	0.425021	1.643281	-2.403869
6	1.107870	2.536283	-3.201174
6	2.183738	3.224335	-2.664502
6	2.525747	2.991596	-1.346979
6	1.783962	2.086515	-0.613418
1	-0.425792	1.072369	-2.794417

1	0.792720	2.682989	-4.237627
1	2.749227	3.934780	-3.276012
1	3.361980	3.481508	-0.841021
1	2.016414	1.881245	0.436897
7	0.752998	1.415819	-1.133201
7	-0.883859	-1.109800	1.627260
8	4.086996	2.620629	1.467810
1	3.419115	2.321630	2.092367
1	4.463444	1.766169	1.208769

[Ru^{II}(tda-κ-N^3O)Py_2] • □□□□)$_2$ (Closed-shell singlet)

E = -1862.53668537 a.u.

6	-0.003040	2.788907	-0.433759
6	-0.442300	4.097343	-0.535692
6	-1.722050	4.417485	-0.122230
6	-2.528448	3.404529	0.341218
6	-2.013751	2.118785	0.477399
1	0.208192	4.864678	-0.963251
1	-2.087769	5.446260	-0.199239
1	-3.576721	3.555927	0.610168
6	1.287048	2.363797	-0.978881
6	2.250492	3.150677	-1.594487
6	3.388832	2.550978	-2.104614
1	2.119446	4.232231	-1.681189
6	2.590779	0.430498	-1.357538
6	3.564727	1.180815	-1.990659
1	4.152380	3.160156	-2.595443
1	4.464236	0.700485	-2.385891
6	2.611566	-1.008455	-1.087940
6	3.561090	-1.949039	-1.460762
6	1.352798	-2.671215	0.005110
6	3.379353	-3.270545	-1.084736
1	4.436986	-1.655923	-2.047211
6	2.264251	-3.645723	-0.345236
1	4.120640	-4.019482	-1.379172
1	2.081730	-4.678537	-0.036221
7	1.476760	1.041054	-0.871760
7	1.548176	-1.413104	-0.367151
7	-0.764375	1.811353	0.126568
6	-2.942079	1.020373	0.994693
8	-2.415412	0.176132	1.723961
8	-4.091795	1.135020	0.588495
6	0.065513	-2.837850	0.799135
8	-0.255634	-3.942149	1.163520
8	-0.566899	-1.747630	1.001117
44	0.243316	-0.078068	0.074898
6	2.445789	0.512492	2.062106

6	3.011035	0.699645	3.305553
6	2.190805	0.670062	4.418716
6	0.838774	0.455835	4.231494
6	0.346334	0.277376	2.953083
1	3.067388	0.522499	1.159306
1	4.088575	0.861739	3.390261
1	2.604942	0.810476	5.422006
1	0.144975	0.419057	5.074962
1	-0.718435	0.113167	2.732668
6	-0.495602	-0.410273	-2.830326
6	-1.303607	-0.697829	-3.908257
6	-2.587529	-1.162065	-3.675364
6	-3.004461	-1.331222	-2.370070
6	-2.124479	-1.032020	-1.346890
1	0.520732	-0.026724	-2.976041
1	-0.921348	-0.548097	-4.921607
1	-3.257004	-1.386810	-4.512032
1	-4.002887	-1.669917	-2.073229
1	-2.412161	-1.178344	-0.299644
7	-0.891140	-0.569299	-1.567144
7	1.143010	0.308635	1.880377
8	-4.970428	-1.589170	-0.074720
1	-4.515644	-2.091311	0.617802
1	-4.879854	-0.677308	0.232227
8	-3.252105	-2.503981	1.994675
1	-2.967993	-1.577757	2.024630
1	-2.436198	-2.957906	1.761619

[Ru^{II}(tda-κ-N^3)Py_2(OH_2)] (Closed-shell singlet)

E = -1786.11604207 a.u.

6	2.180531	-0.981016	-1.380823
6	3.411024	-1.244329	-1.954922
6	4.556296	-0.724883	-1.384747
6	4.413139	0.060314	-0.267659
6	3.158537	0.235550	0.310938
1	3.471243	-1.827268	-2.876553
1	5.537166	-0.910747	-1.832922
1	5.255485	0.569188	0.207382
6	0.944349	-1.396877	-2.028436
6	0.839147	-2.220332	-3.138055
6	-0.411601	-2.510306	-3.648990
1	1.729886	-2.653058	-3.598196
6	-1.382912	-1.174576	-1.925482
6	-1.534864	-1.986529	-3.039020
1	-0.512126	-3.162480	-4.520504
1	-2.528445	-2.230083	-3.421144
6	-2.457785	-0.568990	-1.148332

6	-3.784210	-0.692531	-1.524632
6	-3.021100	0.730226	0.675486
6	-4.766380	-0.121903	-0.739827
1	-4.048518	-1.237516	-2.433738
6	-4.372838	0.577108	0.375974
1	-5.822745	-0.222051	-1.008784
1	-5.077877	1.046159	1.066888
7	-0.157101	-0.889823	-1.450325
7	-2.066228	0.129342	-0.046766
7	2.042958	-0.280372	-0.221677
6	3.136158	1.069795	1.591474
8	2.542674	0.556195	2.555037
8	3.743080	2.120509	1.495824
6	-2.702945	1.691411	1.832954
8	-3.500153	1.635860	2.747902
8	-1.722136	2.427138	1.628875
44	0.003981	0.031109	0.232264
6	-1.021898	-2.709871	1.013828
6	-1.068248	-3.900188	1.708733
6	-0.091365	-4.160398	2.651187
6	0.889804	-3.208823	2.851019
6	0.868822	-2.043575	2.110362
1	-1.797113	-2.468936	0.280279
1	-1.879311	-4.605796	1.512209
1	-0.101026	-5.090934	3.227065
1	1.683273	-3.351533	3.588726
1	1.621225	-1.253794	2.252100
6	-0.503199	2.241768	-1.699407
6	-0.483374	3.507906	-2.241930
6	0.242122	4.496389	-1.603367
6	0.914067	4.164403	-0.444616
6	0.834251	2.872545	0.030900
1	-1.071682	1.438674	-2.179334
1	-1.042252	3.708108	-3.159470
1	0.278901	5.513771	-2.004335
1	1.505683	4.894911	0.110973
1	1.347687	2.594517	0.953679
7	0.142892	1.914714	-0.582507
7	-0.075484	-1.792245	1.198761
8	0.048333	0.743256	2.158774
1	0.946521	0.865730	2.531266
1	-0.487954	1.565634	2.215460

$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]\bullet$ Conformer 1 (Closed-shell singlet)

E = -1862.52367454 a.u.

6	2.256666	-1.409550	-1.035808
6	3.511490	-1.776398	-1.488153

6	4.628397	-1.119332	-1.011079
6	4.435233	-0.110205	-0.100343
6	3.156617	0.169711	0.375226
1	3.612889	-2.552487	-2.249928
1	5.627563	-1.382733	-1.371418
1	5.254139	0.501962	0.285893
6	1.052051	-1.994245	-1.608196
6	1.000775	-3.077956	-2.470463
6	-0.222478	-3.507574	-2.948827
1	1.913875	-3.602148	-2.760332
6	-1.276618	-1.785947	-1.677380
6	-1.374160	-2.857669	-2.550390
1	-0.278077	-4.362525	-3.627719
1	-2.348704	-3.195059	-2.910306
6	-2.384597	-1.005621	-1.145178
6	-3.706633	-1.267139	-1.465710
6	-2.990560	0.770922	0.196834
6	-4.704138	-0.517614	-0.872666
1	-3.956090	-2.066881	-2.166804
6	-4.336272	0.502763	-0.025243
1	-5.756983	-0.727179	-1.086604
1	-5.067133	1.140386	0.479185
7	-0.076336	-1.371537	-1.229218
7	-2.024035	-0.009260	-0.297202
7	2.065933	-0.460464	-0.079917
6	3.075850	1.233009	1.470378
8	2.440168	0.891375	2.482331
8	3.686214	2.253168	1.211629
6	-2.610103	2.061947	0.898799
8	-3.132649	2.269751	1.986686
8	-1.847501	2.749491	0.208424
44	0.004864	-0.015790	0.133174
6	-1.267568	-2.334489	1.635511
6	-1.413182	-3.292851	2.616192
6	-0.442715	-3.401797	3.593532
6	0.631431	-2.535976	3.538054
6	0.706508	-1.606718	2.518728
1	-2.039260	-2.216460	0.870542
1	-2.296604	-3.936270	2.610042
1	-0.529451	-4.146037	4.391286
1	1.425749	-2.560031	4.288169
1	1.531010	-0.881501	2.462405
6	-0.288830	1.566544	-2.367183
6	-0.183527	2.632226	-3.233576
6	0.558399	3.733345	-2.848831
6	1.163696	3.709979	-1.608621
6	1.004266	2.601608	-0.803182
1	-0.880063	0.684921	-2.635712
1	-0.693193	2.592428	-4.199471
1	0.659518	4.600354	-3.508669

1	1.763937	4.545407	-1.241713
1	1.462424	2.569366	0.188360
7	0.292157	1.538708	-1.171240
7	-0.229841	-1.501728	1.570750
8	-0.007674	1.239523	1.779202
1	0.854507	1.253155	2.246213
1	-0.368003	2.152404	1.856235
8	-0.816926	3.753991	2.439519
1	-1.091904	3.943728	1.530295
1	-1.662348	3.425676	2.781322

[Ru^{II}(tda-κ-N^3)Py_2(OH_2)]•□□ Conformer 2 (Closed-shell singlet)

E = -1862.51707412 a.u.

6	-2.351888	-1.011939	1.284425
6	-3.633843	-1.272309	1.733975
6	-4.716631	-0.870360	0.976261
6	-4.465120	-0.204797	-0.198521
6	-3.155043	-0.031515	-0.637256
1	-3.786467	-1.754483	2.702305
1	-5.738419	-1.052120	1.323454
1	-5.258675	0.209230	-0.825538
6	-1.187208	-1.300891	2.111926
6	-1.173518	-2.031827	3.289145
6	0.021778	-2.207563	3.961951
1	-2.089830	-2.483089	3.675881
6	1.123260	-0.942386	2.264319
6	1.182470	-1.661682	3.447746
1	0.050288	-2.786493	4.888826
1	2.134290	-1.807094	3.963797
6	2.240338	-0.300500	1.581545
6	3.527111	-0.301178	2.090101
6	2.871922	1.003183	-0.229047
6	4.532225	0.319801	1.371451
1	3.743760	-0.786650	3.044533
6	4.196307	0.970730	0.207528
1	5.563969	0.306843	1.737270
1	4.939904	1.497906	-0.396903
7	-0.051502	-0.774422	1.627467
7	1.921374	0.305053	0.406199
7	-2.099011	-0.430230	0.081067
6	-2.985026	0.647444	-1.995409
8	-2.207644	0.070815	-2.779232
8	-3.671151	1.639909	-2.137777
6	2.529813	2.009748	-1.341312
8	3.063255	1.803996	-2.432671
8	1.862103	2.933474	-0.907242
44	-0.034776	0.003985	-0.131221

6	1.352679	-2.657380	-0.567176
6	1.617570	-3.870344	-1.168044
6	0.791044	-4.306005	-2.187835
6	-0.271222	-3.501451	-2.549921
6	-0.474310	-2.302731	-1.894068
1	2.004779	-2.282389	0.227552
1	2.476989	-4.458230	-0.835283
1	0.978712	-5.257439	-2.694658
1	-0.954702	-3.784373	-3.354120
1	-1.294581	-1.621893	-2.169136
6	-0.161129	2.348011	1.698972
6	-0.380634	3.640411	2.119451
6	-0.929276	4.544620	1.228855
6	-1.224556	4.109151	-0.045731
6	-0.961432	2.798985	-0.387429
1	0.280473	1.607137	2.373961
1	-0.112018	3.928396	3.138844
1	-1.115916	5.580934	1.526499
1	-1.648509	4.775372	-0.799435
1	-1.143530	2.440369	-1.401866
7	-0.450331	1.921662	0.472183
7	0.330873	-1.874717	-0.915799
8	0.158590	0.676487	-2.073280
1	-0.668090	0.500404	-2.577855
1	0.882583	0.209878	-2.544574
8	2.270682	-0.608885	-3.206017
1	2.780052	0.215949	-3.050804
1	2.644507	-1.234685	-2.582528

[Ru^{II}(tda-κ-N^2O)Py_2] (Closed-shell singlet)

E = -1786.11505434 a.u.

6	-1.989160	2.101850	0.505989
6	-2.976049	2.950690	1.007715
6	-4.299909	2.668474	0.726638
6	-4.595055	1.533755	0.005263
6	-3.544188	0.753761	-0.469341
1	-2.732769	3.788467	1.665876
1	-5.092578	3.319355	1.111709
1	-5.615713	1.201496	-0.200535
6	-0.593302	2.288777	0.950381
6	-0.196058	3.509934	1.500396
6	0.977347	3.602410	2.211945
1	-0.821308	4.393551	1.357752
6	1.345750	1.303035	1.721913
6	1.724150	2.456313	2.388033
1	1.298262	4.554562	2.644094
1	2.636697	2.466045	2.988735

6	2.139132	0.079996	1.801939
6	3.161061	-0.227173	2.690819
6	2.435846	-1.967692	0.702452
6	3.802659	-1.448527	2.580535
1	3.451084	0.477457	3.475556
6	3.453760	-2.324288	1.558595
1	4.598540	-1.708314	3.284342
1	3.964886	-3.276969	1.394316
7	0.240292	1.231412	0.932839
7	1.784370	-0.811927	0.873109
7	-2.271918	1.047305	-0.246264
6	-3.873061	-0.529770	-1.230787
8	-2.975592	-0.953955	-1.989619
8	-4.972512	-0.997324	-0.999074
6	2.066618	-2.689139	-0.578226
8	2.570647	-3.753465	-0.822693
8	1.270776	-2.015453	-1.335232
44	0.477871	-0.399288	-0.442633
6	-1.500119	-1.399961	1.548934
6	-2.575774	-2.112233	2.026228
6	-3.091853	-3.139668	1.254684
6	-2.479735	-3.426798	0.053824
6	-1.400259	-2.665890	-0.348168
1	-1.081162	-0.556879	2.108416
1	-3.018187	-1.841006	2.987770
1	-3.971214	-3.700115	1.584014
1	-2.854339	-4.210301	-0.607267
1	-0.892998	-2.849821	-1.298815
6	3.069019	0.580652	-1.576646
6	3.925186	1.419641	-2.260013
6	3.424237	2.587326	-2.804179
6	2.078155	2.862194	-2.641131
6	1.291539	1.971460	-1.941652
1	3.423183	-0.365094	-1.153097
1	4.976821	1.142836	-2.368265
1	4.074138	3.272231	-3.357143
1	1.625306	3.764114	-3.060428
1	0.214271	2.121119	-1.811373
7	1.774585	0.845998	-1.410385
7	-0.921711	-1.654137	0.373599
8	-0.658091	-0.082099	-2.158099
1	-1.651188	-0.302263	-2.021972
1	-0.358842	-0.748763	-2.787224

[Ru^{II}(tda-κ-N^2O)Py_2(OH_2)]•□□□ (Closed-shell singlet)

E = -1862.52551087 a.u.

6	1.537158	2.421168	-0.281680

6	2.357755	3.341837	-0.934699
6	3.727749	3.176737	-0.869519
6	4.225705	2.087791	-0.190556
6	3.331180	1.228476	0.439502
1	1.931020	4.144702	-1.542217
1	4.392859	3.881613	-1.380047
1	5.291006	1.852590	-0.131533
6	0.082065	2.542010	-0.515322
6	-0.461352	3.800474	-0.775537
6	-1.720915	3.914705	-1.321076
1	0.123212	4.691451	-0.533666
6	-1.845256	1.536050	-1.292124
6	-2.389725	2.756490	-1.656232
1	-2.163704	4.895967	-1.513871
1	-3.359205	2.792459	-2.159105
6	-2.493964	0.268641	-1.615170
6	-3.579025	0.037356	-2.450856
6	-2.360302	-2.018321	-1.101694
6	-4.026202	-1.261139	-2.624357
1	-4.073710	0.862855	-2.970559
6	-3.426657	-2.303442	-1.925251
1	-4.871045	-1.457558	-3.290745
1	-3.782231	-3.335981	-1.982175
7	-0.662677	1.426139	-0.622726
7	-1.901542	-0.766238	-1.010924
7	2.016270	1.398553	0.412371
6	3.892600	0.000765	1.147517
8	3.112810	-0.603124	1.911077
8	5.051591	-0.273766	0.867608
6	-1.743993	-2.966291	-0.087211
8	-2.060287	-4.125745	-0.102513
8	-0.978995	-2.377800	0.765981
44	-0.562283	-0.466676	0.294785
6	1.298499	-0.622218	-2.031666
6	2.468870	-0.916213	-2.693340
6	3.354172	-1.813484	-2.118825
6	3.007068	-2.417031	-0.926869
6	1.801456	-2.075921	-0.344123
1	0.585166	0.107331	-2.430767
1	2.688024	-0.423305	-3.644000
1	4.313022	-2.035434	-2.596688
1	3.678908	-3.086949	-0.379548
1	1.481731	-2.528044	0.598806
6	-3.179963	-0.314370	1.755203
6	-4.111149	0.162439	2.655223
6	-3.792215	1.264077	3.426383
6	-2.545420	1.840975	3.262622
6	-1.674739	1.303152	2.338764
1	-3.386915	-1.200702	1.146376
1	-5.074918	-0.343748	2.750314

1	-4.504450	1.664504	4.154127
1	-2.234296	2.706252	3.853054
1	-0.664948	1.700708	2.190909
7	-1.982098	0.242854	1.588836
7	0.970459	-1.172096	-0.861107
8	0.598492	-0.362502	2.026204
1	1.592099	-0.268589	1.904918
1	0.493424	-1.213616	2.466506
8	4.720886	-2.993155	1.650588
1	4.012123	-2.497721	2.077336
1	5.234045	-2.239053	1.330662

$[Ru^{II}(tda\text{-}\kappa\text{-}N^3)Py_2(OH)]^-$ (Closed-shell singlet)

E = -1785.54795323 a.u.

6	-2.074519	-0.035758	1.780562
6	-3.287313	0.000039	2.445474
6	-4.442473	0.254273	1.730938
6	-4.335238	0.465969	0.380054
6	-3.089064	0.446755	-0.255697
1	-3.328922	-0.178646	3.522487
1	-5.414509	0.280351	2.236787
1	-5.215225	0.660930	-0.239948
6	-0.831592	-0.335066	2.481895
6	-0.700446	-0.627711	3.825964
6	0.552284	-0.924032	4.347854
1	-1.575796	-0.639502	4.480768
6	1.484829	-0.605026	2.170948
6	1.653215	-0.911874	3.511743
1	0.664243	-1.167051	5.408148
1	2.645752	-1.145296	3.908362
6	2.516735	-0.495912	1.159844
6	3.866640	-0.591009	1.473830
6	3.000036	-0.061959	-1.061378
6	4.807821	-0.366473	0.493579
1	4.170636	-0.808734	2.501438
6	4.360267	-0.064170	-0.775005
1	5.877758	-0.416332	0.726531
1	5.033146	0.169590	-1.604122
7	0.254510	-0.331773	1.672612
7	2.072608	-0.256781	-0.110485
7	-1.970260	0.193452	0.438142
6	-3.166427	0.758572	-1.767922
8	-3.063838	1.953976	-2.017587
8	-3.493174	-0.210970	-2.443567
6	2.624837	0.071513	-2.544115
8	3.277900	0.916803	-3.140984
8	1.788075	-0.751921	-2.923102

44	-0.008156	0.009902	-0.202916
6	0.381173	-2.951918	-0.102799
6	0.189138	-4.280010	-0.419244
6	-0.799928	-4.609002	-1.328257
6	-1.548443	-3.585824	-1.874974
6	-1.295502	-2.276220	-1.510538
1	1.163301	-2.651631	0.602614
1	0.824541	-5.041128	0.042079
1	-0.979715	-5.653151	-1.607339
1	-2.344148	-3.779838	-2.598935
1	-1.854302	-1.431174	-1.939165
6	1.041249	2.599001	0.888061
6	1.229016	3.959915	1.003693
6	0.563449	4.797350	0.126555
6	-0.257436	4.225033	-0.824382
6	-0.390279	2.849702	-0.884670
1	1.549997	1.904494	1.565953
1	1.897840	4.348268	1.776843
1	0.686231	5.884403	0.187945
1	-0.816681	4.833354	-1.539822
1	-1.027604	2.344169	-1.622008
7	0.253209	2.046878	-0.031687
7	-0.339831	-1.967029	-0.629218
8	-0.508078	0.340207	-2.032074
1	0.191414	0.036301	-2.629451

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2]^{2+}$ (Doublet)

E = -1709.81169293 a.u.

