Supporting Information

Effect of the Electronic Structure on the Robustness of Ruthenium(II) Bis-phenanthroline Compounds for Photodissociation of Co-ligand: Synthesis, Structural Characterization, and Density Functional Theory Study

Megha S. Deshpande,*[a] Sudesh M. Morajkar,[a] Bikshandarkoil R. Srinivasan,[a]

Mini Bharati Ahirwar,[b] and Milind M. Deshmukh*[b]

[a]School of Chemical Sciences, Goa University, Goa 403206, India

[b]Department of Chemistry, Dr. Harisingh Gour Vishwavidyalaya (A Central University), Sagar, 470003, India

Email: d_megha9@yahoo.co.in, milind.deshmukh@gmail.com, mdeshmukh@dhsgsu.edu.in

ORCID Number:

Megha S. Deshpande: 0000-0002-4307-7898

Milind M. Deshmukh: 0000-0003-3518-7859

Table of Contents

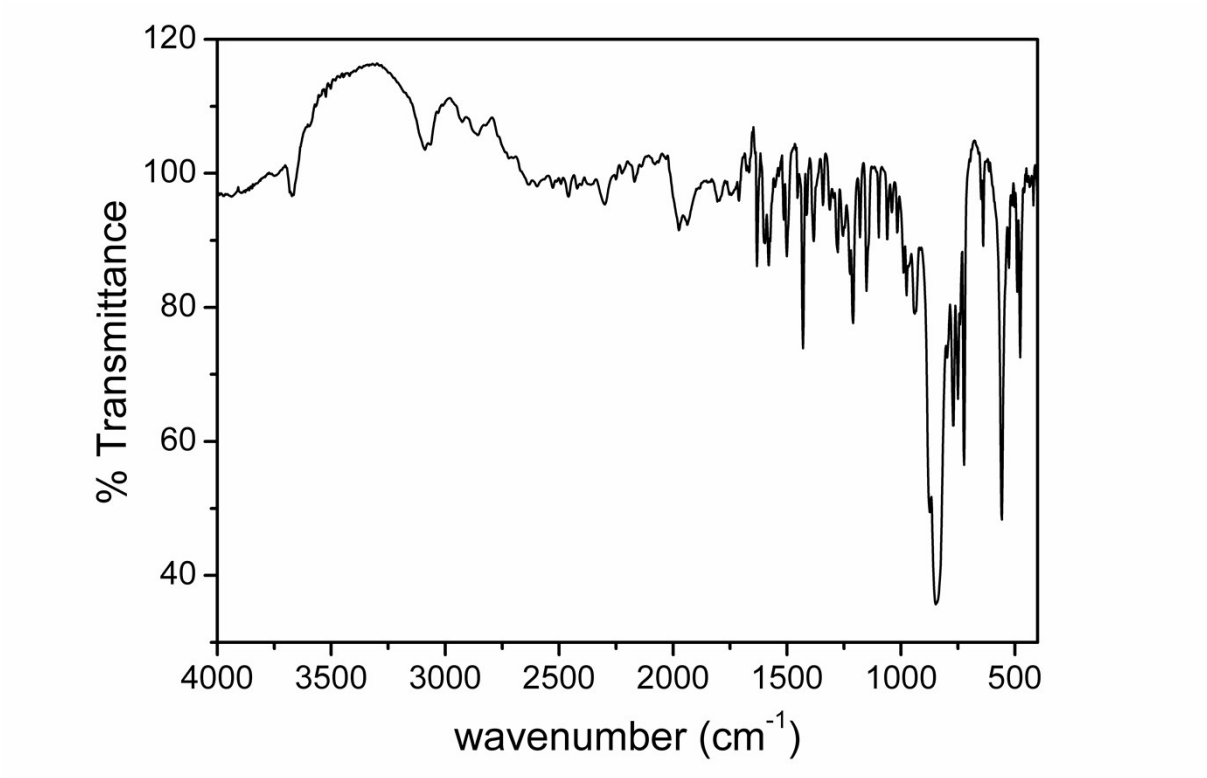


Fig. S1. IR spectrum of **1**.

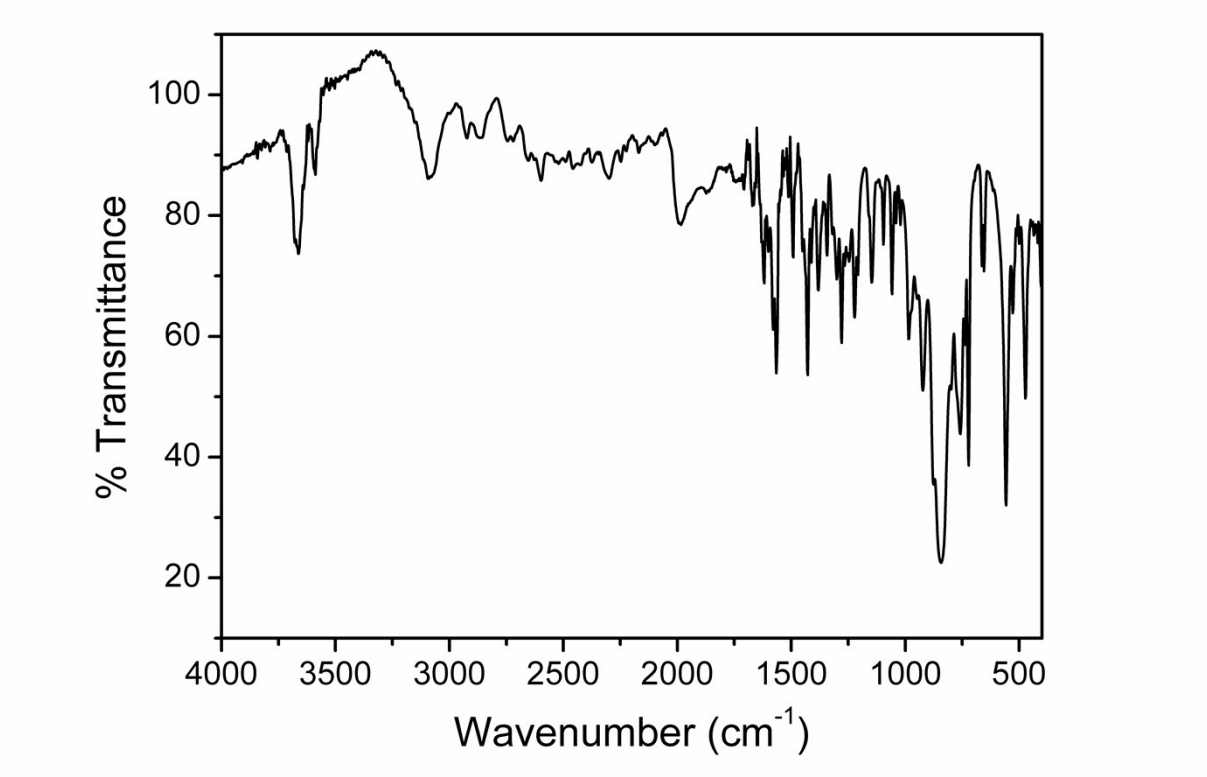


Fig. S2. IR spectrum of **2**.

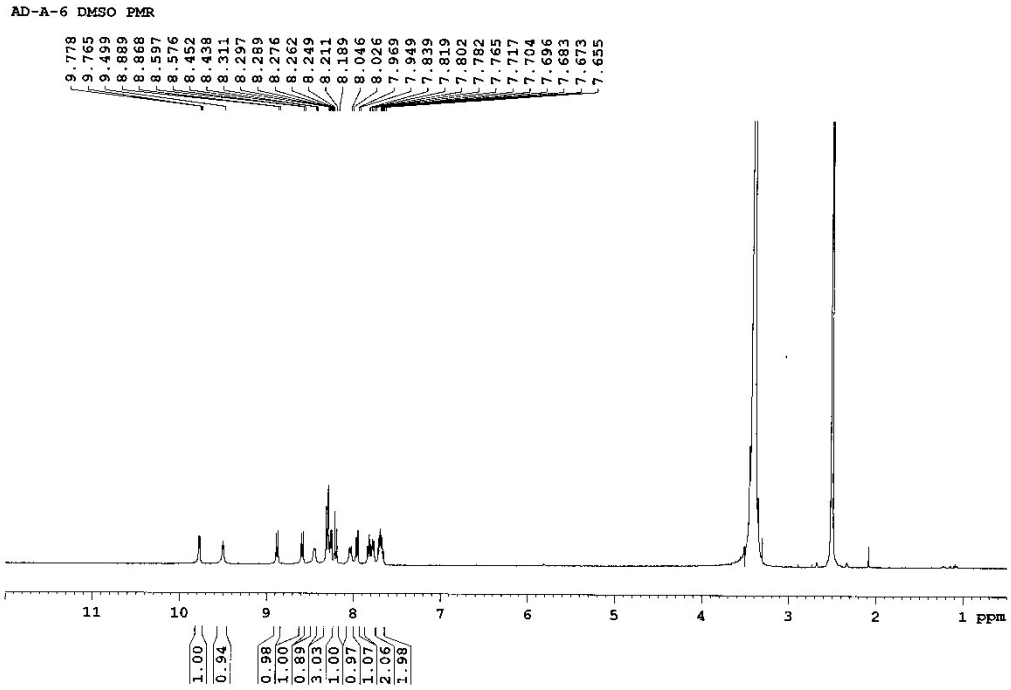


Fig. S3. ^{1}H NMR spectrum of **1** in DMSO-d_6.

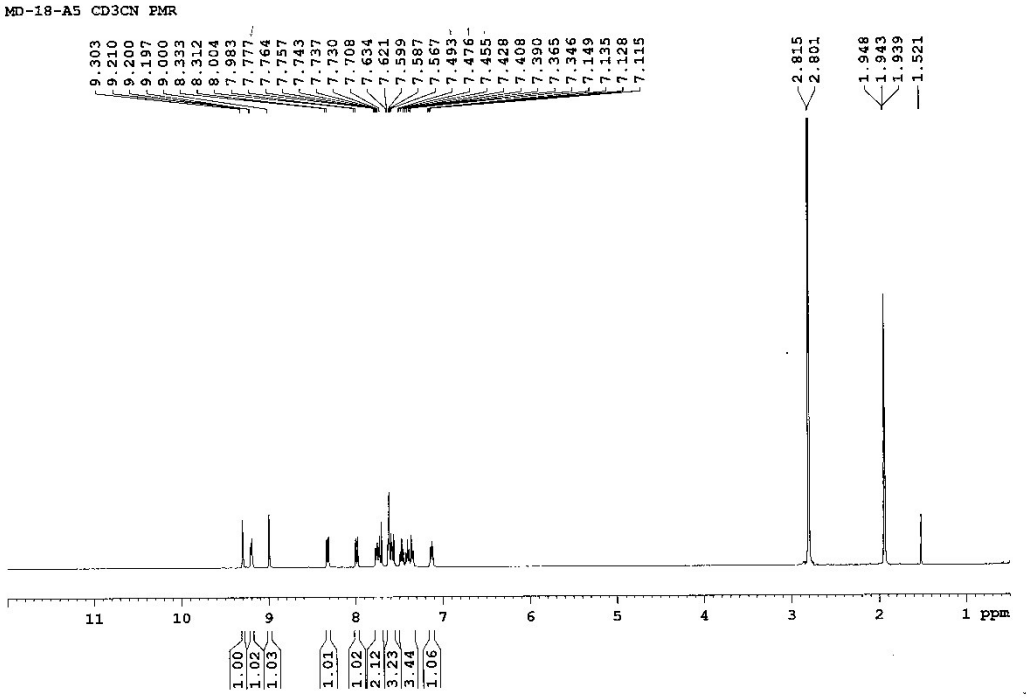


Fig. S4. ^{1}H NMR spectrum of **2** in CD_3CN.

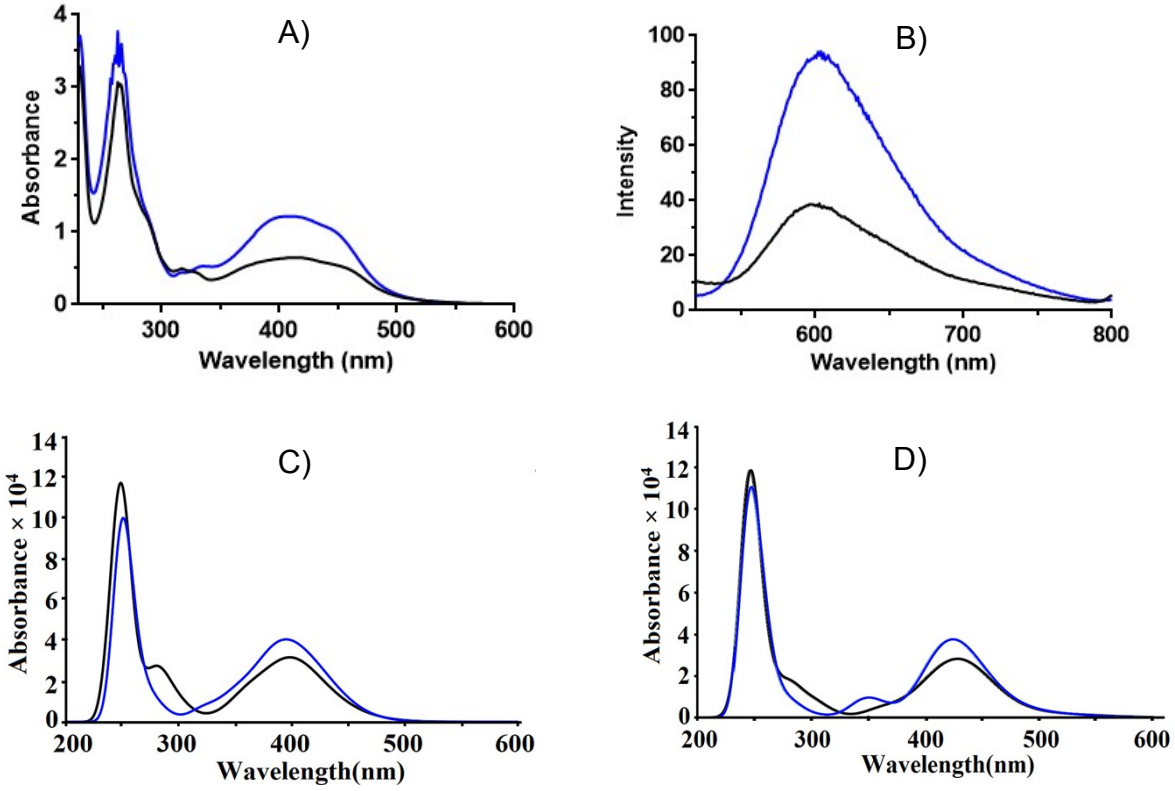


Fig. S5. A) Experimental absorption and B) steady state emission spectra of **1** (black line) and **2** (blue line) in acetonitrile at room temperature ([Ru] = 50 μM); C) TD-DFT simulated absorption spectra of **1** and **2;** D) TD-DFT simulated absorption spectra of **1a** and **2a** in acetonitrile.

Table S1. Crystal data and structure refinement for **2**.

Empirical formula	$C_{40}H_{28}F_{12}N_8P_2Ru$	
Formula weight	1011.71	
T (K)	293(2)	
λ (Å)	0.71073	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 18.6540(5) Å	α = 90°
	b = 10.7253(3) Å	β = 90°
	c = 20.2024(6) Å	γ = 90°
V (Å^3)	4041.9(2)	
Z	4	
d_{calc} (g/cm^3)	1.663	
μ (MoKα) (mm^{-1})	0.565	
F (000)	2024	
θ range (°)	2.98 to 27.48	
Reflections collected/unique	35415/8723 [R(int) = 0.0253]	
Completeness to θ	99.6 %	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	8723/1/568	
GOF on F^2	1.051	
R_1, wR_2 [I>2σ(I)]	R_1 = 0.0289, wR_2 = 0.0672	
R_1, wR_2 (all data)	R_1 = 0.0356, wR_2 = 0.0732	
Largest diff. peak and hole	0.407 and -0.395	

Table S2. Selected bond lengths (Å) and bond angles (°) of **2**.

Bond lengths (Å)			
Phenanthroline		Phthalazine	
Ru1–N1	2.075(3)	Ru1–N5	2.084(3)
Ru1–N2	2.063(3)	Ru1–N6	2.079(3)
Ru1–N3	2.072(3)		
Ru1–N4	2.063(3)		
Bond angles (°)			
N4–Ru1–N2	95.24(13)	N3–Ru1–N6	173.90(13)
N4–Ru1–N3	79.93(12)	N1–Ru1–N6	86.33(13)
N2–Ru1–N3	84.38(12)	N4–Ru1–N5	87.72(13)
N4–Ru1–N1	174.91(13)	N2–Ru1–N5	174.20(13)
N2–Ru1–N1	79.84(13)	N3–Ru1–N5	91.24(12)
N3–Ru1–N1	98.20(13)	N1–Ru1–N5	97.08(14)
N4–Ru1–N6	95.22(12)	N6–Ru1–N5	92.27(12)
N2–Ru1–N6	92.43(13)		

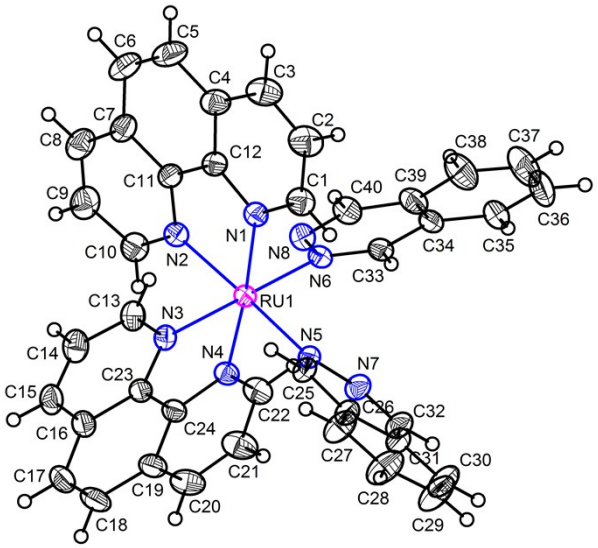


Fig. S6. The crystal structure of **2** depicts the atom labeling scheme. Displacement ellipsoids are drawn at the 30 % probability level (Counter anions PF_6^- are omitted for clarity).

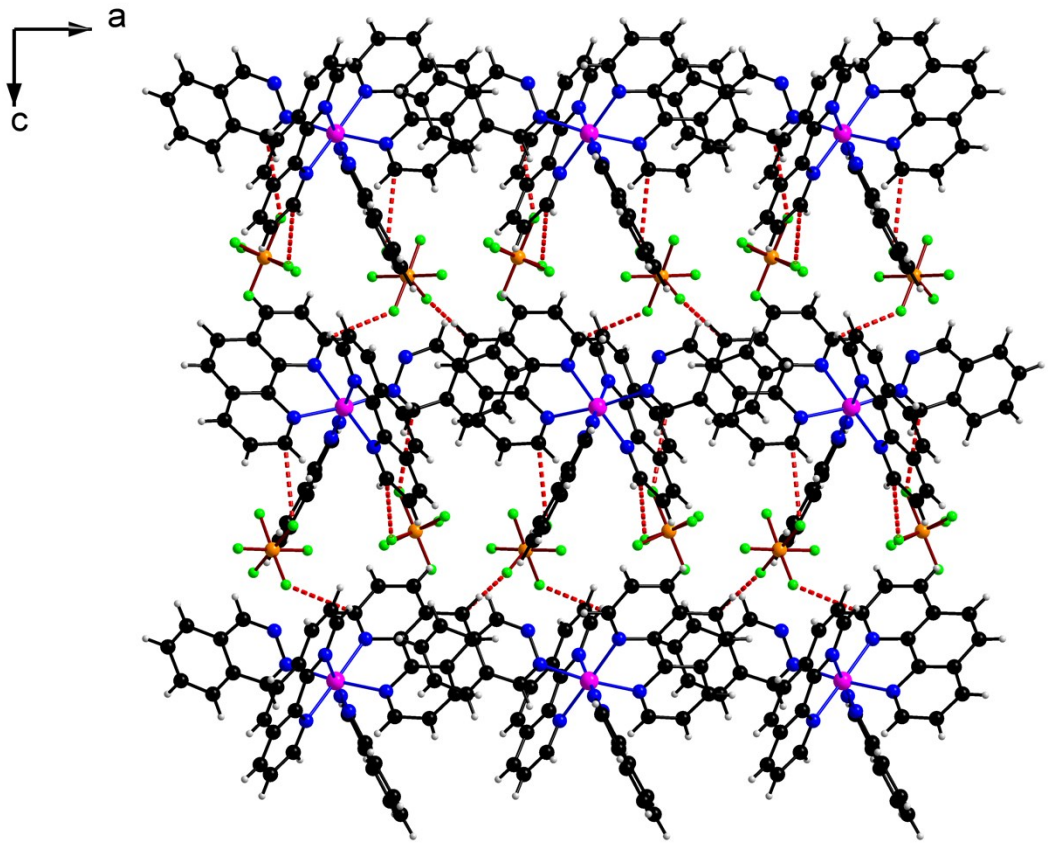


Fig. S7. Packing of molecules in **2** viewed down the crystallographic '*b*' axis depicting C–H···F hydrogen bonding interactions.

