Supporting Information

Ligand photodissociation in Ru(II)-1,4,7-triazacyclononane complexes enhances water oxidation and enables electrochemical generation of surface active species

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Experimental

All solvents and reagents were purchased from Sigma Aldrich or Aladdin and used as received. All solutions were prepared in ultra- pure water (Millipore MilliQ® A10 gradient, 18.25 MΩ cm, 2–4 ppb total organic content). ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and at 100 MHz, respectively, if not otherwise stated using Bruker 500 MHz NMR spectrometer. Non-deuterated trifluoromethanesulfonic acid (TFSA) was used in ^{1}H NMR studies. However, when ^{1}H NMR of TFSA was recorded in D_2O, no peaks for TFSA was observed which might be due to fast H/D exchange with D_2O. UV/Vis spectra were recorded on a Shimadzu UV-1800 spectrophotometer. Time-dependent ^{1}H NMR and UV-vis studies were recorded at room temperature. Field Emission Scanning Electron Microscope (FE-SEM) images and SEM-EDX data were taken on a ZEISS ULTRA PLUS-43-13 on connection to an Energy Dispersive Spectrometer (OXFORD X-Max 50). The acceleration voltage was 15 kV. High-resolution mass spectra were collected on a Bruker Daltonics Solarix 7.0 Tesla Fourier Transform Mass Spectrometer. X-ray photoelectron spectroscopy (XPS) was implemented on a surface analysis system (ESCALAB 250Xi, Thermo Fisher Scientific) with Al Kα radiation (1486.6 eV), analyzing the surface nature and concentration of the active surface. For the wide scan, the energy pass was 100 eV, the energy step was 1 eV and the scan number is 1. For the narrow high-resolution scan, the energy pass was 30 eV, the energy step was 0.1 eV, and the scan number is 5. All binding energies (BE) were referenced to the C 1 s line at 284.8 eV. For calculating the elements ratio, we used the At% data for each element that was determined based on the high-resolution scan of each element. Survey scans were performed to identify the elements, while additional high-resolution spectra were obtained for details on specific elements. For every sample, at least two points were tested. High-resolution spectra taken on the chosen points were processed with Casa XPS Software (V2.3.18, Casa Software Ltd., UK).

Electrochemistry

The electrochemical measurements were performed under complete aqueous conditions in trifluoromethanesulfonic acid (TFSA) of pH 1.0 using glass carbon (GC) as working electrode, Pt wire and Ag/AgCl as counter and reference electrodes, respectively. Prior to use, the electrode was polished 3 times until a mirror-like surface was obtained, then sonicated in acetone and water for one minute each.

Chemical water oxidation

Firstly, 3 mL aqueous solution of Ce^{IV}/CF_3SO_3H (at pH 1.0, the concentration of Ce^{IV} is 0.5 M) was introduced into the reaction flask of a total volume 55 mL. The reaction mixture was stirred and deaerated with argon or nitrogen gas for 30-60 min until no oxygen was detected by the oxygen sensor in the reaction flask. Then, 200 μL of 1 mM catalyst solution (that was also deoxygenated for 30 min) was injected in the reaction flask through a septum using a syringe, so that the final catalyst concentration is 6.25 x 10^{-6} M. For comparing the activities of original complex and its photolyzed form, 500 μL of 1 mM stock solution was injected so that the final concentration is 14.2×10^{-5} M. The oxygen content in the headspace of the flask was monitored directly after injecting the catalyst solution using an oxygen sensor (Ocean Optics FOSPOR-R) and finally calibrated using GC.

DFT Calculations

In this study, we utilized DFT calculations to study the energetics of transition for complex **1** and **2** from **^{3}MLCT** state to **^{3}MC** state using M06-2X [1] DFT functional with Gaussian 09 package [2]. The SDD basis set and effective core potential [3, 4] were used for Ru atom. The 6–31G(d) basis set was used for the other atoms. The reasoning to utilize M06-2X functional is that this functional gives better results in the main-group chemistry [5]. The geometries of reactants, products, and transition states were optimized in the gas phase. Transition states (TS) are validated with the frequency calculations requiring one negative eigenvalue, and reactants and products were validated without any negative eigenvalues.

Synthesis

[Ru([9]a-neN3)(DMSO-S)$_2$Cl]Cl [6].

In glove box, a 280 mg of *cis*-[$RuCl_2(DMSO)_4$] (0.58 mmol) and 78 mg of [9]-aneN3 (0.60 mmol) were suspended in 50 mL of dry toluene, then the suspension was transferred out of the glove box and was refluxed for 3 h under Ar atmosphere. During this time the product gradually formed as a white-gray precipitate. After 3 h, the mixture was cooled down, the solid was collected by filtration, washed with toluene, chloroform and diethyl ether and vacuum dried (198 mg, 75%). Found: C, 26.2; H, 5.99; N, 9.13%. $C_{10}H_{27}Cl_2N_3O_2RuS_2$ (457.45) requires (Calculated): C, 26.3; H, 5.95; N, 9.19%. ^{1}H-NMR (500 MHz, D_2O) δ 6.27 (br s, 1H, NH [9]aneN3 *trans*-Cl), 6.05 (s, 2H, 2 × NH [9]aneN3 trans-S), 3.52 (s, 2H, CH_2 [9]aneN3), 3.29

(dd, *J* = 10.1, 2.0 Hz, 12H, 4 ×CH_3DMSO), 3.22 – 3.03 (m, 4H, CH_2 [9]aneN3), 2.91 (dd, *J* = 36.2, 5.0 Hz, 6H, CH_2 [9]aneN3). ^{13}C-NMR (126 MHz, D_2O) δ 52.37 (CH_2 [9]aneN3), 52.24 (CH_2 [9]aneN3), 49.75 (CH_2 [9]aneN3), 49.70 (CH_3 DMSO), 45.46 (CH_3 DMSO), 45.22 (CH_3 DMSO).

Complex 1, [Ru([9]-aneN3)(bpy) DMSO]$(PF_6)_2$ [7].

To a warm solution of [Ru([9]-aneN3)(DMSO-S)$_2$Cl]Cl (50 mg, 0.11 mmol) in 5 mL dry methanol was added a 35 mg of 2, 2' -bipyridine (0.22 mmol, 2 eq.), then the reaction mixture was refluxed for 4 h. During this time the color of the solution changed from yellow to red. Then a 58 mg of $AgPF_6$ (0.23 mmol, 2.05 eq.), partially dissolved in 5 mL of methanol, was added and the mixture was refluxed for an additional 2 h in the dark. The AgCl precipitate was filtered off over celite and the deep orange filtrate was rotary concentrated to *ca.* 2 mL to induce the formation of the product as a yellow solid. To improve precipitation, the mixture was saturated with diethyl ether. After overnight standing, the solid was collected by filtration, washed with ethanol and diethyl ether and vacuum dried (45 mg, 55%). Found: C, 28.6; H, 3.99; N, 9.19%.$C_{18}H_{29}F_{12}N_5OP_2RuS$ (754.52) requires (Calculated): C, 28.7; H, 3.87; N,9.28%. ^{1}H-NMR (500 MHz, D_2O) δ 8.87 (d, J = 5.3 Hz, 2H,C^6H/$C^{6'}$H), 8.43 (d, J = 8.2 Hz, 2H,C^3H/$C^{3'}$H), 8.15 (t, J = 7.8 Hz, 2H,C^4H/$C^{4'}$H), 7.73 – 7.65 (m, 2H, C^5H/$C^{5'}$H), 6.37 (br s, 2H, 2 × NH [9]aneN3), 5.56 (br s, 1H,NH [9]aneN3), 3.41–3.27 (4 H, m, CH_2 [9]aneN3), 3.07–2.95 (4H, m, CH_2 [9]aneN3), 2.91–2.78 (4 H, m, CH_2 [9]aneN3), 2.67(6 H, s, CH_3 DMSO). ^{13}C-NMR (126MHz, D_2O) δ158.5 (C^2/$C^{2'}$), 154.1 (C^6H/$C^{6'}$H), 139.4 (C^4H/$C^{4'}$H), 128.5 (C^5H/$C^{5'}$H), 125.0 (C^3H/$C^{3'}$H), 51.1 (2× CH_2 [9]aneN3), 50.7 (2 × CH_2 [9]aneN3), 48.8 (2 × CH_2 [9]-aneN3), 44.3 (2 × CH_3 DMSO).

Complex 2, [Ru([9]-aneN3)(pic) DMSO]Cl [7].

To a solution of Ru([9]-aneN3)(DMSO-S)$_2$Cl]Cl (125 mg, 0.275 mmol) in 15 mL of methanol, an equimolar amount of potassium picolinate (46.0 mg, 0.275 mmol) was added and the mixture was refluxed for 5 h yielding an orange solution. The solvent was removed in vacuo, then the orange residue was washed with acetone followed by dissolving in ethanol (*ca.*1 mL), affording the product as an orange solid, which was collected by filtration, washed with acetone and diethyl ether and vacuum dried (85.0 mg, 66%). Found: C, 36.3; H, 5.52; N, 11.98%. $C_{14}H_{25}ClN_4O_3RuS$ (465.96) requires (Calculated): C, 36.1; H, 5.41; N, 12.02%. ^{1}H-NMR (500

MHz, D_2O) δ 8.83 (d, *J* = 4.8 Hz, 1H, C^6H), 8.10 (t, J = 7.6 Hz, 1H, C^4H), 8.04 (d, J = 7.6 Hz, 1H, C^4H), 7.87 – 7.56 (m, 1H), 6.12 (br s, 1H, NH [9]aneN3), 6.05 (br s, 2H, 2 × NH [9]aneN3), 3.45 – 3.11 (m, 4H, CH_2 [9]-aneN3), 3.01 (d, *J* = 11.1 Hz, 4H, CH_2 [9]aneN3), 2.91 (s, 3H, CH_3 DMSO), 2.83 (m, 4H, CH_2 [9]aneN3), 2.80 (s, 3H, CH_3 DMSO). ^{13}C-NMR (126MHz, D_2O) δ176.5 (C=O), 154.9(C^6H), 152.5 (C^2), 139.2 (C^4H), 130.2 (C^5H), 128.2 (C^3H), 54.1(CH_2 [9]aneN3), 52.4 (CH_2 [9]aneN3), 50.0 (CH_2 [9]aneN3),49.5 (CH_2 [9]aneN3), 47.7 (CH_2 [9]aneN3), 47.0 (CH_2 [9]-aneN3), 44.3 (CH_3 DMSO), 44.2 (CH_3 DMSO).

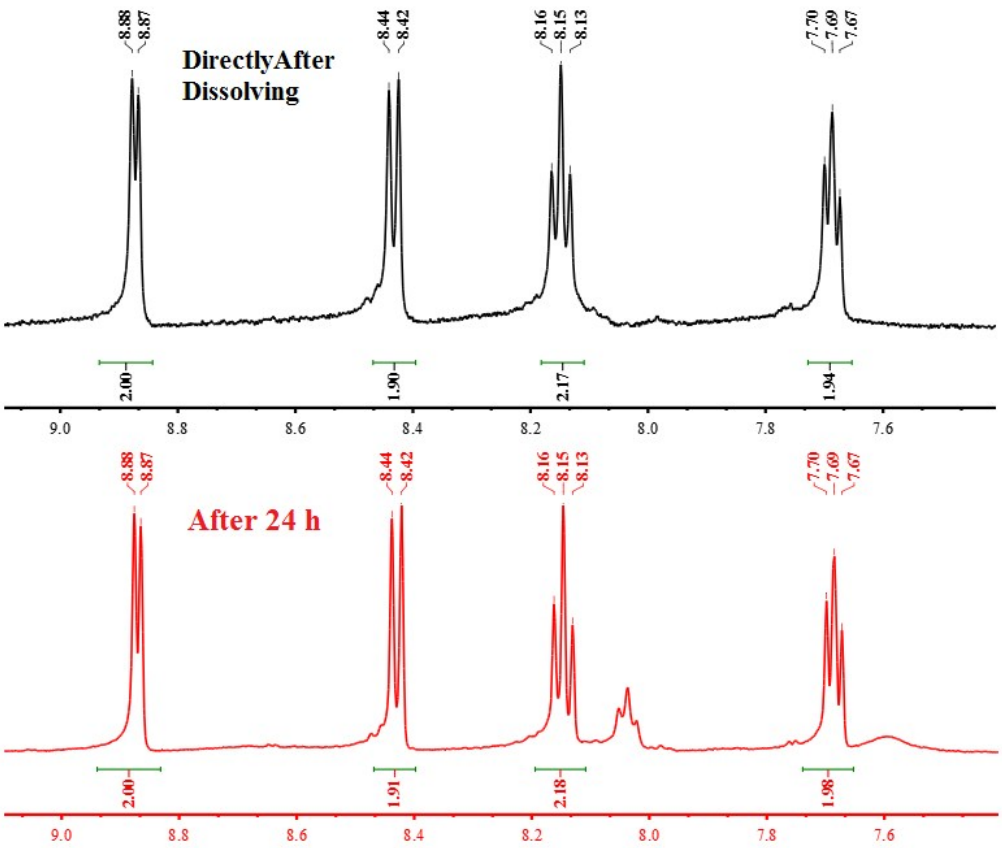


Figure S1. ^{1}H NMR spectrum of complex **1** (15 mM) after dissolving in D_2O, directly after dissolving in D_2O (**Black**) and after 1day of dissolving the complex (**Red**); magnification of the aromatic area**.**