6	-2.201147	-0.061940	1.576039
6	-3.482239	-0.131520	2.105224
6	-4.577039	-0.016600	1.273807
6	-4.353458	0.184940	-0.072898
6	-3.050152	0.249456	-0.531949
1	-3.626501	-0.282589	3.177387
1	-5.592158	-0.076472	1.675227
1	-5.162471	0.302120	-0.799794
6	-0.997077	-0.155830	2.394584
6	-0.952506	-0.252770	3.777734
6	0.274621	-0.294304	4.412047
1	-1.871141	-0.290622	4.366770
6	1.339619	-0.161544	2.284083
6	1.435552	-0.251572	3.661243
1	0.326824	-0.365326	5.501735
1	2.413297	-0.292664	4.147237
6	2.443544	-0.175914	1.333966
6	3.799957	-0.257641	1.604868
6	2.867632	-0.200117	-0.954987

6	4.698102	-0.310960	0.550397
1	4.160063	-0.281710	2.636631
6	4.230126	-0.289382	-0.753111
1	5.770865	-0.374834	0.753271
1	4.890357	-0.338814	-1.624173
7	0.135256	-0.103045	1.681556
7	2.021642	-0.142617	0.062701
7	-1.980944	0.115847	0.257858
6	-2.854608	0.499991	-1.983969
8	-3.736468	0.568241	-2.770259
6	2.165056	-0.154902	-2.279346
8	2.744881	-0.200783	-3.315695
8	0.876091	-0.044067	-2.122907
44	0.084496	0.020370	-0.303251
6	0.255717	-2.929268	0.418193
6	0.133826	-4.289495	0.232058
6	-0.374672	-4.758227	-0.966128
6	-0.734286	-3.837044	-1.932390
6	-0.575487	-2.492991	-1.667331
1	0.660251	-2.532696	1.354955
1	0.443160	-4.971655	1.027358
1	-0.481958	-5.831526	-1.147156
1	-1.129442	-4.148926	-2.901954
1	-0.811373	-1.732860	-2.417494
6	-0.053738	2.838256	0.792174
6	0.019219	4.214087	0.818602
6	0.416513	4.885547	-0.323413
6	0.714947	4.138494	-1.447169
6	0.613184	2.763778	-1.390220
1	-0.371345	2.289379	1.683800
1	-0.238100	4.748104	1.736386
1	0.486606	5.976945	-0.337777
1	1.026928	4.610776	-2.381772
1	0.825460	2.148020	-2.267417
7	0.239717	2.108568	-0.286872
7	-0.094734	-2.036173	-0.508497
8	-1.565967	0.635672	-2.250696
1	-1.439228	0.763339	-3.203572

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^{2+}$ (Doublet)

E = -1786.18549772 a.u.

6	2.237501	-0.896275	1.353950
6	3.487040	-1.160410	1.879822
6	4.622795	-0.704545	1.231733
6	4.452101	0.028899	0.085925
6	3.169442	0.213009	-0.432308
1	3.583431	-1.703903	2.821837

1	5.617292	-0.901271	1.641304
1	5.291301	0.476030	-0.453125
6	1.021933	-1.286924	2.056131
6	0.954549	-2.037311	3.222235
6	-0.280836	-2.308585	3.774679
1	1.857638	-2.417541	3.702661
6	-1.316328	-1.119966	1.989347
6	-1.433274	-1.852805	3.157397
1	-0.350702	-2.891546	4.697075
1	-2.407016	-2.081974	3.593706
6	-2.422295	-0.600423	1.186787
6	-3.744841	-0.840032	1.539558
6	-3.084388	0.600928	-0.650303
6	-4.762550	-0.385314	0.733748
1	-3.978471	-1.401019	2.446521
6	-4.420759	0.353588	-0.381859
1	-5.808828	-0.585427	0.979757
1	-5.181865	0.772118	-1.044098
7	-0.105180	-0.845636	1.482650
7	-2.076848	0.100372	0.079734
7	2.064622	-0.233877	0.176665
6	3.069529	1.010250	-1.718716
8	2.470142	0.520511	-2.677505
8	3.630463	2.092973	-1.602390
6	-2.775660	1.614487	-1.702243
8	-1.854129	2.377039	-1.634504
44	0.014899	0.047870	-0.233478
6	-0.534673	2.283257	1.678686
6	-0.486940	3.543594	2.228948
6	0.293059	4.511786	1.619014
6	0.995583	4.166234	0.479820
6	0.894669	2.879434	-0.002159
1	-1.140041	1.498985	2.142462
1	-1.061550	3.758503	3.132854
1	0.352563	5.523554	2.030403
1	1.632071	4.881557	-0.045778
1	1.443067	2.590678	-0.901374
6	-0.987103	-2.739492	-0.919019
6	-1.024364	-3.957903	-1.558214
6	-0.048161	-4.251015	-2.495050
6	0.924724	-3.301241	-2.745142
6	0.892414	-2.104496	-2.060592
1	-1.755691	-2.485862	-0.184472
1	-1.822090	-4.665916	-1.322305
1	-0.051685	-5.207153	-3.026506
1	1.716483	-3.471341	-3.478409
1	1.638858	-1.324349	-2.253164
7	-0.049766	-1.817291	-1.154064
7	0.143386	1.940890	0.580041
8	0.035946	0.749547	-2.150680

1	0.925644	0.735885	-2.588599
1	-0.375963	1.613964	-2.286183
8	-3.689799	1.618190	-2.629774
1	-3.513449	2.350084	-3.240957

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^3)Py_2(OH)]^+$ (Doublet)

E = -1785.86902372 a.u.

6	-2.134567	0.991159	1.371399
6	-3.363218	1.414163	1.842325
6	-4.520123	0.936165	1.266079
6	-4.398585	-0.009360	0.278003
6	-3.138564	-0.389381	-0.180645
1	-3.417157	2.121617	2.671368
1	-5.501789	1.267302	1.614685
1	-5.268383	-0.503390	-0.158452
6	-0.894775	1.430970	2.009133
6	-0.803271	2.266711	3.110542
6	0.449139	2.613222	3.585117
1	-1.694241	2.656334	3.605048
6	1.432688	1.297743	1.860051
6	1.580659	2.140561	2.952335
1	0.540368	3.274055	4.451087
1	2.571617	2.435542	3.303034
6	2.500793	0.724496	1.054351
6	3.836688	0.879024	1.366219
6	3.005199	-0.568033	-0.799708
6	4.794033	0.322609	0.535407
1	4.132191	1.434702	2.258978
6	4.366967	-0.380546	-0.563544
1	5.858598	0.445622	0.754757
1	5.052716	-0.821167	-1.292421
7	0.211697	0.945574	1.437903
7	2.084474	0.005905	-0.022896
7	-2.010244	0.139774	0.316190
6	-3.245851	-1.542655	-1.179113
8	-2.558795	-1.588692	-2.273571
8	-4.091292	-2.342116	-0.920686
6	2.627487	-1.480641	-1.976172
8	3.300914	-1.291683	-2.964040
8	1.725916	-2.293854	-1.710679
44	0.012944	-0.068118	-0.252738
6	0.689120	-2.139664	1.788489
6	0.798830	-3.375150	2.388512
6	0.252320	-4.475332	1.755188
6	-0.377129	-4.283321	0.541503
6	-0.432687	-3.013741	0.008432
1	1.113961	-1.252483	2.267377

1	1.315965	-3.462569	3.346789
1	0.322215	-5.471631	2.200738
1	-0.819265	-5.111884	-0.015347
1	-0.890563	-2.847360	-0.969061
6	0.778210	2.743922	-1.104209
6	0.725729	3.915302	-1.829708
6	-0.295307	4.089076	-2.744554
6	-1.222465	3.074554	-2.891516
6	-1.091809	1.936614	-2.125364
1	1.591804	2.569571	-0.394189
1	1.496838	4.674631	-1.681554
1	-0.361778	5.001051	-3.344561
1	-2.044062	3.147903	-3.607487
1	-1.792260	1.105006	-2.239232
7	-0.113139	1.763948	-1.237944
7	0.082005	-1.947470	0.619017
8	-0.215991	-0.747391	-1.998921
1	-1.712584	-1.075252	-2.268182
1	0.349609	-1.545411	-2.136923

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (Doublet)

E = -1861.01755710 a.u.

6	2.074810	-1.648124	0.985510
6	2.685129	-2.849680	0.646077
6	3.875851	-2.813414	-0.058519
6	4.408461	-1.585030	-0.392225
6	3.725165	-0.449167	0.013211
1	2.218319	-3.803055	0.915358
1	4.379106	-3.741648	-0.345641
1	5.341036	-1.473317	-0.951554
6	0.820012	-1.634531	1.764017
6	0.735225	-2.404130	2.916950
6	-0.385393	-2.324800	3.715790
1	1.587487	-3.028437	3.198597
6	-1.268126	-0.737773	2.165363
6	-1.391487	-1.460826	3.339232
1	-0.466191	-2.913243	4.633544
1	-2.291510	-1.357726	3.949588
6	-2.305248	0.177804	1.696621
6	-3.432718	0.610899	2.381764
6	-2.888764	1.473309	-0.150054
6	-4.290706	1.504130	1.763073
1	-3.640922	0.267594	3.398153
6	-4.022934	1.946333	0.476155
1	-5.178724	1.856636	2.295336
1	-4.668999	2.647281	-0.059230
7	-0.178688	-0.835284	1.361098

7	-2.072003	0.625436	0.464511
7	2.590223	-0.466088	0.690631
6	4.264274	0.903187	-0.348167
8	5.205081	1.035581	-1.063250
8	3.613798	1.907092	0.193992
6	-2.457017	1.783071	-1.564090
8	-3.082165	2.550711	-2.234788
8	-1.413652	1.108366	-1.923320
44	-0.451057	0.092382	-0.520850
6	0.564999	2.268044	1.280825
6	1.051678	3.501386	1.655976
6	1.342069	4.430867	0.672197
6	1.120599	4.081123	-0.644289
6	0.632658	2.823178	-0.936786
1	0.338398	1.502569	2.030100
1	1.203371	3.721743	2.715245
1	1.738921	5.415949	0.932967
1	1.329912	4.773685	-1.462310
1	0.446993	2.502966	-1.964431
6	-2.593794	-1.701455	-1.588755
6	-3.187015	-2.841219	-2.089725
6	-2.439104	-3.999629	-2.180044
6	-1.120340	-3.962837	-1.766149
6	-0.607246	-2.780696	-1.275960
1	-3.150896	-0.762506	-1.529008
1	-4.228594	-2.805173	-2.416760
1	-2.876458	-4.919638	-2.578385
1	-0.477791	-4.844137	-1.829307
1	0.441690	-2.695772	-0.971467
7	-1.327604	-1.663853	-1.178543
7	0.368227	1.918688	0.007378
8	0.961487	-0.472474	-1.655179
8	1.906731	0.498235	-1.971084
1	2.869051	1.529588	0.687913
1	2.274782	0.129339	-2.785820

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 1 (Quartet)

E = -1860.95740151 a.u.

6	2.220671	-1.482454	1.166503
6	3.072356	-2.527057	0.822344
6	4.242814	-2.240352	0.143070
6	4.526178	-0.923958	-0.159160
6	3.621894	0.043921	0.247894
1	2.802794	-3.561414	1.057664
1	4.927074	-3.043445	-0.147010
1	5.431352	-0.616614	-0.689382
6	0.943431	-1.751119	1.855646

6	0.840311	-2.743066	2.823779
6	-0.378592	-2.949654	3.438909
1	1.721092	-3.320649	3.117766
6	-1.265997	-1.192771	2.102017
6	-1.455326	-2.166771	3.074387
1	-0.489708	-3.721454	4.205968
1	-2.436932	-2.332199	3.525054
6	-2.347464	-0.322240	1.626558
6	-3.509912	-0.087119	2.348294
6	-3.095811	1.032173	-0.080847
6	-4.483354	0.742588	1.825114
1	-3.640967	-0.533705	3.337073
6	-4.276282	1.307528	0.581893
1	-5.397951	0.943378	2.390640
1	-4.998099	1.965353	0.090416
7	-0.092300	-0.993491	1.508217
7	-2.146862	0.249412	0.432775
7	2.491442	-0.213663	0.886147
6	3.919861	1.486542	-0.037879
8	4.808774	1.817792	-0.754818
8	3.136428	2.334679	0.589775
6	-2.819626	1.573545	-1.466456
8	-3.588541	2.358610	-1.947570
8	-1.756198	1.086598	-1.983636
44	-0.363244	0.156361	-0.706460
6	0.061048	2.358822	1.320212
6	0.285859	3.622931	1.818325
6	0.473470	4.664811	0.925812
6	0.422138	4.395613	-0.427498
6	0.210048	3.097916	-0.845706
1	-0.085570	1.498126	1.982995
1	0.309902	3.783161	2.898680
1	0.654630	5.681347	1.286632
1	0.553039	5.183324	-1.172327
1	0.166264	2.831866	-1.905083
6	-2.009867	-2.143925	-1.731149
6	-2.318687	-3.374245	-2.270256
6	-1.296338	-4.277247	-2.498474
6	-0.001314	-3.903824	-2.188725
6	0.223797	-2.647903	-1.665977
1	-2.782700	-1.389229	-1.554611
1	-3.356573	-3.610201	-2.515541
1	-1.506746	-5.261867	-2.926442
1	0.843047	-4.574108	-2.365416
1	1.234589	-2.286644	-1.445619
7	-0.763122	-1.784565	-1.429241
7	0.043501	2.093751	0.013051
8	1.113539	0.005444	-1.874236
8	1.977235	1.110597	-1.882796
1	2.480842	1.809299	1.073746

1	2.463026	0.949787	-2.703116

[Ru^{III}(Htda-κ-N^2O)Py_2(OOH)]$^+$ Conformer 2 (Doublet)

E = -1861.00544635 a.u.

6	2.035289	-1.765951	0.773450
6	2.639147	-2.960343	0.387631
6	3.864126	-2.903757	-0.245373
6	4.455089	-1.667811	-0.431183
6	3.758263	-0.541120	-0.017503
1	2.140120	-3.919282	0.561355
1	4.355928	-3.816512	-0.593764
1	5.413902	-1.585248	-0.954092
6	0.791423	-1.768858	1.574052
6	0.715258	-2.621049	2.666900
6	-0.352282	-2.531882	3.535667
1	1.536074	-3.318600	2.854784
6	-1.204181	-0.773238	2.162508
6	-1.310193	-1.572873	3.288306
1	-0.424354	-3.186078	4.408398
1	-2.164616	-1.455492	3.958793
6	-2.208883	0.228346	1.816410
6	-3.256398	0.693922	2.599799
6	-2.849545	1.625610	0.064776
6	-4.103185	1.657888	2.079118
1	-3.409813	0.321548	3.615862
6	-3.906828	2.133043	0.790843
1	-4.927934	2.038333	2.688463
1	-4.552532	2.885461	0.330021
7	-0.172725	-0.882655	1.285929
7	-2.038109	0.714652	0.588766
7	2.567586	-0.577403	0.555915
6	4.277024	0.848781	-0.248847
8	3.549272	1.759710	-0.496259
8	5.579990	1.019867	-0.183495
6	-2.509364	1.952701	-1.370664
8	-3.139178	2.775754	-1.968742
8	-1.539724	1.231961	-1.829356
44	-0.524466	0.128455	-0.522834
6	0.888434	2.159300	1.185422
6	1.480331	3.353994	1.529403
6	1.646846	4.321884	0.556265
6	1.206859	4.048219	-0.723462
6	0.614937	2.830236	-0.985081
1	0.766004	1.357577	1.919671
1	1.815367	3.512634	2.557050
1	2.121225	5.278375	0.793810
1	1.317519	4.771222	-1.534419

1	0.247395	2.571049	-1.982891
6	-2.829621	-1.520849	-1.475073
6	-3.513685	-2.609712	-1.973110
6	-2.831613	-3.795602	-2.167940
6	-1.485286	-3.836381	-1.856783
6	-0.879510	-2.701371	-1.361128
1	-3.333167	-0.560285	-1.336161
1	-4.573905	-2.511867	-2.217118
1	-3.341765	-4.676196	-2.568822
1	-0.892056	-4.741093	-2.008661
1	0.193772	-2.674159	-1.144180
7	-1.535603	-1.558385	-1.163709
7	0.455580	1.891161	-0.046303
8	0.792798	-0.505783	-1.733768
8	1.881980	0.239325	-2.111534
1	6.016584	0.224995	0.141745
1	2.039839	0.854594	-1.370537

$[Ru^{III}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ Conformer 2 (Quartet)

E = -1860.94459970 a.u.

6	2.443772	-0.957789	1.061585
6	3.552487	-1.728097	0.710843
6	4.647952	-1.100189	0.156817
6	4.613223	0.274381	0.007255
6	3.451084	0.942909	0.369468
1	3.540052	-2.814654	0.839308
1	5.524653	-1.674842	-0.155753
1	5.458233	0.807871	-0.441531
6	1.262486	-1.578727	1.696249
6	1.398171	-2.657354	2.560985
6	0.265275	-3.185060	3.150454
1	2.387855	-3.053901	2.804162
6	-1.006628	-1.554977	1.971354
6	-0.961999	-2.633748	2.848424
1	0.339883	-4.029852	3.841100
1	-1.879345	-3.056616	3.266126
6	-2.269905	-0.956647	1.527110
6	-3.446507	-1.027081	2.259763
6	-3.349563	0.150878	-0.174855
6	-4.605347	-0.482002	1.740343
1	-3.446157	-1.484944	3.252583
6	-4.558317	0.108764	0.492646
1	-5.537715	-0.521028	2.311093
1	-5.429404	0.551822	0.002571
7	0.083253	-1.033593	1.419222
7	-2.226560	-0.357965	0.330649
7	2.376385	0.348939	0.860562

6	3.338992	2.431067	0.202377
8	2.345859	2.976473	-0.167944
8	4.420505	3.128125	0.478309
6	-3.227100	0.774738	-1.544357
8	-4.192774	1.276720	-2.046766
8	-2.043550	0.690424	-2.028459
44	-0.473299	0.124128	-0.802894
6	-0.313820	2.252463	1.399489
6	-0.408300	3.484708	2.010016
6	-0.836683	4.566527	1.263612
6	-1.154196	4.367539	-0.066464
6	-1.023672	3.104349	-0.606055
1	0.044291	1.370910	1.940492
1	-0.140363	3.587295	3.064243
1	-0.920518	5.559222	1.715841
1	-1.501041	5.186082	-0.701203
1	-1.239656	2.898109	-1.658912
6	-0.837982	-2.870458	-1.220562
6	-0.590893	-4.159510	-1.641114
6	0.616069	-4.436639	-2.257846
6	1.520652	-3.405733	-2.431927
6	1.187538	-2.140036	-1.993978
1	-1.784939	-2.604928	-0.738275
1	-1.348392	-4.932363	-1.492291
1	0.844184	-5.447448	-2.609161
1	2.480958	-3.567945	-2.927160
1	1.850845	-1.281129	-2.146724
7	0.029673	-1.873446	-1.391101
7	-0.608568	2.063200	0.116187
8	0.936589	0.581381	-1.946271
8	0.936354	1.922377	-2.339320
1	5.095830	2.572216	0.882964
1	1.442008	2.334870	-1.616930

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] (Doublet)

E = -1860.58547364 a.u.