Table S3. Analysis of potential hydrogen bonds in **2**.

Donor–H····Acceptor	D–H	H····A	D–A	D–H····A
C1–H1····F8^{i}	0.93	2.51	3.2461(1)	137
C13–H13····F2^{i}	0.93	2.49	3.1414(1)	128
C18–H18····F5^{ii}	0.93	2.41	3.1923(1)	142
C22–H22····F6^{iii}	0.93	2.37	3.1935(1)	147
C29–H29····F2^{iv}	0.93	2.52	3.2205(1)	132
C33–H33····F7^{i}	0.93	2.48	3.3745(1)	160'

Translation of ARU–code to CIF and equivalent position code.

^{i}1/2-x,-1/2+y,1/2+z; ^{ii} 1/2+x,1/2-y,z; ^{iii} x,-1+y,z; ^{iv} 1/2-x,-3/2+y,1/2+z

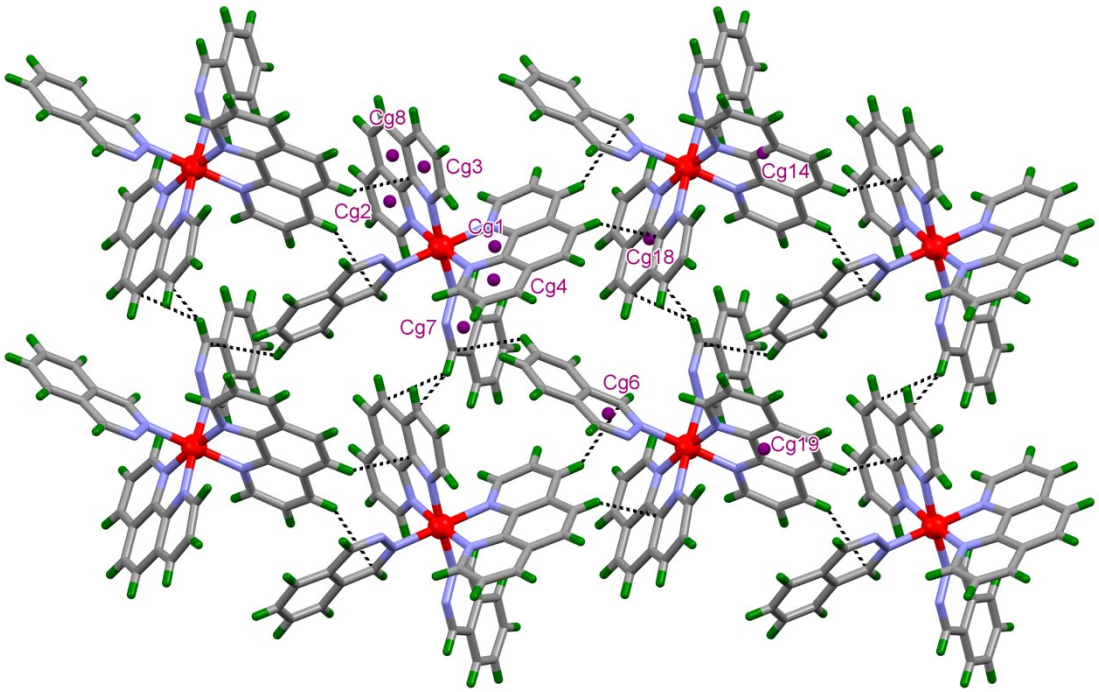


Fig. S8. Cationic units of the composition $[Ru(phen)_2(phthz)_2]^{2+}$ showing C–H···π interactions viewed down crystallographic '*c*' axis.

Table S4. Analysis of C–H$\cdots\pi$ interactions (H$\cdots$Cg < 4 Å, γ < 40°) for **2**.

X–H(I) Res(I) Cg(J)	H$\cdots$Cg	H–Perp	γ	X–H$\cdots$Cg	X$\cdots$Cg
C10–H10 [1] -> Cg2[i]	2.80	2.67	17.91	98	3.0734(1)
C13–H13 [1] -> Cg1 [i]	2.90	2.78	16.71	97	3.1593(1)
C15–H15 [1] -> Cg3 [ii]	2.96	-2.93	8.16	123	3.5495(1)
C15–H15 [1] -> Cg8 [ii]	2.78	2.73	10.36	128	3.4329(1)
C17–H17 [1] -> Cg4 [ii]	2.98	-2.77	21.46	139	3.7324(1)
C17–H17 [1] -> Cg14 [ii]	2.77	-2.76	5.76	125	3.3920(1)
C17–H17 [1] -> Cg19 [ii]	2.93	-2.76	19.55	123	3.5264(1)
C36–H36 [1] -> Cg7 [iii]	2.77	2.71	11.77	149	3.5973(1)
C36–H36 [1] -> Cg17 [iii]	2.95	2.72	22.92	140	3.7150(1)

Symmetry transformations used to generate equivalent atoms: [i] X,Y,Z; [ii] 1/2+X,1/2-Y,Z; [iii] -1/2+X,-1/2-Y,Z; Where Cg1 = Ru1–N1–C12–C11–N2; Cg2 = Ru1–N3–C23–C24–N4; Cg3 = N1–C1–C2–C3–C4–C12; Cg4 = N2–C10–C9–C8–C7–C11; Cg7 = N5–N7–C32–C31–C26– C25; Cg8 = N6–N8–C40–C39–C34–C33; Cg14 = N2–C10–C9–C8–C7–C6–C5–C4–C12–C11; Cg17 = N5–N7– C32–C31–C30–C29–C28–C27–C26–C25; Cg19 = N1–C1–C2–C3–C4–C5– C6–C7–C8–C9–C10–N2–C11–C12

Table S5. Analysis of short ring–interactions with Cg–Cg distances < 4.4 Å, α < 20° and β < 60° for **2**.

Cg(I) Res(I) Cg(J)	Cg–Cg	*A*	*B*	γ	CgI_Perp	CgJ_Perp
Cg1 [1] -> Cg5[i]	3.9377(1)	78	31.9	69.6	1.3726	3.3419
Cg1 [1] -> Cg8 [i]	3.8249(1)	87	26.7	63	1.7375	3.4165
Cg1 [1] -> Cg15[i]	4.3768(1)	78	47.1	72.2	1.3401	2.9787
Cg2 [1] -> Cg4[i]	3.8839(1)	78	29.6	70.5	1.2946	3.3767
Cg2 [1] -> Cg7 [i]	3.8574(1)	89	27.1	63.2	1.7406	3.4351
Cg2 [1] -> Cg14 [i]	4.3639(1)	79	44.7	74.1	1.1967	3.1017
Cg2 [1] -> Cg19 [i]	4.2544(1)	80	58.7	74.7	1.1246	2.2113
Cg5 [1] -> Cg18 [vii]	4.4577(1)	47	50.6	8	4.4148	2.8312
Cg9 [1] -> Cg10 [ii]	4.3915(1)	40	13.9	50.7	2.783	4.2636
Cg9 [1] -> Cg15 [ii]	4.4192(1)	39	12.2	50.4	2.8181	4.3195
Cg10 [1] -> Cg9 [vii]	4.3915(1)	40	50.7	13.9	4.2636	2.783
Cg15 [1] -> Cg9 [vii]	4.4192(1)	39	50.4	12.2	4.3195	2.8181
Cg18 [1] -> Cg5 [ii]	4.4577(1)	47	8	50.6	2.8312	4.4148

Symmetry transformations used to generate equivalent atoms: [i] X,Y,Z; [ii] -1/2+X,1/2-Y,Z; [iii] 1/2+X,-1/2-Y,Z; [iv] 1/2-X,1/2+Y,1/2+Z; [v] X,1+Y,Z; [vi] 1/2-X,1/2+Y,-1/2+Z; [vii] 1/2+X,1/2-Y,Z; [viii] 1/2-X,-1/2+Y,1/2+Z; [ix] -1/2+X,-1/2-Y,Z, [X] X,-1+Y,Z Where Cg1 = Ru1–N1– C12–C11–N2; Cg2 = Ru1–N3–C23–C24–N4; Cg4 = N2–C10–C9–C8–C7–C11; Cg5 = N3–C13–C14–C15–C16–C23; Cg7 = N5–N7–C32–C31–C26–C25; Cg8 = N6–N8–C40 –C39–C34–C33; Cg9 = C4–C5–C6–C7–C11–C12; Cg10 = C16–C17–C18–C19–C24 –C23; Cg14 = N2–C10–C9–C8–C7–C6–C5–C4–C12–C11; Cg15 = N3–C13–C14–C15 –C16–C17–C18–C19– C24–C23; Cg18 = N6–N8–C40–C39–C38–C37–C36–C35–C34 –C33; Cg19 = N1–C1–C2–C3–C4–C5–C6–C7–C8–C9–C10–N2–C11–C12

Table S6. Analysis of anion····π interactions (X····Cg < 4.0 Å, γ < 30°) for **2**.

Y–X(I) Res(I) Cg(J)	X····Cg	X–Perp	γ	Y–X····Cg	Y····Cg
P1–F6 [2] -> Cg8[i]	3.3836(1)	-3.144	21.68	139.89(1)	4.6918(1)
P1–F6 [2] -> Cg18 [i]	3.6355(1)	-3.153	29.86	124.85(1)	4.7096(1)
P2–F7 [3] -> Cg7 [ii]	3.1209(1)	-3.101	6.41	137.75(1)	4.4057(1)
P2–F7 [3] -> Cg17 [ii]	3.3197(1)	-3.096	21.18	118.78(1)	4.2968(1)
P2–F10 [3] -> Cg10 [iii]	3.4160(1)	3.260	17.38	135.70(1)	4.6430(1)
P2–F10 [3] -> Cg16 [iii]	3.6243(1)	3.262	25.85	117.08(1)	4.5363(1)
P2–F10 [3] -> Cg20 [iii]	3.7319(1)	3.248	29.49	130.83(1)	4.8785(1)
P2–F12 [3] -> Cg6 [iii]	3.6428(1)	3.557	12.45	127.58(1)	4.7478(1)
P2–F12 [3] -> Cg11 [ii]	3.4837(1)	-3.462	6.45	123.35(1)	4.5233(1)
P2–F12 [3] -> Cg16 [iii]	3.7376(1)	3.541	18.68	111.36(1)	4.5363(1)
P2–F12 [3] -> Cg17 [ii]	3.6396(1)	-3.469	17.63	104.50(1)	4.2968(1)

Symmetry transformations used to generate equivalent atoms: [i] X,1+Y,Z; [ii] 1/2-X,1/2+Y,-1/2+Z; [iii] X,Y,Z; Where Cg6 = N4–C22–C21–C20–C19–C24; Cg7 = N5–N7–C32–C31–C26–C25; Cg8 = N6–N8–C40–C39–C34–C33; Cg10 = C16–C17–C18–C19–C24–C23; Cg11= C26–C27–C28 –C29–C30–C31; Cg16 = N4–C22– C21–C20–C19–C18–C17–C16–C23–C24; Cg17 = N5–N7–C32–C31–C30–C29–C28–C27–C26–C25; Cg18 = N6–N8–C40–C39–C38 –C37–C36–C35–C34–C33

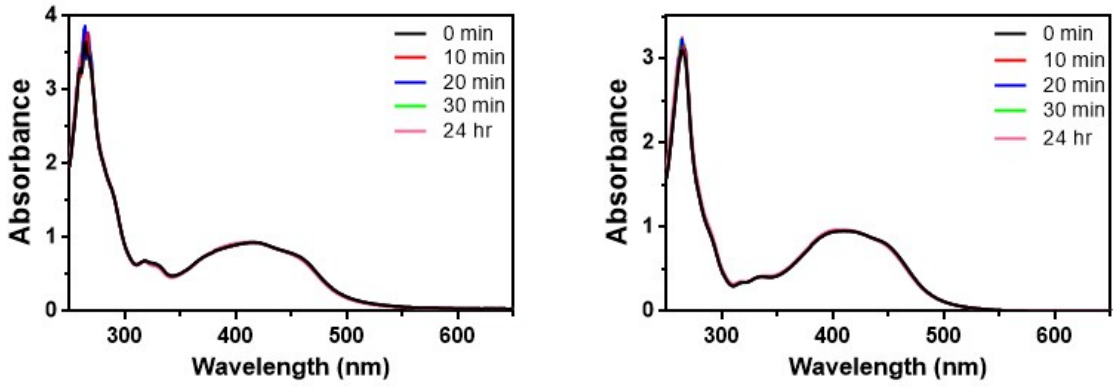


Fig. S9. Time-dependent UV-vis absorption spectra of **1** and **2** in acetonitrile in the dark at 37 °C.

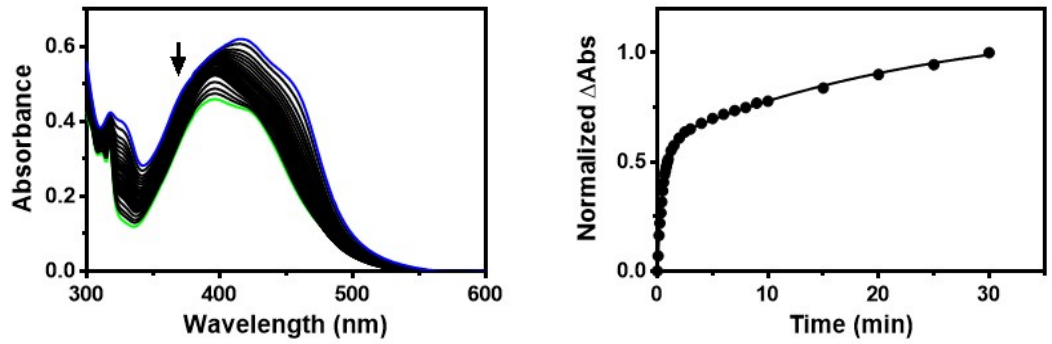


Fig. S10. UV-Visible absorption spectra monitoring photodissociation of **1** (50 μM) in acetonitrile upon irradiation (λ_{irr} = 470 nm) for 0–30 min; 0 min (blue line), 30 min (green line). The normalized change in extinction coefficient was plotted versus time and fitted to a bi-exponential equation using Prism software.

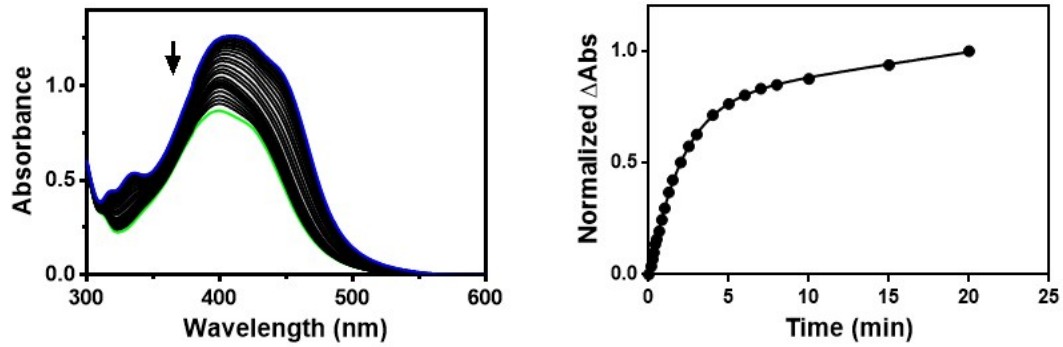


Fig. S11. UV-Visible absorption spectra monitoring photodissociation of **2** (50 μM) in acetonitrile upon irradiation (λ_{irr} = 470 nm) for 0–35 min; 0 min (blue line), 35 min (green line). The normalized change in extinction coefficient was plotted versus time and fitted to a mono exponential equation using Prism software.

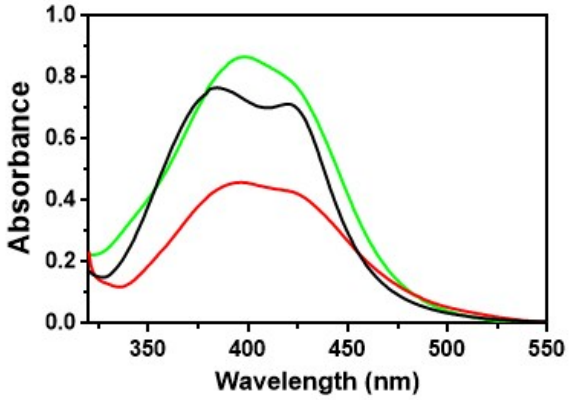


Fig. S12. UV-Visible absorption spectra monitoring photodissociation of **1** and **2** (50 μM) in acetonitrile upon irradiation (λ_{irr} = 470 nm) **1**: 30 min (red line); **2**: 35 min (green line) and absorption spectra of *cis*-[Ru(phen)$_2$(acetonitrile)$_2$](PF$_6$)$_2$ (50 μM) prepared separately in acetonitrile in the dark at 37 °C (black line).

Table S7. Half-lives and quantum yields of first and second co-ligand dissociation for compounds **1–2** in CH_2Cl_2 with 10 mM Bu_4NCl upon irradiation (λ_{irr} = 470 nm).