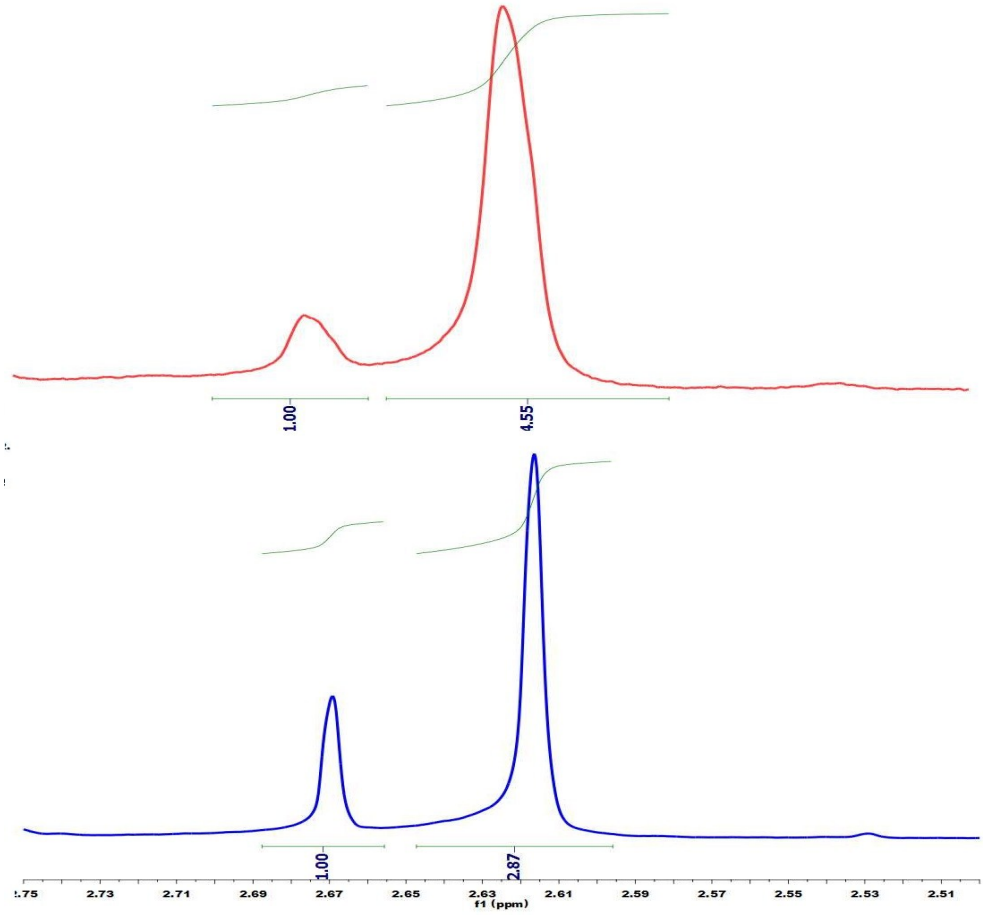


Figure S2. ^{1}H NMR spectrum of complex **1** (15 mM) after dissolving in D_2O, directly after dissolving in D_2O (**Red**) and after 1day of dissolving the complex (**Blue**); magnification of the aromatic area**.**

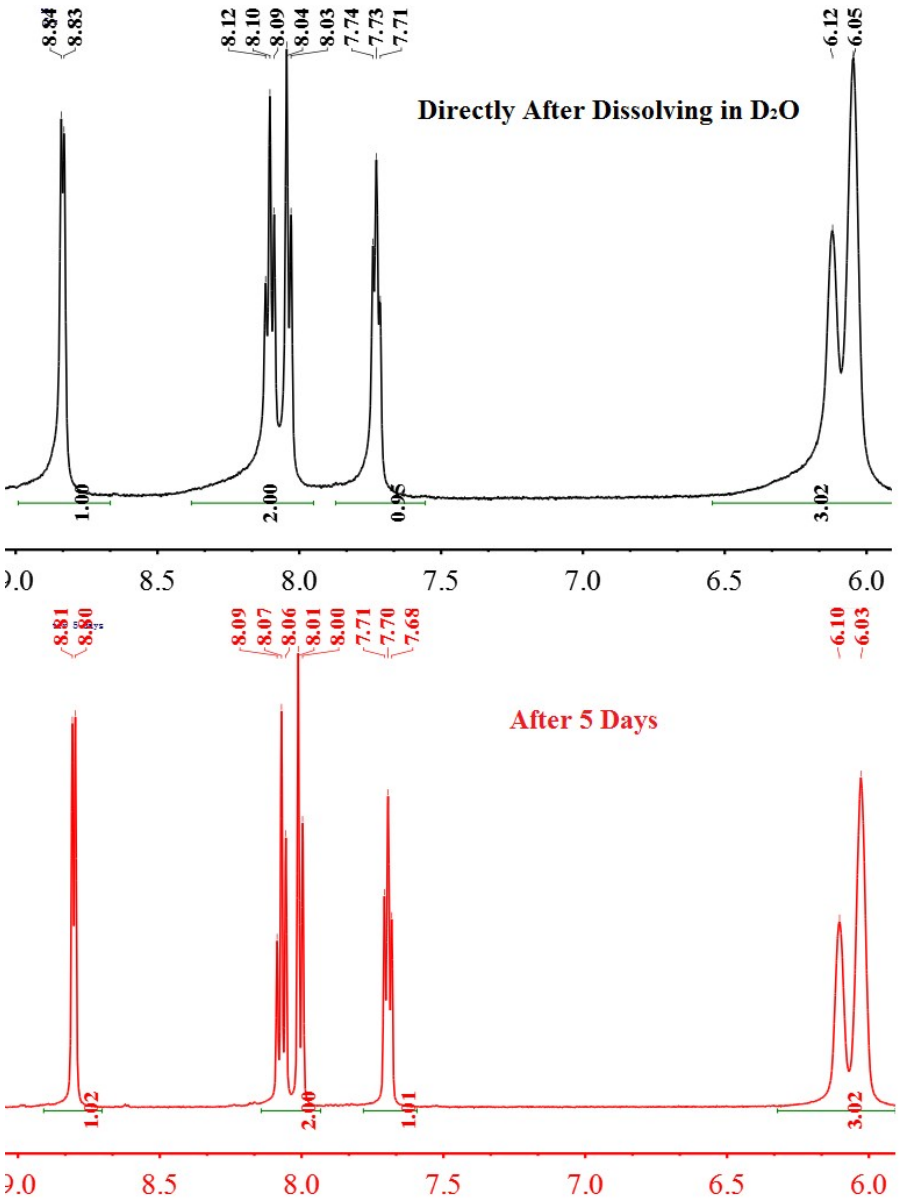


Figure S3. ^{1}H NMR spectrum of complex **2** (25 mM); directly after dissolving in D_2O (**Upper**) and after 5 days of dissolving the complex (**Lower**); magnification of the aromatic area.

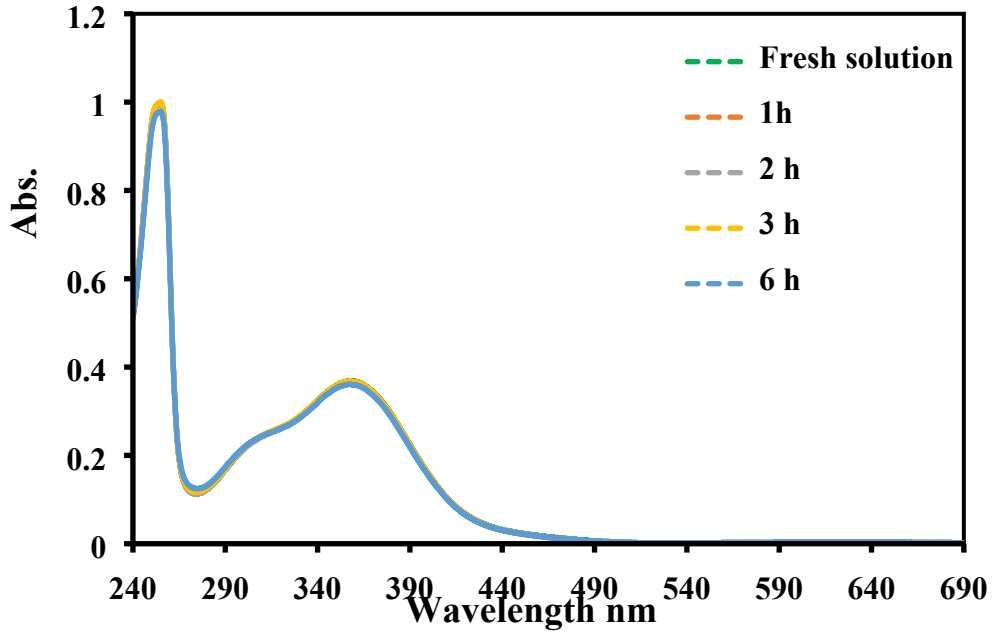


Figure S4. Time-dependent UV-Vis absorption spectra of complex **2** in TFSA aqueous solution (pH 1).

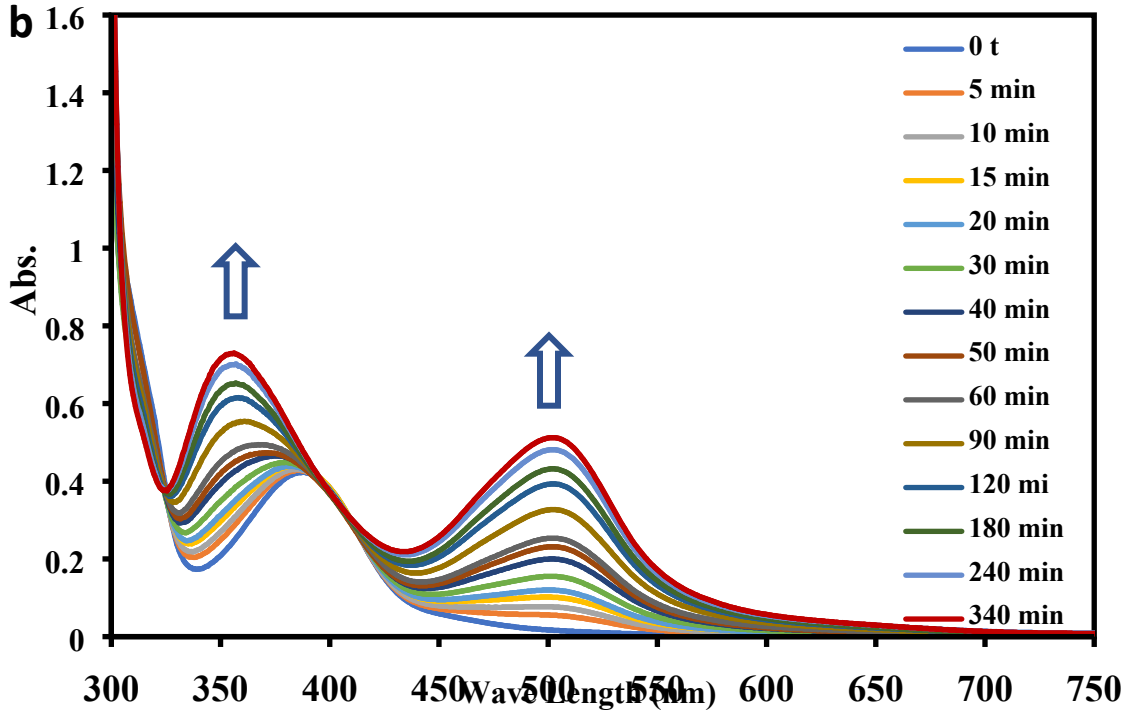


Figure S5. Time-dependent UV-Vis absorption spectra of complex **1** in an aqueous solution of sodium triflate (0.1 M).

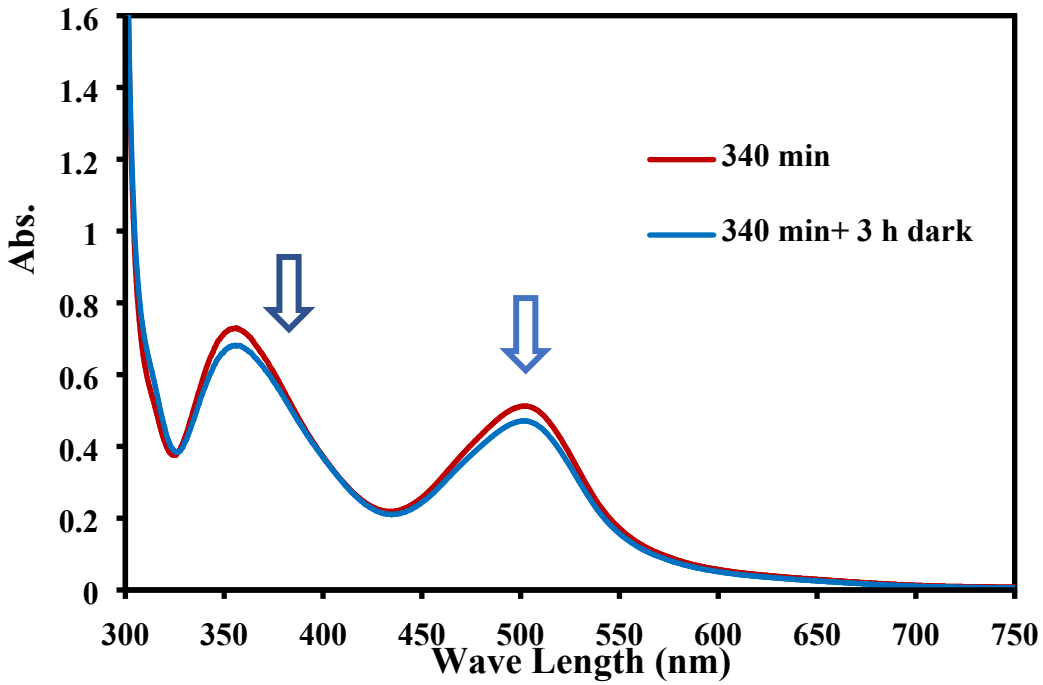
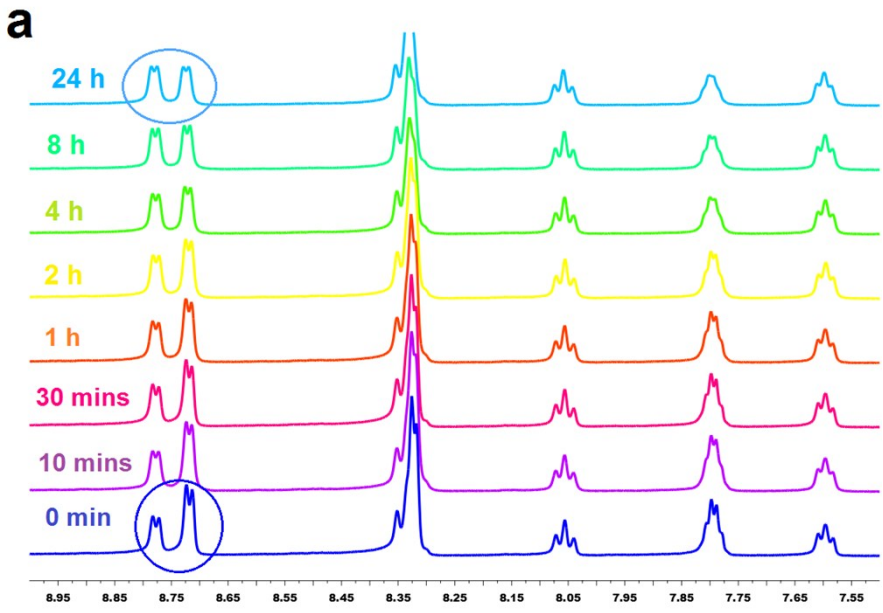


Figure S6. UV-Vis absorption spectra of complex **1** in an aqueous solution of sodium triflate (0.1 M), after exposure for 340 min to light (**red**), and then stored for 3 h in dark (**blue**).