6	2.113427	-1.660706	0.793904
6	2.756668	-2.848988	0.460938
6	3.996370	-2.781857	-0.147589
6	4.547612	-1.540480	-0.381049
6	3.794483	-0.419828	-0.058295
1	2.281180	-3.813222	0.670895
1	4.528986	-3.696493	-0.427414
1	5.538199	-1.408053	-0.822993
6	0.878251	-1.686697	1.603405
6	0.844545	-2.513548	2.719099
6	-0.227103	-2.462926	3.585582

1	1.702963	-3.160337	2.920976
6	-1.173726	-0.790616	2.163398
6	-1.236710	-1.567341	3.308360
1	-0.264518	-3.096655	4.475819
1	-2.101887	-1.481378	3.970684
6	-2.238314	0.138799	1.799340
6	-3.322527	0.551614	2.563943
6	-2.937825	1.479133	0.015786
6	-4.218346	1.455361	2.018881
1	-3.466609	0.184991	3.584371
6	-4.032699	1.925306	0.724425
1	-5.071891	1.795147	2.612943
1	-4.717758	2.630380	0.245423
7	-0.131330	-0.860280	1.284279
7	-2.081420	0.620246	0.565346
7	2.606606	-0.464146	0.519673
6	4.379217	0.943251	-0.302931
8	5.555804	1.128532	-0.214717
8	3.513212	1.878466	-0.578116
6	-2.608774	1.809550	-1.427877
8	-3.325101	2.571429	-2.025808
8	-1.584719	1.183529	-1.881555
44	-0.534328	0.125838	-0.502392
6	0.707884	2.233803	1.229661
6	1.272453	3.447132	1.559158
6	1.470969	4.382242	0.560991
6	1.091070	4.057362	-0.726305
6	0.536790	2.818229	-0.975203
1	0.558415	1.456105	1.985292
1	1.566916	3.640926	2.593337
1	1.927979	5.350950	0.784027
1	1.234004	4.752516	-1.556597
1	0.235769	2.504402	-1.977951
6	-2.691445	-1.688435	-1.482785
6	-3.281044	-2.826922	-1.991536
6	-2.498546	-3.945527	-2.207315
6	-1.151187	-3.868270	-1.907644
6	-0.642151	-2.690420	-1.400879
1	-3.275169	-0.777340	-1.320853
1	-4.348378	-2.820336	-2.225625
1	-2.932177	-4.864022	-2.614410
1	-0.480417	-4.714764	-2.075102
1	0.426391	-2.563643	-1.195166
7	-1.396961	-1.613279	-1.181164
7	0.344546	1.913437	-0.010542
8	0.903593	-0.408348	-1.716977
8	1.853916	0.425293	-2.020980
1	2.668642	1.445572	-0.845079

[Ru^{III}(Htda-κ-N^2O)Py_2(OO)] (Quartet)

E = -1860.54972846 a.u.

6	2.072082	-1.691461	0.894939
6	2.606010	-2.910269	0.483544
6	3.784789	-2.921841	-0.239935
6	4.398587	-1.720117	-0.526158
6	3.792851	-0.565185	-0.059374
1	2.080070	-3.838871	0.728933
1	4.216184	-3.868019	-0.582463
1	5.326185	-1.642282	-1.098149
6	0.833082	-1.651600	1.698682
6	0.779191	-2.422856	2.838457
6	-0.344360	-2.330227	3.675514
1	1.641907	-3.037361	3.106501
6	-1.260766	-0.718072	2.141534
6	-1.339832	-1.467272	3.324691
1	-0.409154	-2.919443	4.593901
1	-2.226735	-1.361909	3.956849
6	-2.270883	0.179668	1.716380
6	-3.441066	0.586821	2.386837
6	-2.872331	1.576802	-0.101536
6	-4.286721	1.491752	1.799939
1	-3.669463	0.191948	3.381050
6	-4.012805	2.015227	0.524275
1	-5.186636	1.808146	2.336911
1	-4.662055	2.730394	0.016548
7	-0.156197	-0.837025	1.298846
7	-2.057812	0.705504	0.482335
7	2.665932	-0.536626	0.630871
6	4.428629	0.764386	-0.323403
8	5.443937	0.884282	-0.934234
8	3.776327	1.779327	0.200372
6	-2.439261	1.930864	-1.507311
8	-3.052525	2.741746	-2.147532
8	-1.416326	1.253205	-1.911047
44	-0.498022	0.129536	-0.517438
6	0.603159	2.221965	1.309573
6	1.187030	3.416562	1.673192
6	1.613662	4.283375	0.681549
6	1.429142	3.917688	-0.636173
6	0.832660	2.705056	-0.919996
1	0.257479	1.499686	2.056481
1	1.306069	3.656211	2.732627
1	2.089357	5.234488	0.937968
1	1.749856	4.560631	-1.458558
1	0.646660	2.376002	-1.946567
6	-2.748970	-1.513245	-1.579447
6	-3.411160	-2.627277	-2.051314

6	-2.737576	-3.832182	-2.119705
6	-1.416602	-3.865635	-1.711452
6	-0.831179	-2.707539	-1.247836
1	-3.246764	-0.541372	-1.528432
1	-4.452450	-2.534930	-2.369193
1	-3.233134	-4.732861	-2.493905
1	-0.828497	-4.785722	-1.752443
1	0.217627	-2.683262	-0.931252
7	-1.479774	-1.544384	-1.175635
7	0.434355	1.864698	0.035596
8	1.020561	-0.330004	-1.617254
8	1.950211	0.214264	-2.241853
1	2.989259	1.408896	0.635968

[Ru^{III}(tda-κ-N^2O)Py_2(OOH)] (Doublet)

E = -1860.57736614 a.u.

6	2.046647	-1.821346	0.735981
6	2.758782	-2.982288	0.464267
6	4.025798	-2.849313	-0.082336
6	4.522550	-1.582602	-0.293344
6	3.697450	-0.482411	-0.059562
1	2.330646	-3.970411	0.666025
1	4.619503	-3.738303	-0.321944
1	5.536252	-1.397347	-0.659030
6	0.795201	-1.857475	1.511964
6	0.687530	-2.753888	2.571871
6	-0.385869	-2.690295	3.430959
1	1.501857	-3.462643	2.741889
6	-1.193516	-0.860888	2.132029
6	-1.328109	-1.706434	3.219540
1	-0.473868	-3.380311	4.274821
1	-2.187959	-1.603122	3.885452
6	-2.184310	0.166245	1.827283
6	-3.225404	0.612677	2.630697
6	-2.823235	1.628716	0.128328
6	-4.068929	1.598506	2.149158
1	-3.372414	0.207199	3.635232
6	-3.876045	2.112150	0.875078
1	-4.886713	1.965259	2.776466
1	-4.519906	2.879893	0.437820
7	-0.158543	-0.945610	1.257384
7	-2.010135	0.696299	0.617194
7	2.476002	-0.604082	0.438306
6	4.198445	0.933954	-0.346047
8	5.387828	1.105488	-0.157049
8	3.309775	1.719983	-0.732035
6	-2.506383	1.997750	-1.302119

8	-3.175958	2.821329	-1.865895
8	-1.533576	1.316740	-1.794181
44	-0.501829	0.164225	-0.513667
6	1.000072	2.047798	1.253549
6	1.653635	3.194133	1.643309
6	1.799317	4.222101	0.731936
6	1.279559	4.053471	-0.533604
6	0.635170	2.874683	-0.843722
1	0.902590	1.194440	1.929897
1	2.068841	3.259218	2.651598
1	2.334112	5.137436	1.002042
1	1.387965	4.818653	-1.305053
1	0.228695	2.686890	-1.841606
6	-2.778751	-1.498200	-1.515766
6	-3.438091	-2.587926	-2.044905
6	-2.724893	-3.747082	-2.285842
6	-1.375111	-3.759968	-1.988945
6	-0.794138	-2.625887	-1.460214
1	-3.304029	-0.555350	-1.336255
1	-4.503397	-2.511859	-2.275370
1	-3.214650	-4.628558	-2.710645
1	-0.757772	-4.642362	-2.173929
1	0.279370	-2.575287	-1.245975
7	-1.482098	-1.510378	-1.217847
7	0.484941	1.885118	0.037190
8	0.764502	-0.374270	-1.832180
8	1.793399	0.377273	-2.275537
1	2.188186	0.891799	-1.497932

[Ru^{III}(tda-κ-N^2O)Py_2(OOH)] (Quartet)

E = -1860.51713176 a.u.

6	1.988653	-1.890557	0.712176
6	2.719034	-3.048654	0.466308
6	4.000499	-2.925519	-0.039371
6	4.507200	-1.662819	-0.260796
6	3.666128	-0.572482	-0.069120
1	2.284568	-4.031648	0.674289
1	4.602186	-3.817656	-0.243728
1	5.529372	-1.483939	-0.604593
6	0.720204	-1.927697	1.455712
6	0.572779	-2.843343	2.471914
6	-0.552072	-2.781242	3.310940
1	1.384140	-3.544266	2.677582
6	-1.290822	-0.873325	2.055898
6	-1.456552	-1.782164	3.108734
1	-0.681652	-3.500915	4.123289
1	-2.338922	-1.692187	3.749216

6	-2.211480	0.158340	1.767144
6	-3.322892	0.604253	2.511241
6	-2.735388	1.741728	0.098094
6	-4.105520	1.618603	2.028081
1	-3.551936	0.151449	3.480283
6	-3.828065	2.211549	0.781591
1	-4.960376	1.964862	2.616757
1	-4.444655	2.998677	0.344429
7	-0.194014	-0.968885	1.197894
7	-1.967935	0.777646	0.587927
7	2.436411	-0.682234	0.390798
6	4.165422	0.847174	-0.364938
8	5.359328	1.016789	-0.159633
8	3.308423	1.646020	-0.766577
6	-2.319832	2.135695	-1.290628
8	-2.836220	3.035873	-1.886204
8	-1.384026	1.361233	-1.779120
44	-0.446613	0.189214	-0.515779
6	1.012865	1.962721	1.368158
6	1.665177	3.080639	1.835293
6	1.867713	4.146180	0.978263
6	1.413680	4.042097	-0.319102
6	0.778332	2.884625	-0.714789
1	0.847802	1.085948	2.000207
1	2.019876	3.100703	2.868201
1	2.391266	5.044642	1.318066
1	1.565841	4.840682	-1.047749
1	0.419597	2.746347	-1.739632
6	-2.821035	-1.348243	-1.495270
6	-3.543127	-2.411117	-1.995241
6	-2.895656	-3.610892	-2.221421
6	-1.545073	-3.693778	-1.941182
6	-0.895521	-2.582478	-1.446347
1	-3.293734	-0.379293	-1.311495
1	-4.607152	-2.284551	-2.207292
1	-3.439203	-4.473397	-2.618738
1	-0.980642	-4.613775	-2.109168
1	0.179388	-2.589198	-1.236381
7	-1.522341	-1.429629	-1.221914
7	0.569798	1.864675	0.116274
8	0.752405	-0.417250	-1.893343
8	1.795357	0.298433	-2.352569
1	2.181753	0.816530	-1.584588

$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+$ (Doublet)

E = -1709.53019396 a.u.

6	-2.299306	-0.111048	1.674835

6	-3.617950	-0.130994	2.105074
6	-4.640467	-0.058255	1.179808
6	-4.307184	0.031517	-0.156013
6	-2.969929	0.044974	-0.501630
1	-3.846457	-0.202958	3.171153
1	-5.684691	-0.071985	1.504259
1	-5.043620	0.092692	-0.961968
6	-1.146339	-0.180942	2.563499
6	-1.193910	-0.287982	3.947780
6	0.000037	-0.341826	4.640364
1	-2.144305	-0.330536	4.484453
6	1.146377	-0.180942	2.563479
6	1.193972	-0.287986	3.947759
1	0.000047	-0.426885	5.730690
1	2.144376	-0.330549	4.484415
6	2.299328	-0.111051	1.674795
6	3.617978	-0.130970	2.105014
6	2.969918	0.044916	-0.501684
6	4.640481	-0.058251	1.179732
1	3.846502	-0.202894	3.171092
6	4.307177	0.031473	-0.156087
1	5.684711	-0.071959	1.504168
1	5.043600	0.092626	-0.962056
7	0.000013	-0.130936	1.903115
7	1.977375	-0.022629	0.378735
7	-1.977375	-0.022592	0.378773
6	-2.536207	0.136160	-1.926175
8	-1.254701	0.130785	-2.040015
8	-3.328817	0.202226	-2.818925
6	2.536177	0.136071	-1.926225
8	3.328774	0.202084	-2.818990
8	1.254669	0.130726	-2.040047
44	0.000001	0.033844	-0.552591
6	0.000045	-2.907502	0.161169
6	0.000037	-4.266423	-0.065489
6	-0.000049	-4.724121	-1.371465
6	-0.000122	-3.795029	-2.393440
6	-0.000106	-2.449668	-2.082501
1	0.000111	-2.503102	1.178643
1	0.000097	-4.955402	0.782468
1	-0.000059	-5.796381	-1.587847
1	-0.000191	-4.099144	-3.442613
1	-0.000160	-1.673829	-2.853827
6	0.000035	2.853056	0.544338
6	0.000039	4.230071	0.500849
6	0.000027	4.857757	-0.732466
6	0.000007	4.073414	-1.869368
6	0.000002	2.698581	-1.740667
1	0.000039	2.316368	1.498653
1	0.000051	4.799887	1.432996

1	0.000030	5.949309	-0.803815
1	-0.000009	4.514985	-2.868568
1	-0.000020	2.031973	-2.608396
7	0.000021	2.094081	-0.550596
7	-0.000024	-2.009053	-0.822566

[Ru^{III}(tda-κ-N^2O^2)Py_2]$^+$ • □□□□) (Doublet)

E = -1785.93220232 a.u.

6	-0.714284	2.705351	-0.775270
6	-1.513946	3.816091	-1.003707
6	-2.833659	3.801863	-0.597632
6	-3.313992	2.669987	0.029978
6	-2.447041	1.614025	0.231067
1	-1.105419	4.692815	-1.512167
1	-3.478153	4.667245	-0.775623
1	-4.344665	2.565436	0.379399
6	0.677453	2.593085	-1.194941
6	1.423751	3.590125	-1.809788
6	2.728003	3.304730	-2.164747
1	1.001497	4.577639	-2.009558
6	2.427151	1.114204	-1.290058
6	3.245426	2.049033	-1.912130
1	3.346301	4.067296	-2.646557
1	4.273199	1.809814	-2.194468
6	2.796649	-0.255843	-0.958013
6	4.016096	-0.834366	-1.277687
6	2.091452	-2.194217	0.025565
6	4.262918	-2.147709	-0.929695
1	4.775523	-0.254720	-1.808076
6	3.276669	-2.842694	-0.260298
1	5.218291	-2.617758	-1.179042
1	3.380555	-3.882121	0.063104
7	1.183248	1.397481	-0.936413
7	1.838325	-0.933980	-0.313940
7	-1.176300	1.614993	-0.156139
6	-2.868548	0.367281	0.928065
8	-1.887876	-0.427261	1.131170
8	-4.009703	0.184156	1.262022
6	0.997547	-2.868797	0.784765
8	1.094223	-4.004014	1.146449
8	0.007209	-2.077040	1.004759
44	-0.131927	-0.276230	0.286370
6	1.413714	1.388286	2.303848
6	1.843136	1.790544	3.549820
6	1.362654	1.129065	4.665937
6	0.470144	0.091458	4.479966
6	0.089649	-0.249688	3.197328

1	1.769794	1.887406	1.397075
1	2.551030	2.618299	3.635525
1	1.682674	1.421582	5.670219
1	0.059193	-0.466632	5.324393
1	-0.611951	-1.064413	2.996355
6	-0.609255	-0.773787	-2.650709
6	-1.192807	-1.339501	-3.761952
6	-2.184175	-2.290930	-3.584100
6	-2.538513	-2.639250	-2.296628
6	-1.894111	-2.038157	-1.232025
1	0.171413	-0.011299	-2.744469
1	-0.871068	-1.026995	-4.758337
1	-2.674646	-2.751344	-4.447071
1	-3.323496	-3.367817	-2.080863
1	-2.167479	-2.289779	-0.201620
7	-0.950402	-1.110151	-1.406071
7	0.553469	0.387810	2.120610
8	-4.160208	-2.695565	0.666176
1	-4.114013	-3.248368	1.447466
1	-4.293818	-1.808587	1.021343

$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O^2)Py_2]^+ \bullet$ □□□□)$_2$ (Doublet)

E = -1862.33811808 a.u.

6	0.671164	2.909133	0.183830
6	0.434371	4.268983	0.325282
6	-0.843453	4.715215	0.598127
6	-1.852416	3.780749	0.718514
6	-1.531737	2.445734	0.572837
1	1.252845	4.984222	0.213477
1	-1.046117	5.784011	0.709069
1	-2.894397	4.040817	0.923648
6	1.970213	2.328288	-0.134254
6	3.157673	3.031647	-0.291319
6	4.300717	2.322796	-0.606382
1	3.198623	4.116400	-0.169430
6	3.004729	0.329550	-0.579275
6	4.233781	0.951280	-0.758631
1	5.253011	2.844577	-0.736288
1	5.130136	0.381049	-1.012696
6	2.747020	-1.100612	-0.702385
6	3.711172	-2.044731	-1.025083
6	1.149224	-2.727843	-0.554270
6	3.360544	-3.377067	-1.115398
1	4.743240	-1.735615	-1.207215
6	2.047746	-3.727098	-0.870691
1	4.109463	-4.131822	-1.370970
1	1.679437	-4.755852	-0.910858

7	1.912623	1.012589	-0.271681
7	1.473330	-1.440280	-0.474519
7	-0.304153	2.004129	0.315853
6	-2.558814	1.373588	0.697245
8	-2.039343	0.202426	0.620034
8	-3.720641	1.622045	0.862941
6	-0.280625	-3.022397	-0.253622
8	-0.727067	-4.133342	-0.262391
8	-0.939819	-1.953384	0.015794
44	-0.197844	-0.160668	0.082062
6	1.254394	0.010803	2.730533
6	1.484596	-0.191624	4.073422
6	0.567286	-0.926539	4.803615
6	-0.541614	-1.424243	4.148854
6	-0.700294	-1.177611	2.798759
1	1.954779	0.591387	2.122263
1	2.380212	0.229866	4.536051
1	0.717450	-1.106149	5.872228
1	-1.302388	-2.009227	4.670827
1	-1.571024	-1.561293	2.254805
6	0.020281	0.451423	-2.864554
6	-0.382838	0.549614	-4.177578
6	-1.680879	0.195906	-4.506108
6	-2.513894	-0.246121	-3.498511
6	-2.032535	-0.324928	-2.205278
1	1.038383	0.720737	-2.565301
1	0.323185	0.902945	-4.932977
1	-2.033582	0.266280	-5.539409
1	-3.551379	-0.535455	-3.682407
1	-2.692324	-0.661384	-1.396244
7	-0.783468	0.026246	-1.888685
7	0.185979	-0.469433	2.093794
8	-4.721289	-0.721142	-0.720824
1	-4.801045	-1.476172	-0.126208
1	-4.759180	0.034136	-0.123806
8	-3.470157	-2.413688	1.207944
1	-3.027325	-3.175460	0.820495
1	-3.015394	-1.678055	0.782823

$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(OH_2)]^+$ (Doublet)

E = -1785.86502648 a.u.