	$t_{1/2}$ (first step) min	$t_{1/2}$ (second step) min	ϕ_{ps} (1)	(2)
1	1.49	3.08	0.19	0.031
2	2.17	5.75	0.16	0.018

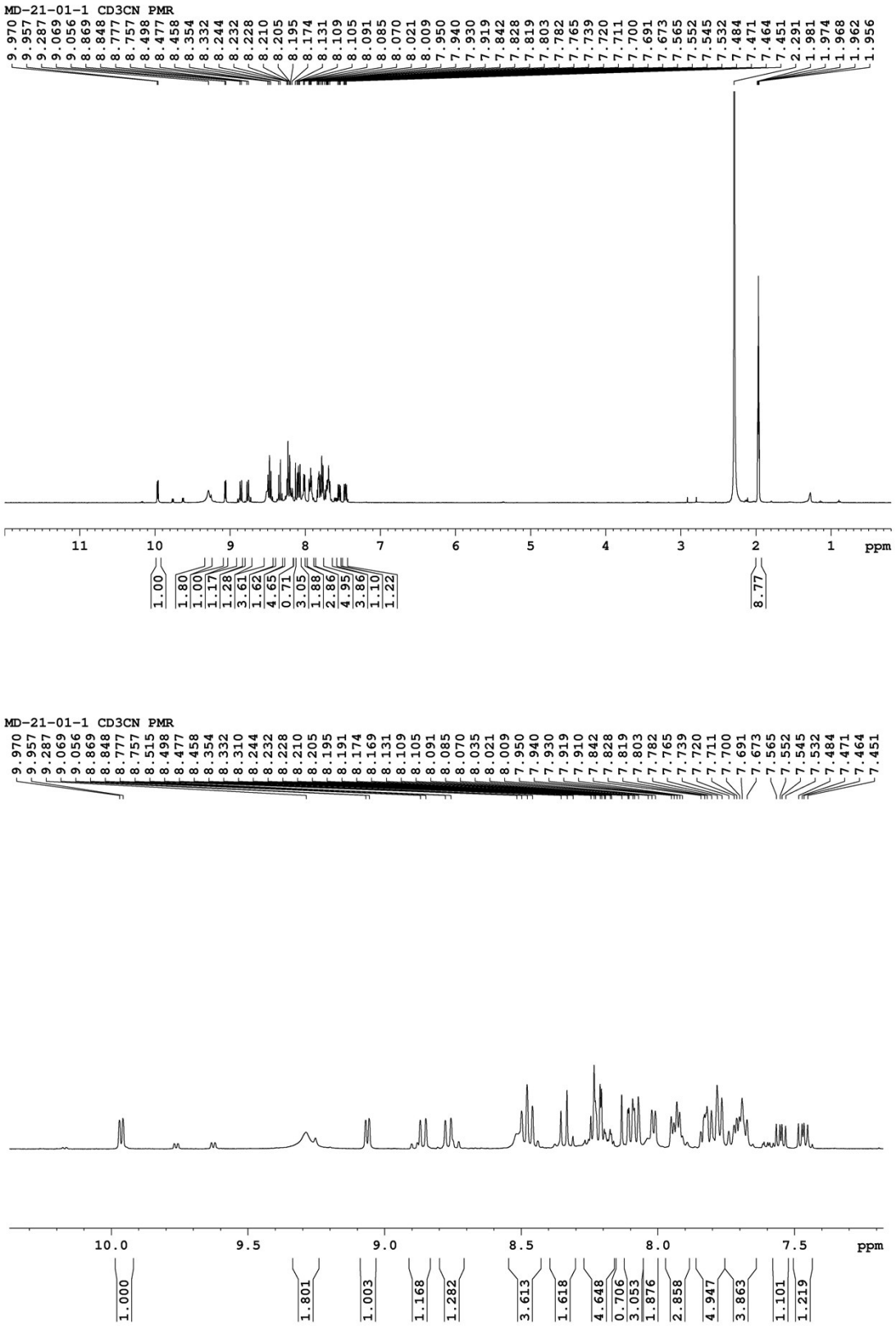


Fig. S13. ^{1}H NMR spectrum of **1** after irradiation for 45 min in acetonitrile-d3.

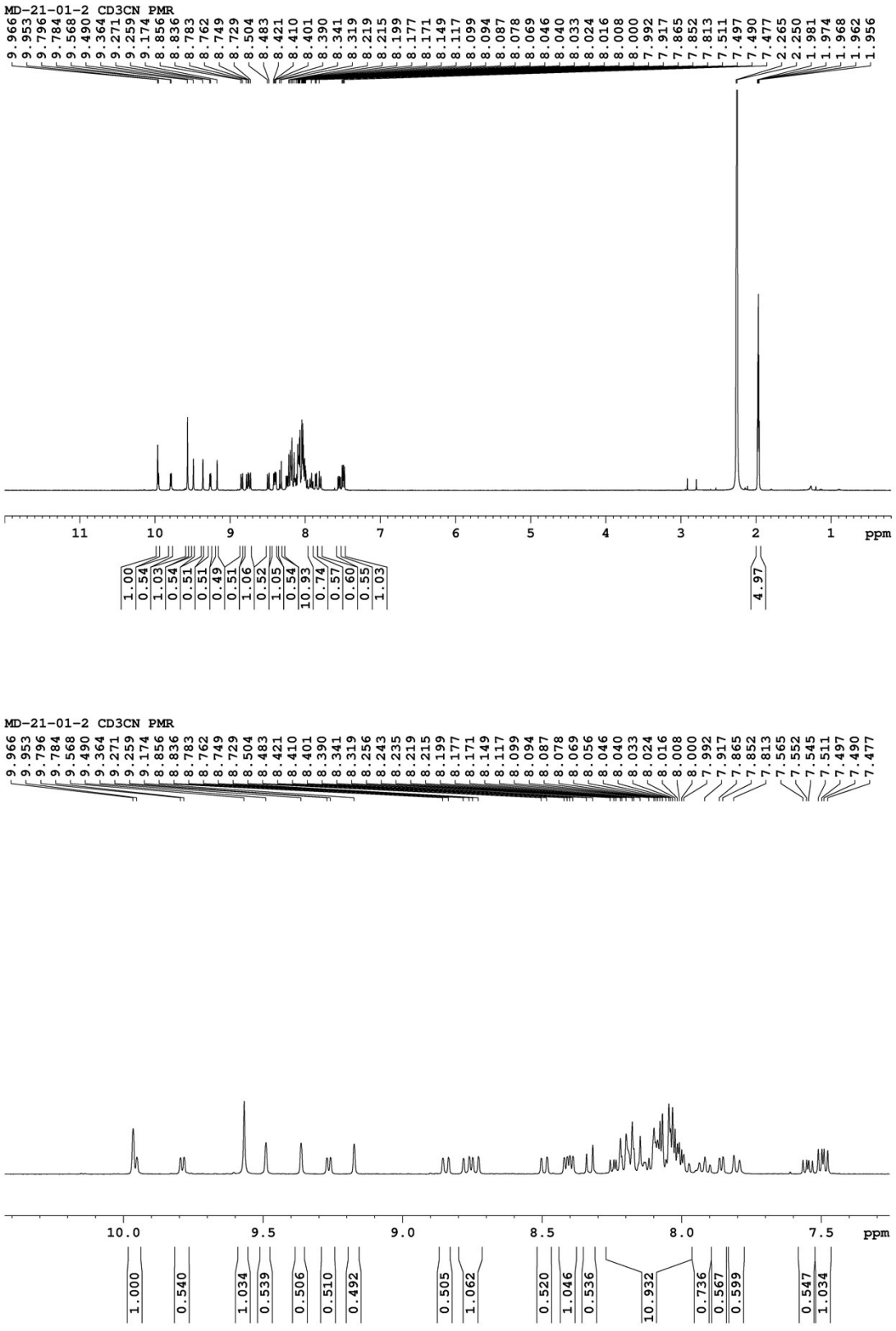


Fig. S14. ^{1}H NMR spectrum of **2** after irradiation for 45 min in acetonitrile-d3.

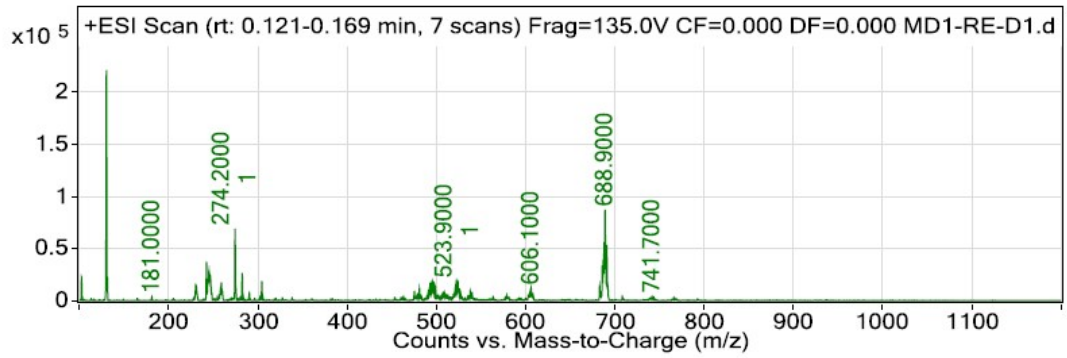


Fig. S15. ESI-LC-MS of **1** after photodissociation in acetonitrile upon irradiation (λ_{irr} = 470 nm) for 30 min; The ion at m/z 130 is the isoquinoline ligand liberated from the compound. The ion at m/z 688.9 is the PF_6- salt of the $[Ru(phen)_2(CH_3CN)_2]$ compound and the ion at m/z 606.1 is the ligand deficient PF_6- salt of the $[Ru(phen)_2]$ compound.

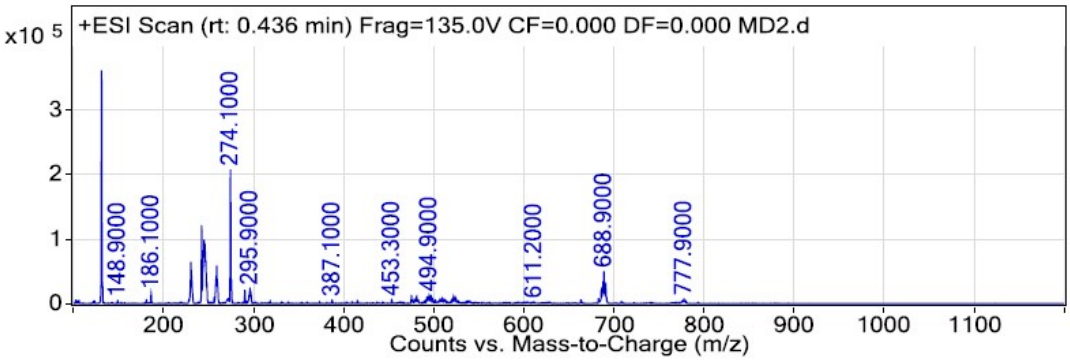


Fig. S16. ESI-LC-MS of **2** after photodissociation in acetonitrile upon irradiation (λ_{irr} = 470 nm) for 35 min; The ion at m/z 131 is the phthalazine ligand liberated from the compound. The ion at m/z 688.9 is the PF_6- salt of the $[Ru(phen)_2(CH_3CN)_2]$ compound and the ion at m/z 777.9 is the mono-substituted PF_6- salt of the $[Ru(phen)_2(phthz)(CH_3CN)]$ compound.

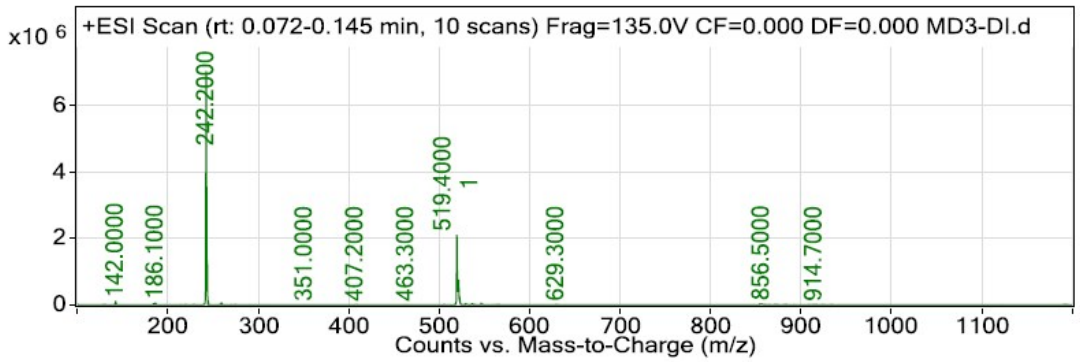


Fig. S17. ESI-LC-MS of **1** in CH_2Cl_2 with 10 mM Bu_4NCl upon irradiation (λ_{irr} = 470 nm) for 25 min. The ion at m/z 519.4 is the sodium adduct of the $[Ru(phen)_2Cl]$ compound. The peak at m/z 242.2 is the tetrabutyl ammonium ion.

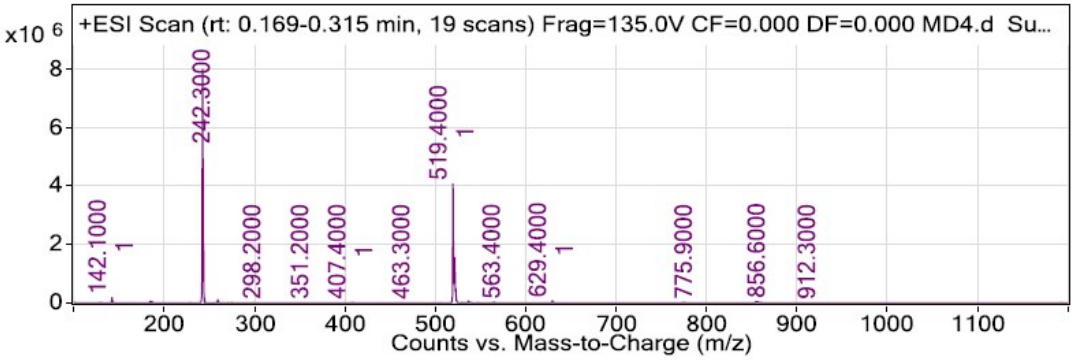


Fig. S18. ESI-LC-MS of **2** in CH_2Cl_2 with 10 mM Bu_4NCl upon irradiation (λ_{irr} = 470 nm) for 35 min . The ion at m/z 519.4 is the sodium adduct of the $[Ru(phen)_2Cl]$ compound. The peak at m/z 242.2 is the tetrabutyl ammonium ion.

1) Detailed methods for determination of quantum yields

Quantum yields were determined as has been described previously by E. C. Glazer et al. *Chem. Commun. 54*, 2018, 12487-12490. In all cases, the light source was a 470 nm LED array from Elixa. The photon flux of the light source was determined by ferrioxalate actinometery.

Part A

1) Procedure for Ferrioxilate Actinometry Method:

The literature procedures reported by C. G. Hatchard et. al. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, 235*, No. 1203, 1956, 518-536 and E. C. Glazer et al. *Chem. Commun. 54*, 2018, 12487-12490 has been adapted for the calculation of the photon flux of light source. The reported values for the fraction of light absorbed was 0.85 and the quantum yield at 468 nm was 0.92.

The procedure is as follows-

1) Solution A: A solution of potassium ferrioxalate (0.15 M, prepared by dissolving 0.7369 g potassium ferrioxalate in 10 ml 0.05 M sulfuric acid) was used as an actinometer.

2) Solution B: A solution of 1% 1,10-phenanthroline was prepared in buffer (1.125 sodium acetate trihydrate, 50 mg 1,10-phenanthroline, 0.14 ml of H_2SO_4 in water, diluted to 5 ml).

3) Solution A (3 ml) was used for irradiation for set times. At each time point, 150 µl aliquots of Solution A, 450 µl of Solution B, and 2400 µl of H_2O were combined to determine the absorbance of Fe^{2+}complex at 510 nm. This complex forms as a result of photolysis of the ferrioxalate.

2) Photon flux of the light source was determined as given below using two approaches.

Approach 1

Table S8. Photon flux determination of the light source: Experiment 1

Time (sec)	Abs. 510 nm	ΔAbs 510 nm	C(Fe^{2+})	Moles	Moles irradiated	Abs. 470 nm	F	Photon flux
0	0.272228	0	0	0	0	0.4091	0.61	
5	0.331639	0.059411	0.000005401	1.50e-008	3.00e-007			1.068000e-007
10	0.381460	0.109232	0.0000099302	3.00e-008	6.00e-007			1.069000e-007
15	0.427324	0.155096	0.0000140996	4.20e-008	8.40e-007			9.900000e-008
20	0.472480	0.200252	0.0000182047	5.40e-008	1.08e-006			9.600000e-008
30	0.545232	0.273004	0.0000248185	7.50e-008	1.50e-006			8.900000e-008
40	0.609845	0.337617	0.0000306925	9.30e-008	1.86e-006			8.288000e-008
50	0.667881	0.395653	0.0000359684	1.08e-007	2.16e-006			7.697700e-008
60	0.720422	0.448194	0.0000407449	1.23e-007	2.46e-006			7.305700e-008
80	0.831456	0.559228	0.0000508389	1.53e-007	3.06e-006			6.815700e-008
100	0.930189	0.657961	0.0000598146	1.80e-007	3.60e-006			6.414000e-008
120	1.027413	0.755185	0.0000686532	2.07e-007	4.14e-006			6.147540e-008
140	1.173820	0.901592	0.0000819629	2.46e-007	4.92e-006			6.262000e-008
								6.462025e-008

Approach 1

Table S9. Photon flux determination of the light source: Experiment 2

Time (sec)	Abs. 510 nm	ΔAbs 510 nm	C(Fe^{2+})	Moles	Moles irradiated	Abs. 470 nm	F	Photon flux
0	0.308288	0	0	0	0	0.4503	0.64	
5	0.358295	0.050007	0.0000045461	1.50e-008	3.00e-007			1.019022e-007
10	0.419489	0.111201	0.0000101091	3.00e-008	6.00e-007			1.019022e-007
15	0.474723	0.166435	0.0000151304	4.50e-008	9.00e-007			1.019022e-007
20	0.527385	0.219097	0.0000199179	6.00e-008	1.20e-006			1.019021e-007
30	0.614912	0.306624	0.0000278749	8.40e-008	1.68e-006			9.624090e-008
40	0.666456	0.358168	0.0000325607	9.90e-008	1.98e-006			8.491000e-008
50	0.726587	0.418299	0.0000380272	1.14e-007	2.28e-006			7.812500e-008
60	0.810924	0.502636	0.0000456942	1.38e-007	2.76e-006			7.925000e-008
80	0.953578	0.645290	0.0000586627	1.77e-007	3.54e-006			7.430000e-008
100	1.008894	0.700606	0.000066369	1.98e-007	3.96e-006			6.793000e-008
120	1.136546	0.828258	0.00007529	2.25e-007	4.50e-006			6.368000e-008
								4.984300e-008

3) Approach 2: The change in absorbance of Fe^{2+} at 510 nm was plotted against irradiation time.

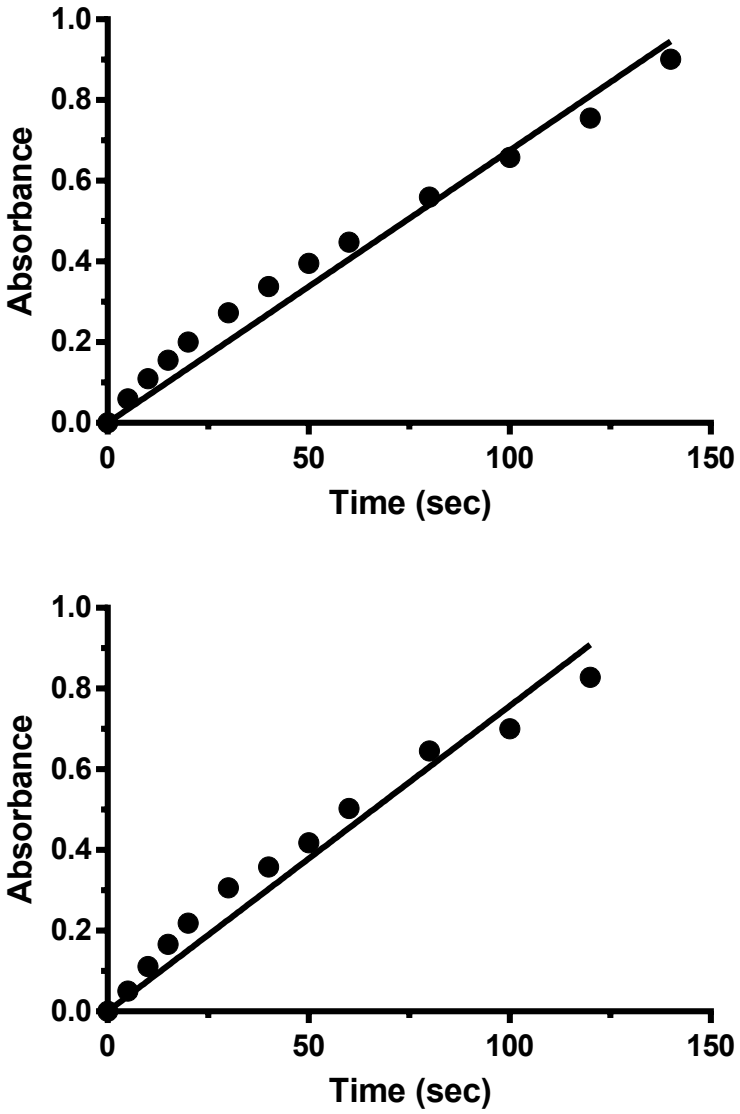


Fig. S19. Linear regression plot of absorbance vs. time for $[Fe(phen)_3]^{2+}$ complex formation.