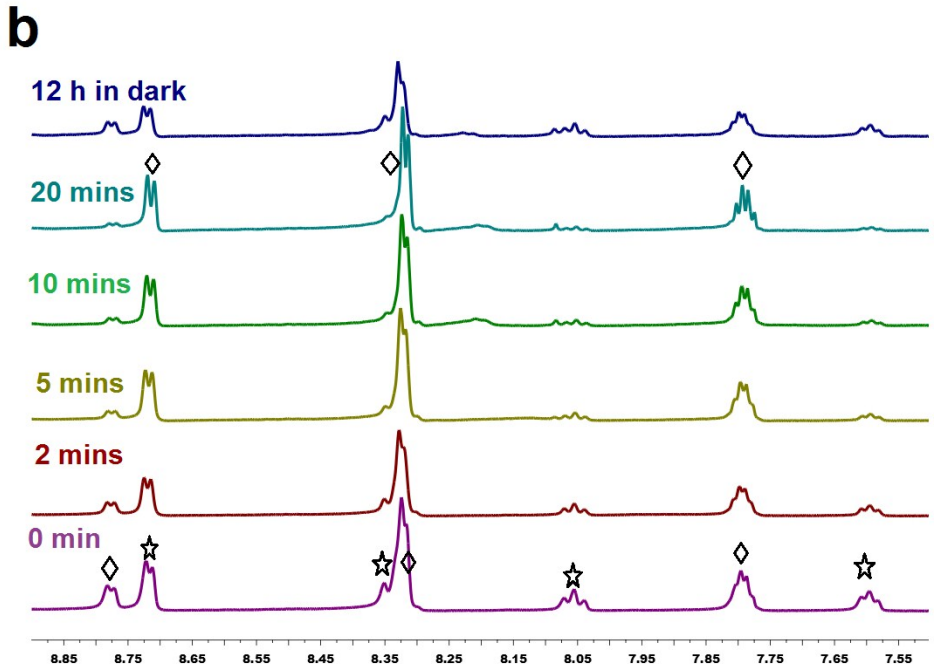


Figure S7. Time dependent ^{1}H-NMR spectrum of complex **1** (15 mM) after dissolving in TFSA/D_2O (p*D* 1.0); magnification of the aromatic area. (a) under dark conditions and (b) under visible light irradiation (diamonds show new peaks (Form **B**), and stars show peaks from original structure (Form **A**).

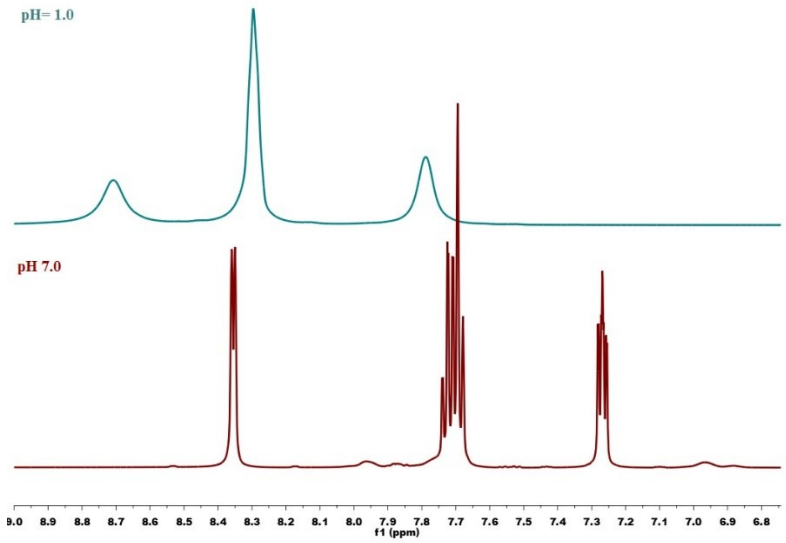


Figure S8. ^{1}H NMR spectra of bpy in D_2O (**Blue**) and TFSA/D_2O (**Red**). The figure indicates the protonation of bpy in pH 1 solution and the changes in the chemical shifts and peaks shape after

protonation. This behavior is different from the new peaks appear in case of ligand partial dissociation in the complex.

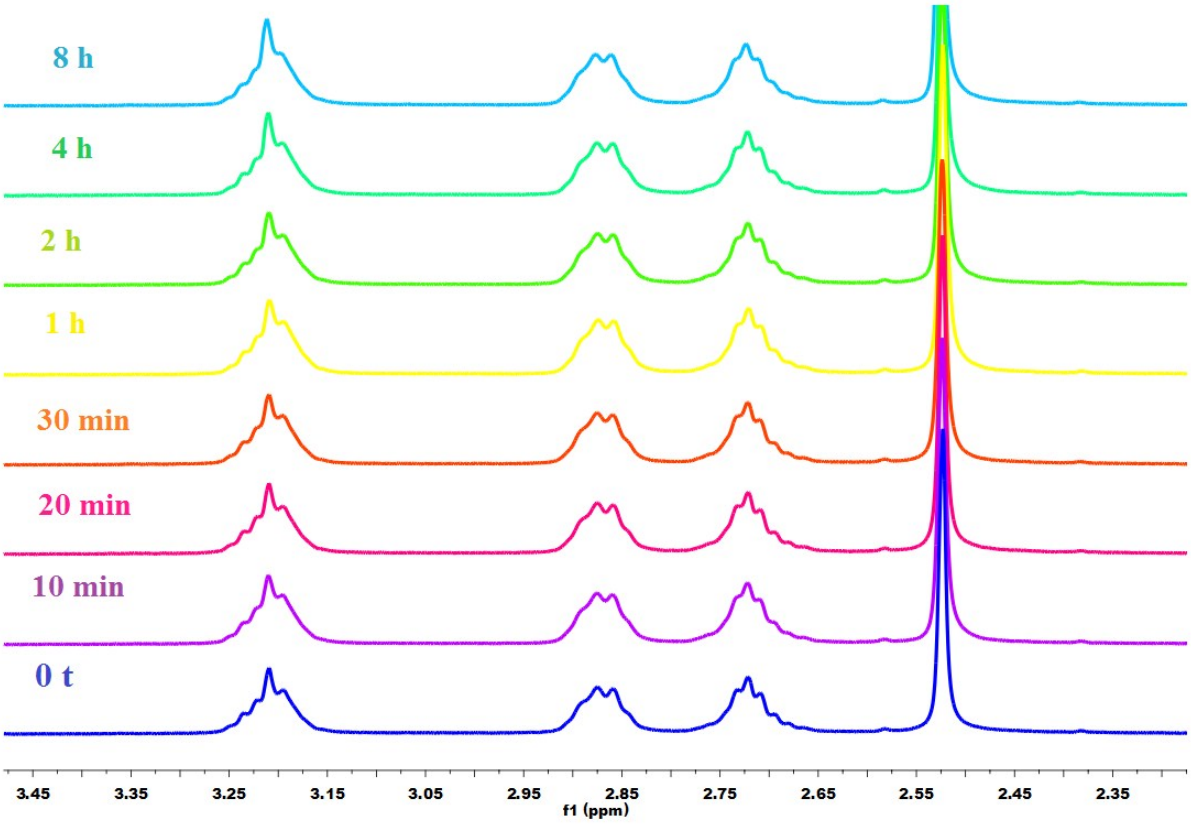


Figure S9. Time dependent ^{1}H-NMR spectrum of complex **1** (15 mM) after dissolving in TFSA/D_2O (p*D* 1.0) under dark conditions, magnification of the aliphatic area. The spectrum shows that no free DMSO ligand is released in acidic conditions, which omits the change in ^{1}H NMR spectra of the complex to be as result of DMSO dissociation.

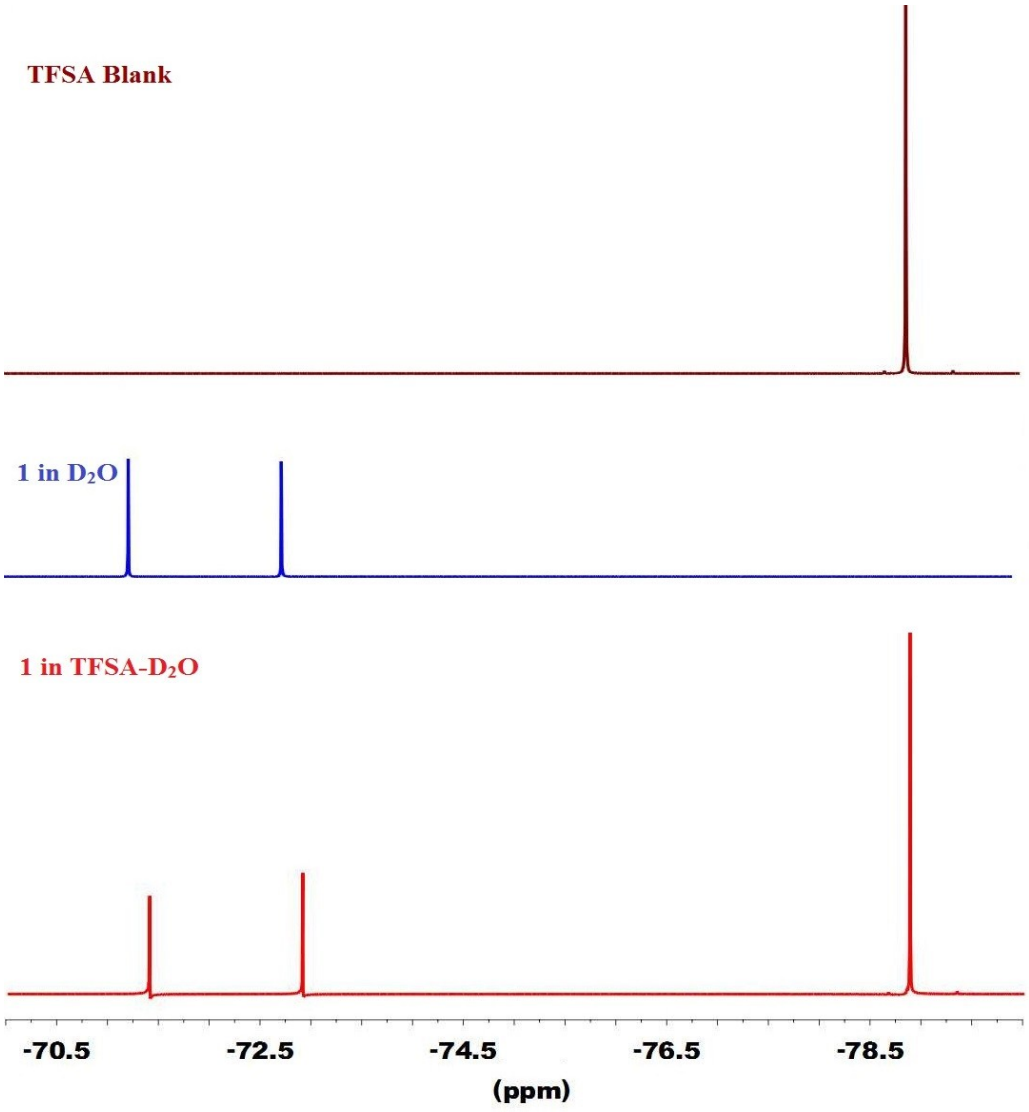


Figure S10. ^{19}F NMR of complex **1** in D_2O and TFSA/D_2O (p*D*= 1.0) as compared to blank TFSA.

