Impacts of Terminal Modification of $[Ru(phen)_2dppz]^{2+}$ on the Luminescence Properties: a Theoretical Study

Xing Gao, Shuo Shi*, Jun-Liang Yao, Juan Zhao, and Tian-Ming Yao*
[a]Department of Chemistry, Tongji University, Shanghai 200092, PR China[1]

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* Corresponding author. Tel.: +86-21-6598-3292; fax: +86-21-6598-2287.
E-mail address: shishuo@tongji.edu.cn (S. Shi) tmyao@tongji.edu.cn (T.M. Yao)

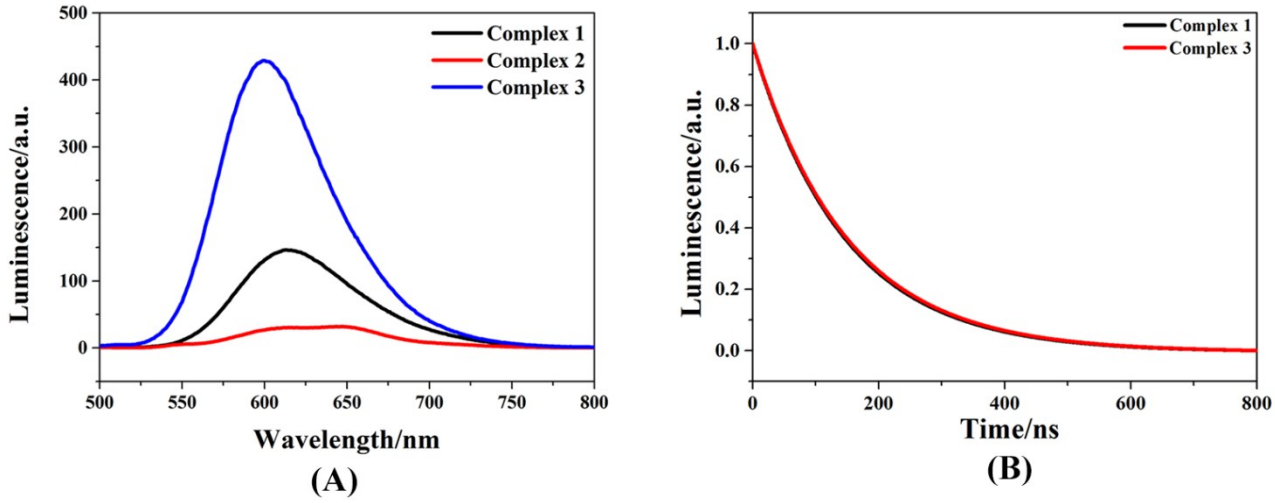

Figure S1 (A) Emission spectra (λ_{ex}=440 nm) of 5.0 μM $[Ru(phen)_2dppz]^{2+}$(**1**), $[Ru(phen)_2dppzi]^{2+}$(**2**), and $[Ru(phen)_2dppz\text{-}idzo]^{2+}$(**3**) in acetonitrile; (B) Luminescence decays for $[Ru(phen)_2dppz]^{2+}$ (**1**, black curve) and $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (**3**, red curve) in acetonitrile..

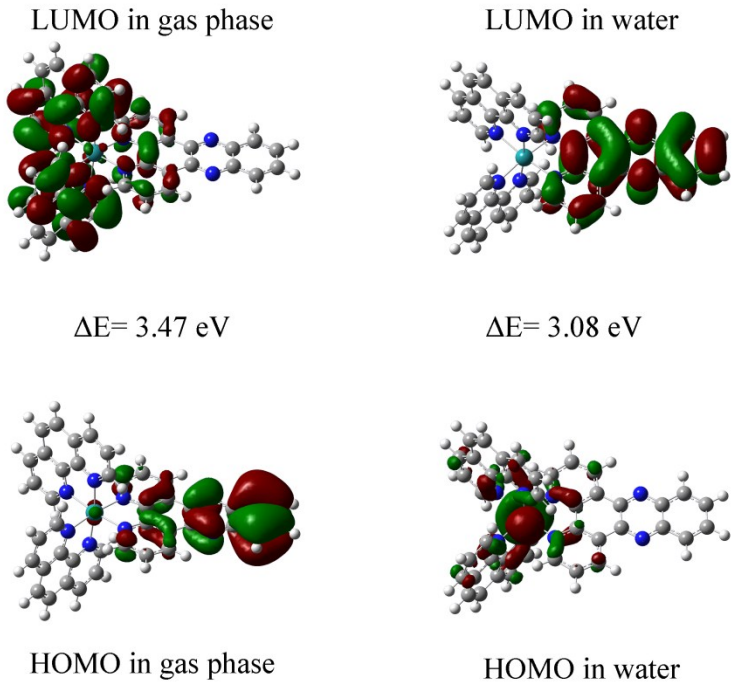

Figure S2 The composition and energy gap of HOMO and LUMO of complex 1 in both gas phase and water.