The slope corresponds to the *dA/dt* value and the equation for the photon flux is as follows-

$$q = \frac{dA}{dt} \times \frac{V1}{\varepsilon \times l} \times \frac{V3}{V2 \times \phi \times F}$$

Where *q* is photon flux (Einstein/s), *dA/dt* is slope, *V1*-volume of irradiated actinometer (0.15 M, 3000 μL), *V2* is the aliquot of actinometer taken to determine the concentration of $[Fe(phen)_3]^{2+}$ (150 μL), *V3* is the volume of the solution measured after complexation (3000 μL), ε is the extinction coefficient of $[Fe(phen)_3]^{2+}$ (11000) as previously reported by Oktavia, B.; Lim, L. W.; Takeuchi, T., *Anal. Sci.* **2008,** *24* (11), 1487-1492, *l* is the path

length, ϕ is the quantum yield of actinometer at 468 nm (0.92) determined by C. G. Hatchard *et. al. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, 235* (1203), **1956**, 518-536 and F=1−1/10^$A_{(470)}$ is the photon absorption probability for the actinometer. For all subsequent quantum yield determinations, we used q = 6.785E-08 (average of values obtained by Approach 2).

Part B

Quantum Yield Determination for 1-2

1) For compounds **1–2** in CH_2Cl_2 in the presence of 10 mM Bu_4NCl, the change in absorbance upon irradiation possessed clear isosbestic points for both steps (Fig. 3 and 4) of photosubstitution. As a result, the moles of decreasing reactant were determined based on the changes in normalized corrected Δ Absorbance (reactant vs. product) over time, which is used in the $t_{1/2}$ determinations. To calculate the photosubstitution quantum yield for Step 1, the average absorbance for the first five time points at 470 nm was measured and used for the calculation of the photon absorption probability (F) for each compound. Similarly for the second step of the photochemical reaction, the average absorbance at 470 nm was measured for the first five time points and was used for calculation of the photon absorption probability (F) of the intermediate photosubstitution (Step 2) for compounds **1–2**.

Table S10. Photon absorption probability (F) for **1-2**.

Compound	**1**		**2**	
Step	1	2	1	2
Abs 470nm	0.4164	0.3925	0.5738	0.5528
F	0.616	0.594	0.733	0.719

2) The corrected change in absorbance (*ΔAcorr*) was calculated for each time point for **1**, **step 1** as:

$\Delta A_{corr} = A_t^{542} - A_t^{420} - (A_0^{542} - A_0^{420})$

Were A_t^{542} is the MLCT absorbance of photoproduct/intermediate (Step 1) at each time point (t) increasing over time, A_t^{420} is MLCT absorbance of **1** at each time point (t) decreasing over time, A_0^{542} is the initial MLCT absorbance of photoproduct/intermediate (Step 1), and A_0^{420} is initial MLCT absorbance for **1**.

The normalized corrected change in absorbance has been calculated for each time point as:

$Normalized\ \Delta A_{corr} = 1 - \Delta A_{corr} / \Delta A_{corr}^{max}$

Where ΔA_{corr}^{max} is maximum corrected change in absorbance.

We calculated the moles of the starting compound and product at each time point.

The initial moles (*mol*) has been calculated as-

$mol = A_0^{420} * V / (\varepsilon * l)$

Where A_0^{420} is initial MLCT absorbance for **1,** step 1, V is the aliquot irradiated (3000 μL), ε is the extinction coefficient for **1** and l is the path length. Similarly we calculated the moles at each time points for **1** and **2** for Step 1 and 2. The moles of photon absorbed have been calculated as the product of photons irradiated and photon absorption probability (F).

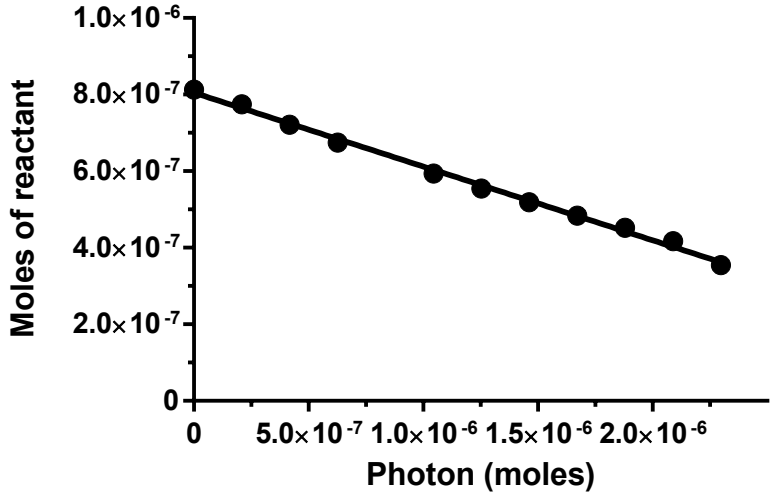


Fig. S20. Linear regression plot of moles of reactant vs. moles of photons absorbed for compound **1**, **Step 1**.

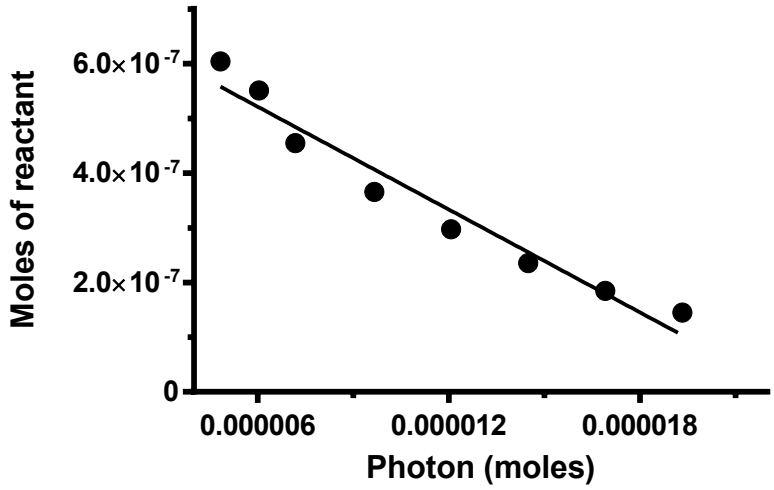


Fig. S21. Linear regression plot of moles of reactant vs. moles of photons absorbed for compound **1**, **Step 2**.

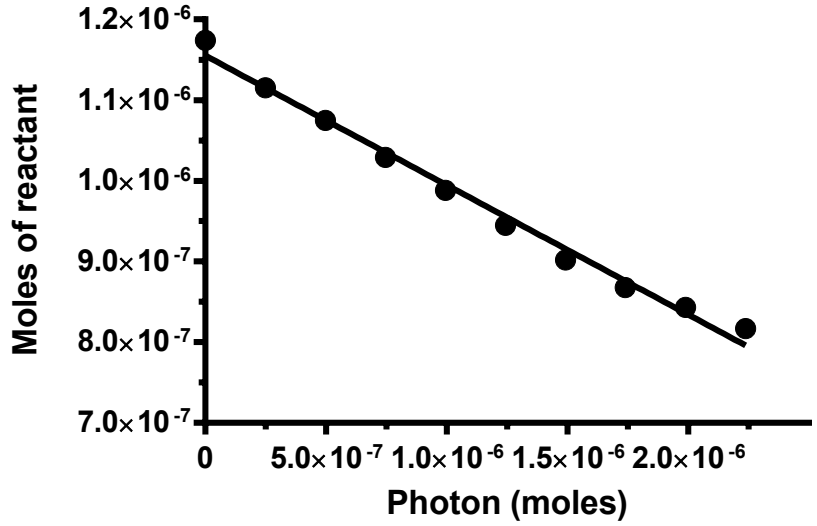


Fig. S22. Linear regression plot of moles of reactant vs. moles of photons absorbed for compound **2**, **Step 1**.

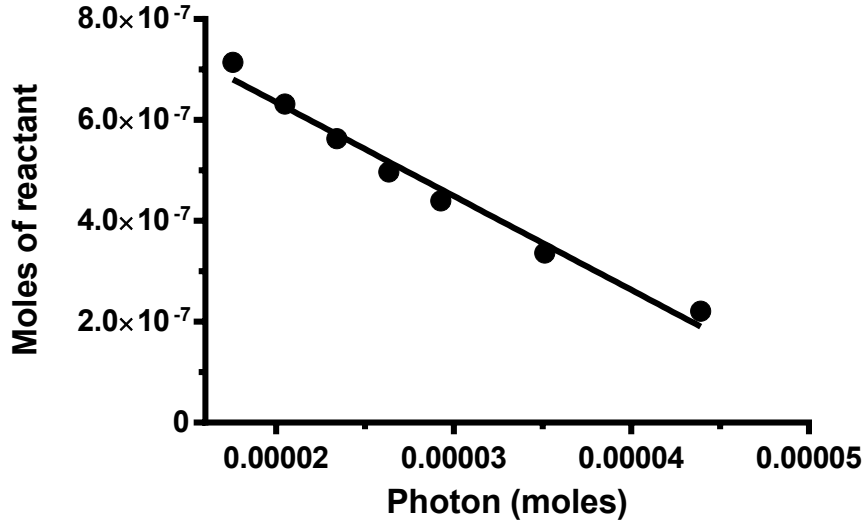
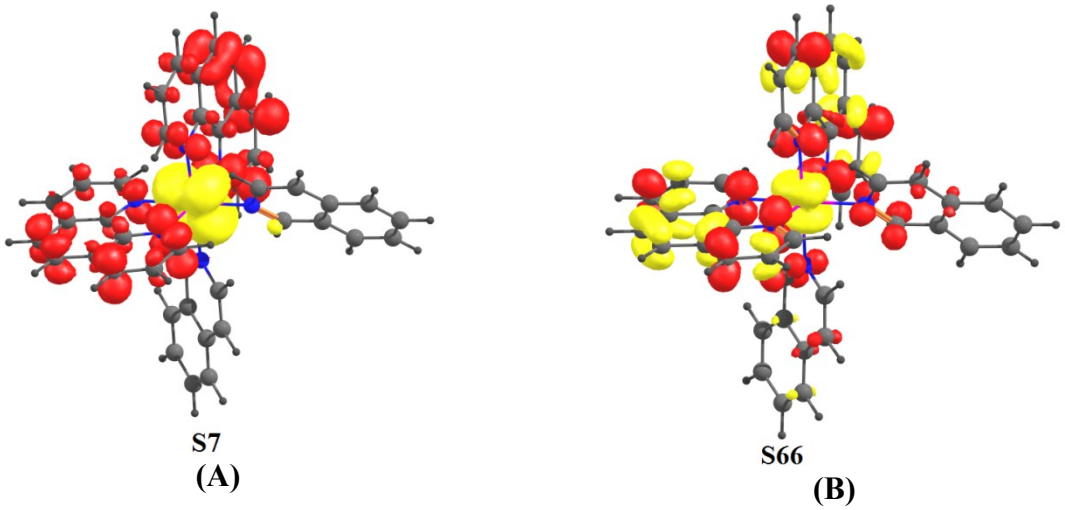
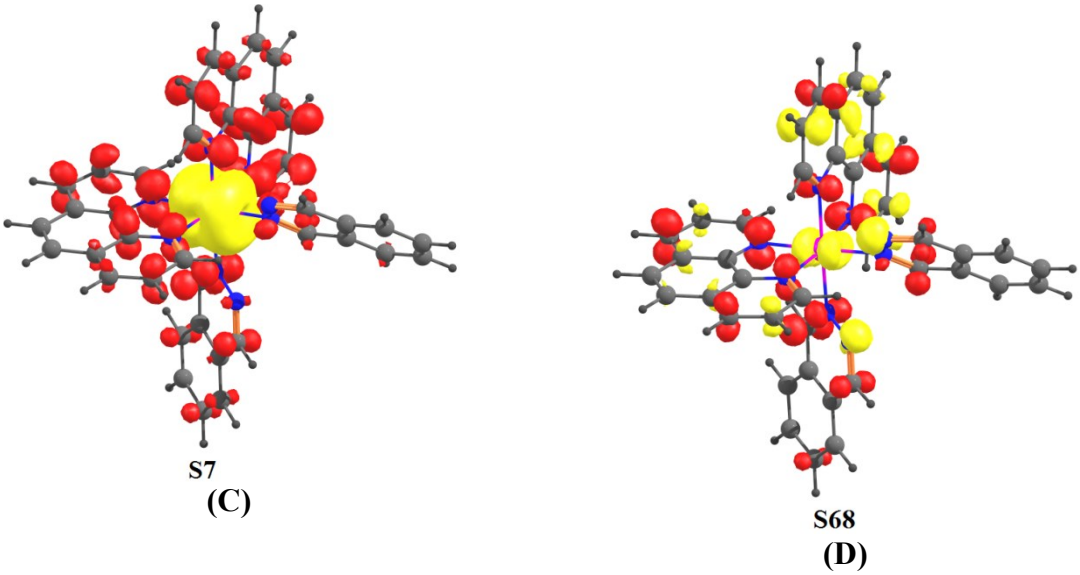


Fig. S23. Linear regression plot of moles of reactant vs. moles of photons absorbed for compound **2**, **Step 2**.

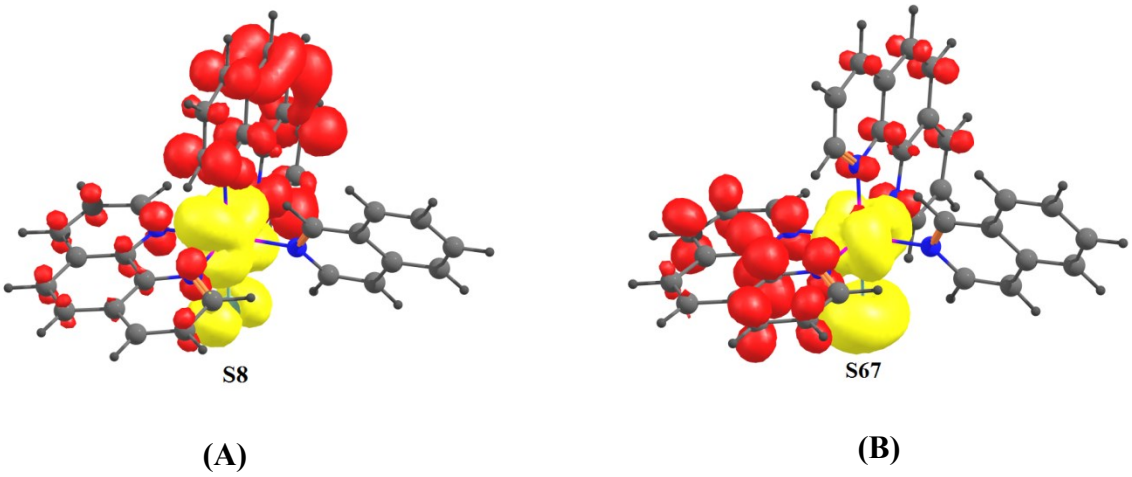


cis-[Ru(phen)$_2$(isoq)$_2$]$^{2+}$ **1**



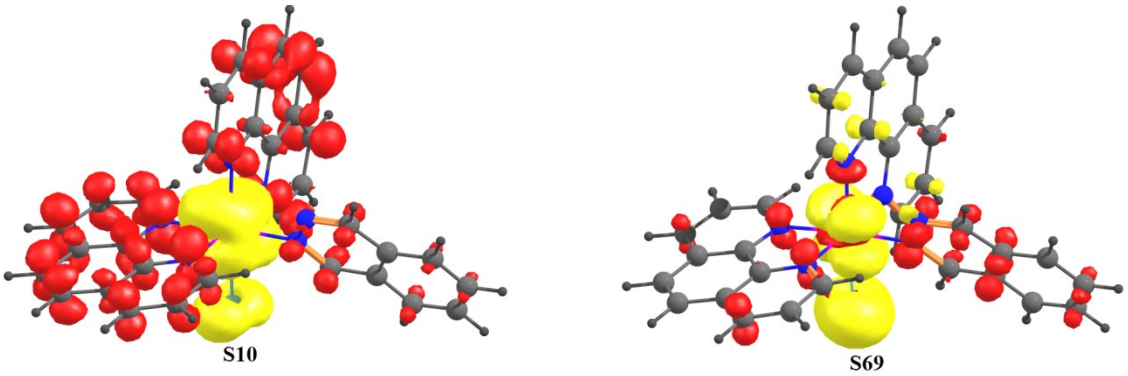
cis-[Ru(phen)$_2$(phthz)$_2$]$^{2+}$ **2**

Fig. S24. The electron difference density plots (iso-surface value = 0.001247 au) of two low energy singlet-singlet transitions in TD-DFT calculations for **1–2**. The yellow regions indicate the depletion of electron density and red regions indicates the increase in electron density.



(A) **(B)**

cis-[Ru(phen)$_2$(isoq)Cl]$^{1+}$ **1a**



(C) **(D)**

cis-[Ru(phen)$_2$(phthz)Cl]$^{1+}$ **2a**

Fig. S25. The electron difference density plots (iso-surface value = 0.001247 au) of two low energy singlet-singlet transitions in TD-DFT calculations for **1a–2a**. The yellow regions indicate the depletion of electron density and red regions indicates the increase in electron density.

Table S11. Calculated bond lengths (Å) and bond angles (°) in the optimized geometry S_0(DFT), ^{3}MLCT, ^{3}MC and ^{3}TS states of **1a** and **2a** in acetonitrile.