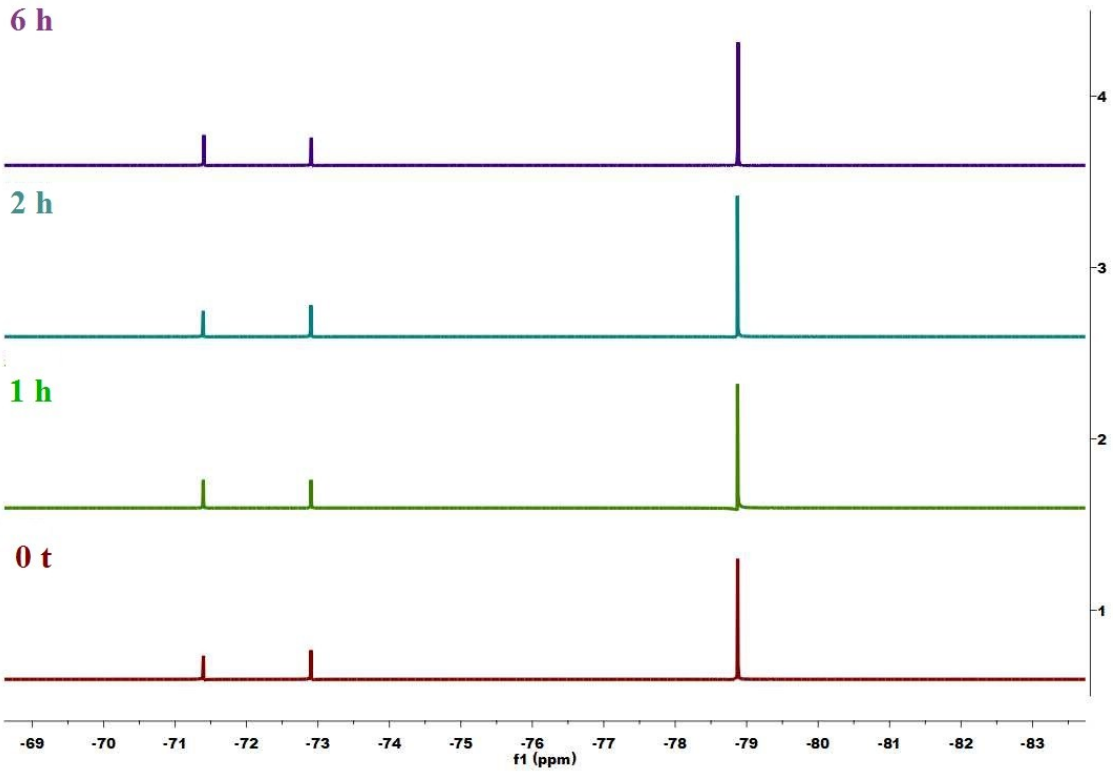


Figure S11. Time dependent ^{19}F NMR of complex **1** in TFSA-D_2O under light conditions.

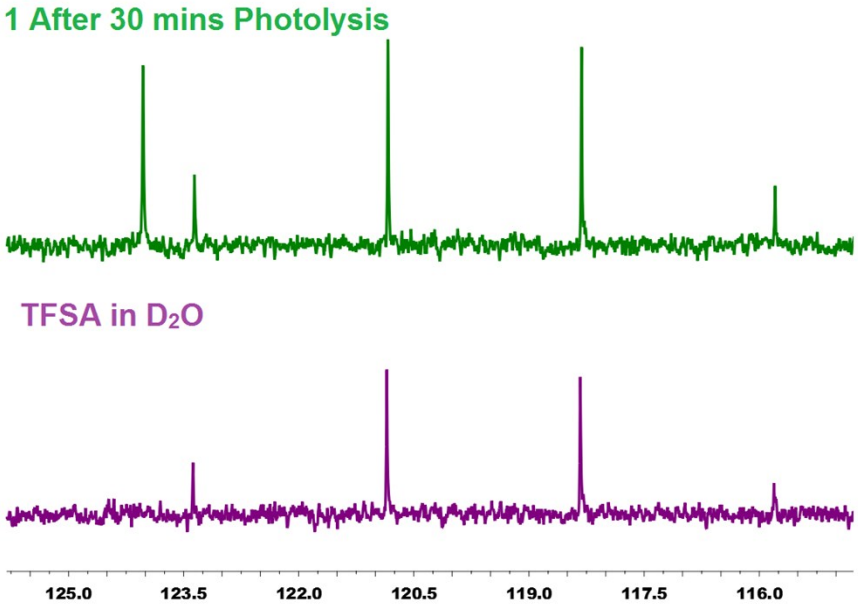


Figure S12. ^{13}C NMR comparison of complex **1** after photolysis for 20 mins and TFSA in D_2O (p*D*= 1.0).

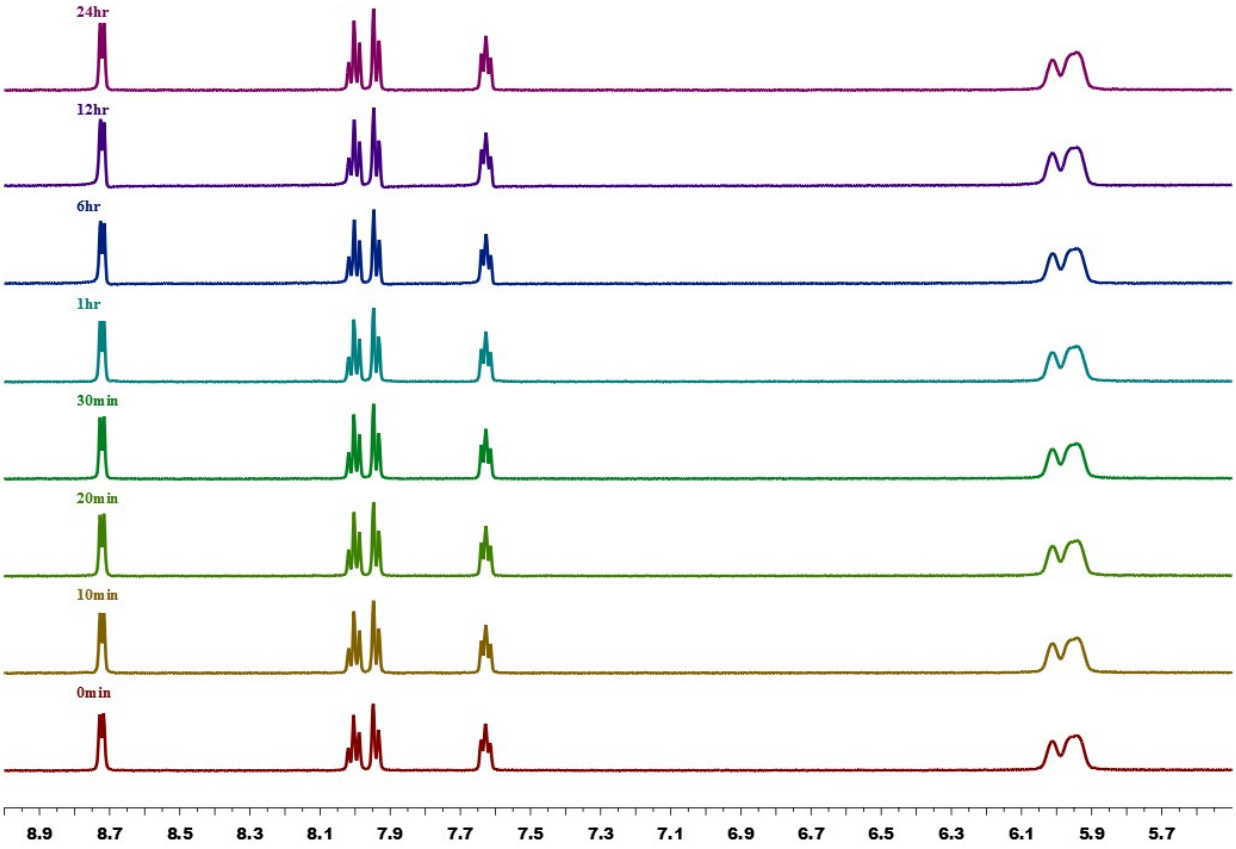


Figure S13. Time dependent ^{1}H-NMR spectrum of complex **2** (15 mM) after dissolving in TFSA/D_2O (p*D* 1.0), in the range 5.5 to 9.0 ppm. Both dark and light samples showed identical spectra, here we show the dark sample.

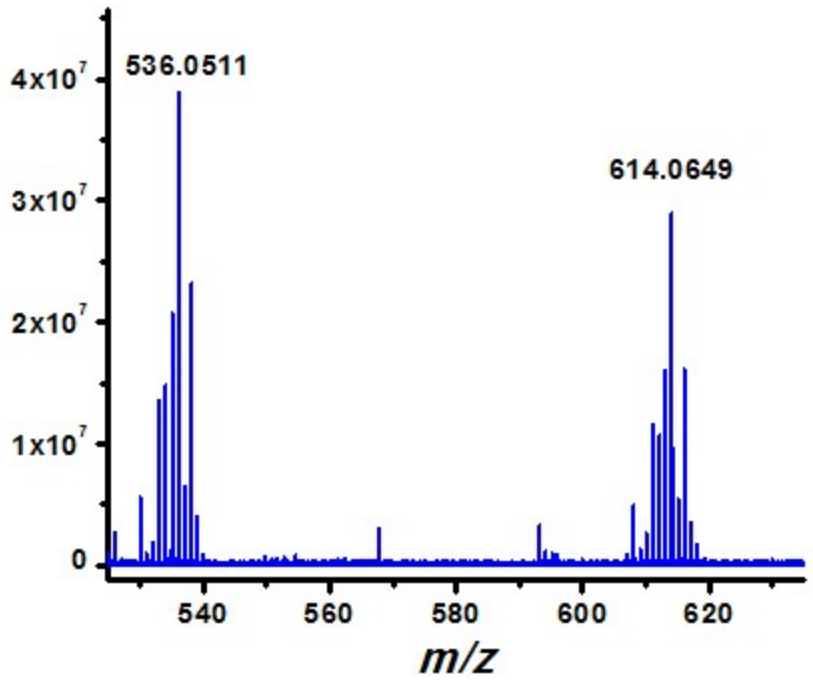


Figure S14. HR-ESI-MS of complex **1** after 24 h of dissolution in TFSA/D_2O (p*D*=1.0) for the dark sample.

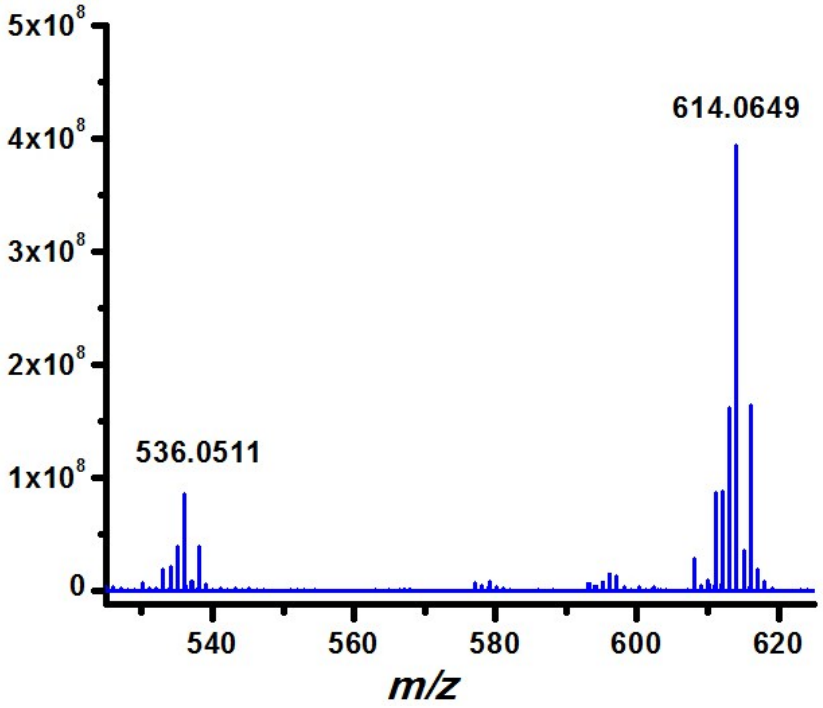


Figure S15. HR-ESI-MS of complex **1** after 20 mins photolysis in TFSA/D_2O (p*D*=1.0).

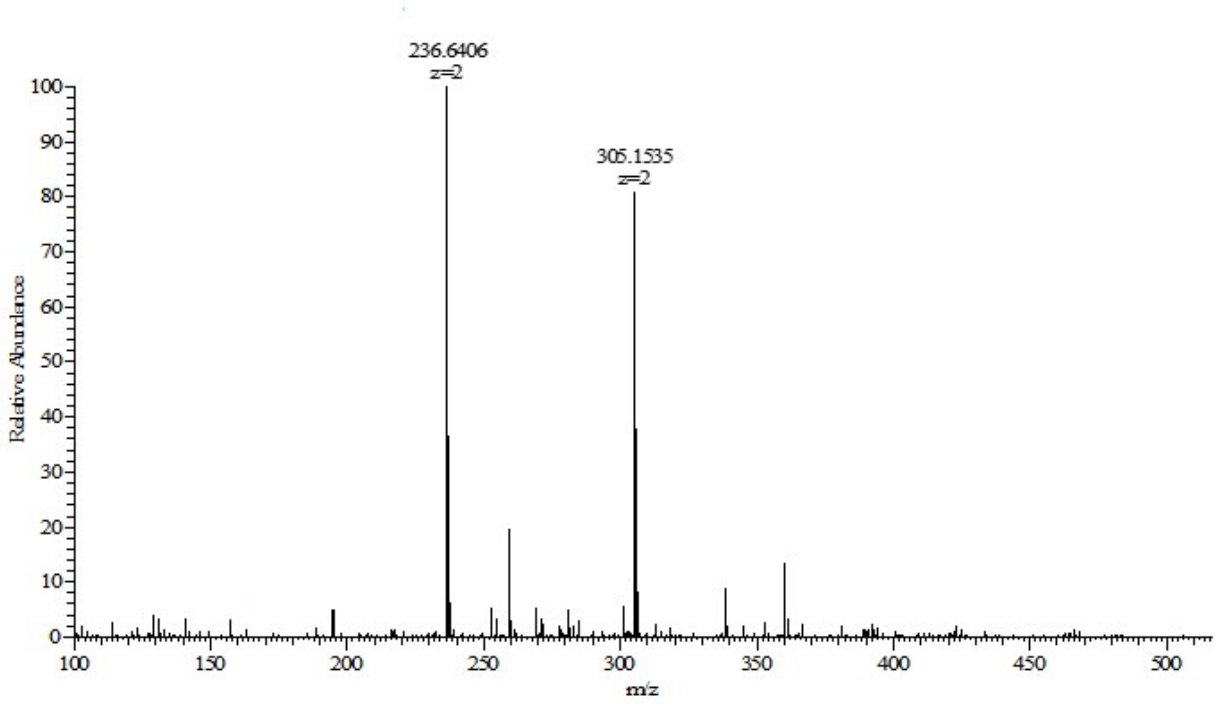


Figure S16. ESI-MS of complex **1** solution (light sample) after 5 days of dissolution in TFSA/D_2O. m/z= 305.1535 ([Ru([9]-aneN3)(bpy) DMSO]OTf - 4H, Z= 2, calculated 305.017).