6	-2.050533	0.045170	1.824561
6	-3.192167	0.263800	2.564230
6	-4.279435	0.896800	1.981456
6	-4.185910	1.259563	0.664042
6	-2.987411	1.068394	-0.025481
1	-3.245885	-0.067222	3.603243

1	-5.191215	1.076352	2.557926
1	-5.022905	1.708585	0.123564
6	-0.909180	-0.684447	2.371120
6	-0.844786	-1.299544	3.612418
6	0.301248	-1.989711	3.960622
1	-1.686602	-1.258568	4.305947
6	1.254887	-1.419635	1.854838
6	1.364248	-2.057904	3.080299
1	0.364407	-2.485779	4.932699
1	2.270965	-2.602013	3.352760
6	2.282702	-1.325202	0.824061
6	3.540692	-1.869440	0.963299
6	2.895883	-0.252121	-1.136710
6	4.505105	-1.610189	-0.000562
1	3.783625	-2.481065	1.835087
6	4.190728	-0.758198	-1.028618
1	5.504483	-2.045856	0.087255
1	4.930680	-0.462289	-1.776663
7	0.133887	-0.757907	1.537909
7	1.934618	-0.580919	-0.266198
7	-1.926067	0.480003	0.537343
6	-2.970903	1.467603	-1.495174
8	-2.208384	2.364295	-1.854981
8	-3.771695	0.793192	-2.130088
6	2.560712	0.798105	-2.175515
8	2.863157	1.917411	-1.780658
8	2.030435	0.424709	-3.220795
44	-0.029029	0.033800	-0.224933
6	-0.190596	-2.950261	-0.702061
6	-0.644240	-4.136788	-1.231323
6	-1.709672	-4.110401	-2.114279
6	-2.267709	-2.887280	-2.427973
6	-1.745227	-1.741836	-1.863882
1	0.655497	-2.947376	-0.010774
1	-0.154768	-5.072246	-0.951052
1	-2.094915	-5.034728	-2.554513
1	-3.108870	-2.795926	-3.118524
1	-2.160552	-0.765652	-2.118739
6	1.702022	1.957210	1.282459
6	2.286424	3.153134	1.626726
6	1.808233	4.317801	1.054518
6	0.743574	4.227043	0.180595
6	0.210468	2.989599	-0.112259
1	2.069415	1.022792	1.715045
1	3.122214	3.159986	2.329730
1	2.262942	5.284388	1.289858
1	0.316972	5.111367	-0.297771
1	-0.648724	2.887673	-0.784355
7	0.684969	1.860974	0.422570
7	-0.721626	-1.763741	-1.004520

8	-0.298187	0.673527	-2.172424
1	-0.838804	1.467980	-2.345468
1	0.471290	0.650879	-2.784804

[Ru^{III}(tda-κ-N^3)Py_2(OH)] (Doublet)

E = -1785.44748634 a.u.

6	-2.109779	0.051907	1.765346
6	-3.219631	0.358847	2.523203
6	-4.085548	1.346146	2.080908
6	-3.805425	1.974515	0.896327
6	-2.652287	1.652907	0.171379
1	-3.408943	-0.167389	3.461213
1	-4.972144	1.608121	2.666851
1	-4.462556	2.747353	0.488530
6	-1.176304	-1.003099	2.142188
6	-1.326364	-1.900313	3.187271
6	-0.373128	-2.886990	3.367069
1	-2.192730	-1.847590	3.849779
6	0.811751	-2.045886	1.477775
6	0.701462	-2.973153	2.504139
1	-0.477350	-3.605435	4.184798
1	1.452748	-3.755192	2.634133
6	1.881722	-1.960935	0.494715
6	2.957988	-2.822867	0.472585
6	2.882096	-0.536676	-1.033178
6	4.014985	-2.556953	-0.382771
1	2.987623	-3.684749	1.143822
6	4.006478	-1.365595	-1.064472
1	4.868643	-3.238924	-0.439532
1	4.876143	-1.011766	-1.622787
7	-0.110622	-1.082048	1.333243
7	1.785378	-0.905323	-0.365391
7	-1.818105	0.705388	0.609010
6	-2.431393	2.428622	-1.139323
8	-1.724535	3.418819	-1.019174
8	-3.090668	1.970088	-2.064594
6	3.096341	0.906321	-1.553758
8	4.092159	1.334343	-0.985660
8	2.342657	1.408143	-2.378196
44	-0.051835	0.061791	-0.278391
6	-0.919346	-2.713052	-1.221144
6	-1.649560	-3.642778	-1.929654
6	-2.678504	-3.200794	-2.740985
6	-2.919009	-1.843775	-2.805786
6	-2.138122	-0.973408	-2.068046
1	-0.087202	-3.036314	-0.589173
1	-1.398203	-4.702940	-1.844850

1	-3.278941	-3.909648	-3.319919
1	-3.711670	-1.428164	-3.432462
1	-2.300551	0.111843	-2.124722
6	1.872576	1.402012	1.562603
6	2.702122	2.374402	2.069930
6	2.667177	3.635139	1.503979
6	1.781804	3.865900	0.472822
6	0.973344	2.840385	0.023685
1	1.888631	0.385788	1.970832
1	3.385933	2.127446	2.885104
1	3.329765	4.427714	1.864649
1	1.706266	4.841261	-0.012202
1	0.231175	2.997551	-0.765574
7	1.023318	1.618191	0.557348
7	-1.152961	-1.404530	-1.276083
8	-0.135993	0.881417	-1.952186
1	0.693416	1.333007	-2.218514

[Ru^{III}(tda-κ-N^3)Py_2(OH)]•(H_2O) (Doublet)

E = -1861.86313255 a.u.

6	-2.643333	-0.667546	1.137899
6	-3.983805	-0.938632	1.336114
6	-4.774383	-1.252176	0.244234
6	-4.185253	-1.317459	-0.996177
6	-2.816330	-1.099382	-1.134739
1	-4.413144	-0.886198	2.339462
1	-5.844113	-1.444272	0.374756
1	-4.746912	-1.538865	-1.907557
6	-1.715447	-0.368677	2.221110
6	-1.976348	-0.449327	3.580225
6	-0.947925	-0.214814	4.473818
1	-2.974307	-0.706458	3.942016
6	0.522122	0.168016	2.636055
6	0.315715	0.092185	4.004277
1	-1.132925	-0.275469	5.549755
1	1.134341	0.283278	4.701757
6	1.756401	0.544103	1.960156
6	2.961710	0.736577	2.606589
6	2.660845	1.180641	-0.083936
6	4.069433	1.098100	1.858483
1	3.042387	0.573515	3.683927
6	3.915671	1.315982	0.510089
1	5.046469	1.207730	2.339262
1	4.758404	1.584461	-0.132513
7	-0.487915	-0.058183	1.783168
7	1.622180	0.740884	0.628116
7	-2.071632	-0.736238	-0.089021

6	-2.157886	-1.337840	-2.501222
8	-1.146717	-2.044104	-2.434670
8	-2.761733	-0.819957	-3.424815
6	2.437293	1.675357	-1.521542
8	3.105222	1.108583	-2.386191
8	1.674271	2.626656	-1.541212
44	-0.139535	0.027173	-0.167046
6	1.921201	-1.942796	-0.834330
6	2.602316	-3.140297	-0.913666
6	2.056026	-4.256582	-0.313290
6	0.844250	-4.129465	0.343287
6	0.235873	-2.894822	0.383019
1	2.311954	-1.045690	-1.329334
1	3.561294	-3.146081	-1.436423
1	2.565373	-5.224339	-0.358302
1	0.358748	-4.983866	0.821173
1	-0.728704	-2.751893	0.881766
6	-0.709274	2.881445	0.495008
6	-1.137560	4.175913	0.306001
6	-1.847833	4.477335	-0.841070
6	-2.101490	3.464554	-1.743492
6	-1.638053	2.191970	-1.477584
1	-0.118711	2.604550	1.375168
1	-0.891017	4.939874	1.046925
1	-2.191700	5.498444	-1.032621
1	-2.646752	3.646099	-2.672233
1	-1.789697	1.369557	-2.185407
7	-0.956214	1.904425	-0.370509
7	0.764188	-1.815449	-0.185658
8	0.161144	0.170376	-2.004242
1	0.160024	-0.705746	-2.435462
8	4.845833	-0.932780	-1.761836
1	4.253691	-0.192391	-1.986366
1	5.322795	-1.074307	-2.580581

[Ru^{II}(tda-κ-N^2O)Py_2(OH)] (Doublet)

E = -1785.46785542 a.u.

6	2.314960	0.885756	1.085892
6	3.488262	1.584583	1.268763
6	3.543250	2.911133	0.867919
6	2.384678	3.497680	0.428368
6	1.230166	2.729723	0.237899
1	4.349021	1.108495	1.744677
1	4.468020	3.487372	0.972519
1	2.327371	4.570860	0.228025
6	2.076203	-0.436149	1.660669
6	2.945217	-1.141174	2.489283
6	2.491803	-2.308625	3.072582

1	3.954432	-0.778695	2.699568
6	0.427084	-2.001729	1.951071
6	1.206744	-2.753534	2.818346
1	3.149351	-2.879987	3.734927
1	0.834148	-3.681073	3.262060
6	-0.903913	-2.351583	1.456145
6	-1.759875	-3.293689	2.006295
6	-2.307795	-2.009385	-0.312279
6	-2.952803	-3.566051	1.360073
1	-1.499908	-3.801276	2.940143
6	-3.224854	-2.930985	0.163027
1	-3.653150	-4.293546	1.782447
1	-4.115467	-3.134513	-0.437413
7	0.860505	-0.881707	1.403458
7	-1.199872	-1.695247	0.336475
7	1.237250	1.411804	0.461987
6	-0.085671	3.528158	0.076054
8	-0.662313	3.613616	-1.003424
8	-0.319551	4.016902	1.173269
6	-2.390452	-1.395702	-1.680883
8	-3.332773	-1.635724	-2.391399
8	-1.346666	-0.723293	-1.976177
44	-0.135371	0.135685	-0.636240
6	-1.959062	1.345968	1.362529
6	-3.067488	1.994242	1.859819
6	-4.023439	2.450674	0.972083
6	-3.826536	2.240787	-0.378515
6	-2.686083	1.589134	-0.796335
1	-1.158997	0.980665	2.016829
1	-3.158936	2.156147	2.935959
1	-4.911285	2.979405	1.332051
1	-4.542807	2.593000	-1.123770
1	-2.468094	1.411430	-1.854461
6	1.423758	-2.196996	-1.600662
6	2.434650	-2.908396	-2.211469
6	3.521987	-2.219239	-2.717199
6	3.540359	-0.843088	-2.595887
6	2.483847	-0.206758	-1.974888
1	0.532016	-2.692699	-1.202492
1	2.356198	-3.995196	-2.294165
1	4.341944	-2.750638	-3.210207
1	4.367037	-0.247052	-2.990661
1	2.415984	0.882890	-1.894364
7	1.444304	-0.872582	-1.474999
7	-1.769004	1.140567	0.060855
8	0.233825	1.353097	-1.997132
1	-0.172978	2.229104	-1.814853

$[Ru^{III}(tda\text{-}\kappa\text{-}N^2O)Py_2(OH)]\bullet(H_2O)$ (Doublet)

E = -1861.87546235 a.u.

6	-0.727139	-2.389125	1.045624
6	-0.836966	-3.758618	1.160190
6	0.208293	-4.550007	0.712180
6	1.355021	-3.921786	0.297322
6	1.390769	-2.529676	0.172732
1	-1.724877	-4.207292	1.612367
1	0.144529	-5.641400	0.762029
1	2.264820	-4.483399	0.070146
6	-1.661225	-1.459544	1.679071
6	-2.681030	-1.801901	2.562296
6	-3.365882	-0.783594	3.197602
1	-2.923005	-2.845211	2.779316
6	-2.023846	0.777003	2.022504
6	-3.034344	0.534626	2.942386
1	-4.167178	-1.021396	3.903837
1	-3.571167	1.353663	3.429124
6	-1.597957	2.083547	1.524398
6	-1.880719	3.311917	2.102303
6	-0.613948	3.083389	-0.277731
6	-1.475167	4.463265	1.450971
1	-2.404259	3.366385	3.061534
6	-0.852044	4.351430	0.222399
1	-1.671291	5.444397	1.894643
1	-0.555415	5.212711	-0.381934
7	-1.367434	-0.199065	1.423355
7	-0.937402	1.978673	0.373019
7	0.316383	-1.782021	0.439733
6	2.803619	-1.927250	0.019057
8	3.180986	-1.401384	-1.025886
8	3.396871	-2.138563	1.072931
6	-0.116110	2.828258	-1.670207
8	0.163044	3.750759	-2.391114
8	-0.132059	1.586750	-1.973334
44	-0.030749	0.111247	-0.638965
6	2.100002	0.851265	1.285262
6	3.329782	1.285437	1.724693
6	4.221050	1.805239	0.804554
6	3.822054	1.905408	-0.514091
6	2.579389	1.436297	-0.876863
1	1.369323	0.396679	1.964957
1	3.595817	1.171170	2.777725
1	5.227203	2.103334	1.107573
1	4.488586	2.304035	-1.281838
1	2.232320	1.443061	-1.915654
6	-2.860843	0.074607	-1.532053
6	-4.020457	-0.376619	-2.126102
6	-4.040985	-1.651054	-2.662806

6	-2.890740	-2.412805	-2.588053
6	-1.769896	-1.883042	-1.980275
1	-2.786806	1.082626	-1.110003
1	-4.894063	0.278322	-2.171098
1	-4.943161	-2.041670	-3.143622
1	-2.845813	-3.419978	-3.009881
1	-0.814980	-2.416845	-1.935888
7	-1.755331	-0.661280	-1.450400
7	1.732272	0.905440	0.006510
8	0.774173	-0.860898	-2.012977
1	1.730693	-0.987154	-1.843535
8	5.754497	-0.664552	0.263031
1	5.191319	-0.738016	-0.515569
1	5.226742	-1.198015	0.869324

$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^-$ (Doublet)

E = -1784.88810110 a.u.

6	-2.226399	-0.647218	1.493387
6	-3.510103	-0.843606	1.979011
6	-4.586309	-0.389749	1.244603
6	-4.344540	0.263303	0.057539
6	-3.037968	0.480425	-0.377305
1	-3.660232	-1.361814	2.929360
1	-5.608923	-0.550187	1.605342
1	-5.159083	0.634254	-0.570806
6	-1.043393	-1.114943	2.186714
6	-1.004604	-1.806195	3.381897
6	0.218680	-2.192575	3.912782
1	-1.930733	-2.052645	3.908865
6	1.304083	-1.206026	2.021033
6	1.380547	-1.899494	3.214541
1	0.264375	-2.735665	4.860469
1	2.350282	-2.218691	3.607298
6	2.401911	-0.852855	1.145106
6	3.719686	-1.197723	1.415715
6	3.014367	0.180836	-0.849305
6	4.697890	-0.894260	0.493056
1	3.966742	-1.717973	2.344776
6	4.333021	-0.221687	-0.652651
1	5.739795	-1.182201	0.676533
1	5.048133	0.037725	-1.437891
7	0.103703	-0.798523	1.533811
7	2.051811	-0.175710	0.014369
7	-1.996708	0.009559	0.321113
6	-2.851891	1.314507	-1.655311
8	-2.589721	2.487234	-1.419973
8	-3.099936	0.695777	-2.686778

6	2.770326	1.165874	-2.007797
8	2.326515	2.238552	-1.603911
8	3.180845	0.776806	-3.091418
44	0.003043	0.092351	-0.217486
6	0.403105	-2.847406	-0.820565
6	0.245830	-4.043202	-1.489924
6	-0.618579	-4.090273	-2.568290
6	-1.285277	-2.934544	-2.922968
6	-1.071790	-1.771363	-2.206418
1	1.086360	-2.768667	0.031954
1	0.809686	-4.921538	-1.164436
1	-0.767618	-5.021480	-3.125804
1	-1.982275	-2.910074	-3.764551
1	-1.573407	-0.827009	-2.466191
6	0.357636	2.282787	1.794993
6	0.467650	3.561813	2.294276
6	0.357777	4.623524	1.412959
6	0.147287	4.349759	0.079457
6	0.056343	3.036952	-0.347083
1	0.434842	1.411803	2.454944
1	0.637832	3.712065	3.363873
1	0.437408	5.656532	1.770464
1	0.052883	5.147441	-0.660603
1	-0.102367	2.752597	-1.389927
7	0.155163	2.020761	0.507021
7	-0.235127	-1.734464	-1.165059
8	-0.130354	0.771724	-1.855393

$[Ru^{III}(tda\text{-}\kappa\text{-}N^3)Py_2(O)]^-$ (Quartet)

E = -1784.86499154 a.u.

6	-2.216954	-0.583741	1.499781
6	-3.512965	-0.743216	1.986583
6	-4.577973	-0.265092	1.261434
6	-4.333197	0.377383	0.060264
6	-3.025958	0.549110	-0.383930
1	-3.671846	-1.253786	2.940360
1	-5.600858	-0.395074	1.633644
1	-5.142804	0.767056	-0.561747
6	-1.052898	-1.058925	2.191505
6	-1.010671	-1.726152	3.404751
6	0.209681	-2.130562	3.922139
1	-1.931746	-1.941661	3.954564
6	1.307338	-1.217919	2.007830
6	1.388737	-1.891970	3.206176
1	0.250261	-2.653044	4.881965
1	2.348607	-2.240639	3.595862
6	2.404433	-0.899991	1.110569

6	3.716492	-1.276128	1.363081
6	3.024729	0.126290	-0.888686
6	4.694324	-0.992289	0.434018
1	3.959085	-1.804763	2.288828
6	4.335398	-0.304841	-0.708297
1	5.730627	-1.303937	0.608858
1	5.047983	-0.054001	-1.498282
7	0.116188	-0.788592	1.546131
7	2.063018	-0.209252	-0.018362
7	-1.990170	0.066323	0.308662
6	-2.804807	1.333565	-1.685292
8	-2.474926	2.499236	-1.502435
8	-3.068767	0.687710	-2.698141
6	2.778085	1.120375	-2.038197
8	2.284754	2.172973	-1.635327
8	3.217578	0.757680	-3.119586
44	0.004281	0.115821	-0.265094
6	0.346502	-2.860229	-0.766561
6	0.130155	-4.079631	-1.374048
6	-0.786159	-4.155250	-2.406605
6	-1.442523	-3.000832	-2.784058
6	-1.171208	-1.814103	-2.129394
1	1.071229	-2.761570	0.047862
1	0.687833	-4.956023	-1.033558
1	-0.981995	-5.106872	-2.912533
1	-2.176381	-2.994923	-3.593792
1	-1.674790	-0.874259	-2.408485
6	0.416419	2.244614	1.805241
6	0.547801	3.512233	2.328427
6	0.440534	4.594459	1.473188
6	0.208981	4.353346	0.136704
6	0.097022	3.051651	-0.315574
1	0.487925	1.359088	2.444514
1	0.731767	3.636456	3.398889
1	0.537298	5.618130	1.851912
1	0.113310	5.166721	-0.585594
1	-0.083780	2.810016	-1.363857
7	0.196100	2.013876	0.513475
7	-0.285798	-1.749423	-1.130453
8	-0.115313	0.755335	-1.897980

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 1 (Closed-shell singlet)

E = -1785.57012892 a.u.

6	-1.905383	-1.550718	1.109699
6	-2.821932	-2.564130	1.306866
6	-2.534031	-3.818183	0.802024
6	-1.307910	-4.022068	0.203188

6	-0.439996	-2.952392	0.018390
1	-3.750607	-2.378929	1.851560
1	-3.241780	-4.643499	0.920373
1	-0.992245	-5.020777	-0.112324
6	-1.948976	-0.243039	1.724950
6	-2.794172	0.128711	2.757915
6	-2.565568	1.315078	3.426112
1	-3.605416	-0.534278	3.066894
6	-0.696694	1.682734	1.995740
6	-1.480929	2.087613	3.061841
1	-3.214814	1.621803	4.250498
1	-1.246439	3.012750	3.593830
6	0.428059	2.391949	1.442649
6	1.058504	3.521635	1.941117
6	1.752862	2.429544	-0.439700
6	2.099695	4.084380	1.225056
1	0.734311	3.959477	2.888926
6	2.439307	3.543561	-0.003942
1	2.619658	4.965738	1.611042
1	3.205856	3.973191	-0.655972
7	-0.946338	0.549801	1.321172
7	0.811423	1.845679	0.285943
7	-0.771130	-1.721892	0.406421
6	0.990695	-3.330146	-0.348865
8	1.324219	-3.450476	-1.596384
8	1.688768	-3.634526	0.562183
6	1.823591	1.850759	-1.808746
8	2.602654	2.178899	-2.641013
8	0.834540	1.014202	-1.967051
44	0.033574	0.066568	-0.443543
6	2.194662	-0.769029	1.434321
6	3.421967	-1.223875	1.856377
6	4.377817	-1.539046	0.905298
6	4.067750	-1.372397	-0.431099
6	2.815676	-0.907745	-0.775230
1	1.395019	-0.538108	2.147555
1	3.615180	-1.346381	2.924304
1	5.358457	-1.917940	1.206983
1	4.784296	-1.608899	-1.220616
1	2.513523	-0.781113	-1.819708
6	-1.967335	2.032684	-1.453829
6	-3.096720	2.529884	-2.067753
6	-4.058174	1.641324	-2.515442
6	-3.845454	0.287136	-2.329630
6	-2.687141	-0.127563	-1.706270
1	-1.170499	2.700707	-1.111073
1	-3.206498	3.608229	-2.203797
1	-4.961391	2.001526	-3.016421
1	-4.565316	-0.457103	-2.678190
1	-2.457059	-1.190509	-1.574977

7	-1.763086	0.729053	-1.268720
7	1.890968	-0.620721	0.143588
8	0.009995	-1.213228	-1.853485
1	0.713305	-2.918477	-2.129943
1	-0.160086	-0.708764	-2.662098

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^{2+}$ Conformer 1 (Triplet)

E = -1785.54510774 a.u.