	Ru1–N1	Ru1–N2	Ru1–N3	Ru1–N4	Ru1–N5	Ru1–Cl6	N1–Ru1–N3	N2–Ru1–N3	N4–Ru1–N3	N1–Ru1–N5	N2–Ru1–N5	N4–Ru1–N5	N3–Ru1–Cl6
1a													
S_0	2.063	2.043	2.056	2.064	2.117	2.441	96	91	80	87	91	96	175
^{3}MLCT	2.080	2.027	2.068	2.077	2.117	2.392	98	87	80	85	90	97	176
^{3}MC	2.064	2.103	2.383	2.109	2.545	2.408	106	87	74	87	88	92	164
^{3}TS	2.062	2.159	2.229	2.084	2.384	2.429	102	86	77	87	88	94	167
2a													
S_0	2.062	2.043	2.062	2.065	2.069	2.444	96	94	80	89	90	96	176
^{3}MLCT	2.077	2.040	2.071	2.088	2.069	2.382	96	89	79	86	91	98	178
^{3}MC	2.065	2.099	2.378	2.104	2.472	2.421	105	90	74	87	88	93	167
^{3}TS	2.070	2.161	2.337	2.073	2.245	2.514	102	87	76	87	103	96	168

Table S12. Selected TD-DFT singlet-singlet transitions along with oscillator strength (f) and orbital contribution in **1a** and **2a**.[a]

Transition	Energy (eV)	Wavelength (nm)	Oscillator Strength (*f*)	Major Contributions	Orbital transitions
1a					
S7	2.78	446	0.0916	H-2 →LUMO (29%), H-1→L+2 (23%), HOMO→LUMO (10%), HOMO→L+3 (23%)	d_{xy} →π*(Phen) d_z^2 →π*(Phen) d_{xz} →π*(Phen) d_{xz} →π*(Phen)
S8	2.86	433	0.1115	H-1→L+1 (14%), H-1→L+2 (61%)	d_z^2 →π*(Phen) d_z^2 →π*(Phen)
S13	3.11	398	0.0908	H-2→L+2 (33%), H-2→L+4 (18%), H-1→L+1 (12%)	d_{xy} →π*(Phen) d_{xy} →π*(Isoq) d_z^2 →π*(Phen)
S59	4.99	248	0.0997	H-1→L+9 (39%)	d_z^2 →π*(Phen)
S62	5.04	245	0.295	H-8→L+1 (17%), H-2→L+8 (11%)	p-(Cl) →π*(Phen) d_{xy} →π*(Phen)
S65	5.08	243	0.2021	HOMO→L+10 (38%), HOMO→L+11 (10%)	d_{xz} → d_z^2* d_{xz} → d_z^2*
S66	5.10	243	0.1018	H-2→L+9 (35%), HOMO→L+10 (18%)	d_{xy} →π*(Phen) d_{xz} → d_z^2*
S67	5.11	242	0.3471	H-2→L+9 (31%)	d_{xy} →π*(Phen)
S68	5.12	242	0.1108	H-9→L+2 (39%) H-8→L+2 (11%) H-8→L+3 (10%) H-7→L+3 (15%)	p-(Cl) →π*(Phen) p-(Cl) →π*(Phen) p-(Cl) →π*(Phen) p-(Cl) →π*(Phen)
2a					
S10	2.89	429	0.168	H-1->L+1 (19%), H-1->L+2 (34%), HOMO->L+3 (19%)	d_{yz} → π*(Phen) d_{yz} → π*(Phen) d_{xz} → π*(Phen)
S11	2.96	418	0.1006	H-1->L+2 (15%), H-1->L+3 (26%), H-1->L+4 (30%)	d_{yz} → π*(Phen) d_{yz} → π*(Phen) d_{yz} → π*(Phthz)
S12	2.99	415	0.1157	H-2->L+2 (30%), H-1->L+3 (45%)	d_{xy} → π*(Phen) d_{yz} → π*(Phen)
S19	3.56	348	0.119	H-2->L+5 (56%), HOMO->L+5 (10%)	d_{xy} → π*(Phen) d_{xz} → π*(Phthz)
S55	4.94	251	0.0956	H-7->L+1 (16%), H-6->L+1 (18%)	π(Phen) → π*(Phen) π(Phen) → π*(Phen)
S56	4.95	250	0.1096	H-7->LUMO (16%), HOMO->L+9 (12%)	π(Phen) → π*(Phen) d_{xz} → π*(Phen)
S64	5.04	245	0.1325	H-9->L+2 (10%)	p-(Cl) → π*(Phen)
S69	5.12	242	0.2350	HOMO->L+10 (32%)	d_{xz} → d_z^2*
S76	5.17	239	0.1054	H-8->L+2 (10%), H-8->L+3 (13%), H-8->L+4 (25%)	p-(Cl) → π*(Phen) p-(Cl) → π*(Phen) p-(Cl) → π*(Phthz)

[a] **Abbreviations:** Phen= phenanthroline, Phthz= phthalazine, Isoq= isoquinoline

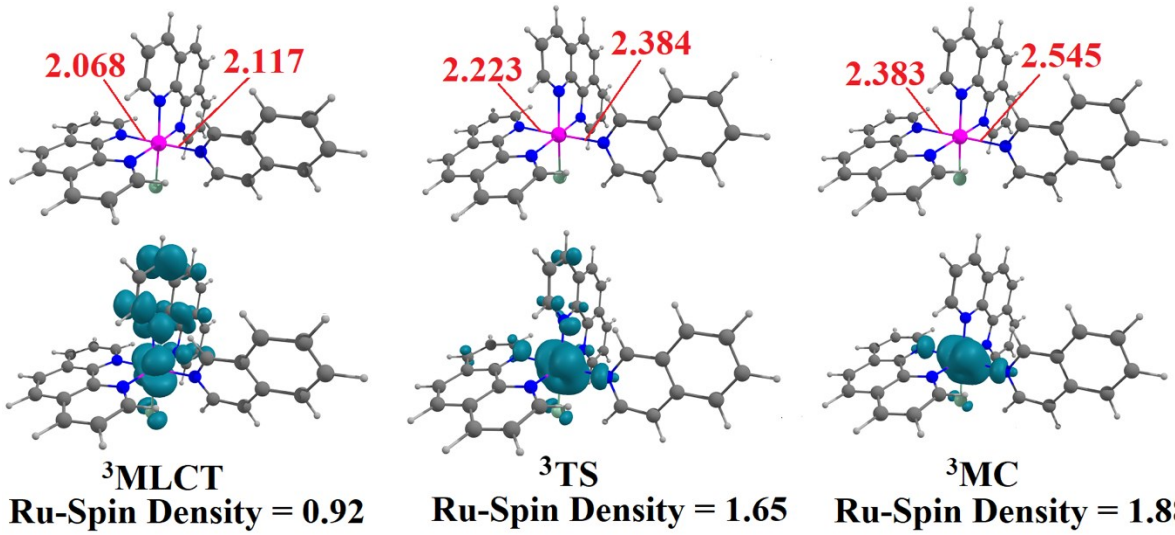


Fig. S26. Optimized structures and spin density plots (iso-surface value = 0.004 au) of the triplet states for the *cis*-$[Ru(phen)_2(isoq)Cl]^{1+}$ **1a** in acetonitrile. The respective Ru–N distances are shown in red color.

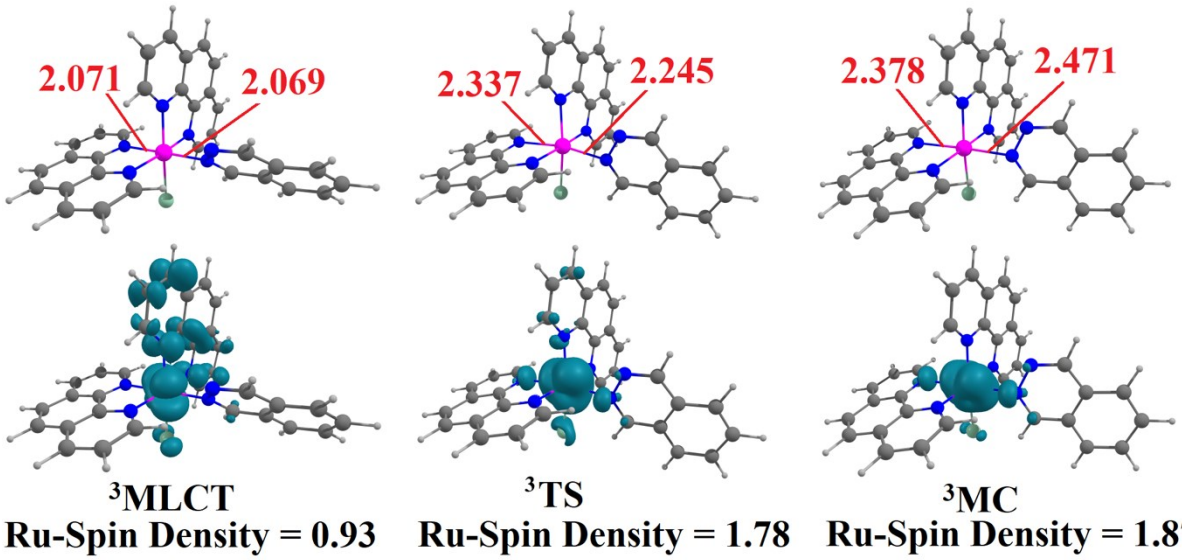
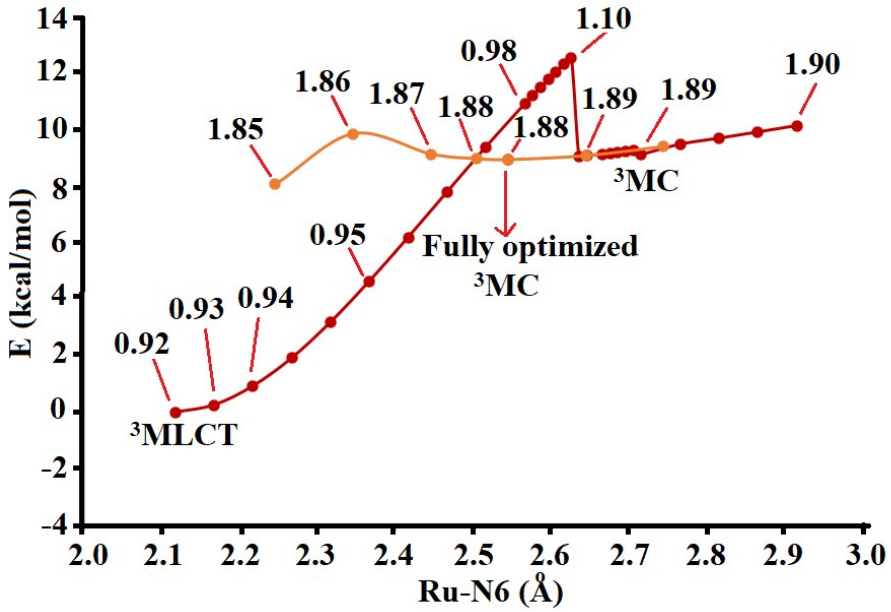
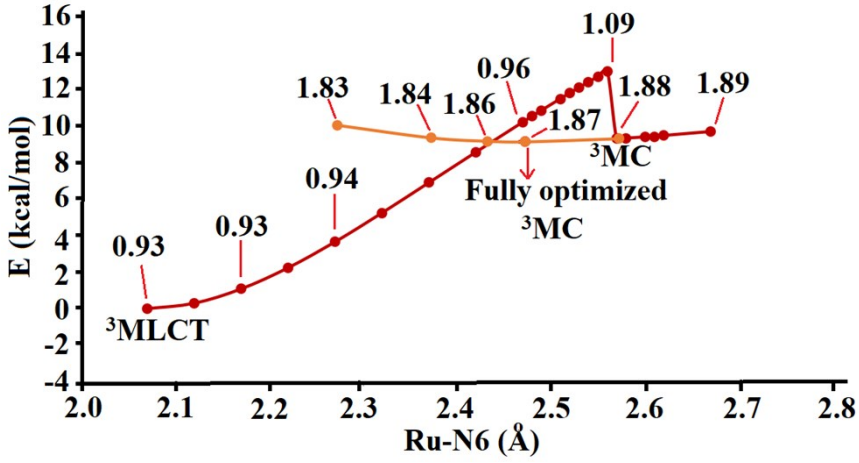


Fig. S27. Optimized structures and spin density plots (iso-surface value = 0.004 au) of the triplet states for the *cis*-$[Ru(phen)_2(phthz)Cl]^{1+}$ **2a** in acetonitrile. The respective Ru–N distances are shown in red color.



(A)



(B)

Fig. S28. Relaxed potential energy scans from the ^{3}MLCT towards ^{3}MC (red line) and from ^{3}MC towards ^{3}MLCT (orange line) states of A) *cis*-[Ru(phen)$_2$(isoq)Cl]$^{1+}$ **1a** in acetonitrile for stretching the Ru−N5(isoq)Cl coordinate and B) *cis*-[Ru(phen)$_2$(phthz)Cl]$^{1+}$ **2a** in acetonitrile for stretching the Ru−N5(phthz)Cl coordinate. The numbers along the PES lines corresponds to the spin density values on the Ru-centre.

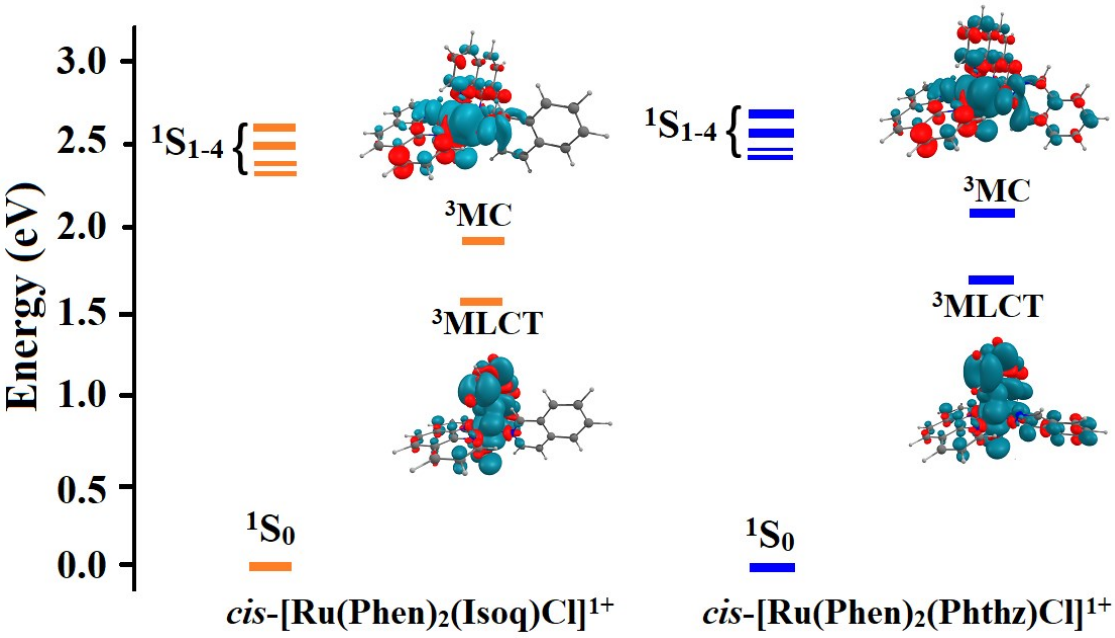


Fig. S29. Jablonski diagram obtained using DFT (triplets) and TD-DFT (singlets) data for *cis*-[Ru(phen)$_2$(isoq)Cl]$^{1+}$ **1a** and *cis*-[Ru(phen)$_2$(phthz)Cl]$^{1+}$ **2a**. Spin densities are plotted for ^{3}MLCT and ^{3}MC states (iso-surface value = 0.004 au).

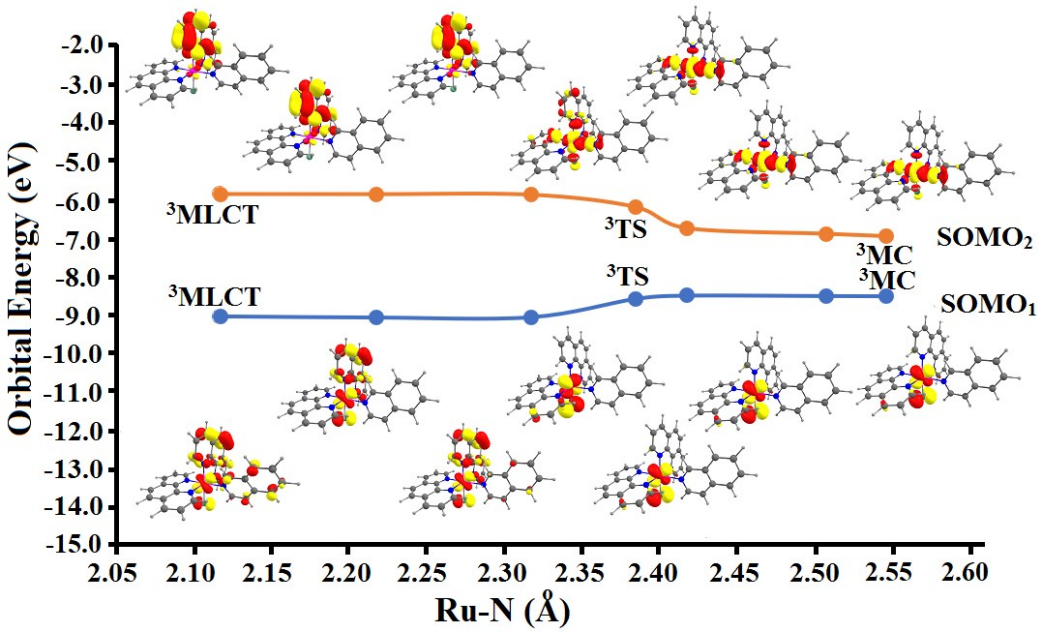


Fig. S30. MO diagram for the relaxed PES scan of the triplet state of **1a** in acetonitrile along the Ru−N5(isoq)Cl coordinate. Selected isosurface plots (iso-surface value = 0.04 au) of SOMOs are present to show the changes in electron population and geometry.

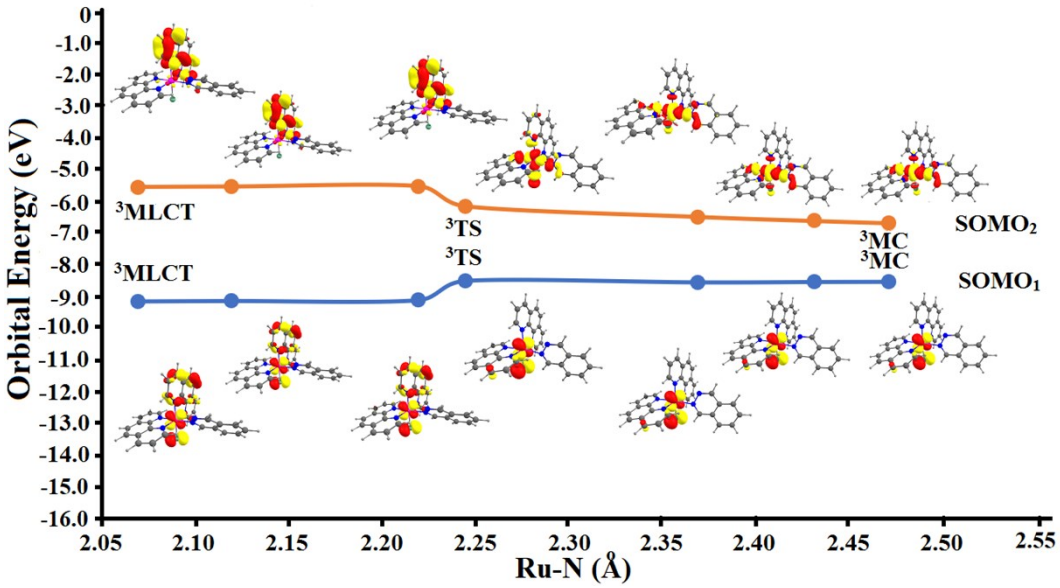


Fig. S31. MO diagram for the relaxed PES scan of the triplet state of **2a** in acetonitrile along the Ru−N5(phthz)Cl coordinate. Selected isosurface plots (iso-surface value = 0.04 au) of SOMOs are present to show the changes in electron population and geometry.

Cartesian coordinates:

***cis*-[Ru(phen)$_2$(Isoq)$_2$]$^{2+}$: $^1S_0$**

E(RPBE1PBE) = –2038.98628016 A.U.