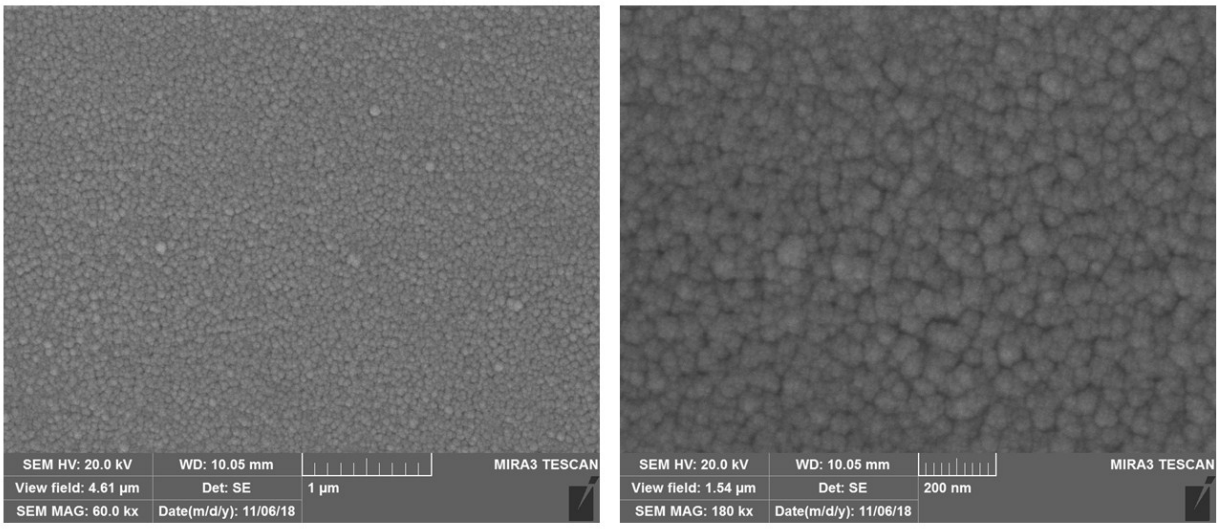


Figure S17. FESEM taken for the electrodeposited film after 100 CV cycles of 1mM of **1** in TFSA solution (pH 1) after 20 mins photolysis, in the potential window 0.2 to 1.89 V (*vs.* NHE).

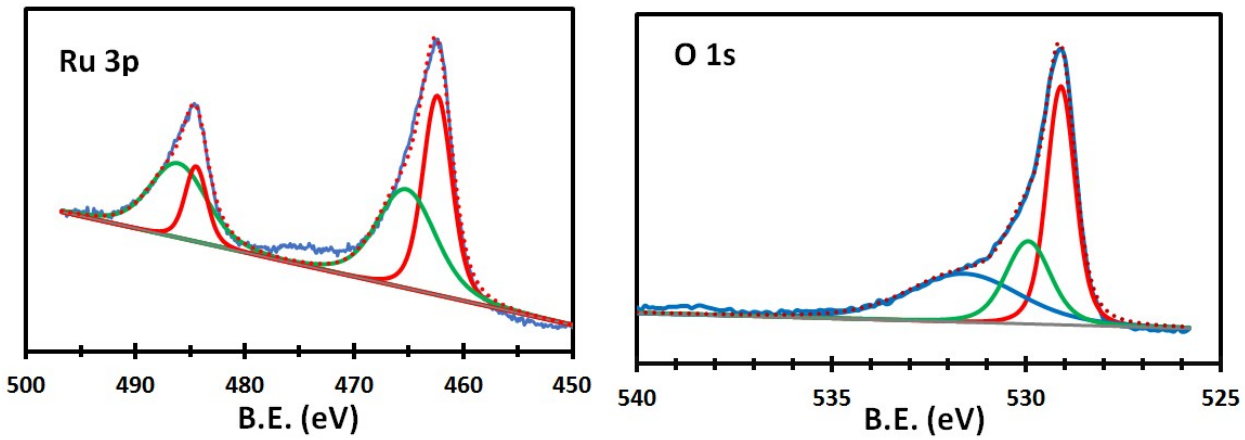


Figure S18. High resolution X-ray photoelectron spectra of Ru 3p and O 1s of commercial available RuO_2 (20% RuO_2/C).

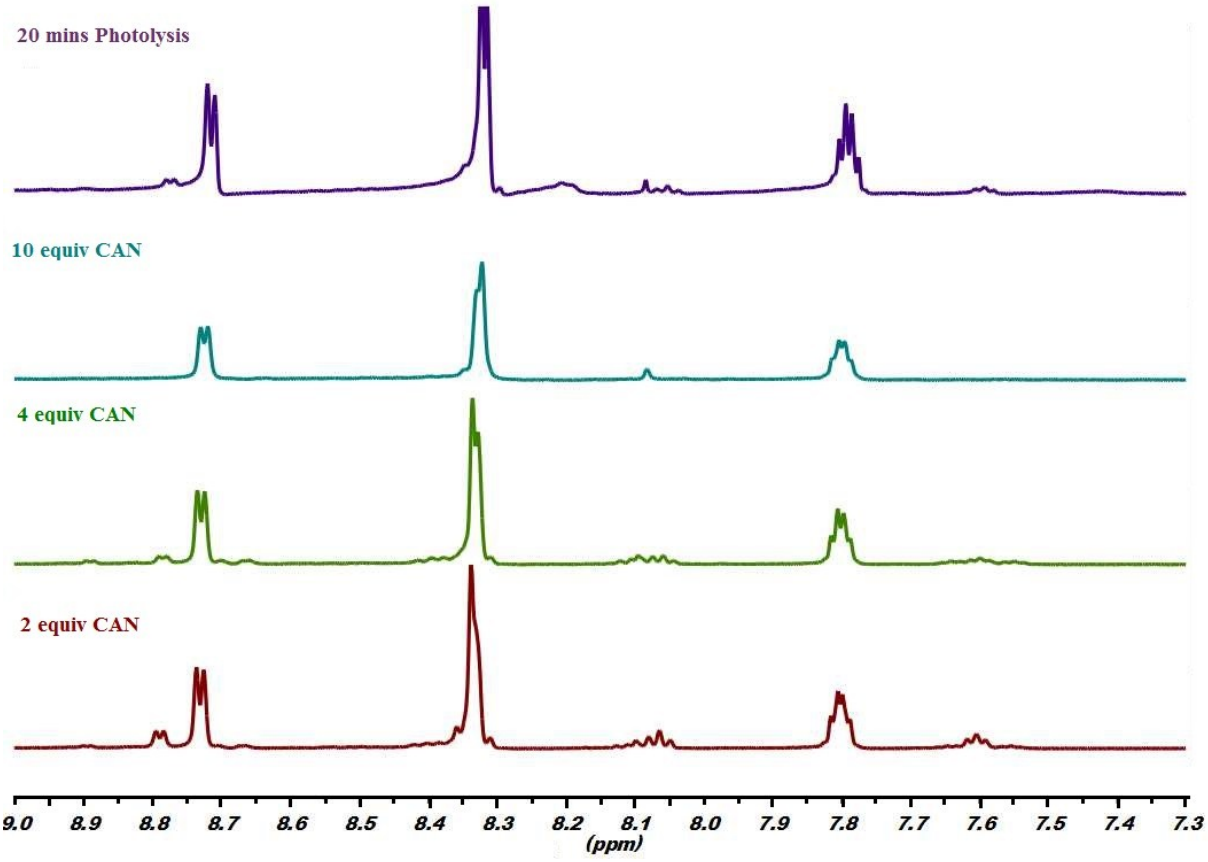


Figure S19. Time dependent ^{1}H-NMR spectrum of complex **1** (15 mM) after dissolving in TFSA/D_2O (p*D* 1.0), in the range 7.3 to 9.0 ppm. After adding different amounts of CAN and its comparison to photolyzed sample (20 mins).

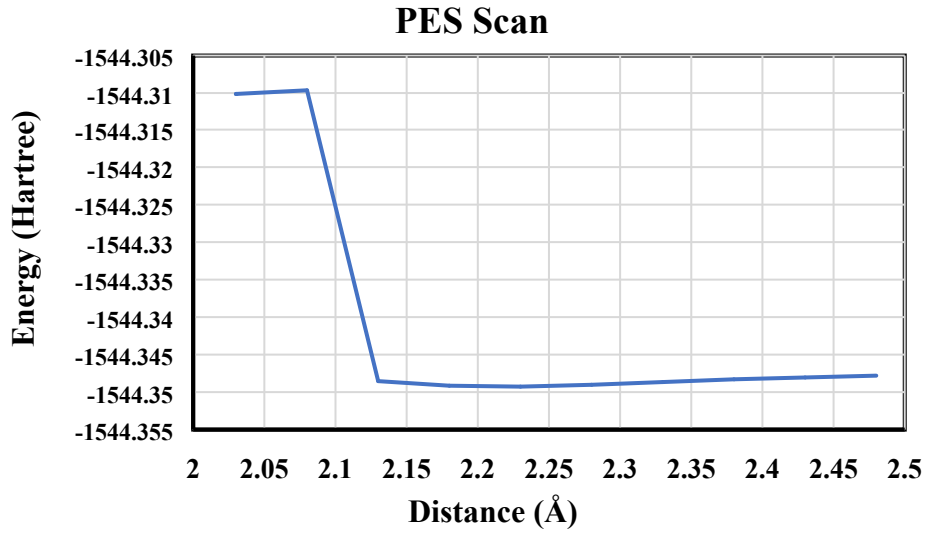


Figure S20. The Potential energy surface (PES) scan plot of 1-^{3}MLCT for N1-Ru bond in gas phase using M06-2X density functional theory with the SDD basis set and effective core potential on Ru and the 6–31G(d) basis set for the rest of the atoms.

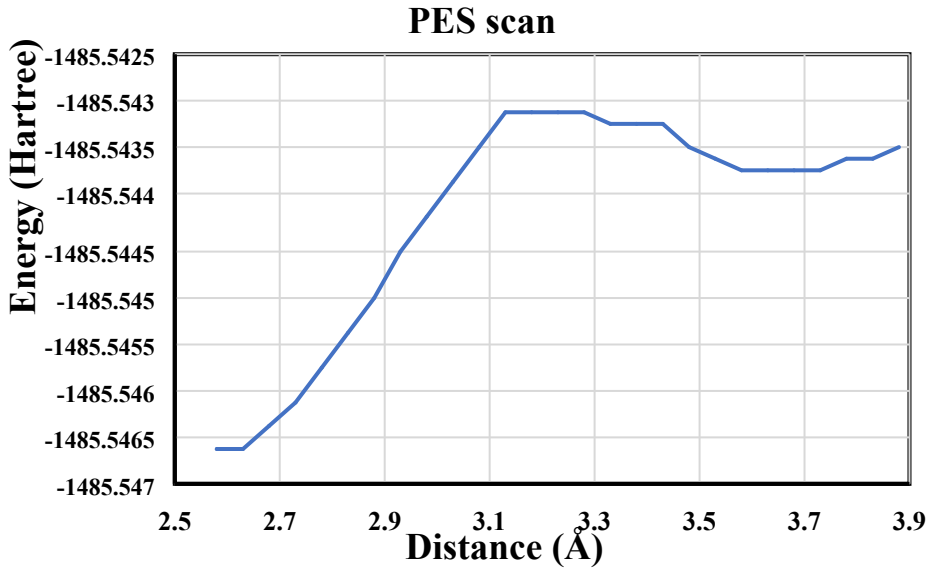


Figure S21. The Potential energy surface (PES) scan plot of **2-^{3}MLCT** for N1-Ru bond in gas phase using M06-2X density functional theory with the SDD basis set and effective core potential on Ru and the 6–31G(d) basis set for the rest of the atoms.