6	2.167278	-1.711738	0.760795
6	3.092982	-2.749021	0.686954
6	4.330270	-2.496241	0.124814
6	4.603586	-1.216385	-0.312475
6	3.580273	-0.276380	-0.274120
1	2.853416	-3.749264	1.058828
1	5.082091	-3.287456	0.054610
1	5.583760	-0.924388	-0.700108
6	0.927343	-1.838650	1.536994
6	0.877554	-2.715153	2.619658
6	-0.217218	-2.730934	3.451940
1	1.740514	-3.348134	2.837374
6	-1.146608	-0.998396	2.108913
6	-1.240228	-1.838142	3.202846
1	-0.262186	-3.411207	4.306736
1	-2.117382	-1.803707	3.852509
6	-2.195221	-0.046557	1.768355
6	-3.307323	0.301052	2.523534
6	-2.869103	1.401051	0.071766
6	-4.195566	1.238898	2.023931
1	-3.482638	-0.145666	3.505050
6	-3.984644	1.801036	0.771451
1	-5.069181	1.526821	2.616379
1	-4.665292	2.531195	0.324117
7	-0.090515	-1.008999	1.264856
7	-2.007638	0.523471	0.579373
7	2.382954	-0.512034	0.234947
6	3.892919	1.121051	-0.737876
8	2.929641	1.765108	-1.341513
8	4.964569	1.589804	-0.528784
6	-2.516461	1.825459	-1.323673
8	-3.120166	2.652078	-1.921583
8	-1.510820	1.124494	-1.798309
44	-0.388058	0.175134	-0.542454
6	0.914884	2.095438	1.329134
6	1.489911	3.265602	1.766237
6	1.492214	4.366977	0.925247
6	0.911611	4.248654	-0.323840
6	0.356082	3.043072	-0.691254

1	0.914889	1.194772	1.949113
1	1.942156	3.304605	2.759778
1	1.951924	5.308075	1.240832
1	0.896896	5.080423	-1.031385
1	-0.088170	2.903270	-1.681412
6	-2.488152	-1.705314	-1.613852
6	-3.007741	-2.842330	-2.194884
6	-2.156149	-3.890194	-2.491946
6	-0.811127	-3.755610	-2.192164
6	-0.371490	-2.589905	-1.604803
1	-3.130484	-0.849012	-1.390437
1	-4.074896	-2.888674	-2.423302
1	-2.535108	-4.801398	-2.963731
1	-0.092668	-4.544871	-2.425122
1	0.688542	-2.423847	-1.383955
7	-1.194970	-1.579370	-1.315946
7	0.354439	1.978866	0.120739
8	0.905502	0.068460	-1.906956
1	2.202060	1.146810	-1.544305
1	0.497336	0.218618	-2.774288

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^{2+}$ Conformer 2 (Closed-shell singlet)

E = -1785.55579276 a.u.

6	2.460873	-0.409768	0.998868
6	3.827431	-0.659034	1.002004
6	4.671782	0.308978	0.506206
6	4.119020	1.519558	0.123729
6	2.740095	1.667273	0.107623
1	4.219297	-1.610640	1.370285
1	5.751740	0.144276	0.455790
1	4.759218	2.344289	-0.207652
6	1.480211	-1.236661	1.686895
6	1.799930	-2.069818	2.744390
6	0.785508	-2.615160	3.508792
1	2.846049	-2.248521	3.003667
6	-0.771490	-1.491660	2.098841
6	-0.518691	-2.298293	3.197512
1	1.015106	-3.267139	4.355876
1	-1.348867	-2.696351	3.785992
6	-2.075316	-1.183808	1.565838
6	-3.313530	-1.435447	2.135731
6	-3.059581	-0.455747	-0.373897
6	-4.457478	-1.148466	1.411527
1	-3.384411	-1.857563	3.141700
6	-4.330995	-0.672679	0.117728
1	-5.444072	-1.328650	1.847858
1	-5.186784	-0.480444	-0.536259

7	0.211876	-0.975761	1.347489
7	-1.969591	-0.667283	0.341135
7	1.910385	0.684359	0.469053
6	2.180124	3.023281	-0.255009
8	2.789415	4.034728	0.306453
8	1.273625	3.207128	-1.006260
6	-2.718669	-0.104005	-1.777448
8	-3.520137	0.148496	-2.617358
8	-1.432576	-0.198389	-1.952793
44	-0.145743	-0.005203	-0.495940
6	-0.938569	2.278697	1.254073
6	-1.446167	3.509283	1.606880
6	-2.003645	4.308236	0.621799
6	-2.025090	3.839994	-0.677599
6	-1.489888	2.597864	-0.950830
1	-0.483865	1.612288	1.996842
1	-1.403853	3.833512	2.649382
1	-2.414600	5.291439	0.868414
1	-2.445677	4.431171	-1.494072
1	-1.463284	2.200087	-1.972295
6	-0.097239	-2.903108	-1.161846
6	0.278814	-4.089285	-1.752400
6	1.461264	-4.128835	-2.469900
6	2.215386	-2.974082	-2.561633
6	1.764378	-1.825400	-1.944211
1	-1.038106	-2.825266	-0.606423
1	-0.364664	-4.967092	-1.660110
1	1.784530	-5.049850	-2.963623
1	3.147192	-2.945212	-3.131095
1	2.299756	-0.876238	-2.037669
7	0.629011	-1.789426	-1.248545
7	-0.956924	1.828664	-0.000727
8	0.799203	0.731199	-1.875918
1	3.434245	3.761406	0.969364
1	0.853411	1.702817	-1.788372

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OH)]^{2+}$ Conformer 2 (Triplet)

E = -1785.54895767 a.u.

6	2.255422	-1.608278	0.843954
6	3.054727	-2.733124	0.638580
6	4.283440	-2.566509	0.031658
6	4.667158	-1.292514	-0.351058
6	3.771651	-0.254874	-0.140905
1	2.712297	-3.731654	0.927401
1	4.934318	-3.425366	-0.155337
1	5.622292	-1.129864	-0.861744
6	0.994313	-1.704315	1.609010

6	0.977101	-2.546307	2.716469
6	-0.122922	-2.591497	3.542772
1	1.870181	-3.131263	2.950228
6	-1.120385	-0.946797	2.131726
6	-1.180501	-1.758276	3.251565
1	-0.146160	-3.247716	4.416945
1	-2.067516	-1.748432	3.888233
6	-2.224419	-0.056523	1.785471
6	-3.329942	0.261021	2.564710
6	-3.004711	1.327958	0.080035
6	-4.273376	1.144409	2.066460
1	-3.458984	-0.160576	3.564025
6	-4.120559	1.691402	0.798673
1	-5.142269	1.406748	2.677425
1	-4.843439	2.384533	0.359018
7	-0.056036	-0.929223	1.289637
7	-2.099947	0.491705	0.579427
7	2.594173	-0.398262	0.446706
6	3.973350	1.115575	-0.709865
8	5.162145	1.646637	-0.701435
8	3.044533	1.692832	-1.203520
6	-2.670101	1.753567	-1.320582
8	-3.327343	2.533261	-1.928159
8	-1.612192	1.132373	-1.784482
44	-0.476933	0.166619	-0.545071
6	0.729226	2.216248	1.278062
6	1.298818	3.415116	1.636969
6	1.422562	4.409426	0.679860
6	0.970947	4.159387	-0.603275
6	0.409318	2.934623	-0.886431
1	0.630242	1.395669	1.994087
1	1.643330	3.563176	2.662877
1	1.872709	5.373492	0.934474
1	1.054892	4.904766	-1.396877
1	0.047328	2.686561	-1.889230
6	-2.508768	-1.728556	-1.698519
6	-2.994312	-2.860759	-2.315656
6	-2.126008	-3.904049	-2.577329
6	-0.800342	-3.768568	-2.205478
6	-0.393816	-2.606871	-1.587177
1	-3.164436	-0.876313	-1.501346
1	-4.047707	-2.905515	-2.600825
1	-2.476860	-4.811278	-3.077409
1	-0.068433	-4.553707	-2.407831
1	0.653677	-2.439277	-1.316411
7	-1.233157	-1.601187	-1.332867
7	0.284192	1.978246	0.041103
8	0.957864	-0.051164	-1.656748
1	5.790055	1.125227	-0.187540
1	1.717675	0.563575	-1.528502

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(O)]^+$ (Triplet)

E = -1785.26274627 a.u.

6	2.340694	-1.474563	0.851955
6	3.167431	-2.581205	0.676807
6	4.393358	-2.401226	0.062144
6	4.741790	-1.133790	-0.358403
6	3.811678	-0.117572	-0.196746
1	2.850195	-3.576227	1.004928
1	5.068994	-3.248664	-0.086858
1	5.701873	-0.910620	-0.831425
6	1.099589	-1.587369	1.643083
6	1.132860	-2.384689	2.784547
6	0.041381	-2.450178	3.618414
1	2.056804	-2.913241	3.031285
6	-1.049466	-0.920888	2.146252
6	-1.061886	-1.689710	3.296754
1	0.056149	-3.067240	4.520731
1	-1.948099	-1.701990	3.934586
6	-2.213133	-0.113467	1.769826
6	-3.335869	0.163637	2.539165
6	-3.068460	1.144222	0.006558
6	-4.333612	0.958923	1.997944
1	-3.438909	-0.217198	3.557882
6	-4.211937	1.460446	0.710721
1	-5.219862	1.189280	2.596689
1	-4.973827	2.088182	0.241195
7	0.012785	-0.877808	1.300951
7	-2.122832	0.387932	0.545044
7	2.645413	-0.268503	0.406959
6	4.109046	1.251247	-0.734154
8	3.038347	1.934518	-1.071608
8	5.218423	1.662038	-0.843408
6	-2.758645	1.553293	-1.414972
8	-3.523399	2.242592	-2.022537
8	-1.649044	1.058741	-1.861277
44	-0.450906	0.138193	-0.571671
6	0.592617	2.305910	1.257188
6	1.068318	3.547043	1.616517
6	1.109706	4.547335	0.661754
6	0.666940	4.262132	-0.614733
6	0.199660	2.995292	-0.894941
1	0.575321	1.476892	1.970651
1	1.418266	3.715375	2.637392
1	1.496300	5.539706	0.910936
1	0.693212	5.008737	-1.411028
1	-0.146004	2.712837	-1.894132

6	-2.378021	-1.929435	-1.599433
6	-2.804082	-3.113666	-2.163270
6	-1.869739	-4.090965	-2.448105
6	-0.541755	-3.837224	-2.157019
6	-0.200186	-2.627967	-1.590912
1	-3.086708	-1.124297	-1.386469
1	-3.863966	-3.250206	-2.388805
1	-2.171845	-5.037725	-2.905048
1	0.241223	-4.565234	-2.380955
1	0.841688	-2.362314	-1.380869
7	-1.102604	-1.688348	-1.307883
7	0.160562	2.030388	0.027587
8	0.962698	0.018042	-1.595608
1	2.269926	1.336982	-1.041895

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (Closed-shell singlet)

E = -1860.65768215 a.u.

6	2.006041	-1.653984	1.057162
6	2.691787	-2.837711	0.813780
6	3.911337	-2.773296	0.159914
6	4.391796	-1.536507	-0.222765
6	3.636578	-0.416061	0.091730
1	2.268654	-3.801966	1.114131
1	4.477641	-3.685575	-0.049528
1	5.340913	-1.409471	-0.751413
6	0.723078	-1.655065	1.781003
6	0.586434	-2.442742	2.918782
6	-0.561317	-2.378399	3.677913
1	1.429816	-3.066083	3.227790
6	-1.381042	-0.756070	2.137546
6	-1.553040	-1.501996	3.288308
1	-0.673475	-2.986369	4.579806
1	-2.473766	-1.408203	3.868321
6	-2.370839	0.180102	1.634704
6	-3.508309	0.639138	2.284957
6	-2.842585	1.514623	-0.190934
6	-4.314065	1.574221	1.659705
1	-3.762215	0.279909	3.285270
6	-3.978820	2.029451	0.393569
1	-5.209747	1.947596	2.164488
1	-4.575860	2.763925	-0.154571
7	-0.267464	-0.840080	1.376542
7	-2.070147	0.626202	0.416558
7	2.468904	-0.458652	0.716388
6	4.110958	0.938744	-0.347794
8	4.902271	1.062901	-1.223207
8	3.555056	1.948872	0.283899

6	-2.350115	1.826279	-1.566596
8	-2.831194	2.630703	-2.288797
8	-1.348359	1.027538	-1.860231
44	-0.366958	0.061874	-0.534830
6	0.558129	2.245351	1.313337
6	1.000199	3.485819	1.717043
6	1.281198	4.442666	0.755181
6	1.095609	4.112266	-0.572436
6	0.648154	2.846830	-0.894842
1	0.344953	1.460525	2.045809
1	1.122812	3.693305	2.782851
1	1.641411	5.434661	1.041966
1	1.299348	4.824892	-1.374642
1	0.491147	2.553803	-1.935952
6	-2.486149	-1.747811	-1.640724
6	-3.065820	-2.883513	-2.164502
6	-2.310779	-4.037885	-2.258738
6	-0.998724	-4.004565	-1.821205
6	-0.497346	-2.827578	-1.308964
1	-3.049893	-0.813362	-1.578243
1	-4.102511	-2.848059	-2.506895
1	-2.738026	-4.953516	-2.677621
1	-0.353569	-4.883865	-1.883777
1	0.544864	-2.755583	-0.977746
7	-1.224031	-1.713303	-1.213218
7	0.393071	1.917621	0.028326
8	0.953137	-0.398791	-1.705052
8	1.923340	0.502428	-1.990095
1	2.941615	1.591006	0.941098
1	2.311628	0.134401	-2.803746

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^{2+}$ (Triplet)

E = -1860.65355720 a.u.

6	2.016043	-1.728331	1.024805
6	2.693257	-2.909664	0.741931
6	3.896824	-2.836381	0.061585
6	4.375013	-1.592934	-0.304172
6	3.632860	-0.477311	0.056538
1	2.270204	-3.878694	1.026293
1	4.452895	-3.746249	-0.182860
1	5.315546	-1.457378	-0.846018
6	0.737401	-1.739078	1.752514
6	0.582915	-2.550767	2.870347
6	-0.568161	-2.469588	3.623078
1	1.405898	-3.204304	3.171821
6	-1.353029	-0.799305	2.110813
6	-1.540561	-1.562015	3.247193

1	-0.699766	-3.088947	4.514767
1	-2.456321	-1.459331	3.833713
6	-2.347581	0.162748	1.636970
6	-3.503909	0.594782	2.276920
6	-2.814377	1.541390	-0.186531
6	-4.307075	1.533324	1.649712
1	-3.780922	0.214287	3.263230
6	-3.970032	2.020550	0.393058
1	-5.215321	1.884447	2.148078
1	-4.583760	2.751145	-0.141561
7	-0.230571	-0.899704	1.349760
7	-2.048768	0.660659	0.442855
7	2.481363	-0.528471	0.703755
6	4.114022	0.888767	-0.339045
8	4.915028	1.040545	-1.201247
8	3.557978	1.877259	0.325798
6	-2.298027	1.860957	-1.558857
8	-2.773316	2.683504	-2.265022
8	-1.268978	1.090247	-1.905303
44	-0.409086	0.121992	-0.513142
6	0.533880	2.251609	1.366891
6	1.028911	3.463307	1.792549
6	1.385284	4.411198	0.846428
6	1.225430	4.100612	-0.489751
6	0.733027	2.860341	-0.838874
1	0.250994	1.475243	2.084970
1	1.128406	3.657733	2.863101
1	1.781682	5.383518	1.152360
1	1.485816	4.809936	-1.278345
1	0.595698	2.575680	-1.885493
6	-2.565555	-1.662980	-1.599482
6	-3.151821	-2.787552	-2.136571
6	-2.391350	-3.934167	-2.280077
6	-1.067564	-3.902933	-1.879006
6	-0.555430	-2.735682	-1.356338
1	-3.134831	-0.734917	-1.497050
1	-4.197065	-2.750069	-2.451472
1	-2.824219	-4.841665	-2.710898
1	-0.419412	-4.775999	-1.982766
1	0.496089	-2.659715	-1.059540
7	-1.290198	-1.631033	-1.210409
7	0.399533	1.942159	0.072207
8	0.988460	-0.447010	-1.697107
8	1.899415	0.510595	-2.009617
1	2.941293	1.492251	0.965136
1	2.336285	0.133598	-2.792165

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (Broken-symmetry singlet)

E = -1860.38041178 a.u.

6	1.989944	-1.726059	0.925155
6	2.509069	-2.943757	0.503130
6	3.691936	-2.947964	-0.217019
6	4.314750	-1.744045	-0.470818
6	3.721273	-0.589687	0.017373
1	1.981010	-3.877325	0.725778
1	4.119198	-3.888769	-0.576328
1	5.247145	-1.662348	-1.035146
6	0.750360	-1.662247	1.726309
6	0.641336	-2.437580	2.872734
6	-0.453797	-2.293104	3.698176
1	1.457329	-3.118720	3.128734
6	-1.269939	-0.638864	2.183714
6	-1.409429	-1.359816	3.356504
1	-0.551399	-2.885221	4.611967
1	-2.284857	-1.202766	3.990746
6	-2.252124	0.345263	1.737080
6	-3.319119	0.870079	2.453502
6	-2.792030	1.661585	-0.102931
6	-4.125965	1.820755	1.850950
1	-3.517943	0.554196	3.480678
6	-3.865932	2.228686	0.551419
1	-4.966504	2.246672	2.406185
1	-4.472355	2.973056	0.028377
7	-0.209813	-0.802858	1.354157
7	-2.024682	0.758424	0.492709
7	2.586836	-0.566780	0.698233
6	4.378972	0.736351	-0.229880
8	5.372898	0.838142	-0.871547
8	3.766458	1.753325	0.335428
6	-2.376521	1.925906	-1.528961
8	-2.954795	2.727978	-2.198395
8	-1.393675	1.167713	-1.900437
44	-0.454414	0.090447	-0.538954
6	0.666017	2.306537	1.155424
6	1.241031	3.523896	1.448818
6	1.674285	4.324205	0.405504
6	1.506081	3.868471	-0.886278
6	0.922603	2.634855	-1.094755
1	0.321519	1.639223	1.952984
1	1.349595	3.832808	2.491111
1	2.142563	5.292628	0.602183
1	1.831119	4.456152	-1.747223
1	0.769355	2.236900	-2.100988
6	-2.755682	-1.556151	-1.529436
6	-3.448676	-2.652005	-1.998861
6	-2.798368	-3.868587	-2.082224
6	-1.473276	-3.932093	-1.693588

6	-0.856751	-2.786807	-1.236436
1	-3.234218	-0.574585	-1.476202
1	-4.489931	-2.536556	-2.308083
1	-3.316368	-4.756309	-2.456311
1	-0.904718	-4.862950	-1.754372
1	0.202304	-2.784928	-0.957741
7	-1.481962	-1.613716	-1.145498
7	0.514066	1.857694	-0.091669
8	0.884006	-0.588583	-1.647351
8	1.921805	0.034224	-1.983571
1	2.986372	1.400472	0.791446

$[Ru^{IV}(Htda\text{-}\kappa\text{-}N^2O)Py_2(OO)]^+$ (Triplet)

E = -1860.37784857 a.u.