Ru	-0.013002000	-0.390045000	-0.101135000	H	3.243387000	-0.809903000	4.883005000
N	-1.075703000	-0.565970000	-1.886643000	C	1.819602000	0.411199000	3.828342000
C	-0.765216000	-0.088408000	-3.102669000	H	1.785863000	1.193364000	4.576793000
H	0.181274000	0.428074000	-3.195380000	C	1.027641000	0.532167000	2.675654000
N	-1.656508000	-1.469795000	0.545304000	H	0.386170000	1.391286000	2.529034000
C	-1.611861000	-0.246319000	-4.210995000	C	3.444465000	-2.886136000	3.069060000
H	-1.308825000	0.159744000	-5.168251000	H	4.073043000	-3.035414000	3.940099000
N	1.009731000	-2.183777000	-0.261946000	C	3.412449000	-3.818339000	2.072278000
C	-2.815421000	-0.914492000	-4.071294000	H	4.013753000	-4.718104000	2.142818000
H	-3.479713000	-1.047342000	-4.918128000	C	-1.875750000	1.575726000	1.268541000
N	1.017753000	-0.398950000	1.708597000	H	-1.900566000	0.769460000	1.992729000
C	-3.174285000	-1.428056000	-2.805700000	C	-1.790830000	3.554013000	-0.634797000
N	-1.082406000	1.406081000	0.204812000	H	-1.731449000	4.308649000	-1.411347000
C	-2.272917000	-1.222191000	-1.738301000	C	-2.631295000	3.760892000	0.488526000
C	-1.051668000	2.404607000	-0.747541000	C	-2.670892000	2.724140000	1.473469000
C	-2.575990000	-1.718280000	-0.440567000	C	-3.497355000	2.873816000	2.617702000
N	1.651463000	0.649693000	-0.885793000	H	-3.528527000	2.084401000	3.362453000
C	-3.766775000	-2.441993000	-0.212176000	C	-4.252387000	4.014130000	2.773051000
C	2.397040000	0.092728000	-1.906277000	H	-4.885444000	4.133567000	3.644835000
C	-3.989687000	-2.935672000	1.091800000	C	-4.212491000	5.041989000	1.797380000
H	-4.890492000	-3.498392000	1.310726000	H	-4.816174000	5.931189000	1.940111000
C	-3.045304000	-2.698112000	2.075426000	C	-3.419891000	4.921652000	0.675860000
H	-3.184480000	-3.073136000	3.081892000	H	-3.392957000	5.709360000	-0.069525000
C	-1.890178000	-1.961113000	1.772404000	C	2.062836000	1.812206000	-0.369790000
H	-1.138189000	-1.761232000	2.524983000	H	1.466310000	2.228947000	0.432435000
C	-4.672088000	-2.637460000	-1.308265000	C	3.522921000	0.691016000	-2.409554000
H	-5.590370000	-3.186307000	-1.130441000	H	4.073875000	0.211054000	-3.210960000
C	-4.389773000	-2.147267000	-2.550696000	C	3.973523000	1.929762000	-1.884782000
H	-5.081937000	-2.300251000	-3.371429000	C	3.207897000	2.504441000	-0.822197000
C	0.937920000	-3.091090000	-1.248938000	C	3.610881000	3.742147000	-0.257279000
H	0.284606000	-2.855407000	-2.079178000	H	3.027588000	4.177688000	0.548123000
C	1.670548000	-4.287544000	-1.220021000	C	4.734082000	4.379860000	-0.733942000
H	1.576783000	-4.984432000	-2.043731000	H	5.045835000	5.325788000	-0.306063000
C	2.502795000	-4.561594000	-0.148743000	C	5.493475000	3.809364000	-1.785853000
H	3.081330000	-5.478181000	-0.114706000	H	6.374809000	4.328658000	-2.145088000
C	2.589382000	-3.633391000	0.911584000	C	5.123979000	2.608131000	-2.353108000
C	1.813393000	-2.457581000	0.814165000	H	5.707153000	2.174173000	-3.158344000
C	1.831267000	-1.495451000	1.860746000	H	2.046559000	-0.858522000	-2.280443000
C	2.648638000	-1.694090000	2.995068000	H	-0.403875000	2.227984000	-1.593362000
C	2.628395000	-0.698702000	3.996754000				

cis-$[Ru(phen)_2(Isoq)_2]^{2+}$: ^{3}MLCT

E(UPBE1PBE) = -2038.90712035 A.U.

Ru	-0.011399000	-0.330094000	-0.108419000	H	3.136454000	-0.828909000	4.938001000
N	-1.046313000	-0.486814000	-1.920521000	C	1.764615000	0.442152000	3.862166000
C	-0.738656000	0.013177000	-3.128925000	H	1.742426000	1.221699000	4.613063000
H	0.200480000	0.545667000	-3.213576000	C	0.999118000	0.587495000	2.701209000
N	-1.621459000	-1.431984000	0.509835000	H	0.385687000	1.466771000	2.547155000
C	-1.576009000	-0.141835000	-4.239143000	C	3.292778000	-2.917828000	3.134724000
H	-1.277705000	0.280543000	-5.190259000	H	3.906428000	-3.089662000	4.012316000
N	0.918619000	-2.146019000	-0.238272000	C	3.228469000	-3.855300000	2.143728000
C	-2.775064000	-0.837097000	-4.109494000	H	3.789436000	-4.779623000	2.228315000
H	-3.431057000	-0.969113000	-4.963047000	C	-1.919615000	1.599493000	1.252709000
N	0.978787000	-0.342661000	1.730926000	H	-1.963365000	0.774691000	1.954642000
C	-3.131916000	-1.374874000	-2.861691000	C	-1.772313000	3.628720000	-0.599480000
N	-1.096584000	1.465308000	0.206270000	H	-1.688626000	4.404383000	-1.352463000
C	-2.238235000	-1.171627000	-1.776109000	C	-2.650495000	3.802930000	0.500719000
C	-1.031445000	2.482241000	-0.723347000	C	-2.723502000	2.739659000	1.456902000
C	-2.530049000	-1.688699000	-0.499129000	C	-3.590647000	2.855704000	2.574770000
N	1.711244000	0.632936000	-0.880083000	H	-3.646651000	2.046172000	3.295740000
C	-3.699562000	-2.454990000	-0.279248000	C	-4.353726000	3.990230000	2.732475000
C	2.412018000	0.046455000	-1.915368000	H	-5.018789000	4.085175000	3.583042000
C	-3.904610000	-2.984093000	1.008347000	C	-4.280490000	5.043861000	1.786611000
H	-4.787174000	-3.578044000	1.216315000	H	-4.891513000	5.927744000	1.931121000
C	-2.952002000	-2.749766000	2.009483000	C	-3.447387000	4.956499000	0.691035000
H	-3.084225000	-3.162381000	3.001891000	H	-3.396671000	5.764437000	-0.030889000
C	-1.828756000	-1.981802000	1.737348000	C	2.181043000	1.764289000	-0.343927000
H	-1.074543000	-1.786791000	2.488465000	H	1.616375000	2.194975000	0.474102000
C	-4.596139000	-2.649556000	-1.385506000	C	3.564545000	0.593800000	-2.414381000
H	-5.498886000	-3.227597000	-1.220920000	H	4.086767000	0.095610000	-3.223540000
C	-4.328397000	-2.126879000	-2.618839000	C	4.079899000	1.801061000	-1.876403000
H	-5.017333000	-2.283454000	-3.441680000	C	3.353422000	2.402751000	-0.799639000
C	0.788785000	-3.081281000	-1.218866000	C	3.825594000	3.609734000	-0.220840000
H	0.137796000	-2.830238000	-2.046149000	H	3.273695000	4.064349000	0.595864000
C	1.462987000	-4.291928000	-1.162862000	C	4.978161000	4.191750000	-0.698209000
H	1.341189000	-5.004129000	-1.969334000	H	5.344430000	5.112967000	-0.259976000
C	2.296283000	-4.584982000	-0.073370000	C	5.697531000	3.595426000	-1.764133000
H	2.830746000	-5.526886000	-0.027302000	H	6.602979000	4.071501000	-2.123223000
C	2.423023000	-3.651866000	0.970539000	C	5.260748000	2.423127000	-2.344827000
C	1.704440000	-2.436494000	0.861545000	H	5.814929000	1.969645000	-3.159512000
C	1.751368000	-1.478872000	1.891594000	H	2.012297000	-0.882126000	-2.297002000
C	2.547618000	-1.695071000	3.048947000	H	-0.362573000	2.324796000	-1.556771000
C	2.541324000	-0.701278000	4.040374000				

***cis*-[Ru(phen)$_2$(Isoq)$_2$]$^{2+}$: ^{3}MC**

E(UPBE1PBE) = -2038.90619393 A.U.

Ru	-0.211728000	-0.204466000	0.137732000	H	3.167366000	0.323895000	5.024084000
N	-1.298670000	-0.557793000	-1.667518000	C	1.588395000	1.237463000	3.882925000
C	-1.026641000	0.104431000	-2.803034000	H	1.467564000	2.086178000	4.544656000
H	-0.199730000	0.801010000	-2.762056000	C	0.776187000	1.136556000	2.744896000
N	-1.944478000	-1.780780000	0.676950000	H	0.034270000	1.890012000	2.514819000
C	-1.756839000	-0.092794000	-3.983698000	C	3.594183000	-1.909957000	3.452638000
H	-1.491874000	0.467574000	-4.871653000	H	4.253161000	-1.879154000	4.313356000
N	0.993999000	-1.927798000	0.173428000	C	3.656057000	-2.951177000	2.571861000
C	-2.798261000	-1.001675000	-3.996084000	H	4.365014000	-3.757514000	2.724502000
H	-3.372149000	-1.178759000	-4.899271000	C	-2.476365000	1.645777000	0.908581000
N	0.874805000	0.105985000	1.885846000	H	-2.802448000	0.737053000	1.403323000
C	-3.121958000	-1.700480000	-2.812781000	C	-1.577396000	3.891924000	-0.403797000
N	-1.321522000	1.588051000	0.237365000	H	-1.193472000	4.754022000	-0.937998000
C	-2.350430000	-1.437420000	-1.654583000	C	-2.801080000	3.988762000	0.307218000
C	-0.876557000	2.713294000	-0.423938000	C	-3.262510000	2.815565000	0.985342000
C	-2.677095000	-2.095755000	-0.424905000	C	-4.483089000	2.855651000	1.707859000
N	1.844302000	0.651418000	-1.218394000	H	-4.830973000	1.964284000	2.220422000
C	-3.739005000	-3.031971000	-0.382909000	C	-5.213849000	4.021321000	1.753256000
C	2.347143000	-0.061559000	-2.281284000	H	-6.146656000	4.057970000	2.304138000
C	-4.009106000	-3.652758000	0.857414000	C	-4.757184000	5.183676000	1.082337000
H	-4.813881000	-4.376631000	0.929964000	H	-5.349413000	6.090513000	1.131400000
C	-3.246560000	-3.331302000	1.966494000	C	-3.575501000	5.172074000	0.372275000
H	-3.434286000	-3.795498000	2.926885000	H	-3.229865000	6.063173000	-0.140784000
C	-2.216117000	-2.384271000	1.837680000	C	2.612807000	1.591196000	-0.670835000
H	-1.599048000	-2.107836000	2.685396000	H	2.199170000	2.135748000	0.174065000
C	-4.487257000	-3.297286000	-1.576364000	C	3.597929000	0.162838000	-2.801198000
H	-5.298216000	-4.016260000	-1.534009000	H	3.950924000	-0.420760000	-3.644681000
C	-4.193699000	-2.651646000	-2.740982000	C	4.431374000	1.164157000	-2.238263000
H	-4.769929000	-2.846810000	-3.638839000	C	3.915067000	1.904220000	-1.127862000
C	1.006630000	-2.946902000	-0.697305000	C	4.707715000	2.916996000	-0.529717000
H	0.294376000	-2.897162000	-1.510716000	H	4.310681000	3.478855000	0.310300000
C	1.890710000	-4.028022000	-0.565637000	C	5.966724000	3.182757000	-1.019127000
H	1.864195000	-4.827071000	-1.296114000	H	6.575193000	3.957867000	-0.567270000
C	2.783724000	-4.062446000	0.492620000	C	6.479132000	2.449967000	-2.119035000
H	3.474205000	-4.890840000	0.607903000	H	7.472393000	2.676783000	-2.490038000
C	2.786371000	-3.008810000	1.431672000	C	5.730696000	1.460293000	-2.719007000
C	1.866932000	-1.955927000	1.228624000	H	6.125319000	0.903009000	-3.562082000
C	1.803277000	-0.872820000	2.143766000	H	1.694560000	-0.820714000	-2.694758000
C	2.658228000	-0.837671000	3.267483000	H	0.055161000	2.605519000	-0.962447000
C	2.531448000	0.257809000	4.147994000				

cis-$[Ru(phen)_2(Isoq)_2]^{2+}$: ^{3}TS

E(UPBE1PBE) = -2038.89739882 A.U.

Ru	-0.014683000	-0.389017000	-0.076412000	H	3.139079000	-0.898566000	4.961394000
N	-1.029668000	-0.408492000	-1.941563000	C	1.658555000	0.282090000	3.937219000
C	-0.680950000	0.223318000	-3.073084000	H	1.539670000	1.005146000	4.734574000
H	0.274528000	0.732223000	-3.071416000	C	0.898776000	0.420808000	2.768965000
N	-1.570653000	-1.831220000	0.246238000	H	0.194062000	1.234326000	2.654599000
C	-1.510603000	0.248793000	-4.202809000	C	3.545224000	-2.839299000	3.041340000
H	-1.181112000	0.774994000	-5.089954000	H	4.150557000	-2.997641000	3.927082000
N	1.191155000	-2.112305000	-0.339319000	C	3.600720000	-3.720059000	2.000441000
C	-2.750478000	-0.371838000	-4.160020000	H	4.248248000	-4.588599000	2.050096000
H	-3.416207000	-0.337400000	-5.015679000	C	-2.106870000	1.263151000	1.327530000
N	1.003532000	-0.436203000	1.737961000	H	-2.133908000	0.363655000	1.935198000
C	-3.147853000	-1.045816000	-2.988665000	C	-1.983923000	3.495942000	-0.274342000
N	-1.200734000	1.307304000	0.342819000	H	-1.904460000	4.358543000	-0.926581000
C	-2.237035000	-1.067339000	-1.903599000	C	-2.953708000	3.479651000	0.761017000
C	-1.147302000	2.425920000	-0.461421000	C	-3.013864000	2.311416000	1.586305000
C	-2.561535000	-1.751305000	-0.708014000	C	-3.968029000	2.238410000	2.634699000
N	1.838188000	0.749372000	-0.921317000	H	-4.012981000	1.350117000	3.257044000
C	-3.835338000	-2.337604000	-0.539872000	C	-4.827722000	3.291213000	2.851235000
C	2.619289000	0.252313000	-1.939690000	H	-5.558751000	3.241777000	3.650009000
C	-4.108719000	-2.965456000	0.695589000	C	-4.768051000	4.448737000	2.034736000
H	-5.074713000	-3.425591000	0.868941000	H	-5.455218000	5.265780000	2.223742000
C	-3.115045000	-3.003445000	1.673079000	C	-3.851253000	4.545362000	1.009168000
H	-3.292265000	-3.504402000	2.617462000	H	-3.809741000	5.432589000	0.386495000
C	-1.858720000	-2.453048000	1.419592000	C	2.216327000	1.876922000	-0.319175000
H	-1.046401000	-2.542083000	2.131238000	H	1.586472000	2.241108000	0.486723000
C	-4.759406000	-2.279218000	-1.637254000	C	3.763432000	0.881924000	-2.361570000
H	-5.737036000	-2.732525000	-1.513802000	H	4.348543000	0.456428000	-3.169629000
C	-4.422243000	-1.680408000	-2.818313000	C	4.184776000	2.088084000	-1.743767000
H	-5.125744000	-1.660464000	-3.643520000	C	3.375871000	2.599659000	-0.679633000
C	1.176983000	-2.980981000	-1.361369000	C	3.751091000	3.801673000	-0.026515000
H	0.518782000	-2.746147000	-2.188540000	H	3.134666000	4.187361000	0.779645000
C	1.971639000	-4.134704000	-1.362823000	C	4.889450000	4.468574000	-0.419273000
H	1.938794000	-4.802105000	-2.214942000	H	5.180640000	5.388083000	0.075408000
C	2.795067000	-4.404004000	-0.279196000	C	5.691701000	3.962297000	-1.472652000
H	3.422268000	-5.288764000	-0.268390000	H	6.584108000	4.503740000	-1.765902000
C	2.805661000	-3.523178000	0.821895000	C	5.350498000	2.796342000	-2.124305000
C	1.972673000	-2.382192000	0.750942000	H	5.966981000	2.412524000	-2.930160000
C	1.892411000	-1.480509000	1.845218000	H	2.284004000	-0.673278000	-2.387678000
C	2.678050000	-1.695586000	3.001585000	H	-0.406352000	2.409698000	-1.247781000
C	2.548255000	-0.773772000	4.060589000				

***cis*-[Ru(phen)$_2$(Isoq)Cl]$^{1+}$: $^1S_0$**

E(RPBE1PBE) = -2097.92118423 A.U.

Ru	-0.433434000	-0.013359000	-0.473786000	H	-6.170078000	1.465202000	-0.117089000
N	0.418631000	1.754499000	-1.108419000	C	-4.651803000	-0.060836000	0.127981000
C	0.567317000	2.194906000	-2.368027000	C	-3.263830000	-0.296636000	0.037866000
H	0.138150000	1.564976000	-3.139008000	C	-2.732826000	-1.585893000	0.308757000
N	0.047389000	0.816679000	1.330227000	C	-3.588697000	-2.652366000	0.655405000
C	1.232311000	3.399367000	-2.652225000	C	-2.998508000	-3.915413000	0.873381000
H	1.329899000	3.711968000	-3.684649000	H	-3.619097000	-4.764968000	1.136544000
N	-2.367171000	0.671102000	-0.328168000	C	-1.629108000	-4.052820000	0.728475000
C	1.750517000	4.170705000	-1.625440000	H	-1.148826000	-5.013406000	0.868357000
H	2.263525000	5.103264000	-1.834120000	C	-0.843811000	-2.942558000	0.382968000
N	-1.373750000	-1.725623000	0.191894000	H	0.224320000	-3.031046000	0.241014000
C	1.598607000	3.733589000	-0.291417000	C	-4.997407000	-2.393990000	0.749855000
N	1.491613000	-0.878418000	-0.637011000	H	-5.655899000	-3.213243000	1.017891000
C	0.927961000	2.510597000	-0.084008000	C	-5.506361000	-1.152299000	0.499633000
C	2.055329000	-1.074567000	-1.881686000	H	-6.573952000	-0.972743000	0.567449000
C	0.714053000	2.015588000	1.229406000	C	2.207800000	-1.209295000	0.441528000
C	1.147352000	2.754174000	2.351463000	H	1.744835000	-1.043774000	1.407028000
C	0.853931000	2.230998000	3.628921000	C	3.316842000	-1.590038000	-2.038912000
H	1.167136000	2.765078000	4.519169000	H	3.712956000	-1.731064000	-3.038459000
C	0.154116000	1.038635000	3.723330000	C	4.097541000	-1.948045000	-0.911529000
H	-0.098267000	0.618943000	4.689626000	C	3.511483000	-1.748390000	0.375750000
C	-0.234370000	0.354533000	2.562761000	C	4.244529000	-2.091607000	1.541991000
H	-0.774518000	-0.582344000	2.610586000	H	3.794773000	-1.936208000	2.518145000
C	1.844500000	3.988630000	2.123522000	C	5.512314000	-2.614109000	1.428014000
H	2.191157000	4.551671000	2.983452000	H	6.075300000	-2.877514000	2.316427000
C	2.064520000	4.455136000	0.858779000	C	6.094518000	-2.813348000	0.150671000
H	2.589481000	5.391832000	0.704260000	H	7.094578000	-3.227227000	0.082478000
C	-2.830535000	1.894563000	-0.615130000	C	5.404918000	-2.488388000	-0.996855000
H	-2.098958000	2.628849000	-0.923221000	H	5.851015000	-2.642145000	-1.973929000
C	-4.195700000	2.209905000	-0.539865000	H	1.417123000	-0.829771000	-2.718861000
H	-4.518611000	3.214275000	-0.784332000	Cl	-1.040191000	-0.729006000	-2.727803000
C	-5.110616000	1.239713000	-0.170225000				

***cis*-[Ru(phen)$_2$(Isoq)Cl]$^{1+}$: ^{3}MLCT**

E(UPBE1PBE) = -2097.86269702 A.U.