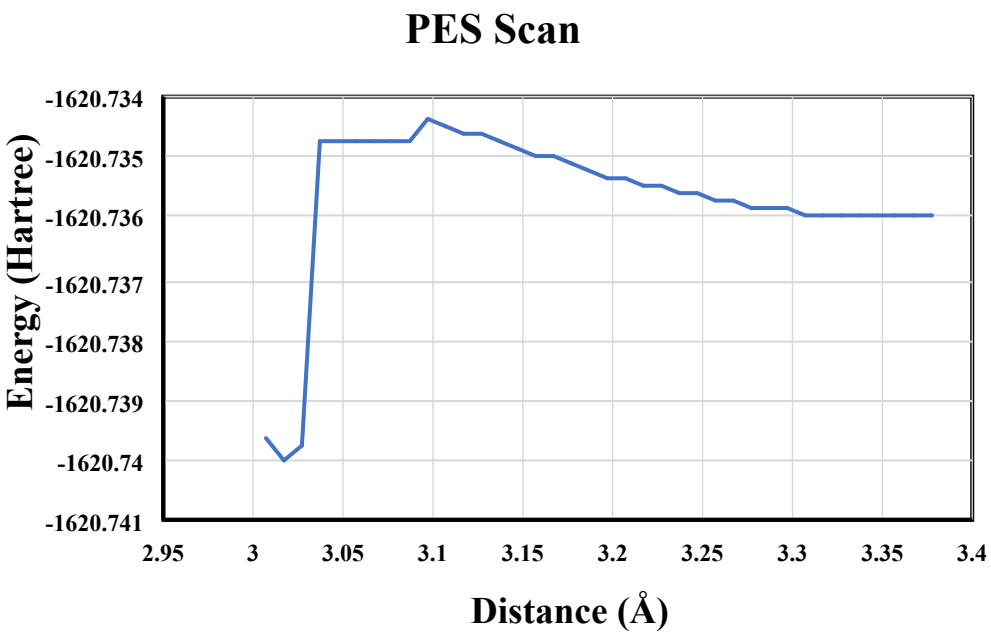


Figure S22. The PES scan plot of H2O-**1-^{3}MC** for Ru-O1 bond in gas phase using M06-2X density functional theory with the SDD basis set and effective core potential on Ru and the 6–31G(d) basis set for the rest of the atoms.

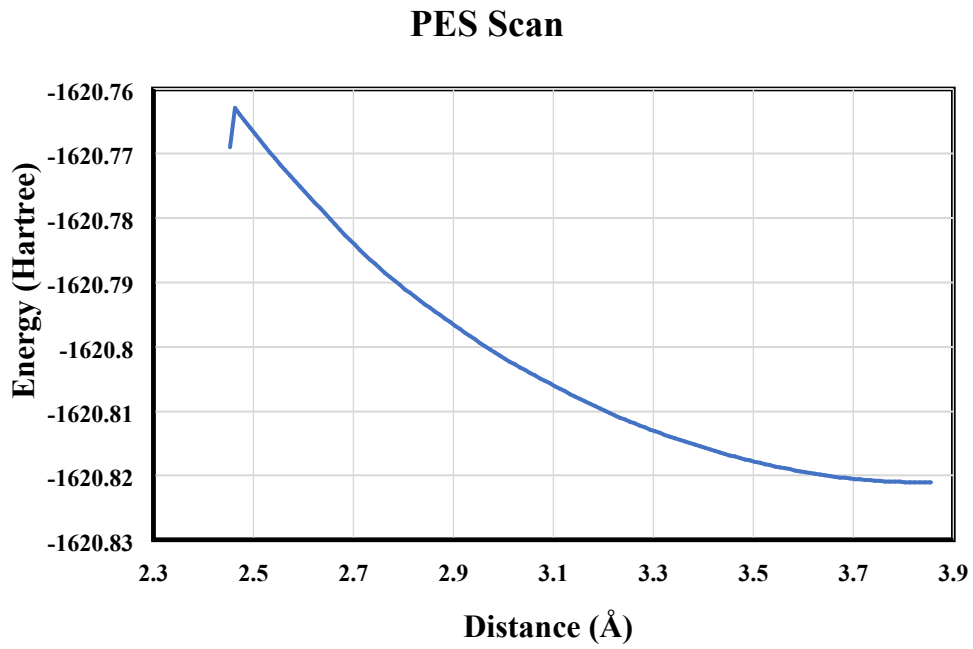
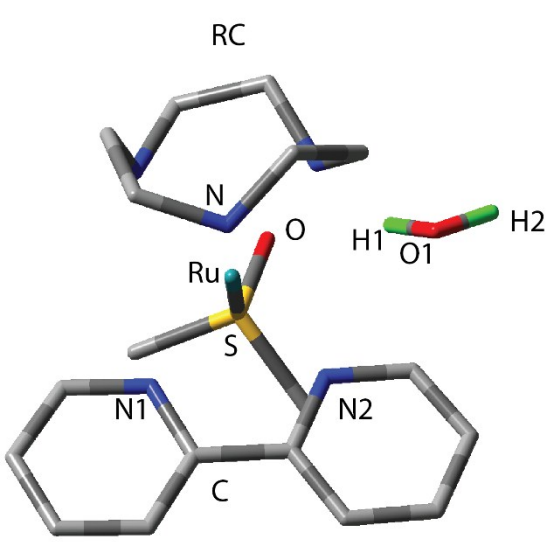
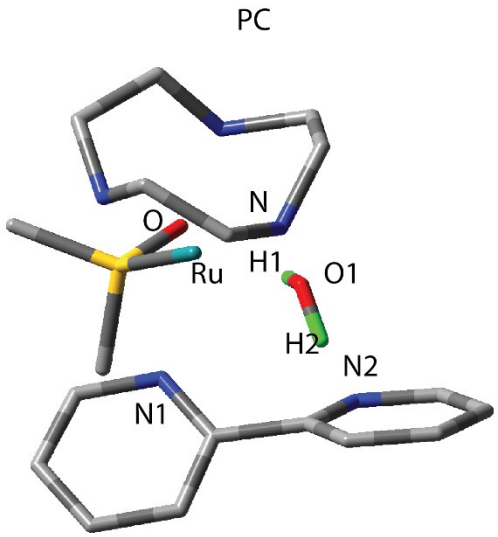


Figure S23. The PES scan plot of H2O-**1-^{1}MC** for Ru-O1 bond in gas phase using M06-2X density functional theory with the SDD basis set and effective core potential on Ru and the 6–31G(d) basis set for the rest of the atoms.





Bond	Distance (Å)
Ru-S	2.30
Ru-N	2.18
Ru-N1	2.14
Ru-N2	2.13
Ru-O1	3.85
O-H1	1.91

Bond	Distance (Å)
Ru-S	2.37
Ru-N	2.14
Ru-N1	2.23
Ru-N2	3.50
Ru-O1	2.17
O-H1	2.04
N2-H2	1.74

Figure S24. The optimized structures of RC and PC for the dissociation of bpy unit in singlet state by a water molecule for complex 1 in gas phase using M06-2X density functional theory with the SDD basis set and effective core potential on Ru and the 6–31G(d) basis set for the rest of the atoms using tube model excluding H atoms except the ones shown with green color.

Cartesian Coordinates

1-^{3}MLCT

Ru	-0.47337500	0.04061100	-0.02817800
N	-0.98472500	0.71853900	-1.99836700
N	-2.06759800	-1.36371900	-0.48034000
N	-2.22407400	1.26171400	0.44650700
C	-1.92701500	-0.23485900	-2.67886000
H	-2.91331300	0.23400100	-2.71388200
H	-1.61626100	-0.38759900	-3.71539100
C	-1.98495000	-1.57876800	-1.95518000
H	-1.07827200	-2.15074500	-2.16100000
H	-2.84053100	-2.16203600	-2.31354600
C	-3.40844400	-0.85408200	-0.04521300
H	-3.96871600	-0.55529200	-0.93473400
H	-3.97412200	-1.65925600	0.42977800
C	-3.27010200	0.30887400	0.92790200
H	-2.94899800	-0.06971100	1.90238800
H	-4.23439100	0.81375700	1.05480700
C	-2.65077600	2.05246000	-0.75787300
H	-3.56556500	1.60333700	-1.15294900
H	-2.90951400	3.07410700	-0.46739000
C	-1.55846000	2.08355800	-1.82409100
H	-0.73760300	2.74072500	-1.52642900
H	-1.96769200	2.45680100	-2.76974200
C	0.88011600	2.70314800	0.55872500
H	-0.11069400	2.98459500	0.90710200
C	1.90535100	3.60194900	0.55782000
H	1.74642600	4.61282200	0.91191400
C	3.18011000	3.17329500	0.07735700

H	4.01077400	3.86971600	0.05054700
C	3.34641300	1.88759400	-0.35435200
C	2.26299800	0.96675300	-0.32193100
C	2.32336500	-0.38739200	-0.72743900
C	3.50272000	-1.06839900	-1.14023200
C	3.47414400	-2.41280900	-1.38894300
H	4.37549500	-2.93108700	-1.69709100
C	2.26096400	-3.13421500	-1.21616800
H	2.21157400	-4.20492900	-1.37064100
C	1.14008500	-2.44105900	-0.84779200
H	0.19886600	-2.95850400	-0.68047400
N	1.02147000	1.40794300	0.14625300
N	1.13123900	-1.09606900	-0.64698100
H	4.30903000	1.56059100	-0.72955300
H	4.43034700	-0.51648200	-1.23759400
S	-0.12000800	-0.94740100	2.10645600
C	1.53713100	-1.57634900	2.38322200
H	1.58843600	-1.93676000	3.41386200
H	1.70469500	-2.39819100	1.68452600
H	2.25240200	-0.76842100	2.20207700
C	-0.23973500	0.24187600	3.44878400
H	-1.23820500	0.68405000	3.42542500
H	-0.10408600	-0.29423900	4.39226600
H	0.52885000	1.00887300	3.31645100
O	-1.13772100	-2.03019200	2.27568500
H	-0.12954700	0.79636700	-2.55317800
H	-2.05119000	1.92170900	1.20567400
H	-1.89546200	-2.24343900	0.01392300

Transition State for 1-^{3}MLCT to 1-^{3}MC

Ru	-0.48071800	0.05703100	-0.00739400
N	-0.86480900	0.95834300	-1.92034500
N	-2.09094400	-1.22776500	-0.66587000
N	-2.20991900	1.29799200	0.49366900
C	-1.79650500	0.10685200	-2.73476200
H	-2.76667100	0.60827500	-2.77358600
H	-1.43825700	0.04081100	-3.76510200
C	-1.93356600	-1.29951500	-2.15056500
H	-1.03636900	-1.88396400	-2.36485000
H	-2.78696900	-1.81359800	-2.60662600
C	-3.43795100	-0.71007000	-0.25425900
H	-3.93521500	-0.30579400	-1.13955400
H	-4.05504000	-1.53565800	0.10833400
C	-3.31373100	0.34808300	0.83310400
H	-3.06049600	-0.13239800	1.78214900
H	-4.26399700	0.87905900	0.95858800
C	-2.54835900	2.22515300	-0.63922900
H	-3.45694900	1.85350400	-1.11909700
H	-2.78614200	3.22014600	-0.25386600
C	-1.40079000	2.31887600	-1.64127800
H	-0.57549300	2.90942000	-1.23550400
H	-1.74625600	2.80234700	-2.56242500
C	1.08209800	2.63116200	0.83814400
H	0.12568000	2.92392700	1.26694000
C	2.14684400	3.49098700	0.84162600
H	2.05086500	4.47728100	1.27817900
C	3.36842300	3.04878200	0.26356500
H	4.22657100	3.71103500	0.23562900
C	3.45484800	1.78934400	-0.26352300

C	2.33285300	0.91510800	-0.22921800
C	2.31865200	-0.41735100	-0.71602800
C	3.46815200	-1.13856600	-1.14000700
C	3.38394100	-2.46674500	-1.45331800
H	4.26647200	-3.01250000	-1.76754400
C	2.13463000	-3.14085400	-1.32444200
H	2.03977000	-4.20072100	-1.52600800
C	1.04425700	-2.41803300	-0.93644100
H	0.07884300	-2.89865700	-0.79918100
N	1.15132000	1.37169300	0.33437800
N	1.08809000	-1.07408100	-0.69335100
H	4.37832800	1.45317200	-0.72028300
H	4.42456700	-0.63033600	-1.18349400
S	-0.27582700	-1.13589100	2.00724000
C	1.35897200	-1.81319500	2.30716700
H	1.36196600	-2.24786100	3.31002000
H	1.54273300	-2.58635600	1.55895300
H	2.09383700	-1.00789100	2.21353700
C	-0.44438300	-0.08138200	3.45516400
H	-1.42486600	0.39894200	3.42204300
H	-0.38535100	-0.71640600	4.34352500
H	0.35635800	0.66412700	3.45135500
O	-1.31251600	-2.21121700	2.03330500
H	0.02254500	1.05753800	-2.41791200
H	-2.03466300	1.86767100	1.32320600
H	-1.97734300	-2.15555900	-0.24793100

1-^{3}MC

Ru	-0.52763500	-0.05803100	-0.03406700
N	-1.11777300	0.58327300	-2.05144100

N	-2.17591800	-1.43385000	-0.42993200
N	-2.57973700	1.31581800	0.31950500
C	-1.98508200	-0.45683600	-2.69544800
H	-2.99214100	-0.04768500	-2.80670900
H	-1.62815200	-0.67540400	-3.70538300
C	-2.01376300	-1.74593400	-1.87512900
H	-1.06670100	-2.28193000	-1.99042500
H	-2.81413600	-2.40412800	-2.23408400
C	-3.54551500	-0.94014300	-0.08813700
H	-4.07351600	-0.73115100	-1.02206500
H	-4.10175000	-1.73494300	0.41496300
C	-3.53004700	0.29306800	0.80886900
H	-3.21450800	-0.00046000	1.81495500
H	-4.55392500	0.68347200	0.87815300
C	-2.94112300	1.92405200	-0.98337200
H	-3.79763700	1.38962900	-1.40490200
H	-3.27237000	2.95897800	-0.85285600
C	-1.76853500	1.91851200	-1.96617800
H	-0.99811900	2.62207900	-1.63462400
H	-2.11690100	2.24624400	-2.95342600
C	0.81653200	2.66977900	0.56054100
H	-0.21589100	2.84104000	0.85463500
C	1.74828100	3.69550000	0.60434500
H	1.45571400	4.68366300	0.93997300
C	3.04944900	3.41526200	0.19803900
H	3.80970900	4.18962500	0.19885200
C	3.36442400	2.12643900	-0.21316100
C	2.38049000	1.13572700	-0.21237000
C	2.66876000	-0.27262100	-0.60627500
C	3.97068500	-0.74938400	-0.76873400