6	2.054838	-1.688704	0.945334
6	2.603985	-2.904328	0.556539
6	3.780608	-2.901488	-0.174141
6	4.368318	-1.690485	-0.474896
6	3.748745	-0.537832	-0.016883
1	2.102099	-3.843845	0.812142
1	4.230547	-3.842410	-0.504577
1	5.294188	-1.603306	-1.049272
6	0.817308	-1.643012	1.752958
6	0.743670	-2.401361	2.914007
6	-0.360735	-2.297702	3.733032
1	1.589371	-3.040432	3.182543
6	-1.249223	-0.711437	2.185184
6	-1.360997	-1.421506	3.368021
1	-0.433733	-2.877863	4.656678
1	-2.246814	-1.299260	3.995586
6	-2.278406	0.222907	1.732854
6	-3.389820	0.678366	2.428955
6	-2.852562	1.551788	-0.108084
6	-4.231468	1.596607	1.822936
1	-3.598378	0.332783	3.444513
6	-3.968468	2.043676	0.536149
1	-5.105088	1.966365	2.367283
1	-4.604910	2.763163	0.013831
7	-0.176487	-0.833904	1.359514
7	-2.055919	0.678873	0.499625
7	2.621414	-0.522812	0.674639
6	4.362457	0.798493	-0.314185
8	5.342364	0.913691	-0.974783
8	3.721637	1.813108	0.226268
6	-2.430378	1.858982	-1.531934
8	-3.055828	2.649697	-2.175915
8	-1.413661	1.164393	-1.919360

44	-0.497361	0.111290	-0.491086
6	0.610924	2.299286	1.246495
6	1.193098	3.508889	1.555537
6	1.595699	4.339590	0.522842
6	1.387629	3.922374	-0.775887
6	0.790750	2.697953	-1.002454
1	0.294013	1.606349	2.033308
1	1.332937	3.788699	2.602328
1	2.070706	5.301681	0.733802
1	1.687642	4.534588	-1.628795
1	0.585409	2.337830	-2.014964
6	-2.703553	-1.586206	-1.599060
6	-3.330613	-2.697077	-2.123586
6	-2.628526	-3.883773	-2.210219
6	-1.319125	-3.905044	-1.765358
6	-0.772373	-2.750248	-1.249119
1	-3.223450	-0.625957	-1.545746
1	-4.362058	-2.615124	-2.473675
1	-3.092659	-4.780992	-2.629571
1	-0.710389	-4.810185	-1.824943
1	0.269505	-2.717216	-0.910386
7	-1.446550	-1.603414	-1.159184
7	0.414697	1.889986	-0.008624
8	1.022825	-0.359886	-1.599402
8	1.913316	0.172546	-2.264501
1	2.968953	1.446662	0.717234

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ (Closed-shell singlet)

E = -1709.19195915 a.u.

6	-2.314358	-0.005210	1.552019
6	-3.638983	-0.006121	1.960765
6	-4.646430	-0.002830	1.013939
6	-4.296094	0.001225	-0.322648
6	-2.955554	0.001833	-0.645858
1	-3.885527	-0.009372	3.025191
1	-5.695475	-0.003454	1.322692
1	-5.024499	0.003951	-1.139458
6	-1.153826	-0.008154	2.401897
6	-1.184288	-0.013339	3.786229
6	0.000050	-0.015776	4.492475
1	-2.142880	-0.015549	4.309262
6	1.153884	-0.007527	2.401876
6	1.184374	-0.012710	3.786207
1	0.000062	-0.020018	5.585685
1	2.142977	-0.014401	4.309222
6	2.314399	-0.003841	1.551977
6	3.639031	-0.004075	1.960698

6	2.955550	0.004023	-0.645910
6	4.646459	-0.000004	1.013855
1	3.885596	-0.007411	3.025119
6	4.296096	0.004160	-0.322725
1	5.695510	-0.000103	1.322589
1	5.024485	0.007523	-1.139547
7	0.000022	-0.005460	1.707807
7	1.987930	0.000228	0.255285
7	-1.987916	-0.001190	0.255320
6	-2.419195	0.005626	-2.024596
8	-1.119721	0.004616	-1.987636
8	-3.079292	0.008961	-3.009916
6	2.419164	0.007799	-2.024637
8	3.079240	0.011837	-3.009968
8	1.119692	0.005835	-1.987654
44	0.000001	0.000865	-0.380895
6	0.000923	-2.908873	0.515924
6	0.001463	-4.278862	0.379042
6	0.001940	-4.823374	-0.893725
6	0.001835	-3.964314	-1.975492
6	0.001274	-2.601070	-1.757601
1	0.000529	-2.451832	1.510403
1	0.001502	-4.909136	1.271423
1	0.002379	-5.907692	-1.037665
1	0.002178	-4.336227	-3.002773
1	0.001135	-1.886023	-2.585119
6	-0.000882	2.905458	0.532280
6	-0.001448	4.276203	0.403040
6	-0.002005	4.827801	-0.866673
6	-0.001952	3.974831	-1.953241
6	-0.001361	2.610398	-1.742973
1	-0.000428	2.442838	1.524191
1	-0.001444	4.901528	1.298889
1	-0.002469	5.912908	-1.004547
1	-0.002362	4.352499	-2.978429
1	-0.001269	1.899957	-2.574465
7	-0.000841	2.078899	-0.516132
7	0.000834	-2.076434	-0.527813

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ • □□□□) (Closed-shell singlet)

E = -1785.59553065 a.u.

6	-0.874100	2.487608	-1.044151
6	-1.713955	3.546082	-1.354847
6	-2.984273	3.591208	-0.812105
6	-3.378395	2.572387	0.035023
6	-2.479025	1.562672	0.303941
1	-1.375798	4.336154	-2.029558

1	-3.658989	4.417751	-1.051720
1	-4.364171	2.529053	0.507938
6	0.455875	2.268818	-1.547289
6	1.136201	3.126748	-2.394656
6	2.402823	2.793158	-2.826182
1	0.667840	4.059989	-2.714598
6	2.216628	0.776838	-1.560847
6	2.943689	1.595471	-2.408473
1	2.961058	3.458037	-3.490503
1	3.937826	1.288631	-2.740404
6	2.652818	-0.505520	-1.076103
6	3.838313	-1.150890	-1.390842
6	2.008015	-2.257633	0.250630
6	4.095896	-2.401602	-0.860870
1	4.562770	-0.675883	-2.056742
6	3.157449	-2.969779	-0.020521
1	5.025678	-2.923557	-1.103723
1	3.279824	-3.951787	0.446724
7	0.991061	1.111294	-1.115131
7	1.753742	-1.065289	-0.260685
7	-1.262792	1.513443	-0.216275
6	-2.720196	0.426841	1.220405
8	-1.637083	-0.268577	1.347080
8	-3.750738	0.211919	1.777349
6	0.931487	-2.700183	1.165809
8	0.913837	-3.737437	1.740717
8	0.033649	-1.766026	1.264005
44	-0.035624	-0.111346	0.226168
6	1.680381	1.856031	1.821653
6	2.228874	2.442373	2.940240
6	1.887985	1.949896	4.188046
6	1.006633	0.888403	4.255038
6	0.498220	0.355108	3.087521
1	1.932998	2.229533	0.824719
1	2.919352	3.281012	2.824512
1	2.305870	2.391697	5.097213
1	0.700410	0.458309	5.211488
1	-0.203604	-0.482997	3.096928
6	-0.836019	-1.036514	-2.548709
6	-1.534469	-1.755327	-3.491196
6	-2.477191	-2.678363	-3.065942
6	-2.668057	-2.846249	-1.709281
6	-1.917909	-2.100025	-0.819855
1	-0.089951	-0.295224	-2.853338
1	-1.338641	-1.583735	-4.552318
1	-3.055151	-3.257379	-3.792264
1	-3.403515	-3.543412	-1.300551
1	-2.059256	-2.223360	0.260508
7	-1.021321	-1.199809	-1.235457
7	0.829713	0.829074	1.882593

8	-3.760374	-2.755839	1.393083
1	-3.870275	-3.460468	2.034234
1	-4.080164	-1.971781	1.848279

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O^2)Py_2]^{2+}$ • □□□□)$_2$ (Closed-shell singlet)

E = -1862.00376448 a.u.

6	1.154031	2.608983	0.749526
6	1.190013	3.929789	1.170247
6	0.010640	4.579069	1.482319
6	-1.178794	3.886375	1.356207
6	-1.128310	2.575287	0.933147
1	2.144744	4.454530	1.253789
1	0.024189	5.620130	1.816607
1	-2.157375	4.325189	1.573107
6	2.281731	1.792389	0.386547
6	3.601678	2.209808	0.406532
6	4.599754	1.327444	0.050590
1	3.844593	3.231989	0.704348
6	2.906252	-0.317096	-0.308492
6	4.242878	0.044647	-0.306781
1	5.648396	1.636124	0.056286
1	5.004170	-0.685930	-0.588515
6	2.406180	-1.622369	-0.648651
6	3.158435	-2.736735	-0.986960
6	0.466153	-2.820183	-0.865907
6	2.520454	-3.930931	-1.266200
1	4.248350	-2.672733	-1.028461
6	1.140476	-3.974708	-1.202252
1	3.101092	-4.818786	-1.531578
1	0.555099	-4.875965	-1.408275
7	1.926886	0.544959	0.024057
7	1.072318	-1.675334	-0.598001
7	-0.000442	1.944749	0.644050
6	-2.300780	1.702121	0.718855
8	-1.917572	0.527906	0.350142
8	-3.436180	2.044762	0.854299
6	-1.005199	-2.683610	-0.784479
8	-1.781719	-3.566822	-0.960870
8	-1.309135	-1.452011	-0.526886
44	-0.077031	-0.033579	-0.022711
6	0.954627	-0.634908	2.767910
6	0.918365	-1.110385	4.058444
6	-0.228946	-1.747488	4.503254
6	-1.288768	-1.875454	3.628318
6	-1.185179	-1.371658	2.344101
1	1.845977	-0.122645	2.391341
1	1.788021	-0.975954	4.705998

1	-0.289986	-2.135926	5.524168
1	-2.222702	-2.364558	3.916603
1	-2.029112	-1.471823	1.639147
6	0.596981	1.116332	-2.763081
6	0.371324	1.538497	-4.053778
6	-0.911442	1.453651	-4.568057
6	-1.909229	0.944512	-3.760583
6	-1.607435	0.536502	-2.475670
1	1.601768	1.168438	-2.331693
1	1.202169	1.928397	-4.646501
1	-1.125727	1.780031	-5.589881
1	-2.940088	0.851644	-4.110040
1	-2.380685	0.121371	-1.817742
7	-0.366957	0.624461	-1.981513
7	-0.071695	-0.760861	1.921757
8	-4.492202	-0.032164	-0.905223
1	-5.404384	-0.140010	-1.185841
1	-4.521166	0.684733	-0.260540
8	-3.749605	-2.140820	0.915007
1	-3.624916	-2.916451	0.361824
1	-4.007858	-1.456235	0.280289

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^+$ (Closed-shell singlet)

E = -1785.25412011 a.u.

6	2.342828	0.845901	1.033105
6	3.558968	1.470133	1.188154
6	3.703970	2.757028	0.688683
6	2.598716	3.379013	0.164611
6	1.407211	2.669822	-0.026285
1	4.380184	0.972423	1.709545
1	4.659452	3.282014	0.775551
1	2.611669	4.436568	-0.111304
6	1.927611	-0.361914	1.705509
6	2.610016	-0.971630	2.748597
6	1.991090	-1.969495	3.470555
1	3.609602	-0.626070	3.020393
6	0.090154	-1.705793	2.066093
6	0.696912	-2.323079	3.145564
1	2.507345	-2.454386	4.303261
1	0.163444	-3.091488	3.709579
6	-1.212528	-2.021480	1.536351
6	-2.186294	-2.822463	2.111957
6	-2.462178	-1.778686	-0.369238
6	-3.352990	-3.068734	1.412086
1	-2.030903	-3.247540	3.106925
6	-3.483849	-2.557787	0.133573
1	-4.140448	-3.685389	1.854430

1	-4.344732	-2.758313	-0.510392
7	0.702855	-0.761241	1.341205
7	-1.378508	-1.480051	0.328440
7	1.323949	1.394130	0.339865
6	0.161483	3.524294	-0.388147
8	-0.419567	3.357516	-1.457935
8	-0.019927	4.284284	0.544159
6	-2.345829	-1.319979	-1.782823
8	-3.209970	-1.498633	-2.588624
8	-1.182083	-0.811979	-1.983336
44	-0.059414	-0.034736	-0.511358
6	-1.739068	1.614307	1.306802
6	-2.754324	2.448917	1.714193
6	-3.668594	2.888642	0.774171
6	-3.527516	2.474105	-0.535341
6	-2.477272	1.644894	-0.866045
1	-0.974075	1.259374	2.006697
1	-2.804349	2.767614	2.757226
1	-4.478461	3.565523	1.060686
1	-4.208531	2.808293	-1.320351
1	-2.296860	1.328246	-1.898586
6	1.313813	-2.571248	-1.248633
6	2.233387	-3.423043	-1.820633
6	3.342872	-2.879598	-2.442798
6	3.479425	-1.504974	-2.467636
6	2.508262	-0.722783	-1.875633
1	0.408537	-2.955343	-0.765971
1	2.065728	-4.501824	-1.786717
1	4.089554	-3.524787	-2.914838
1	4.327972	-1.024124	-2.959499
1	2.541443	0.370135	-1.911313
7	1.447513	-1.248274	-1.269042
7	-1.601572	1.215461	0.042716
8	0.393161	0.988481	-1.948326
1	0.037427	1.923740	-1.896109

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^3O)Py_2(OH)]^+$ (Closed-shell singlet)

E = -1861.65742074 a.u.

6	-0.565803	-2.438135	1.015235
6	-0.629354	-3.808307	1.133073
6	0.430892	-4.557516	0.646951
6	1.534240	-3.888511	0.177295
6	1.510926	-2.498939	0.023140
1	-1.486354	-4.287683	1.612573
1	0.414173	-5.649469	0.704094
1	2.459659	-4.411905	-0.075774
6	-1.433126	-1.502429	1.692638

6	-2.288253	-1.824399	2.736183
6	-2.866159	-0.813007	3.474051
1	-2.456459	-2.871005	2.998394
6	-1.739675	0.748662	2.078297
6	-2.563135	0.496556	3.161326
1	-3.531871	-1.045472	4.309434
1	-2.980581	1.325420	3.737422
6	-1.413199	2.048723	1.550070
6	-1.660068	3.284051	2.127506
6	-0.648523	3.038218	-0.370233
6	-1.347481	4.430063	1.419853
1	-2.093370	3.346132	3.129079
6	-0.858711	4.306037	0.131991
1	-1.518959	5.414786	1.863580
1	-0.651392	5.160454	-0.518463
7	-1.202977	-0.232038	1.340833
7	-0.873821	1.942300	0.334807
7	0.430984	-1.801658	0.367645
6	2.880529	-1.849275	-0.291639
8	3.040501	-1.168092	-1.302714
8	3.649978	-2.176101	0.598899
6	-0.322181	2.715244	-1.787619
8	-0.116820	3.557143	-2.609527
8	-0.390089	1.443703	-1.973568
44	-0.188428	0.109406	-0.493691
6	2.085032	0.778048	1.303803
6	3.333513	1.217715	1.677199
6	4.138541	1.825115	0.729539
6	3.634221	2.006341	-0.544763
6	2.383280	1.521813	-0.846346
1	1.425998	0.259680	2.010196
1	3.682542	1.043546	2.697012
1	5.155713	2.135188	0.975826
1	4.229585	2.473597	-1.331721
1	1.980499	1.567363	-1.863794
6	-3.066945	0.008590	-1.247775
6	-4.232418	-0.419162	-1.845179
6	-4.230288	-1.633725	-2.507438
6	-3.058472	-2.364844	-2.543360
6	-1.933125	-1.860747	-1.923097
1	-3.015085	0.974125	-0.732414
1	-5.125715	0.207752	-1.800176
1	-5.134361	-2.001124	-3.001669
1	-2.998585	-3.322343	-3.065666
1	-0.968024	-2.374479	-1.965006
7	-1.939736	-0.696708	-1.279424
7	1.619232	0.910963	0.062125
8	0.567803	-0.749237	-1.911225
1	1.555026	-0.854256	-1.813692
8	5.751308	-0.300871	-0.099792

1	5.328486	-0.402586	-0.957177
1	5.317167	-1.011040	0.387664

[Ru^{IV}(tda-κ-N^2O)Py_2(O)] (Broken-symmetry singlet)

E = -1784.79760756 a.u.

6	1.738690	-1.986023	0.804839
6	2.139226	-3.209382	0.290331
6	3.308410	-3.231914	-0.453718
6	4.004882	-2.054801	-0.623629
6	3.543422	-0.890767	-0.008748
1	1.536200	-4.112282	0.442655
1	3.661347	-4.167741	-0.901144
1	4.920564	-1.988275	-1.217825
6	0.508972	-1.831507	1.599827
6	0.269612	-2.636984	2.703714
6	-0.770088	-2.341620	3.561642
1	0.961169	-3.458930	2.907416
6	-1.302786	-0.492540	2.151670
6	-1.544051	-1.232376	3.298335
1	-0.956497	-2.953715	4.448678
1	-2.360468	-0.947517	3.966165
6	-2.103275	0.651106	1.749395
6	-3.071427	1.320314	2.485824
6	-2.453920	2.066117	-0.063135
6	-3.725506	2.397025	1.914716
1	-3.307088	1.012133	3.508155
6	-3.420072	2.774825	0.612431
1	-4.482626	2.940244	2.487201
1	-3.916381	3.604593	0.102178
7	-0.304408	-0.806923	1.291617
7	-1.809617	1.047729	0.506383
7	2.422312	-0.858301	0.692139
6	4.352727	0.399892	-0.130361
8	4.114925	1.274152	0.704705
8	5.166963	0.414648	-1.053674
6	-2.055158	2.259786	-1.499023
8	-2.542227	3.130428	-2.164437
8	-1.212908	1.366481	-1.901276
44	-0.383297	0.134431	-0.584812
6	1.160059	2.143220	1.020643
6	1.997856	3.212144	1.236002
6	2.651664	3.771154	0.155889
6	2.430461	3.241884	-1.098713
6	1.562843	2.179877	-1.232749
1	0.655659	1.637532	1.850710
1	2.171331	3.563319	2.255113
1	3.352562	4.598410	0.297116

1	2.948378	3.623150	-1.980718
1	1.352530	1.715373	-2.200040
6	-2.973833	-1.208106	-1.348315
6	-3.820440	-2.202374	-1.792938
6	-3.290985	-3.445921	-2.082541
6	-1.931748	-3.635550	-1.920497
6	-1.154394	-2.586167	-1.473724
1	-3.351722	-0.204844	-1.126957
1	-4.884263	-1.987987	-1.918922
1	-3.932162	-4.257381	-2.440395
1	-1.458714	-4.593576	-2.149925
1	-0.065661	-2.660382	-1.374197
7	-1.668337	-1.391977	-1.183018
7	0.928065	1.649908	-0.189988
8	0.815491	-0.604212	-1.608628

[Ru^{IV}(tda-κ-N^2O)Py_2(O)] (Triplet)

E = -1784.80840453 a.u.