Ru	-0.444864000	-0.044294000	-0.563444000	H	-6.048445000	1.792382000	0.092445000
N	0.522207000	1.695778000	-1.164728000	C	-4.636160000	0.154770000	0.209841000
C	0.764791000	2.133056000	-2.408457000	C	-3.274870000	-0.171744000	0.038803000
H	0.339486000	1.544596000	-3.212690000	C	-2.817775000	-1.498115000	0.256147000
N	-0.025891000	0.751262000	1.253032000	C	-3.725717000	-2.514461000	0.621763000
C	1.517283000	3.289544000	-2.654395000	C	-3.204573000	-3.814833000	0.792428000
H	1.681348000	3.603205000	-3.677306000	H	-3.865258000	-4.629450000	1.068379000
N	-2.342433000	0.747882000	-0.347779000	C	-1.852436000	-4.036758000	0.594018000
C	2.041730000	4.017613000	-1.586179000	H	-1.429228000	-5.027138000	0.705334000
H	2.626782000	4.913696000	-1.766045000	C	-1.011880000	-2.971005000	0.236594000
N	-1.478766000	-1.725942000	0.082719000	H	0.045603000	-3.117212000	0.062595000
C	1.806642000	3.592961000	-0.271822000	C	-5.108351000	-2.167322000	0.789464000
N	1.476498000	-0.928478000	-0.646425000	H	-5.806672000	-2.947514000	1.072068000
C	1.031199000	2.409077000	-0.087949000	C	-5.543881000	-0.887532000	0.596766000
C	2.057688000	-1.204193000	-1.866803000	H	-6.591690000	-0.639426000	0.726161000
C	0.738106000	1.918583000	1.185030000	C	2.167225000	-1.176231000	0.470545000
C	1.181556000	2.597910000	2.347409000	H	1.686949000	-0.929572000	1.409672000
C	0.810460000	2.080948000	3.600825000	C	3.320117000	-1.730176000	-1.963848000
H	1.129730000	2.572816000	4.511847000	H	3.737126000	-1.933858000	-2.943668000
C	-0.017025000	0.926464000	3.653689000	C	4.078348000	-2.008114000	-0.798829000
H	-0.341877000	0.534487000	4.610203000	C	3.471157000	-1.715900000	0.461032000
C	-0.425798000	0.303763000	2.499679000	C	4.183856000	-1.968484000	1.662376000
H	-1.064449000	-0.570647000	2.510358000	H	3.718308000	-1.737474000	2.615471000
C	1.972219000	3.783704000	2.153143000	C	5.453547000	-2.495836000	1.607511000
H	2.327818000	4.308544000	3.033824000	H	6.003189000	-2.689214000	2.521714000
C	2.273060000	4.258805000	0.904327000	C	6.055937000	-2.788866000	0.357996000
H	2.868663000	5.158798000	0.791000000	H	7.057711000	-3.203650000	0.337216000
C	-2.717659000	2.013030000	-0.565699000	C	5.386422000	-2.551202000	-0.822770000
H	-1.944020000	2.701804000	-0.876697000	H	5.850483000	-2.774300000	-1.777696000
C	-4.052022000	2.416546000	-0.407908000	H	1.447111000	-0.996212000	-2.733544000
H	-4.316626000	3.449083000	-0.597266000	Cl	-1.062701000	-0.668407000	-2.788795000
C	-5.012098000	1.494765000	-0.024739000				

***cis*-[Ru(phen)$_2$(Isoq)Cl]$^{1+}$: ^{3}MC**

E(UPBE1PBE) = -2097.84840801 A.U.

Ru	-0.528795000	-0.007416000	-0.521704000	H	-6.541838000	1.524877000	-0.116264000
N	0.598206000	1.543075000	-1.287607000	C	-4.983910000	0.050468000	0.169071000
C	0.874293000	1.785840000	-2.582273000	C	-3.583167000	-0.143585000	0.111747000
H	0.435113000	1.097548000	-3.294198000	C	-3.025564000	-1.433250000	0.385043000
N	0.013515000	1.006988000	1.239120000	C	-3.880469000	-2.502501000	0.743181000
C	1.676298000	2.866399000	-2.975793000	C	-3.294607000	-3.759466000	1.001682000
H	1.868564000	3.016480000	-4.031015000	H	-3.923778000	-4.599662000	1.275140000
N	-2.724636000	0.861226000	-0.201837000	C	-1.924697000	-3.903234000	0.889471000
C	2.209631000	3.725393000	-2.028014000	H	-1.444568000	-4.856742000	1.070999000
H	2.829325000	4.565162000	-2.323011000	C	-1.141502000	-2.802495000	0.515825000
N	-1.670021000	-1.593995000	0.272207000	H	-0.069913000	-2.880833000	0.392295000
C	1.934614000	3.497407000	-0.663975000	C	-5.295272000	-2.273699000	0.811404000
N	1.638409000	-1.324503000	-0.305500000	H	-5.937607000	-3.104825000	1.082388000
C	1.124810000	2.387167000	-0.340275000	C	-5.827513000	-1.050756000	0.529574000
C	2.023752000	-1.984605000	-1.450547000	H	-6.899996000	-0.892813000	0.570816000
C	0.804485000	2.103540000	1.011368000	C	2.529758000	-1.157351000	0.666626000
C	1.279236000	2.932595000	2.053092000	H	2.192174000	-0.636143000	1.558064000
C	0.905137000	2.595599000	3.370190000	C	3.294089000	-2.478835000	-1.618165000
H	1.246842000	3.204086000	4.200638000	H	3.556762000	-2.997864000	-2.533710000
C	0.097804000	1.489069000	3.588718000	C	4.264543000	-2.313850000	-0.595891000
H	-0.206310000	1.212962000	4.590860000	C	3.864202000	-1.624515000	0.590740000
C	-0.333592000	0.714630000	2.503134000	C	4.797542000	-1.437157000	1.642360000
H	-0.966826000	-0.152555000	2.638709000	H	4.485378000	-0.914781000	2.541858000
C	2.103740000	4.055588000	1.707650000	C	6.081501000	-1.917262000	1.518469000
H	2.472707000	4.692276000	2.504592000	H	6.796636000	-1.777162000	2.321441000
C	2.418701000	4.323330000	0.406367000	C	6.480442000	-2.600438000	0.342331000
H	3.042301000	5.175526000	0.157901000	H	7.496154000	-2.972439000	0.263582000
C	-3.209304000	2.069513000	-0.490588000	C	5.594277000	-2.796148000	-0.694091000
H	-2.483157000	2.833982000	-0.741611000	H	5.901121000	-3.320421000	-1.593305000
C	-4.587238000	2.346407000	-0.475757000	H	1.256637000	-2.081183000	-2.209330000
H	-4.939141000	3.340509000	-0.722852000	Cl	-1.098835000	-0.894874000	-2.686826000
C	-5.473304000	1.338474000	-0.140611000				

***cis*-[Ru(phen)$_2$(Isoq)Cl]$^{1+}$: ^{3}TS**

E(UPBE1PBE) = -2097.84598412 A.U.

Ru	-0.463895000	-0.110881000	-0.491883000	H	-6.302344000	1.503672000	-0.316642000
N	0.571455000	1.487241000	-1.283799000	C	-4.798011000	-0.000208000	0.087948000
C	0.843657000	1.698531000	-2.584051000	C	-3.404187000	-0.231533000	0.092616000
H	0.488953000	0.937957000	-3.268922000	C	-2.889903000	-1.518146000	0.421906000
N	0.078445000	0.975262000	1.293431000	C	-3.770733000	-2.557654000	0.797679000
C	1.526877000	2.841665000	-3.020430000	C	-3.207029000	-3.811904000	1.111428000
H	1.727301000	2.959135000	-4.078128000	H	-3.850707000	-4.634734000	1.403001000
N	-2.498253000	0.741142000	-0.215415000	C	-1.836185000	-3.977845000	1.026836000
C	1.923878000	3.807789000	-2.108514000	H	-1.374615000	-4.931512000	1.250663000
H	2.438744000	4.704464000	-2.436073000	C	-1.027376000	-2.906152000	0.621974000
N	-1.534537000	-1.700534000	0.327145000	H	0.043254000	-3.013249000	0.514121000
C	1.643797000	3.618761000	-0.740944000	C	-5.180926000	-2.293700000	0.814290000
N	1.627393000	-1.242603000	-0.325591000	H	-5.852257000	-3.097481000	1.096929000
C	0.981400000	2.426529000	-0.365451000	C	-5.675238000	-1.071314000	0.462944000
C	1.969709000	-2.081211000	-1.364085000	H	-6.744924000	-0.891172000	0.458698000
C	0.674959000	2.175618000	0.997327000	C	2.545154000	-0.949104000	0.591778000
C	0.971198000	3.141492000	1.989177000	H	2.236903000	-0.287087000	1.394069000
C	0.597321000	2.847444000	3.315395000	C	3.223977000	-2.627416000	-1.476414000
H	0.809678000	3.558989000	4.105960000	H	3.452600000	-3.286341000	-2.307025000
C	-0.045942000	1.646772000	3.595397000	C	4.221800000	-2.334005000	-0.511059000
H	-0.343682000	1.400088000	4.607161000	C	3.864497000	-1.459400000	0.561700000
C	-0.290501000	0.733686000	2.565068000	C	4.825106000	-1.137226000	1.554715000
H	-0.771546000	-0.218566000	2.750612000	H	4.546174000	-0.473059000	2.367261000
C	1.635589000	4.349438000	1.588372000	C	6.093919000	-1.665789000	1.482675000
H	1.870283000	5.087423000	2.348067000	H	6.830191000	-1.422590000	2.240601000
C	1.968955000	4.570514000	0.283391000	C	6.450004000	-2.532191000	0.418933000
H	2.476605000	5.484702000	-0.005618000	H	7.454748000	-2.938566000	0.379666000
C	-2.941951000	1.953296000	-0.571374000	C	5.536647000	-2.861191000	-0.558760000
H	-2.188014000	2.694433000	-0.807894000	H	5.811134000	-3.524966000	-1.372102000
C	-4.310224000	2.256551000	-0.627581000	H	1.185009000	-2.269550000	-2.086265000
H	-4.624903000	3.250177000	-0.922216000	Cl	-1.052939000	-1.033329000	-2.659855000
C	-5.240031000	1.286179000	-0.290541000				

***cis*-[Ru(phen)$_2$(phthz)$_2$]$^{2+}$: $^1S_0$**

E(RPBE1PBE) = -2070.95486607 A.U.

Ru	-0.001280000	-0.346655000	0.048384000	C	-2.544922000	-0.927006000	-4.078265000
N	1.074472000	-0.451245000	1.830079000	H	-3.133846000	-1.099133000	-4.972506000
C	0.848139000	0.207393000	2.974440000	C	-1.638082000	0.117104000	-4.016445000
H	-0.029285000	0.834980000	2.999488000	H	-1.499248000	0.783011000	-4.859369000
N	1.524063000	-1.651124000	-0.502901000	C	-0.886536000	0.322942000	-2.849229000
C	1.690038000	0.069979000	4.091289000	H	-0.172511000	1.133930000	-2.780021000
H	1.459376000	0.621830000	4.994075000	C	-3.615891000	-2.877182000	-2.908468000
N	-1.225679000	-1.975949000	0.405104000	H	-4.223451000	-3.085819000	-3.782217000
C	2.790928000	-0.764394000	4.031887000	C	-3.726664000	-3.650829000	-1.788697000
H	3.444166000	-0.887085000	4.888936000	H	-4.424380000	-4.480816000	-1.763291000
N	-1.005828000	-0.466623000	-1.769234000	C	2.116992000	1.347065000	-1.324560000
C	3.061940000	-1.462371000	2.833691000	H	2.200609000	0.466966000	-1.951397000
N	1.184422000	1.305106000	-0.376153000	C	1.798051000	3.427376000	0.348728000
C	2.178486000	-1.262387000	1.751421000	H	1.613260000	4.224821000	1.060111000
N	1.015491000	2.371106000	0.488308000	C	2.814617000	3.558054000	-0.633474000
C	2.407181000	-1.920073000	0.511289000	C	2.978922000	2.454011000	-1.516968000
N	-1.531492000	0.850185000	0.759175000	C	3.972513000	2.501937000	-2.521607000
C	3.497051000	-2.806386000	0.362438000	H	4.103180000	1.660974000	-3.194860000
N	-2.086554000	0.437556000	1.952484000	C	4.770031000	3.623572000	-2.631820000
C	3.651514000	-3.445320000	-0.887250000	H	5.535256000	3.669871000	-3.398323000
H	4.472359000	-4.136734000	-1.043142000	C	4.604462000	4.721235000	-1.753444000
C	2.744331000	-3.182165000	-1.898910000	H	5.244955000	5.588945000	-1.862458000
H	2.832841000	-3.664334000	-2.864672000	C	3.640516000	4.694371000	-0.764254000
C	1.692976000	-2.279541000	-1.677312000	H	3.513281000	5.533682000	-0.088785000
H	0.971009000	-2.058877000	-2.452767000	C	-2.002498000	1.917642000	0.128000000
C	4.377298000	-3.005629000	1.477630000	H	-1.506201000	2.186981000	-0.795017000
H	5.215466000	-3.684000000	1.361987000	C	-3.106690000	1.118339000	2.445577000
C	4.171349000	-2.355920000	2.660631000	H	-3.494901000	0.740221000	3.384943000
H	4.846001000	-2.510199000	3.495713000	C	-3.683050000	2.262079000	1.833736000
C	-1.326289000	-2.691463000	1.531706000	C	-3.090821000	2.684547000	0.610898000
H	-0.704203000	-2.379905000	2.358614000	C	-3.601330000	3.819809000	-0.058776000
C	-2.205338000	-3.781237000	1.643233000	H	-3.152330000	4.144873000	-0.991630000
H	-2.246578000	-4.332605000	2.574320000	C	-4.669966000	4.504026000	0.485393000
C	-3.006896000	-4.135616000	0.572769000	H	-5.068421000	5.376028000	-0.020696000
H	-3.690376000	-4.974599000	0.644168000	C	-5.257847000	4.082338000	1.701830000
C	-2.933123000	-3.386525000	-0.622463000	H	-6.096035000	4.637925000	2.106580000
C	-2.022460000	-2.309456000	-0.656873000	C	-4.774445000	2.975747000	2.372450000
C	-1.908245000	-1.501022000	-1.820911000	H	-5.223233000	2.650784000	3.305154000
C	-2.701697000	-1.772042000	-2.957618000				

cis-$[Ru(phen)_2(phthz)_2]^{2+}$: ^{3}MLCT

E(UPBE1PBE) = -2070.87862800 A.U.

Ru	0.005813000	-0.238512000	-0.031247000	C	-2.907195000	-0.966199000	-3.912390000
N	1.151898000	-0.370997000	1.680117000	H	-3.559638000	-1.185658000	-4.750600000
C	1.053554000	0.321405000	2.839195000	C	-2.077674000	0.140133000	-3.931545000
H	0.266525000	1.060292000	2.892546000	H	-2.062629000	0.809225000	-4.782893000
N	1.412806000	-1.558687000	-0.682305000	C	-1.235327000	0.405376000	-2.838560000
C	1.888851000	0.076810000	3.921703000	H	-0.583771000	1.269172000	-2.813089000
H	1.761363000	0.652669000	4.829265000	C	-3.722444000	-2.986152000	-2.659004000
N	-1.114336000	-1.917654000	0.427124000	H	-4.389316000	-3.240749000	-3.475296000
C	2.880629000	-0.919373000	3.836885000	C	-3.670347000	-3.767549000	-1.539664000
H	3.526310000	-1.122758000	4.684182000	H	-4.295156000	-4.649963000	-1.456922000
N	-1.201412000	-0.390093000	-1.760660000	C	2.518694000	1.394577000	-0.387377000
C	3.034095000	-1.638356000	2.653053000	H	2.926946000	0.535915000	0.130073000
N	1.212195000	1.375669000	-0.631923000	C	1.339899000	3.448123000	-1.673994000
C	2.158238000	-1.334127000	1.565458000	H	0.800004000	4.233525000	-2.191473000
N	0.605577000	2.415723000	-1.299205000	C	2.737244000	3.560967000	-1.447070000
C	2.286043000	-1.965526000	0.331355000	C	3.354383000	2.467681000	-0.774108000
N	-1.500710000	0.989062000	0.799626000	C	4.743601000	2.490796000	-0.517757000
C	3.273838000	-2.968542000	0.115458000	H	5.213331000	1.657721000	-0.005813000
N	-1.977185000	0.481610000	1.990678000	C	5.486237000	3.581854000	-0.925601000
C	3.350843000	-3.556710000	-1.146741000	H	6.552829000	3.612415000	-0.735226000
H	4.089584000	-4.323601000	-1.348804000	C	4.871535000	4.667620000	-1.592724000
C	2.453174000	-3.141304000	-2.162937000	H	5.478272000	5.511239000	-1.901609000
H	2.504022000	-3.583194000	-3.150091000	C	3.513082000	4.664115000	-1.854147000
C	1.513001000	-2.168410000	-1.906690000	H	3.044432000	5.497169000	-2.366895000
H	0.822206000	-1.833474000	-2.669386000	C	-2.038656000	2.065784000	0.240892000
C	4.130804000	-3.295572000	1.227987000	H	-1.567766000	2.404780000	-0.674685000
H	4.882711000	-4.064338000	1.084253000	C	-3.003482000	1.085183000	2.562594000
C	4.020235000	-2.661658000	2.431376000	H	-3.332515000	0.638617000	3.494194000
H	4.685383000	-2.921201000	3.248324000	C	-3.653500000	2.235506000	2.039447000
C	-1.037298000	-2.640312000	1.551785000	C	-3.134253000	2.753287000	0.819075000
H	-0.357467000	-2.285922000	2.312990000	C	-3.719393000	3.901261000	0.239313000
C	-1.818733000	-3.791906000	1.732715000	H	-3.325786000	4.298232000	-0.690451000
H	-1.726294000	-4.351496000	2.654883000	C	-4.791961000	4.504942000	0.866174000
C	-2.692084000	-4.198201000	0.738897000	H	-5.248641000	5.385828000	0.429572000
H	-3.298584000	-5.088415000	0.865722000	C	-5.307450000	3.988174000	2.078147000
C	-2.794157000	-3.443039000	-0.451890000	H	-6.149576000	4.481745000	2.549649000
C	-1.976900000	-2.298659000	-0.561936000	C	-4.748705000	2.867172000	2.663185000
C	-2.026048000	-1.486186000	-1.726827000	H	-5.142117000	2.471597000	3.593497000
C	-2.901089000	-1.817527000	-2.784602000				

***cis*-[Ru(phen)$_2$(phthz)$_2$]$^{2+}$: ^{3}MC**

E(UPBE1PBE) = -2070.87531567 A.U.