C	4.16610500	-2.08217100	-1.11684500
H	5.17084300	-2.47061300	-1.24613400
C	3.05960300	-2.90679100	-1.28557600
H	3.16483200	-3.95206000	-1.55305800
C	1.79779800	-2.35558200	-1.09135500
H	0.90741900	-2.97227200	-1.19138900
N	1.11416800	1.42329300	0.15865000
N	1.60217500	-1.07484700	-0.76303900
H	4.36992200	1.90082500	-0.54575300
H	4.82814900	-0.10639200	-0.61168900
S	-0.28819300	-0.95968900	2.07902900
C	1.33594800	-1.62948800	2.46082800
H	1.31404800	-2.01558000	3.48302200
H	1.52810200	-2.44328600	1.75900800
H	2.08803100	-0.84354100	2.34847300
C	-0.42902000	0.24709400	3.40502900
H	-1.41058000	0.71816000	3.31983100
H	-0.35686400	-0.27866600	4.36068800
H	0.36382900	0.99350900	3.30485000
O	-1.31448100	-2.03086300	2.28946100
H	-0.27550100	0.69108300	-2.61659100
H	-2.53305000	2.04817800	1.02466800
H	-2.00632400	-2.26777600	0.13918900

2-^{3}MLCT

Ru	0.43122900	-0.08961100	0.03959100
N	1.29406600	-2.00847500	0.63019100
N	1.91488800	-0.33159400	-1.54850200
N	2.54678000	0.52390100	1.12147200
C	2.10066800	-2.57157900	-0.48974300

H	3.15689400	-2.54123900	-0.20936000
H	1.85474100	-3.62503600	-0.65209800
C	1.87484400	-1.79720800	-1.79368500
H	0.88295000	-2.02712500	-2.19734800
H	2.62034200	-2.10111100	-2.53974800
C	3.28045500	0.17830600	-1.21908300
H	3.93448600	-0.68424700	-1.06023200
H	3.68193200	0.72250300	-2.07787800
C	3.30639800	1.09823900	0.00268400
H	2.83579500	2.04962400	-0.26421300
H	4.35680900	1.29602000	0.25996200
C	3.10982100	-0.69520400	1.73008100
H	3.94210500	-1.05017700	1.11377400
H	3.53437400	-0.48519100	2.71714100
C	2.04873300	-1.78682300	1.89023100
H	1.30870100	-1.47318600	2.63268800
H	2.52379300	-2.71460000	2.23458100
C	-1.94132800	0.36348300	1.65538400
C	-2.68044500	-0.47792600	0.62104100
C	-4.06841900	-0.56570500	0.65113400
C	-4.70806200	-1.30582500	-0.33776100
H	-5.78855300	-1.40669000	-0.34004400
C	-3.93996800	-1.90699700	-1.33113100
H	-4.39742700	-2.48493600	-2.12621700
C	-2.55829700	-1.74663100	-1.29152300
H	-1.92636200	-2.18814100	-2.05862100
N	-1.93538100	-1.05486600	-0.33247400
H	-4.60724800	-0.05198300	1.43925000
S	-0.19830100	1.98973500	-0.70486600
C	-1.90664300	2.19349800	-1.23502200

H	-1.99549500	3.19495300	-1.66349600
H	-2.11556300	1.43564900	-1.99243000
H	-2.56913900	2.07356700	-0.37273100
C	-0.17895400	3.19139800	0.63291900
H	0.84521900	3.23659800	1.00887000
H	-0.47302000	4.16475100	0.23282100
H	-0.85960000	2.84992100	1.42076300
O	0.70339600	2.45368300	-1.81366900
O	-0.67810400	0.08476200	1.78608600
O	-2.55199400	1.23866900	2.24248600
H	0.51519700	-2.63198300	0.83983500
H	2.38961900	1.22954200	1.83621100
H	1.58650000	0.17379800	-2.37280100

Transition State for 2-^{3}MLCT to 2-^{3}MC

Ru	0.52754200	0.01650300	0.04458100
N	0.65001100	-2.10197400	0.39930000
N	1.93921600	-0.50759700	-1.51711200
N	2.55499300	-0.18241500	1.27134900
C	1.30617900	-2.78587800	-0.74586300
H	2.28731000	-3.14239900	-0.42031700
H	0.73869900	-3.67149400	-1.04662900
C	1.44998700	-1.84648800	-1.95083800
H	0.47317500	-1.69230400	-2.42098200
H	2.12042100	-2.29194400	-2.69630900
C	3.35986300	-0.51710900	-1.05041300
H	3.67926700	-1.55913300	-0.95919600
H	3.99636100	-0.05829800	-1.81137300
C	3.56105700	0.22271500	0.27209400
H	3.43882700	1.29621800	0.09939700

H	4.58806200	0.04136500	0.61811000
C	2.65950700	-1.57641500	1.76024700
H	3.40055200	-2.10804700	1.15443600
H	3.03244700	-1.60139000	2.78864800
C	1.30583100	-2.29271800	1.71186600
H	0.62770900	-1.85767000	2.45165600
H	1.44203000	-3.35717500	1.94248200
C	-1.93539800	0.70121000	1.28087900
C	-2.88627900	-0.17515900	0.48253400
C	-4.22360800	0.19918400	0.38484400
C	-5.08572100	-0.59857900	-0.36032900
H	-6.13758000	-0.34584300	-0.44631100
C	-4.57100900	-1.72343900	-0.99482200
H	-5.20105200	-2.37441900	-1.59042900
C	-3.21401600	-2.00448600	-0.85166800
H	-2.78170900	-2.87431600	-1.34135700
N	-2.37810700	-1.25936600	-0.12442100
H	-4.55587800	1.09617500	0.89514700
S	0.50325500	2.24016300	-0.54906500
C	-1.01157600	2.79801300	-1.33969100
H	-0.86785800	3.83891100	-1.64046900
H	-1.17006900	2.17099000	-2.21947400
H	-1.83663300	2.69680500	-0.62893500
C	0.53231600	3.34339000	0.86529400
H	1.45768400	3.14261600	1.40941500
H	0.52546800	4.37495300	0.50492100
H	-0.34177300	3.11346200	1.48446500
O	1.66131300	2.53751500	-1.46063700
O	-0.79233700	0.14596600	1.58623600
O	-2.26054500	1.84438800	1.55837500

H	-0.33948900	-2.35720100	0.46533500
H	2.57996000	0.46258400	2.05724800
H	1.86712200	0.15986500	-2.28641900

2-^{3}MC

Ru	-0.62834300	0.03176500	0.01019200
N	-0.04461700	-2.03709300	-0.07502700
N	-2.07168500	-0.77765400	1.42000800
N	-2.24329800	-0.87442900	-1.44586000
C	-0.65669800	-2.79622500	1.04456400
H	-1.41209000	-3.47362100	0.63564900
H	0.08863900	-3.42516300	1.54087800
C	-1.28850900	-1.85998100	2.08386100
H	-0.50376000	-1.37077100	2.66998700
H	-1.91763400	-2.43682800	2.77330100
C	-3.31777700	-1.26795900	0.75212600
H	-3.28828400	-2.36112100	0.74250100
H	-4.18820500	-0.98099100	1.34730800
C	-3.48690100	-0.72088800	-0.66452100
H	-3.70863200	0.34886800	-0.60771900
H	-4.33641800	-1.23275700	-1.13679200
C	-1.85521900	-2.26947900	-1.76031300
H	-2.50183100	-2.94904600	-1.19605700
H	-2.02627200	-2.49169900	-2.81795900
C	-0.38309100	-2.52744000	-1.42991200
H	0.26106300	-1.96995700	-2.11615200
H	-0.16157300	-3.59744000	-1.53474500
C	1.90528700	1.07276400	-0.76764800
C	3.10543600	0.27875100	-0.29452000
C	4.33678900	0.91775500	-0.18546400

C	5.43026700	0.18346000	0.26069000
H	6.40890400	0.64448800	0.34587500
C	5.24176600	-1.15110200	0.59934200
H	6.06188200	-1.76567200	0.95320400
C	3.96399500	-1.69415500	0.47888700
H	3.78387700	-2.73215500	0.74788700
N	2.90872700	-1.00761400	0.03538300
H	4.41128900	1.96604600	-0.45127500
S	-1.32884600	2.20971400	0.29078400
C	-0.31268500	3.16468300	1.42191100
H	-0.76637300	4.15312100	1.52893200
H	-0.32321200	2.64359400	2.38157600
H	0.69991100	3.21944100	1.01421500
C	-1.17962800	3.21166400	-1.18935400
H	-1.78417000	2.73633900	-1.96455100
H	-1.56323600	4.21123400	-0.97093500
H	-0.12262500	3.22002200	-1.46973500
O	-2.74809200	2.22874700	0.78796400
O	0.93107200	0.34338600	-1.24489900
O	1.89399600	2.29073000	-0.66393300
H	0.98163500	-1.97355400	0.00516400
H	-2.31953000	-0.33475400	-2.30464400
H	-2.34264500	-0.07714500	2.11062600

RC-1-H_2O-^{3}MC State

Ru	-0.51793400	0.06143500	0.00383200
N	-0.79294600	0.85474800	-2.00523400
N	-2.49790500	-0.78784100	-0.51709300
N	-2.12812200	1.95869700	0.27386400
C	-1.87526000	0.12399400	-2.73873800

H	-2.71098800	0.81045100	-2.89518600
H	-1.52654500	-0.17044200	-3.73220900
C	-2.31613900	-1.10794500	-1.96091800
H	-1.55804800	-1.89468200	-2.01096400
H	-3.24149400	-1.51300500	-2.38901400
C	-3.67966900	0.07755700	-0.25703000
H	-4.06530300	0.43600800	-1.21539300
H	-4.48295300	-0.51473200	0.19108300
C	-3.37342500	1.26201400	0.65865400
H	-3.24016200	0.91480900	1.68738900
H	-4.23921000	1.93753300	0.65076500
C	-2.20408700	2.66792200	-1.02646600
H	-3.15218400	2.42333100	-1.51524200
H	-2.21699200	3.75218800	-0.87839500
C	-1.02513400	2.32268300	-1.93651700
H	-0.10630000	2.76997100	-1.54692400
H	-1.20010100	2.73343900	-2.93837900
C	1.30387600	2.59298700	0.78322800
H	0.32951000	2.90553100	1.14854900
C	2.39579400	3.44519700	0.85921900
H	2.28833500	4.43385900	1.29025800
C	3.61585300	2.98995400	0.36713200
H	4.49708600	3.62198400	0.39778100
C	3.69367900	1.70777700	-0.16140300
C	2.55318900	0.90227000	-0.19383000
C	2.57754100	-0.50365700	-0.68909500
C	3.73375900	-1.13286100	-1.14747700
C	3.66555300	-2.46766200	-1.53839500
H	4.55575900	-2.97394300	-1.89701400
C	2.45331800	-3.14146800	-1.45119600

H	2.36478300	-4.18487400	-1.73106500
C	1.34143600	-2.44634100	-0.98544500
H	0.37088300	-2.92808800	-0.87644300
N	1.36987200	1.35673300	0.26848200
N	1.40559000	-1.15887800	-0.62726700
H	4.63931600	1.34113900	-0.54047000
H	4.67977600	-0.60813300	-1.19836000
S	-0.23569700	-0.93423500	2.09718500
C	1.30301800	-0.44457100	2.88403600
H	1.37907300	-0.99315600	3.82601800
H	2.11147000	-0.74390300	2.21332500
H	1.31684600	0.63582000	3.04604800
C	-1.40464000	-0.46291200	3.37993600
H	-2.39148500	-0.80807500	3.06389300
H	-1.11907300	-0.97350200	4.30321000
H	-1.39507800	0.62253600	3.51182900
O	-0.22289300	-2.43548700	2.04220900
H	0.08320600	0.71166800	-2.50850700
H	-1.92839400	2.63562200	1.00628500
H	-2.60736700	-1.70318900	-0.06342900
O	-1.72946400	-3.39829400	-0.00698900
H	-1.21160200	-3.33946200	0.82176300
H	-2.09106800	-4.29569500	-0.04993900

TS-1-H_2O-^{3}MC State

Ru	0.62602400	-0.07848500	0.01786200
N	-0.40859700	-1.77034000	0.90953500
N	1.92572700	-1.75453300	-0.63737300
N	1.98427500	-0.62803100	1.98541600
C	0.06004000	-3.06832400	0.32610800

H	0.60312000	-3.62080700	1.09717300
H	-0.79836700	-3.68625300	0.04897000
C	0.93398200	-2.83651800	-0.90018600
H	0.33242700	-2.50266000	-1.74922700
H	1.43810400	-3.76890000	-1.18272600
C	3.00085000	-2.15798200	0.31419000
H	2.71561700	-3.11043700	0.76878700
H	3.93321400	-2.34637900	-0.22604200
C	3.24993800	-1.11130400	1.40013300
H	3.75872500	-0.24007000	0.97235400
H	3.91956200	-1.54278000	2.15582400
C	1.24287600	-1.63652500	2.77964300
H	1.71249400	-2.61512200	2.64548800
H	1.30893000	-1.41632600	3.84935800
C	-0.23327500	-1.68871000	2.38593300
H	-0.73893600	-0.77333000	2.71206000
H	-0.71797300	-2.53803800	2.88271300
C	-0.46431400	2.44117400	1.29401100
H	0.59219100	2.42106100	1.54169600
C	-1.25229000	3.51098800	1.68279900
H	-0.81172500	4.34069100	2.22357700
C	-2.60129800	3.48894000	1.34477600
H	-3.25319400	4.31883400	1.59670800
C	-3.09971900	2.37459200	0.68461200
C	-2.25166200	1.31590200	0.34950500
C	-2.85724900	0.09354800	-0.25897100
C	-4.05328300	-0.39968000	0.27001800
C	-4.63407900	-1.52866700	-0.30351900
H	-5.56385500	-1.92531300	0.09088500
C	-4.00710800	-2.12936600	-1.38873100