6	-1.739616	2.038309	0.713447
6	-2.115198	3.244366	0.145688
6	-3.273250	3.250815	-0.618811
6	-3.974741	2.075723	-0.766104
6	-3.554284	0.936102	-0.075372
1	-1.502225	4.145155	0.266315
1	-3.602463	4.170876	-1.114586
1	-4.857290	1.996330	-1.406501
6	-0.514375	1.894826	1.514186
6	-0.262795	2.732841	2.593700
6	0.770488	2.449951	3.460669
1	-0.939852	3.573589	2.768751
6	1.272955	0.544674	2.116055
6	1.524783	1.314787	3.237221
1	0.966813	3.087055	4.327721
1	2.329546	1.035603	3.921715
6	2.054264	-0.644630	1.779322
6	2.992122	-1.309932	2.558632
6	2.376734	-2.162918	0.031589
6	3.610167	-2.434918	2.037966
1	3.233154	-0.968641	3.568835
6	3.312696	-2.872755	0.753403
1	4.341801	-2.975323	2.646361
1	3.788663	-3.744387	0.296855
7	0.285954	0.852862	1.237291
7	1.776410	-1.105513	0.561213
7	-2.453971	0.921822	0.655579
6	-4.364710	-0.367928	-0.191696
8	-4.480039	-0.999020	0.854556

8	-4.758504	-0.569777	-1.339146
6	1.985212	-2.402371	-1.414948
8	2.469072	-3.328107	-2.006526
8	1.185681	-1.511806	-1.887272
44	0.419290	-0.174559	-0.596466
6	-1.260023	-2.013234	1.061717
6	-2.271336	-2.903242	1.323324
6	-3.053098	-3.347708	0.272781
6	-2.745827	-2.932410	-1.007561
6	-1.697639	-2.057898	-1.189380
1	-0.664770	-1.573749	1.868840
1	-2.494105	-3.177691	2.356033
1	-3.915617	-3.992655	0.457105
1	-3.358982	-3.214248	-1.864344
1	-1.430163	-1.666128	-2.174683
6	3.119160	0.945292	-1.385023
6	4.043703	1.874804	-1.814520
6	3.628328	3.174108	-2.034636
6	2.298399	3.484371	-1.819105
6	1.439275	2.494614	-1.388686
1	3.406416	-0.098481	-1.225067
1	5.077645	1.566160	-1.985328
1	4.332996	3.936172	-2.381069
1	1.912009	4.491601	-1.992819
1	0.367255	2.673509	-1.241113
7	1.842384	1.243539	-1.167841
7	-0.976245	-1.596831	-0.169751
8	-0.712419	0.680069	-1.625002

[Ru^{IV}(tda-κ-N^2O)Py_2(O)]•(H_2O) (Triplet)

E = -1861.22724985 a.u.

6	-2.370372	0.282907	1.369492
6	-3.702462	0.107838	1.698449
6	-4.295773	-1.120323	1.469616
6	-3.504176	-2.137062	0.997625
6	-2.156143	-1.910745	0.715685
1	-4.280950	0.933750	2.117923
1	-5.357722	-1.275088	1.687203
1	-3.875860	-3.148939	0.815071
6	-1.660634	1.522883	1.695205
6	-2.167116	2.532318	2.514257
6	-1.347675	3.595458	2.830884
1	-3.176599	2.481548	2.927504
6	0.356881	2.596644	1.521493
6	-0.056555	3.638963	2.336464
1	-1.717864	4.399058	3.474985

1	0.604832	4.478628	2.566702
6	1.662518	2.500817	0.857664
6	2.785513	3.261452	1.144479
6	2.732945	1.428559	-0.852277
6	3.927325	3.062287	0.384701
1	2.779941	3.990830	1.959962
6	3.903862	2.141868	-0.644885
1	4.831933	3.641217	0.596791
1	4.755406	1.957031	-1.304929
7	-0.431376	1.576392	1.219630
7	1.659053	1.593492	-0.108876
7	-1.616199	-0.689551	0.821849
6	-1.317643	-3.162601	0.419331
8	-1.848910	-3.972965	-0.325990
8	-0.277025	-3.202664	1.081409
6	2.535123	0.474838	-1.998124
8	3.422905	0.326390	-2.797993
8	1.369004	-0.039688	-2.038701
44	0.056944	-0.223696	-0.522815
6	1.832078	-1.047778	1.713082
6	2.775186	-1.792078	2.380844
6	3.381181	-2.845605	1.715167
6	3.016228	-3.107019	0.412274
6	2.068477	-2.303399	-0.191951
1	1.286601	-0.232276	2.201576
1	3.009399	-1.560038	3.422526
1	4.119442	-3.472549	2.225050
1	3.408746	-3.958236	-0.146857
1	1.716019	-2.489972	-1.210003
6	-1.118105	2.161309	-1.894475
6	-1.998431	2.911055	-2.645901
6	-3.148421	2.308183	-3.121185
6	-3.364081	0.975567	-2.824916
6	-2.432793	0.296180	-2.066497
1	-0.184633	2.585279	-1.508476
1	-1.768580	3.957166	-2.861974
1	-3.865654	2.870965	-3.726446
1	-4.248335	0.445223	-3.186088
1	-2.533400	-0.769806	-1.830851
7	-1.329494	0.881271	-1.603110
7	1.500504	-1.287405	0.448789
8	-0.495097	-1.611463	-1.359438
8	0.924416	-5.019420	-0.711950
1	0.079431	-4.999597	-1.172003
1	0.650913	-4.587599	0.110519

[Ru^{IV}(tda-κ-N^3O)Py_2(O)] (Triplet)

E = -1784.81563106 a.u.

6	2.263992	-0.460477	1.392446
6	3.592865	-0.507799	1.770644
6	4.413801	0.568567	1.484900
6	3.845063	1.668140	0.896412
6	2.488335	1.675973	0.557591
1	3.991805	-1.388160	2.278567
1	5.477238	0.541657	1.745488
1	4.403059	2.574477	0.646736
6	1.328387	-1.517431	1.782060
6	1.630279	-2.548498	2.673576
6	0.625123	-3.414987	3.045915
1	2.629885	-2.663853	3.096872
6	-0.855750	-2.202552	1.648145
6	-0.649574	-3.246296	2.535829
1	0.835547	-4.230217	3.745084
1	-1.458971	-3.928412	2.809440
6	-2.120966	-1.911655	0.963743
6	-3.366671	-2.429709	1.284337
6	-2.969324	-0.772806	-0.824926
6	-4.449280	-2.072701	0.496069
1	-3.500281	-3.091648	2.145217
6	-4.253465	-1.240423	-0.588849
1	-5.446381	-2.458749	0.731521
1	-5.055335	-0.942207	-1.269251
7	0.112141	-1.370818	1.289011
7	-1.947099	-1.088736	-0.059312
7	1.723992	0.590165	0.740034
6	1.938516	3.050755	0.101436
8	2.712664	3.662189	-0.616793
8	0.869990	3.335436	0.637311
6	-2.592705	0.063204	-2.016994
8	-3.439915	0.345827	-2.826367
8	-1.350924	0.341149	-2.072968
44	0.004150	0.358955	-0.568165
6	-1.519243	1.663705	1.622272
6	-2.302511	2.610747	2.241153
6	-2.752865	3.686325	1.496019
6	-2.395247	3.768236	0.166599
6	-1.602054	2.778962	-0.377490
1	-1.107947	0.806873	2.167893
1	-2.538488	2.508451	3.302891
1	-3.369906	4.463343	1.957750
1	-2.706520	4.606795	-0.459556
1	-1.263174	2.797397	-1.417502
6	0.685326	-2.292543	-1.768484
6	1.401609	-3.247209	-2.459001
6	2.642938	-2.909710	-2.966016

6	3.111260	-1.625520	-2.761820
6	2.331697	-0.729026	-2.059625
1	-0.309948	-2.501455	-1.360935
1	0.975147	-4.242761	-2.603441
1	3.236020	-3.640278	-3.524695
1	4.079102	-1.301039	-3.151263
1	2.635886	0.311716	-1.896680
7	1.139555	-1.059448	-1.565648
7	-1.190189	1.738626	0.339206
8	0.786260	1.550889	-1.516627

$[Ru^{IV}(tda\text{-}\kappa\text{-}N^2O)Py_2(OOH)]^+$ (Triplet)

E = -1860.33636828 a.u.

6	2.017115	-1.852188	0.737346
6	2.744489	-3.000370	0.455644
6	4.011127	-2.858276	-0.086910
6	4.507058	-1.588763	-0.292514
6	3.665387	-0.511195	-0.037471
1	2.328801	-3.992887	0.657746
1	4.613205	-3.740340	-0.325313
1	5.518117	-1.403993	-0.664776
6	0.770665	-1.890657	1.517925
6	0.658048	-2.781899	2.579075
6	-0.420213	-2.702497	3.432950
1	1.462409	-3.499615	2.758080
6	-1.208781	-0.867878	2.130369
6	-1.353493	-1.709974	3.218988
1	-0.518356	-3.389904	4.277448
1	-2.210136	-1.598268	3.887249
6	-2.180449	0.176053	1.816111
6	-3.235168	0.631358	2.597441
6	-2.760360	1.658531	0.113580
6	-4.047553	1.637342	2.103296
1	-3.420610	0.216891	3.591482
6	-3.820358	2.160493	0.838094
1	-4.875319	2.010857	2.712770
1	-4.446595	2.941099	0.397863
7	-0.170563	-0.970633	1.264580
7	-1.975351	0.715595	0.618816
7	2.456257	-0.633353	0.451455
6	4.131740	0.936860	-0.299014
8	5.317667	1.098827	-0.027329
8	3.283366	1.718585	-0.715143
6	-2.402417	2.008810	-1.308588
8	-2.980646	2.868695	-1.899528
8	-1.464112	1.246197	-1.796564
44	-0.465281	0.157521	-0.514299

6	0.931738	2.109287	1.260952
6	1.542034	3.278277	1.652599
6	1.710895	4.288560	0.723107
6	1.262706	4.079039	-0.564589
6	0.662089	2.878440	-0.879085
1	0.806345	1.274581	1.957041
1	1.893072	3.382802	2.681624
1	2.200660	5.226300	1.000259
1	1.384626	4.832401	-1.345372
1	0.302152	2.666115	-1.891003
6	-2.778210	-1.486624	-1.484119
6	-3.458592	-2.561463	-2.014877
6	-2.765249	-3.729504	-2.270974
6	-1.413248	-3.767959	-1.985715
6	-0.809256	-2.647047	-1.457279
1	-3.290746	-0.539304	-1.293917
1	-4.524045	-2.466938	-2.235740
1	-3.272419	-4.598667	-2.699612
1	-0.812595	-4.658535	-2.183698
1	0.266803	-2.620233	-1.255207
7	-1.477500	-1.522401	-1.202060
7	0.490514	1.906125	0.019732
8	0.768653	-0.423597	-1.860228
8	1.811628	0.288559	-2.311147
1	2.140611	0.860713	-1.563982

[Ru^{IV}(tda-κ-N^3)Py_2(O)] (Closed-shell singlet)

E = -1784.78599759 a.u.

6	-2.027455	-1.434445	1.235939
6	-3.233637	-2.014798	1.579746
6	-4.336212	-1.810261	0.771835
6	-4.198208	-1.000230	-0.330455
6	-2.950332	-0.488688	-0.677273
1	-3.315822	-2.602496	2.496946
1	-5.302166	-2.254594	1.031144
1	-5.045303	-0.727161	-0.964643
6	-0.857982	-1.454077	2.093164
6	-0.746842	-2.063695	3.330997
6	0.421651	-1.913560	4.056412
1	-1.574731	-2.649034	3.738046
6	1.309555	-0.591013	2.278265
6	1.460702	-1.168282	3.527507
1	0.523888	-2.381469	5.038756
1	2.390114	-1.046515	4.088816
6	2.310579	0.158839	1.540230
6	3.583363	0.404600	2.025475
6	2.825716	1.148273	-0.499911

6	4.508314	1.024400	1.211051
1	3.849338	0.096018	3.039238
6	4.130907	1.362224	-0.069249
1	5.521192	1.224031	1.574468
1	4.814130	1.810082	-0.794518
7	0.161296	-0.732794	1.587825
7	1.928064	0.563145	0.300417
7	-1.877747	-0.731089	0.082443
6	-2.873215	0.382673	-1.937376
8	-3.631575	1.337415	-1.874291
8	-2.122727	-0.025488	-2.824817
6	2.486181	1.679744	-1.905399
8	1.367435	2.200357	-2.026922
8	3.419346	1.599908	-2.682387
44	0.000338	0.053932	-0.237279
6	1.623351	-2.470763	-0.598602
6	2.091081	-3.601940	-1.231171
6	1.536731	-3.958314	-2.447366
6	0.535718	-3.164633	-2.969560
6	0.118723	-2.043029	-2.277260
1	2.045011	-2.154042	0.361289
1	2.890630	-4.186473	-0.769742
1	1.887145	-4.846804	-2.981887
1	0.065106	-3.396984	-3.927890
1	-0.669333	-1.371164	-2.650358
6	-0.885062	2.203235	1.675503
6	-1.380177	3.410215	2.115647
6	-1.738056	4.361071	1.176399
6	-1.579275	4.054020	-0.158020
6	-1.068663	2.822025	-0.521229
1	-0.599487	1.423466	2.389364
1	-1.484266	3.591626	3.188220
1	-2.140906	5.330171	1.487259
1	-1.855075	4.759014	-0.944975
1	-0.911306	2.533430	-1.563978
7	-0.725846	1.907541	0.386278
7	0.660334	-1.704380	-1.103559
8	-0.098787	0.682484	-1.859196

[Ru^{IV}(tda-κ-N^3)Py_2(O)]•□□□ (triplet)

E = -1861.20613057 a.u.

6	-2.632658	-0.804609	1.039552
6	-3.961003	-1.140278	1.199285
6	-4.733287	-1.375383	0.070049
6	-4.139047	-1.299370	-1.164204
6	-2.775026	-1.010495	-1.273635

1	-4.399235	-1.204321	2.198048
1	-5.796023	-1.617563	0.172574
1	-4.700174	-1.461396	-2.088562
6	-1.722518	-0.582018	2.162272
6	-1.992215	-0.779036	3.509084
6	-0.965384	-0.602128	4.418915
1	-2.985671	-1.079329	3.849105
6	0.508868	-0.045959	2.635159
6	0.300446	-0.240154	3.992540
1	-1.154900	-0.754183	5.485589
1	1.107925	-0.101400	4.714631
6	1.745680	0.395455	1.989555
6	2.945225	0.527358	2.661551
6	2.670415	1.212354	0.022597
6	4.062078	0.951643	1.960047
1	3.016068	0.270779	3.721376
6	3.922172	1.286574	0.634642
1	5.033438	1.018173	2.459941
1	4.767874	1.610804	0.022088
7	-0.499043	-0.213991	1.776142
7	1.623771	0.715460	0.680190
7	-2.057919	-0.728684	-0.186493
6	-2.064991	-1.085633	-2.630410
8	-1.280267	-2.025039	-2.668032
8	-2.435453	-0.235648	-3.428422
6	2.456355	1.844101	-1.362780
8	3.240817	1.470684	-2.232209
8	1.575422	2.690432	-1.334115
44	-0.137519	0.054507	-0.200189
6	1.890295	-1.889387	-1.034599
6	2.571642	-3.078208	-1.192635
6	2.058593	-4.221942	-0.615117
6	0.879090	-4.131770	0.102616
6	0.270861	-2.902253	0.224392
1	2.246325	-0.972159	-1.515562
1	3.504449	-3.060007	-1.759462
1	2.568370	-5.184035	-0.727506
1	0.417793	-5.009242	0.562064
1	-0.671352	-2.787268	0.771263
6	-0.793668	2.827417	0.736613
6	-1.257732	4.121099	0.657431
6	-1.951933	4.505643	-0.474602
6	-2.155242	3.574503	-1.472878
6	-1.662467	2.294499	-1.315643
1	-0.208114	2.488545	1.598364
1	-1.049644	4.820803	1.470099
1	-2.320607	5.530634	-0.580792
1	-2.681707	3.827408	-2.395775
1	-1.783718	1.531799	-2.098996
7	-0.998549	1.929878	-0.219332

7	0.769252	-1.799354	-0.322884
8	0.224787	0.268087	-1.895010
8	4.792447	-0.775802	-1.858217
1	4.264738	0.032930	-1.986135
1	5.223101	-0.876285	-2.708165

[Ru^{IV}(tda-κ-N^3O)Py_2(OO)] (Triplet)

E = -1859.91577312 a.u.

6	2.350668	-0.489634	1.392571
6	3.705712	-0.517595	1.668158
6	4.463747	0.608871	1.404651
6	3.811145	1.728678	0.951281
6	2.434170	1.702462	0.715410
1	4.168718	-1.420685	2.073249
1	5.544948	0.606500	1.580369
1	4.308745	2.680151	0.745121
6	1.471138	-1.600266	1.759431
6	1.825948	-2.665627	2.585976
6	0.857621	-3.589452	2.923058
1	2.836870	-2.762647	2.988227
6	-0.689246	-2.351555	1.625209
6	-0.430803	-3.442053	2.442248
1	1.108854	-4.434599	3.571235
1	-1.207435	-4.172398	2.685040
6	-1.962329	-2.053845	0.970121
6	-3.183061	-2.643366	1.264684
6	-2.888879	-0.855301	-0.742418
6	-4.292499	-2.296313	0.515032
1	-3.267295	-3.361724	2.085302
6	-4.142540	-1.397571	-0.523558
1	-5.267544	-2.740951	0.737297
1	-4.958852	-1.099454	-1.186685
7	0.239758	-1.467753	1.306222
7	-1.834256	-1.155003	-0.003637
7	1.724496	0.577401	0.860521
6	1.779796	3.083166	0.435062
8	2.522231	3.862567	-0.139021
8	0.658930	3.185637	0.926819
6	-2.581856	0.039696	-1.908163
8	-3.447795	0.338652	-2.685886
8	-1.337456	0.330152	-1.980221
44	-0.092897	0.263542	-0.451638
6	-1.585030	1.502663	1.782161
6	-2.375808	2.414139	2.443221
6	-2.911617	3.469776	1.726802
6	-2.627316	3.566257	0.381024
6	-1.822956	2.609483	-0.205234

1	-1.101376	0.669515	2.305241
1	-2.550527	2.302111	3.515923
1	-3.536087	4.219525	2.222357
1	-3.005753	4.390442	-0.227386
1	-1.550355	2.650434	-1.266193
6	0.578823	-2.186726	-1.995296
6	1.283803	-3.055808	-2.800785
6	2.574287	-2.724267	-3.170062
6	3.099136	-1.529595	-2.715913
6	2.324514	-0.718024	-1.912322
1	-0.452544	-2.396740	-1.693272
1	0.810231	-3.979988	-3.140987
1	3.160908	-3.386546	-3.813993
1	4.107275	-1.207641	-2.987389
1	2.691466	0.250860	-1.554735
7	1.083343	-1.038892	-1.548542
7	-1.323719	1.589564	0.483599
8	0.791243	1.650366	-1.439613
8	0.390405	2.184075	-2.498063

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3}O^{2})Py_{2}]^{3+}$ (Doublet)

E = -1708.67489285 a.u.

6	-2.317594	-0.003449	1.566293
6	-3.643603	-0.004081	1.976448
6	-4.654700	-0.001875	1.032729
6	-4.310397	0.000894	-0.309515
6	-2.969987	0.001291	-0.634180
1	-3.890610	-0.006277	3.041460
1	-5.704035	-0.002312	1.344242
1	-5.047136	0.002748	-1.120567
6	-1.155437	-0.005380	2.411913
6	-1.185040	-0.008675	3.799732
6	0.000310	-0.010235	4.506920
1	-2.142958	-0.010055	4.325847
6	1.155785	-0.005045	2.411762
6	1.185568	-0.008333	3.799578
1	0.000382	-0.012899	5.601133
1	2.143555	-0.009423	4.325567
6	2.317831	-0.002750	1.565992
6	3.643893	-0.003040	1.975977
6	2.969941	0.002357	-0.634564
6	4.654868	-0.000478	1.032128
1	3.891036	-0.005249	3.040957
6	4.310392	0.002317	-0.310071
1	5.704243	-0.000652	1.343507
1	5.047026	0.004470	-1.121217
7	0.000129	-0.003682	1.721434

7	1.999792	-0.000050	0.263265
7	-1.999723	-0.000748	0.263525
6	-2.435701	0.003916	-2.011394
8	-1.120976	0.003209	-1.968820
8	-3.063971	0.006723	-3.010518
6	2.435482	0.004989	-2.011710
8	3.063627	0.007915	-3.010913
8	1.120763	0.003772	-1.968969
44	-0.000009	0.000575	-0.396753
6	0.000784	-2.900720	0.506699
6	0.001000	-4.270043	0.373279
6	0.000798	-4.816528	-0.899590
6	0.000365	-3.953425	-1.990883
6	0.000171	-2.588206	-1.778180
1	0.000920	-2.440489	1.498903
1	0.001318	-4.899613	1.266514
1	0.000956	-5.901531	-1.045151
1	0.000164	-4.331094	-3.017173
1	-0.000214	-1.881493	-2.612845
6	-0.000384	2.898398	0.517722
6	-0.000681	4.268215	0.389453
6	-0.001076	4.819492	-0.881354
6	-0.001152	3.960544	-1.975905
6	-0.000835	2.594546	-1.768353
1	-0.000068	2.434434	1.508195
1	-0.000601	4.894443	1.285029
1	-0.001325	5.905038	-1.022814
1	-0.001464	4.342093	-3.000764
1	-0.000887	1.890977	-2.605680
7	-0.000454	2.065753	-0.539457
7	0.000395	-2.064067	-0.547308

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3}O)Py_{2}(OH)]^{2+}$ (Doublet)

E = -1784.87935419 a.u.