Ru	-0.120754000	-0.196431000	0.235629000	C	2.517040000	-0.841168000	4.305060000
N	-1.277994000	-0.277093000	-1.586429000	H	3.110117000	-1.033962000	5.192510000
C	-1.043531000	0.562280000	-2.606207000	C	1.672941000	0.254921000	4.242284000
H	-0.264689000	1.294042000	-2.448584000	H	1.589805000	0.940269000	5.076571000
N	-1.865250000	-1.871182000	0.544763000	C	0.915534000	0.489758000	3.085724000
C	-1.743929000	0.486302000	-3.819342000	H	0.270368000	1.352542000	2.995501000
H	-1.510429000	1.187178000	-4.610950000	C	3.462345000	-2.862339000	3.148591000
N	1.055877000	-1.884311000	-0.131769000	H	4.071866000	-3.091814000	4.015738000
C	-2.709345000	-0.487612000	-3.988434000	C	3.516253000	-3.652666000	2.036498000
H	-3.254322000	-0.576089000	-4.922159000	H	4.170229000	-4.517444000	2.009503000
N	0.970753000	-0.326195000	2.019911000	C	-2.562130000	1.561244000	0.661139000
C	-2.992632000	-1.374764000	-2.926703000	H	-3.073249000	0.646964000	0.385534000
N	-1.236784000	1.494425000	0.723816000	C	-1.117615000	3.732261000	1.338713000
C	-2.257961000	-1.226657000	-1.725063000	H	-0.474189000	4.562161000	1.609708000
N	-0.488156000	2.597252000	1.086542000	C	-2.526562000	3.900064000	1.284217000
C	-2.552451000	-2.078813000	-0.609905000	C	-3.286255000	2.746472000	0.937490000
N	1.649166000	0.928732000	-1.043699000	C	-4.695531000	2.826931000	0.877214000
C	-3.545306000	-3.082372000	-0.727839000	H	-5.277068000	1.949232000	0.615310000
N	2.111380000	0.239196000	-2.147557000	C	-5.317231000	4.028777000	1.153776000
C	-3.793098000	-3.887151000	0.407213000	H	-6.397958000	4.101243000	1.110123000
H	-4.543306000	-4.669136000	0.355838000	C	-4.561125000	5.174811000	1.496204000
C	-3.080331000	-3.667981000	1.572399000	H	-5.075040000	6.105310000	1.708494000
H	-3.254790000	-4.270310000	2.455472000	C	-3.181991000	5.117298000	1.563047000
C	-2.118851000	-2.642576000	1.604452000	H	-2.601591000	5.994841000	1.827358000
H	-1.545151000	-2.439912000	2.501880000	C	2.330997000	1.950212000	-0.546306000
C	-4.251606000	-3.228375000	-1.966241000	H	1.872640000	2.440662000	0.306996000
H	-5.005849000	-4.003586000	-2.047853000	C	3.254479000	0.616017000	-2.695682000
C	-3.988837000	-2.402942000	-3.019506000	H	3.562298000	0.041047000	-3.562355000
H	-4.533276000	-2.509763000	-3.951524000	C	4.055060000	1.691896000	-2.223644000
C	1.105748000	-2.613807000	-1.254203000	C	3.564416000	2.397307000	-1.088911000
H	0.486313000	-2.283487000	-2.075237000	C	4.301021000	3.483313000	-0.565569000
C	1.934641000	-3.740668000	-1.369897000	H	3.926557000	4.022083000	0.298659000
H	1.937406000	-4.300744000	-2.296661000	C	5.492048000	3.846012000	-1.162696000
C	2.735966000	-4.122176000	-0.307988000	H	6.064691000	4.678101000	-0.768926000
H	3.378439000	-4.992849000	-0.382236000	C	5.979520000	3.143670000	-2.290342000
C	2.717850000	-3.360414000	0.880574000	H	6.916697000	3.449758000	-2.741217000
C	1.859341000	-2.240220000	0.918680000	C	5.274649000	2.079832000	-2.818910000
C	1.809497000	-1.413249000	2.070211000	H	5.646368000	1.541938000	-3.684706000
C	2.608199000	-1.710274000	3.196657000				

***cis*-[Ru(phen)$_2$(phthz)$_2$]$^{2+}$: ^{3}TS**

E(UPBE1PBE) = -2070.86827647 A.U.

Ru	0.055030000	-0.192712000	-0.052519000	C	-2.752946000	-1.749381000	-2.910492000
N	1.300046000	-0.332982000	1.634530000	C	-2.805813000	-0.816386000	-3.968221000
C	1.158586000	0.364188000	2.772418000	H	-3.447528000	-1.002972000	-4.822463000
H	0.355527000	1.086877000	2.795089000	C	-2.038404000	0.333664000	-3.895798000
N	1.758639000	-1.485781000	-0.768955000	H	-2.062811000	1.068288000	-4.691134000
C	1.971111000	0.134356000	3.891572000	C	-1.216992000	0.562283000	-2.780927000
H	1.813347000	0.719186000	4.788896000	H	-0.629218000	1.465332000	-2.678211000
N	-0.942853000	-1.994848000	0.280058000	C	-3.523396000	-2.958964000	-2.867038000
C	2.937402000	-0.858622000	3.846756000	H	-4.180114000	-3.184675000	-3.700013000
H	3.550660000	-1.074113000	4.715237000	C	-3.444331000	-3.807540000	-1.799976000
N	-1.131247000	-0.316271000	-1.769423000	H	-4.039327000	-4.713851000	-1.774473000
C	3.118887000	-1.600053000	2.661623000	C	2.521027000	1.576581000	-0.554230000
N	1.198318000	1.526144000	-0.666810000	H	3.007605000	0.661239000	-0.243986000
C	2.299251000	-1.276970000	1.550835000	C	1.139340000	3.746436000	-1.351542000
N	0.485970000	2.627702000	-1.090217000	H	0.520998000	4.575600000	-1.677688000
C	2.469061000	-1.954833000	0.311560000	C	2.547367000	3.897043000	-1.241561000
N	-1.526931000	1.062914000	0.910741000	C	3.273917000	2.742993000	-0.830752000
C	3.366077000	-3.046351000	0.219108000	C	4.680843000	2.803679000	-0.714556000
N	-1.943681000	0.420354000	2.061089000	H	5.236334000	1.925057000	-0.403880000
C	3.451766000	-3.719736000	-1.018244000	C	5.332639000	3.987499000	-0.999508000
H	4.122905000	-4.563860000	-1.129732000	H	6.411707000	4.045347000	-0.913928000
C	2.677393000	-3.279399000	-2.086489000	C	4.609060000	5.133940000	-1.404808000
H	2.735900000	-3.771078000	-3.050139000	H	5.145941000	6.050255000	-1.622085000
C	1.856484000	-2.158578000	-1.937170000	C	3.232599000	5.095453000	-1.527273000
H	1.293748000	-1.757496000	-2.771619000	H	2.678327000	5.973725000	-1.840574000
C	4.153449000	-3.388373000	1.369486000	C	-2.239298000	2.049018000	0.379781000
H	4.843894000	-4.221521000	1.293382000	H	-1.805747000	2.512434000	-0.499032000
C	4.055944000	-2.677412000	2.531252000	C	-3.075838000	0.804344000	2.623556000
H	4.673957000	-2.932272000	3.385416000	H	-3.344549000	0.268553000	3.527323000
C	-0.864475000	-2.778724000	1.366324000	C	-3.910009000	1.840578000	2.121720000
H	-0.197028000	-2.456138000	2.152800000	C	-3.464171000	2.495088000	0.937911000
C	-1.616314000	-3.956489000	1.481761000	C	-4.235122000	3.542437000	0.385254000
H	-1.517692000	-4.560395000	2.375102000	H	-3.896196000	4.044846000	-0.514710000
C	-2.467328000	-4.337697000	0.457148000	C	-5.414286000	3.914994000	1.000247000
H	-3.047538000	-5.251088000	0.530350000	H	-6.011954000	4.717851000	0.583643000
C	-2.582282000	-3.521451000	-0.689150000	C	-5.856652000	3.262411000	2.174982000
C	-1.800010000	-2.347163000	-0.728583000	H	-6.785062000	3.575680000	2.638657000
C	-1.891087000	-1.458590000	-1.829954000	C	-5.117098000	2.237392000	2.733838000
				H	-5.453336000	1.737898000	3.636341000

***cis*-[Ru(phen)$_2$(phthz)Cl]$^{1+}$: $^1S_0$**

E(RPBE1PBE) = -2113.90703813 A.U.

Ru	-0.365720000	-0.075012000	-0.292267000	H	-0.656156000	1.343507000	4.707632000
N	-1.452325000	-1.634312000	0.515422000	C	0.354785000	2.825690000	3.521536000
C	-0.996338000	-2.744778000	1.112028000	H	0.546035000	3.501766000	4.347638000
H	0.067600000	-2.785037000	1.296867000	C	0.786973000	3.160967000	2.220476000
N	-2.283058000	0.584881000	-0.666461000	C	0.506873000	2.242905000	1.186599000
C	-1.850910000	-3.791673000	1.490593000	C	0.904911000	2.520489000	-0.148149000
H	-1.428650000	-4.669586000	1.963826000	C	1.579941000	3.717874000	-0.463587000
N	-0.154902000	1.058344000	1.394668000	C	1.926106000	3.929394000	-1.816462000
C	-3.210563000	-3.698609000	1.251623000	H	2.446162000	4.836240000	-2.105811000
H	-3.882578000	-4.502285000	1.532184000	C	1.590505000	2.971511000	-2.758397000
N	0.581391000	1.575459000	-1.088874000	H	1.839332000	3.109856000	-3.803524000
C	-3.720578000	-2.538722000	0.630831000	C	0.917536000	1.801029000	-2.369453000
Cl	-0.500610000	-1.235515000	-2.438805000	H	0.628102000	1.028242000	-3.073022000
C	-2.798630000	-1.531231000	0.277731000	C	1.863782000	4.637950000	0.600931000
C	-3.244397000	-0.337226000	-0.349574000	H	2.386802000	5.558347000	0.363994000
N	1.490185000	-0.921040000	0.055214000	C	1.484335000	4.370417000	1.885475000
C	-4.614835000	-0.139951000	-0.620844000	H	1.703479000	5.076259000	2.679598000
N	1.825568000	-1.156835000	1.375835000	C	2.340494000	-1.218390000	-0.922737000
C	-4.987253000	1.071558000	-1.240527000	H	1.970939000	-1.053345000	-1.927835000
H	-6.029495000	1.263385000	-1.470957000	C	3.017957000	-1.656274000	1.646799000
C	-4.008478000	1.998840000	-1.551743000	H	3.215906000	-1.815622000	2.701333000
H	-4.262453000	2.935791000	-2.031793000	C	3.996347000	-1.984863000	0.671104000
C	-2.664567000	1.725566000	-1.256069000	C	3.626126000	-1.762967000	-0.682696000
H	-1.880201000	2.425906000	-1.507908000	C	4.532255000	-2.086062000	-1.718918000
C	-5.538459000	-1.176878000	-0.258888000	H	4.244195000	-1.925258000	-2.752429000
H	-6.591170000	-1.029771000	-0.475132000	C	5.769105000	-2.608650000	-1.399425000
C	-5.109695000	-2.326507000	0.339011000	H	6.469361000	-2.861625000	-2.187563000
H	-5.817650000	-3.104522000	0.603929000	C	6.138360000	-2.823956000	-0.050263000
C	-0.549648000	0.764454000	2.641931000	H	7.115923000	-3.236120000	0.173384000
H	-1.051871000	-0.183345000	2.775646000	C	5.266467000	-2.518816000	0.976299000
C	-0.312513000	1.629097000	3.720950000	H	5.544491000	-2.687108000	2.011612000

cis-[Ru(phen)$_2$(phthz)Cl]$^{1+}$: ^{3}MLCT

E(UPBE1PBE) = -2113.84470328 A.U.

u	-0.387198000	-0.135911000	-0.364637000	H	-0.910988000	1.152588000	4.650276000
N	-1.632264000	-1.648490000	0.357684000	C	0.376099000	2.548019000	3.588003000
C	-1.282099000	-2.836657000	0.864191000	H	0.591358000	3.158911000	4.457631000
H	-0.224067000	-2.992778000	1.021391000	C	0.925961000	2.875742000	2.348519000
N	-2.246552000	0.723233000	-0.668473000	C	0.613734000	2.046779000	1.234448000
C	-2.238928000	-3.808123000	1.198363000	C	1.095834000	2.336306000	-0.040177000
H	-1.906732000	-4.756445000	1.601672000	C	1.919273000	3.476014000	-0.281928000
N	-0.216641000	0.935699000	1.362517000	C	2.322215000	3.728948000	-1.592577000
C	-3.585165000	-3.548991000	1.008482000	H	2.945740000	4.588765000	-1.812793000
H	-4.334522000	-4.291782000	1.259822000	C	1.899170000	2.870682000	-2.625323000
N	0.714969000	1.477670000	-1.068399000	H	2.181838000	3.059308000	-3.653304000
C	-3.981919000	-2.301593000	0.481971000	C	1.107504000	1.766503000	-2.331209000
Cl	-0.554216000	-1.148938000	-2.514522000	H	0.763804000	1.084304000	-3.100601000
C	-2.961523000	-1.379849000	0.164334000	C	2.253530000	4.293753000	0.853993000
C	-3.289140000	-0.107098000	-0.370570000	H	2.888043000	5.159668000	0.694526000
N	1.436478000	-1.053073000	-0.025203000	C	1.782817000	4.008291000	2.102069000
C	-4.635294000	0.262114000	-0.574634000	H	2.041585000	4.645397000	2.941653000
N	1.591205000	-1.609306000	1.222140000	C	2.416338000	-1.073781000	-0.921498000
C	-4.878746000	1.549919000	-1.097923000	H	2.189290000	-0.647637000	-1.889230000
H	-5.897946000	1.876192000	-1.274267000	C	2.764156000	-2.125993000	1.538287000
C	-3.810278000	2.384112000	-1.383925000	H	2.826738000	-2.538716000	2.538882000
H	-3.971347000	3.375501000	-1.788018000	C	3.883109000	-2.171035000	0.662854000
C	-2.498017000	1.942313000	-1.160720000	C	3.685665000	-1.633003000	-0.639415000
H	-1.639437000	2.560335000	-1.385885000	C	4.741905000	-1.662913000	-1.578357000
C	-5.660058000	-0.687274000	-0.246458000	H	4.589077000	-1.256030000	-2.572243000
H	-6.695425000	-0.408691000	-0.409611000	C	5.955690000	-2.211464000	-1.215081000
C	-5.345979000	-1.917410000	0.255956000	H	6.771630000	-2.238471000	-1.928404000
H	-6.129274000	-2.628197000	0.495846000	C	6.151685000	-2.743291000	0.080888000
C	-0.746225000	0.651592000	2.583762000	H	7.114624000	-3.168304000	0.340537000
H	-1.381854000	-0.222687000	2.638060000	C	5.130712000	-2.726991000	1.012299000
C	-0.472310000	1.420572000	3.697520000	H	5.277617000	-3.136506000	2.006207000

***cis*-[Ru(phen)$_2$(phthz)Cl]$^{1+}$: ^{3}MC**

E(UPBE1PBE) = -2113.83014258 A.U.

Ru	-0.443246000	-0.050651000	-0.341354000	H	-0.874985000	2.035898000	4.464990000
N	-1.653336000	-1.502448000	0.582644000	C	0.352615000	3.247854000	3.177781000
C	-1.142199000	-2.566337000	1.219924000	H	0.570852000	3.998059000	3.930335000
H	-0.066313000	-2.576088000	1.331772000	C	0.891039000	3.377919000	1.880960000
N	-2.682006000	0.689826000	-0.648158000	C	0.575939000	2.369023000	0.944932000
C	-1.944704000	-3.609490000	1.701843000	C	1.083289000	2.429050000	-0.378062000
H	-1.478463000	-4.446020000	2.207375000	C	1.903836000	3.504605000	-0.780708000
N	-0.224434000	1.302076000	1.249463000	C	2.363887000	3.507407000	-2.114089000
C	-3.312761000	-3.562028000	1.510874000	H	2.996542000	4.314758000	-2.466744000
H	-3.953615000	-4.364097000	1.860927000	C	1.994608000	2.472122000	-2.957828000
N	0.728127000	1.404273000	-1.221095000	H	2.329403000	2.449260000	-3.987647000
C	-3.879140000	-2.455787000	0.843541000	C	1.178308000	1.432986000	-2.488465000
Cl	-0.545635000	-1.427529000	-2.331020000	H	0.868055000	0.605950000	-3.115638000
C	-3.008882000	-1.432253000	0.398917000	C	2.215404000	4.522370000	0.183124000
C	-3.547212000	-0.288344000	-0.272780000	H	2.847362000	5.348460000	-0.125257000
N	1.663090000	-1.114559000	0.393550000	C	1.731669000	4.461796000	1.458427000
C	-4.937585000	-0.202577000	-0.522779000	H	1.975526000	5.238161000	2.175804000
N	2.354780000	-0.460219000	1.397103000	C	2.288182000	-1.958676000	-0.417411000
C	-5.403650000	0.938213000	-1.212481000	H	1.666125000	-2.407395000	-1.186400000
H	-6.462010000	1.036272000	-1.430154000	C	3.647075000	-0.701223000	1.535601000
C	-4.507416000	1.915671000	-1.605237000	H	4.131758000	-0.161911000	2.342423000
H	-4.840310000	2.797136000	-2.139421000	C	4.392910000	-1.592837000	0.716301000
C	-3.144907000	1.758377000	-1.297803000	C	3.672864000	-2.252044000	-0.317100000
H	-2.413401000	2.506342000	-1.580599000	C	4.342365000	-3.153476000	-1.175897000
C	-5.795235000	-1.259044000	-0.072482000	H	3.788785000	-3.653482000	-1.963917000
H	-6.859405000	-1.184917000	-0.269912000	C	5.691697000	-3.383621000	-0.998796000
C	-5.286209000	-2.336276000	0.589729000	H	6.213851000	-4.073873000	-1.651941000
H	-5.939260000	-3.132746000	0.930232000	C	6.408324000	-2.727108000	0.030063000
C	-0.723418000	1.202667000	2.488345000	H	7.467650000	-2.925879000	0.148752000
H	-1.347443000	0.341832000	2.688901000	C	5.773027000	-1.842305000	0.878779000
C	-0.451380000	2.159531000	3.476022000	H	6.320314000	-1.338691000	1.669029000

***cis*-[Ru(phen)$_2$(phthz)Cl]$^{1+}$: ^{3}TS**

E(UPBE1PBE) = -2113.82815427 A.U.

Ru	-0.346177000	-0.077757000	-0.224422000	H	-1.274236000	2.402865000	4.385648000
N	-1.516299000	-1.522096000	0.692375000	C	-0.007468000	3.567549000	3.092348000
C	-1.012686000	-2.511981000	1.446767000	H	0.140010000	4.374578000	3.802009000
H	0.050670000	-2.470182000	1.637895000	C	0.604059000	3.630819000	1.821995000
N	-2.538425000	0.529381000	-0.761622000	C	0.378219000	2.550641000	0.940087000
C	-1.808181000	-3.547266000	1.954121000	C	0.977386000	2.534792000	-0.348256000
H	-1.348186000	-4.321019000	2.556058000	C	1.774938000	3.619072000	-0.775911000
N	-0.416409000	1.486006000	1.264725000	C	2.326014000	3.551820000	-2.073182000
C	-3.160122000	-3.574544000	1.666336000	H	2.941805000	4.365235000	-2.441518000
H	-3.792812000	-4.375062000	2.034143000	C	2.066758000	2.442486000	-2.859770000
N	0.745168000	1.429562000	-1.130547000	H	2.467771000	2.365960000	-3.862969000
C	-3.719244000	-2.547419000	0.878133000	C	1.278347000	1.392997000	-2.363675000
Cl	-0.526379000	-1.408245000	-2.349957000	H	1.045684000	0.510352000	-2.947990000
C	-2.859980000	-1.523345000	0.414558000	C	1.983005000	4.713916000	0.128819000
C	-3.392075000	-0.454107000	-0.371600000	H	2.599366000	5.543958000	-0.199885000
N	1.614616000	-1.084625000	0.200807000	C	1.428687000	4.717178000	1.376479000
C	-4.763928000	-0.443025000	-0.717761000	H	1.602000000	5.547690000	2.052566000
N	2.141254000	-0.693311000	1.417609000	C	2.339498000	-1.768554000	-0.674445000
C	-5.222106000	0.625219000	-1.519085000	H	1.819829000	-2.039520000	-1.589077000
H	-6.265546000	0.663784000	-1.813738000	C	3.394043000	-1.010443000	1.691104000
C	-4.336162000	1.607230000	-1.923796000	H	3.749346000	-0.681094000	2.661434000
H	-4.662439000	2.432247000	-2.545071000	C	4.250359000	-1.731935000	0.813884000
C	-2.992877000	1.527721000	-1.518315000	C	3.689121000	-2.131348000	-0.430494000
H	-2.269196000	2.278109000	-1.813590000	C	4.473578000	-2.862767000	-1.351096000
C	-5.610716000	-1.499773000	-0.247828000	H	4.041147000	-3.169977000	-2.297556000
H	-6.660936000	-1.484373000	-0.519395000	C	5.779053000	-3.177604000	-1.030532000
C	-5.109074000	-2.505143000	0.523962000	H	6.387546000	-3.739519000	-1.730267000
H	-5.754147000	-3.301575000	0.879278000	C	6.337675000	-2.776709000	0.205953000
C	-0.983397000	1.449641000	2.478392000	H	7.365271000	-3.037030000	0.433750000
H	-1.606307000	0.591009000	2.694333000	C	5.587329000	-2.063511000	1.120501000
C	-0.793064000	2.473108000	3.417866000	H	6.012322000	-1.757665000	2.070992000