H	-4.43156400	-2.99846500	-1.87851300
C	-2.81209400	-1.57852600	-1.84532300
H	-2.29206500	-2.00802100	-2.69911600
N	-0.92770000	1.37010500	0.62057800
N	-2.24283000	-0.50078700	-1.29290500
H	-4.14615800	2.32092800	0.40553700
H	-4.51687500	0.08434400	1.12308200
S	1.82245700	1.69240700	-1.09398600
C	2.72883600	2.90042200	-0.10870700
H	3.37892800	3.46992400	-0.77715100
H	1.99711300	3.57890200	0.33205200
H	3.31114900	2.39455400	0.66657500
C	3.20523100	1.01678100	-2.03410400
H	2.79535300	0.29308500	-2.74246900
H	3.66457400	1.83972300	-2.58803200
H	3.93351000	0.54938200	-1.36470400
O	0.94987400	2.44108000	-2.05083700
H	-1.40709700	-1.68279200	0.71972900
H	2.19430000	0.17299200	2.57710900
H	2.34122300	-1.52423700	-1.53973600
O	0.20200600	-0.25789300	-2.54345000
H	-0.74340200	-0.23728100	-2.25866500
H	0.32287500	0.60677300	-2.98104200

PC-1-H_2O-^{3}MC State

Ru	0.66460300	-0.03727200	0.11412100
N	-0.53623900	-1.67990500	0.88155200
N	1.67841600	-1.81957200	-0.86531700
N	2.06028900	-1.00465400	1.81046100
C	-0.29247000	-2.95021500	0.12478800

H	0.22333000	-3.65611100	0.78135900
H	-1.24763100	-3.41377300	-0.13814700
C	0.51332400	-2.69989000	-1.14406500
H	-0.09565100	-2.17976500	-1.88799300
H	0.83324700	-3.65757700	-1.57359000
C	2.74622200	-2.47550500	-0.06526300
H	2.36422000	-3.42893100	0.30986400
H	3.60481300	-2.72113700	-0.69707500
C	3.21028300	-1.59759700	1.09818100
H	3.81757500	-0.76803300	0.72053100
H	3.84673000	-2.19173300	1.76618600
C	1.25499000	-1.98003500	2.58880100
H	1.56653700	-2.99274700	2.31835600
H	1.44910900	-1.87898600	3.66068800
C	-0.23852700	-1.79007800	2.33652400
H	-0.58096100	-0.85689400	2.79752700
H	-0.79972100	-2.61641500	2.78992000
C	-0.45334700	2.65734800	1.02969100
H	0.61380800	2.71356700	1.20282800
C	-1.25348700	3.74034700	1.35690000
H	-0.80483900	4.63651200	1.76894400
C	-2.61835500	3.64394200	1.12389600
H	-3.28366800	4.47320400	1.34067100
C	-3.11494800	2.45632900	0.60062700
C	-2.25118700	1.40034000	0.30944300
C	-2.86713800	0.14444200	-0.21998700
C	-3.97603100	-0.40161900	0.43249000
C	-4.58127000	-1.53960800	-0.09943200
H	-5.44478300	-1.97933400	0.38930600
C	-4.07004900	-2.08906600	-1.26975400

H	-4.52332300	-2.95881500	-1.73178500
C	-2.95866800	-1.48290900	-1.85087800
H	-2.53471900	-1.86800500	-2.77527900
N	-0.91398200	1.50297200	0.51061500
N	-2.36275600	-0.40257200	-1.33612900
H	-4.17293500	2.34431600	0.39020900
H	-4.35505000	0.05507100	1.34119600
S	2.08618400	1.63612200	-0.81162700
C	3.30869300	2.39993600	0.26988200
H	3.85070600	3.14388500	-0.32008800
H	2.78921000	2.89836100	1.09003000
H	3.99257500	1.64114300	0.65878300
C	3.19811800	0.93831200	-2.04460500
H	2.57347300	0.48412500	-2.81752700
H	3.77098600	1.76312300	-2.47675500
H	3.86662900	0.20280100	-1.58827500
O	1.30323400	2.72386000	-1.47752700
H	-1.52810000	-1.45835000	0.80141500
H	2.41339800	-0.28930700	2.44344600
H	2.05149400	-1.53578000	-1.77072100
O	0.07641000	0.25397400	-2.34537000
H	-0.88828900	0.10958500	-2.16265500
H	0.15618600	1.20462900	-2.55520600

RC-1-H_2O- Singlet State

Ru	0.38042800	-0.23963800	-0.06138500
N	0.46255400	-1.09697900	-2.06358500
N	2.22423600	0.62935600	-0.77158800
N	1.76796800	-1.89543200	0.27873000
C	1.55567300	-0.47842600	-2.87864300

H	2.36933600	-1.20253600	-2.96870800
H	1.20544900	-0.27958900	-3.89500500
C	2.05271000	0.81029300	-2.23493400
H	1.31944800	1.60662600	-2.38382600
H	2.98928400	1.12792900	-2.70947600
C	3.42052200	-0.20318200	-0.43713800
H	3.80311600	-0.65187700	-1.35894700
H	4.21932400	0.43266700	-0.04556200
C	3.09135700	-1.27948500	0.59136700
H	3.01396900	-0.82670700	1.58161000
H	3.88206800	-2.03894600	0.60996800
C	1.82138700	-2.80098200	-0.91384800
H	2.77054200	-2.63012800	-1.42820100
H	1.82853600	-3.84818500	-0.59865100
C	0.65031200	-2.55688900	-1.86005300
H	-0.27826200	-2.94641600	-1.43345500
H	0.82795700	-3.07420900	-2.81085100
C	-1.68431600	-2.38883100	0.84176600
H	-0.78619800	-2.88714700	1.19533600
C	-2.92696700	-2.99809300	0.94250500
H	-3.01554500	-3.98441900	1.38318900
C	-4.03802900	-2.31118600	0.46273000
H	-5.02767000	-2.75261500	0.51594400
C	-3.86526800	-1.04358200	-0.08078700
C	-2.58719800	-0.48812000	-0.13963000
C	-2.31497400	0.88056300	-0.64616900
C	-3.31861700	1.74885000	-1.07185100
C	-2.98540400	3.04386300	-1.45423100
H	-3.75634100	3.72911400	-1.79070500
C	-1.65786200	3.44850900	-1.37631500

H	-1.35686300	4.45690000	-1.63596600
C	-0.70605900	2.53080900	-0.94924600
H	0.33670100	2.81201000	-0.82770900
N	-1.50763300	-1.16978600	0.31077800
N	-1.01743600	1.26910300	-0.61577300
H	-4.72420600	-0.49707100	-0.45036800
H	-4.35345200	1.43041200	-1.09883300
S	0.57981900	0.64371700	2.05119100
C	-0.50031000	2.04215300	2.39289300
H	-0.36612800	2.31681900	3.44202100
H	-0.17111200	2.85852000	1.74606800
H	-1.53900700	1.77299500	2.18389700
C	0.03421700	-0.47682400	3.34921900
H	0.65296200	-1.37548800	3.29170400
H	0.19581000	0.01342900	4.31228200
H	-1.01976600	-0.72651800	3.20238200
O	1.97852400	1.07156800	2.42060600
H	-0.42269600	-0.95961300	-2.55182000
H	1.51412100	-2.46316300	1.08590800
H	2.35206600	1.56130400	-0.35609600
O	2.12230400	3.12723700	0.62942700
H	2.61554900	3.96085300	0.60442200
H	2.34359300	2.68873400	1.47533800

TS-1-H_2O- Singlet State

Ru	0.58651500	-0.13854500	0.02602700
N	-0.33377200	-1.77045100	1.09534400
N	2.04048400	-1.66141800	-0.33296300
N	1.66565600	-0.00762900	1.84576300
C	0.37820400	-3.05993000	0.82421200

H	0.96124400	-3.32666400	1.70989100
H	-0.34510400	-3.86622000	0.67581500
C	1.27410100	-2.93255200	-0.40511600
H	0.67383200	-2.87750600	-1.31572600
H	1.94206100	-3.79924400	-0.47704000
C	3.10477400	-1.67412400	0.71360200
H	2.95088500	-2.54202800	1.36030300
H	4.08999000	-1.79673800	0.25638100
C	3.07702800	-0.38593300	1.52904100
H	3.51073000	0.43163300	0.95090300
H	3.66569600	-0.49825300	2.44709800
C	1.07626100	-0.90192100	2.90385300
H	1.74050100	-1.76079600	3.02769200
H	1.05478100	-0.38160300	3.86479400
C	-0.32340100	-1.36097100	2.52046700
H	-1.03759300	-0.53868900	2.62178800
H	-0.64175700	-2.17690500	3.18077600
C	-0.51602500	2.49096600	1.14665400
H	0.55351800	2.55185700	1.32666000
C	-1.34040600	3.54330700	1.51206900
H	-0.92054800	4.42492700	1.98291900
C	-2.70221700	3.43289900	1.24632000
H	-3.38650900	4.23766200	1.49398400
C	-3.16539200	2.26954200	0.64951300
C	-2.27326000	1.24272000	0.32618500
C	-2.77914100	-0.01780300	-0.28160400
C	-4.04096700	-0.51598100	0.05146000
C	-4.47313900	-1.70081500	-0.53950400
H	-5.44968100	-2.10878800	-0.29955700
C	-3.63014300	-2.35022100	-1.43431700

H	-3.92489800	-3.27202200	-1.92337300
C	-2.38190200	-1.78591200	-1.69240300
H	-1.68777500	-2.27231400	-2.37470500
N	-0.94688200	1.36067000	0.55702200
N	-1.95796500	-0.64742500	-1.13398800
H	-4.21615900	2.15837800	0.40690500
H	-4.66818600	-0.00262500	0.77229500
S	1.78934100	1.39912000	-1.30425000
C	0.67344700	2.42329300	-2.28030800
H	1.26362300	2.94299800	-3.03968800
H	-0.06014900	1.76530300	-2.74708300
H	0.16618400	3.13281300	-1.62120300
C	2.80218700	2.72095400	-0.61175000
H	3.60770400	2.27534200	-0.02718000
H	3.23776700	3.26187900	-1.45604700
H	2.19734500	3.39211900	0.00198300
O	2.69241800	0.63176100	-2.23696200
H	-1.30482700	-1.87319900	0.80252700
H	1.68418000	0.93954300	2.22396000
H	2.47128600	-1.47364400	-1.24167700
O	0.40670600	-0.83637200	-2.52362600
H	-0.38013300	-0.59384600	-3.03453200
H	1.19018900	-0.54777000	-3.02983600

PC-1-H_2O- Singlet State

Ru	0.69477500	-0.19664500	-0.04971100
N	-0.50588200	-1.82836300	0.65503300
N	2.08335400	-1.78220100	-0.35873600
N	1.45287900	-0.34684900	1.96276400
C	0.15397100	-3.14007500	0.35770300

H	0.56016900	-3.54069600	1.29009800
H	-0.58508100	-3.86415200	0.00498300
C	1.25138300	-2.97298200	-0.68844900
H	0.81341000	-2.78716300	-1.67080400
H	1.86293200	-3.88119900	-0.74156300
C	2.95195000	-1.98413700	0.84157700
H	2.64753400	-2.91003600	1.33706300
H	3.99313700	-2.12852000	0.53937200
C	2.86292800	-0.80737100	1.81461200
H	3.43461500	0.04497500	1.44071700
H	3.29050800	-1.09499100	2.78292500
C	0.62417900	-1.30073200	2.77414900
H	1.19160100	-2.22703900	2.90013200
H	0.46077100	-0.89968100	3.77770900
C	-0.71567600	-1.58234300	2.10303500
H	-1.37407100	-0.71270000	2.18710400
H	-1.20638000	-2.43314200	2.59146000
C	-0.22226200	2.43291500	1.12273700
H	0.85871800	2.39478300	1.23151300
C	-0.92379700	3.51604000	1.62654600
H	-0.39460800	4.32140200	2.12320300
C	-2.30590000	3.53419300	1.47207800
H	-2.90082000	4.36612700	1.83432000
C	-2.90558300	2.45589100	0.83852500
C	-2.13012500	1.39377800	0.36139700
C	-2.86352400	0.25346300	-0.26918000
C	-3.95592300	-0.30411900	0.40033200
C	-4.68944100	-1.31202400	-0.22316500
H	-5.54305200	-1.75835400	0.27672500
C	-4.31530700	-1.72482600	-1.49656700

H	-4.86461900	-2.49372100	-2.02772500
C	-3.20651900	-1.12226900	-2.08570700
H	-2.87484300	-1.41799200	-3.07745400
N	-0.78305500	1.38287000	0.48820100
N	-2.49378500	-0.15961600	-1.48985500
H	-3.97910400	2.43105100	0.68613400
H	-4.22705600	0.04707100	1.39110900
S	2.12696100	1.30289200	-1.20079500
C	1.35607400	2.82983800	-1.76715200
H	1.99285500	3.23202400	-2.55962900
H	0.37106500	2.57793100	-2.16695800
H	1.25685400	3.54285900	-0.94601200
C	3.63747200	1.98140800	-0.49530800
H	4.30924900	1.14442300	-0.29398000
H	4.09675700	2.63672800	-1.23968200
H	3.41500900	2.53099100	0.42363100
O	2.53037300	0.52933800	-2.43333400
H	-1.41571100	-1.81254500	0.19175900
H	1.47408300	0.54215600	2.46194900
H	2.66269400	-1.56877800	-1.17551000
O	0.02168300	-0.51558900	-2.08638200
H	-0.89302700	-0.13579300	-2.17852800
H	0.65051700	-0.19069600	-2.76116500

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