6	2.482617	-0.242109	1.027779
6	3.869326	-0.280116	1.144005
6	4.604758	0.775272	0.656125
6	3.917544	1.864056	0.145901
6	2.534712	1.799241	0.010152
1	4.364087	-1.136344	1.609129
1	5.696748	0.776234	0.713018
1	4.439290	2.774698	-0.161850
6	1.579828	-1.164415	1.684854
6	1.953472	-2.016038	2.711889
6	0.976852	-2.654662	3.450221
1	3.007922	-2.141823	2.966894
6	-0.650904	-1.588927	2.073441

6	-0.346012	-2.413530	3.144792
1	1.247396	-3.320692	4.273893
1	-1.148435	-2.884268	3.717897
6	-1.971749	-1.341034	1.554645
6	-3.188342	-1.677654	2.126788
6	-3.013840	-0.610180	-0.352490
6	-4.354423	-1.430937	1.423411
1	-3.224465	-2.132275	3.120413
6	-4.266282	-0.910034	0.144240
1	-5.325033	-1.677371	1.863207
1	-5.136696	-0.744919	-0.497994
7	0.296120	-0.983603	1.343465
7	-1.905373	-0.780449	0.345583
7	1.826369	0.734597	0.395317
6	1.876951	3.100240	-0.380991
8	1.026235	3.304172	-1.217485
8	2.367755	4.034677	0.307106
6	-2.711153	-0.207538	-1.751002
8	-3.539788	0.013765	-2.573735
8	-1.426375	-0.214136	-1.939328
44	-0.119244	0.000487	-0.485739
6	-0.899082	2.246891	1.314479
6	-1.431188	3.456109	1.702570
6	-2.096266	4.225799	0.761473
6	-2.197692	3.750193	-0.531565
6	-1.629527	2.532522	-0.844613
1	-0.363687	1.604517	2.023503
1	-1.319463	3.788309	2.737352
1	-2.526195	5.193215	1.036636
1	-2.702223	4.319789	-1.315169
1	-1.654612	2.139041	-1.867285
6	0.039814	-2.869301	-1.265615
6	0.485909	-4.016324	-1.884268
6	1.698766	-3.984786	-2.549783
6	2.412653	-2.801031	-2.565486
6	1.892512	-1.695572	-1.924939
1	-0.927283	-2.846415	-0.752395
1	-0.128194	-4.919209	-1.855097
1	2.076740	-4.873018	-3.064174
1	3.365511	-2.716204	-3.093017
1	2.393452	-0.723625	-1.962934
7	0.728719	-1.728964	-1.277697
7	-0.992737	1.789741	0.063881
8	0.736271	0.790234	-1.889354
1	0.711911	1.773156	-1.867059

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3}O)Py_{2}(O)]^{+}$ (Doublet)

E = -1784.59176143 a.u.

6	2.457055	0.019602	1.144584
6	3.811966	0.186680	1.337499
6	4.411819	1.329956	0.835686
6	3.611876	2.283037	0.251574
6	2.255550	2.028341	0.034852
1	4.395935	-0.562563	1.877468
1	5.486802	1.492164	0.954554
1	3.994713	3.263185	-0.042408
6	1.648055	-1.003029	1.772026
6	2.075158	-1.817184	2.811539
6	1.157179	-2.606225	3.471125
1	3.119423	-1.797113	3.129824
6	-0.516517	-1.744162	2.016499
6	-0.167123	-2.550792	3.085522
1	1.469371	-3.247441	4.299663
1	-0.926223	-3.146634	3.597304
6	-1.838206	-1.643272	1.442570
6	-3.017231	-2.150398	1.966105
6	-2.913656	-0.957776	-0.459433
6	-4.186437	-2.016286	1.239596
1	-3.021480	-2.643933	2.941392
6	-4.131308	-1.428683	-0.010655
1	-5.129721	-2.397569	1.640942
1	-4.997282	-1.336167	-0.671887
7	0.377694	-0.998351	1.354632
7	-1.806414	-1.025082	0.261121
7	1.714114	0.877955	0.425107
6	1.434751	3.244945	-0.423517
8	0.631092	3.157616	-1.358291
8	1.723577	4.214660	0.252170
6	-2.648458	-0.466555	-1.842424
8	-3.520858	-0.358493	-2.653874
8	-1.392146	-0.276441	-2.016680
44	-0.075186	0.054974	-0.511274
6	-1.230990	2.015072	1.416794
6	-1.930643	3.118119	1.850295
6	-2.608193	3.881550	0.915024
6	-2.551445	3.512798	-0.414019
6	-1.815392	2.402236	-0.772024
1	-0.664619	1.384088	2.111604
1	-1.927301	3.378909	2.910690
1	-3.166253	4.770192	1.223827
1	-3.050518	4.093360	-1.192292
1	-1.685225	2.099168	-1.815500
6	0.516277	-2.748188	-1.376312
6	1.157046	-3.797383	-1.999279
6	2.374262	-3.561711	-2.612449
6	2.896426	-2.282618	-2.577434
6	2.186996	-1.288081	-1.936182

1	-0.460270	-2.881055	-0.898272
1	0.690309	-4.784810	-2.012778
1	2.906196	-4.368757	-3.124654
1	3.845832	-2.039341	-3.059668
1	2.534738	-0.249636	-1.918939
7	1.021030	-1.518930	-1.338807
7	-1.179150	1.662506	0.134209
8	0.604580	0.988713	-1.762576

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(O)]^{+}$ Water Nucleophilic Attack TS (Doublet)

E = -1860.96117654 a.u.

6	1.697677	-2.070643	1.012173
6	2.171710	-3.297597	0.575358
6	3.333370	-3.297397	-0.181132
6	3.927764	-2.091428	-0.487483
6	3.394008	-0.921416	0.050228
1	1.630450	-4.226976	0.782346
1	3.744236	-4.236592	-0.564041
1	4.802758	-2.041248	-1.141641
6	0.415760	-1.928411	1.717967
6	0.086806	-2.765123	2.779419
6	-1.052752	-2.531922	3.514987
1	0.779551	-3.568314	3.044752
6	-1.483398	-0.661250	2.100311
6	-1.833861	-1.440901	3.187170
1	-1.316361	-3.172121	4.361275
1	-2.727365	-1.202156	3.768175
6	-2.256118	0.512454	1.693262
6	-3.293778	1.129160	2.379759
6	-2.406518	2.091003	-0.015046
6	-3.872311	2.263741	1.835494
1	-3.644309	0.744292	3.340291
6	-3.432211	2.760281	0.616787
1	-4.683452	2.764791	2.371783
1	-3.865967	3.645268	0.143804
7	-0.391836	-0.921657	1.343918
7	-1.848234	1.018859	0.534818
7	2.318150	-0.918504	0.816652
6	3.930069	0.455076	-0.299104
8	4.396064	1.137605	0.580003
8	3.785699	0.759923	-1.520615
6	-1.849117	2.407347	-1.380268
8	-2.224812	3.353473	-2.000027
8	-0.991810	1.516387	-1.789454
44	-0.336327	0.181493	-0.509227
6	1.219772	1.823790	1.442908
6	2.077421	2.800504	1.885551

6	2.663027	3.644714	0.959502
6	2.331336	3.500969	-0.372534
6	1.442332	2.514247	-0.734439
1	0.785198	1.096935	2.132503
1	2.319331	2.860591	2.948203
1	3.385152	4.402338	1.275186
1	2.777294	4.126188	-1.147654
1	1.143130	2.370845	-1.775413
6	-2.903562	-0.889074	-1.718312
6	-3.787956	-1.800477	-2.255658
6	-3.417422	-3.130206	-2.320935
6	-2.169805	-3.490075	-1.845873
6	-1.345969	-2.515754	-1.324039
1	-3.155528	0.174054	-1.678697
1	-4.753336	-1.454478	-2.631613
1	-4.091098	-3.878417	-2.748478
1	-1.818550	-4.523506	-1.888299
1	-0.334115	-2.749175	-0.974165
7	-1.705634	-1.234409	-1.254130
7	0.902225	1.678098	0.153838
8	0.844912	-0.806159	-1.268343
8	2.054617	-0.379552	-2.741092
1	2.891236	0.123901	-2.156178
1	1.572429	0.318303	-3.201919

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(OO)]^{+}$ (Doublet)

E = -1859.69653810 a.u.

6	2.001993	-1.785843	0.922638
6	2.584428	-2.987957	0.531803
6	3.769343	-2.950810	-0.182128
6	4.328940	-1.720676	-0.465665
6	3.667202	-0.592033	-0.009019
1	2.102022	-3.942402	0.769452
1	4.248040	-3.876355	-0.514990
1	5.261397	-1.613751	-1.027918
6	0.754223	-1.754669	1.711970
6	0.632265	-2.559582	2.836234
6	-0.474502	-2.435880	3.649712
1	1.444008	-3.247788	3.087665
6	-1.266567	-0.741029	2.166147
6	-1.424719	-1.493755	3.317436
1	-0.585499	-3.050475	4.546885
1	-2.308050	-1.352466	3.944475
6	-2.244543	0.257571	1.741314
6	-3.334121	0.745133	2.449653
6	-2.759016	1.652509	-0.065363
6	-4.133576	1.715200	1.868027

1	-3.556976	0.384021	3.456746
6	-3.852184	2.177935	0.590965
1	-4.989120	2.111356	2.422403
1	-4.457673	2.934498	0.084509
7	-0.195923	-0.883708	1.344477
7	-1.998298	0.733775	0.520486
7	2.533944	-0.603229	0.667394
6	4.225257	0.753172	-0.286354
8	5.209690	0.971999	-0.962915
8	3.657951	1.773142	0.209121
6	-2.334336	1.963890	-1.485899
8	-2.927936	2.789479	-2.115902
8	-1.353404	1.228595	-1.891502
44	-0.462224	0.126951	-0.488222
6	0.845861	2.167806	1.281744
6	1.441514	3.359932	1.629512
6	1.748991	4.268108	0.632853
6	1.450065	3.936384	-0.673064
6	0.839873	2.726678	-0.937314
1	0.611127	1.412068	2.037632
1	1.671502	3.560765	2.678261
1	2.227217	5.221696	0.873920
1	1.679758	4.608886	-1.502337
1	0.561934	2.435399	-1.954533
6	-2.736139	-1.476489	-1.612243
6	-3.400210	-2.556254	-2.156271
6	-2.733722	-3.760305	-2.277908
6	-1.421331	-3.830069	-1.847019
6	-0.836768	-2.703968	-1.309598
1	-3.226847	-0.502847	-1.531069
1	-4.432032	-2.436364	-2.494129
1	-3.227859	-4.633386	-2.713643
1	-0.839736	-4.750702	-1.934331
1	0.209166	-2.708889	-0.981349
7	-1.476282	-1.540609	-1.185847
7	0.532033	1.854228	0.024622
8	1.024531	-0.359195	-1.629043
8	1.907644	0.181942	-2.296861

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{2}O)Py_{2}(OO)]^{+}$ (Quartet)

E = -1859.69675396 a.u.

6	2.018437	-1.775416	0.911886
6	2.617404	-2.973608	0.533362
6	3.809521	-2.927803	-0.167742
6	4.360254	-1.693276	-0.449716
6	3.678948	-0.568727	-0.012320
1	2.142652	-3.931861	0.770985

1	4.301809	-3.850101	-0.489743
1	5.300563	-1.579574	-0.997508
6	0.770130	-1.755545	1.700502
6	0.656167	-2.566394	2.821673
6	-0.449749	-2.455162	3.637787
1	1.473840	-3.249044	3.068849
6	-1.257416	-0.759569	2.163713
6	-1.407893	-1.518935	3.311581
1	-0.554132	-3.074616	4.532418
1	-2.291236	-1.387426	3.940694
6	-2.245135	0.232307	1.745970
6	-3.337852	0.706658	2.458655
6	-2.777258	1.629240	-0.054218
6	-4.147773	1.671204	1.882517
1	-3.554972	0.339660	3.464864
6	-3.874078	2.141383	0.606438
1	-5.005744	2.057080	2.440369
1	-4.488435	2.893755	0.104447
7	-0.187033	-0.889774	1.339224
7	-2.006391	0.715955	0.526872
7	2.537632	-0.588617	0.650317
6	4.222981	0.782259	-0.293008
8	5.237823	1.001973	-0.925317
8	3.613224	1.799303	0.148968
6	-2.359002	1.949027	-1.474652
8	-2.961912	2.770174	-2.101421
8	-1.371272	1.225070	-1.885717
44	-0.467512	0.128867	-0.488182
6	0.830971	2.171462	1.284891
6	1.416638	3.367397	1.636028
6	1.707601	4.284859	0.643081
6	1.403544	3.957989	-0.662932
6	0.805384	2.743466	-0.930915
1	0.608600	1.408825	2.037552
1	1.651850	3.563921	2.684409
1	2.177388	5.241943	0.886837
1	1.620996	4.637782	-1.489523
1	0.525425	2.454980	-1.948294
6	-2.725816	-1.495395	-1.614415
6	-3.378020	-2.579742	-2.163503
6	-2.697313	-3.774886	-2.293836
6	-1.383284	-3.831574	-1.865973
6	-0.810940	-2.701794	-1.323181
1	-3.228048	-0.528230	-1.526109
1	-4.411958	-2.470273	-2.498415
1	-3.181789	-4.651210	-2.733913
1	-0.790948	-4.744645	-1.959946
1	0.235684	-2.696442	-0.997013
7	-1.464257	-1.546972	-1.191343
7	0.511322	1.862464	0.027768

8	1.023054	-0.338262	-1.639624
8	1.911755	0.225168	-2.280744

[Ru^{V}(tda-κ-N^{3})Py_2(O)]$^{+}$ (Doublet)

E = -1784.55691103 a.u.

6	-2.313434	-0.154598	1.518488
6	-3.619981	-0.304151	1.931411
6	-4.635849	-0.265726	0.987029
6	-4.317564	-0.037990	-0.330427
6	-2.980913	0.147399	-0.677847
1	-3.851485	-0.463071	2.986968
1	-5.676373	-0.408980	1.292964
1	-5.077184	0.008259	-1.114520
6	-1.162819	-0.118463	2.418484
6	-1.194186	-0.128925	3.804441
6	-0.000365	0.004997	4.490752
1	-2.135295	-0.227933	4.349523
6	1.162399	0.123514	2.418379
6	1.193557	0.137282	3.804311
1	-0.000458	0.006317	5.584396
1	2.134577	0.237666	4.349298
6	2.313102	0.157744	1.518460
6	3.619618	0.308351	1.931070
6	2.980689	-0.148725	-0.677245
6	4.635510	0.268212	0.986780
1	3.851097	0.469433	2.986309
6	4.317300	0.037784	-0.330217
1	5.675996	0.412240	1.292476
1	5.076887	-0.009803	-1.114265
7	-0.000159	0.001754	1.773243
7	2.016079	-0.044757	0.211744
7	-2.016328	0.045054	0.211365
6	-2.637122	0.574501	-2.136635
8	-2.285134	1.737328	-2.169780
8	-2.842201	-0.340483	-2.918577
6	2.637069	-0.579184	-2.135093
8	2.842484	0.334016	-2.919053
8	2.284894	-1.742012	-2.165689
44	-0.000058	-0.000397	-0.271495
6	0.547495	-2.864185	0.497654
6	0.571617	-4.234458	0.367635
6	-0.111167	-4.812786	-0.686749
6	-0.794073	-3.990259	-1.561034
6	-0.770359	-2.625756	-1.361304
1	1.093994	-2.368500	1.307229
1	1.138348	-4.834651	1.082777
1	-0.101633	-5.897250	-0.829442

1	-1.339893	-4.390416	-2.418110
1	-1.276898	-1.939004	-2.050423
6	-0.547375	2.864977	0.492278
6	-0.570852	4.235046	0.360025
6	0.112485	4.811385	-0.695090
6	0.795174	3.987133	-1.567916
6	0.770736	2.622954	-1.366017
1	-1.094292	2.370877	1.302528
1	-1.137543	4.836649	1.074012
1	0.103555	5.895633	-0.839457
1	1.341393	4.385635	-2.425510
1	1.276970	1.934867	-2.054032
7	0.111696	2.070619	-0.346551
7	-0.111737	-2.071492	-0.342605
8	-0.000070	-0.001996	-1.999033

$[Ru^{V}(tda\text{-}\kappa\text{-}N^{3}O)Py_{2}(OO)]^{+}$ (Doublet)

E = -1859.69620644 a.u.

6	2.209346	1.130838	1.215937
6	3.294855	1.952228	1.430718
6	3.237745	3.261043	0.976922
6	2.067501	3.705381	0.411544
6	1.016782	2.810926	0.192804
1	4.176237	1.585085	1.962025
1	4.086711	3.935981	1.118543
1	1.925715	4.754180	0.138319
6	2.049598	-0.189829	1.810525
6	2.872590	-0.747399	2.782596
6	2.476343	-1.922364	3.389377
1	3.797127	-0.252946	3.089239
6	0.524846	-1.892205	2.040697
6	1.270475	-2.501017	3.037869
1	3.102011	-2.380078	4.160655
1	0.927337	-3.417447	3.524117
6	-0.744286	-2.358993	1.503609
6	-1.525599	-3.381898	2.018233
6	-2.176930	-2.097322	-0.268496
6	-2.692651	-3.735574	1.366432
1	-1.222563	-3.896792	2.933718
6	-3.015574	-3.096848	0.184013
1	-3.329089	-4.529253	1.768053
1	-3.886853	-3.357147	-0.423476
7	0.927261	-0.784550	1.436010
7	-1.100220	-1.705240	0.396105
7	1.122890	1.524657	0.522596
6	-0.324753	3.432466	-0.203904
8	-0.737242	3.331556	-1.366774

8	-0.822726	4.033751	0.728815
6	-2.284662	-1.483322	-1.629037
8	-3.207634	-1.699206	-2.354227
8	-1.212721	-0.819289	-1.911353
44	-0.126168	-0.004681	-0.494663
6	-1.972703	1.162391	1.515995
6	-3.067646	1.819489	2.026695
6	-4.008688	2.321498	1.145395
6	-3.819476	2.133536	-0.209275
6	-2.697180	1.459382	-0.642381
1	-1.179353	0.773089	2.164781
1	-3.161846	1.955828	3.105925
1	-4.881720	2.866621	1.515344
1	-4.525613	2.519704	-0.946784
1	-2.487744	1.311909	-1.706380
6	1.381146	-2.286433	-1.660192
6	2.381372	-2.977537	-2.310131
6	3.535966	-2.304570	-2.664063
6	3.638223	-0.961419	-2.353851
6	2.590750	-0.347870	-1.700065
1	0.437397	-2.770865	-1.392159
1	2.239863	-4.034440	-2.546813
1	4.344851	-2.820181	-3.189676
1	4.518345	-0.375792	-2.628387
1	2.619636	0.721371	-1.462862
7	1.481388	-0.996568	-1.348146
7	-1.787364	0.983777	0.208008
8	0.088312	1.282807	-1.870628
8	0.421875	0.999776	-3.021936

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