Table S1 Changes of the Mulliken charges distributions of different parts of the complexes.

	1 in gas phase	1 in aqueous solution	2 in gas phase	2 in aqueous solution	3 in gas phase	3 in aqueous solution
Coligand 1	0.20039	0.20475	0.19505	0.20247	0.19409	0.20129
Coligand 2	0.20038	0.20473	0.19433	0.20244	0.19409	0.20129
Ruthenium(II)	1.37801	1.41126	1.37765	1.40974	1.37744	1.40881
Main ligand	0.22122	0.17926	0.23296	0.18534	0.23438	0.18861

Sum of charges	2.00000	2.00000	1.99999	1.99999	2.00000	2.00000

Table S2 TD-DFT calculated energies, oscillator strengths (*f*), and natural transition orbital analysis results of the ten lowest-energy singlet and triplet excited states of $[Ru(phen)_2dppzi]^{2+}$(2) in gas phase.

Excited State	λabs/nm(eV)	*f*	NTO Results
^{3}ES1	682.44(1.8168)	0.0000	^{3}LLCT(98.8%) [a]
^{3}ES2	514.39(2.4103)	0.0000	^{3}MLCT(94.9%)[b]
^{3}ES3	509.08(2.4355)	0.0000	^{3}MLCT (94.7%)
^{1}ES1	506.90(2.4459)	0.0087	^{1}LLCT(98.9%)[c]
^{3}ES4	505.11(2.4546)	0.0000	^{3}dppzi→phen*+bpy*(98.9%)[d]
^{3}ES5	500.98(2.4748)	0.0000	^{3}metal→phen*+bpy*(31.0%)[e]
			^{3}MLCT(63.1%)
^{1}ES2	492.20(2.5190)	0.0014	^{1}dppzi→L*(99.6%)[f]
^{3}ES6	486.23(2.5499)	0.0000	^{3}MLCT(94.4%)
^{3}ES7	484.28(2.5602)	0.0000	^{3}dppzi→ phen*+bpy*(97.4%)
^{3}ES8	478.20(2.5927)	0.0000	^{3}dppzi→phen*(99.2%)[g]
^{1}ES3	478.07(2.5934)	0.0003	^{1}dppzi→phen*(99.9%)[h]
^{3}ES9	475.42(2.6079)	0.0000	^{3}LLCT(91.9%)
^{1}ES4	472.81(2.6223)	0.0005	^{1}MLCT (99.2%)[i]
^{3}ES10	472.61(2.6234)	0.0000	^{3}Metal→bpy*(95.2%)[j]
^{1}ES5	471.12(2.6317)	0.0002	^{1}MLCT(99.6%)
^{1}ES6	465.60(2.6629)	0.0013	
^{1}ES7	454.94(2.7253)	0.0007	
^{1}ES8	446.70(2.7756)	0.001	
^{1}ES9	445.47(2.7832)	0.0003	
^{1}ES10	444.90(2.7868)	0.0103	

[a] ^{3}LLCT was considered as ^{3}dppzi→dppzi* transition in the context; [b] ^{3}MLCT was referring to ^{3}metal→phen* in the context; [c] ^{1}LLCT was referring as dppzi→dppzi*transition in the context; [d] ^{3}dppzi→phen*+bpy* was considered to be the triplet transition from the π-extended ligand DPPZI to the coligand and bpy part of dppzi. [e] ^{3}Metal→(Phen*+bpy*) was treated as ^{3}Metal→L*, for it contained both coligand and main ligand parts; [f] ^{1}dppzi→L* meant the transition was originating from dppzi ligand to all parts of the ligands; [g] ^{3}Dppzi→phen* was the triplet transition from DPPZI ligand to only coligands; [h] ^{1}dppzi→phen* was the singlet transition from dppzi ligand to only coligands; ; [i] ^{1}MLCT was singlet transition referring ^{1} metal→phen* in the context; [j] ^{3}Metal→bpy* was the triplet transition from metal to bpy part of the dppzi ligand.

Table S3 TD-DFT calculated energies, oscillator strengths (*f*), and natural transition orbital analysis results of the ten lowest-energy singlet and triplet excited states of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$(3) in gas phase.

Excited State	λabs/nm(eV)	*f*	NTO Results
^{3}ES1	557.13(2.2254)	0.0000	^{3}LLCT(92.3%)[a]
^{3}ES2	550.16(2.2536)	0.0000	^{3}LLCT(99.5%)

^{3}ES3	514.82(2.4083)	0.0000	^{3}MLCT (94.8%)[b]
^{3}ES4	509.56(2.4332)	0.0000	^{3}MLCT(94.6%)
^{3}ES5	502.30(2.4683)	0.0000	^{3}metal→phen*+bpy*(35.2%)[c]
			^{3}MLCT(57.5%)
^{3}ES6	491.16(2.5243)	0.0000	^{3}Metal+dppz-idzo→bpy*(91.3%)[d]
^{3}ES7	487.39(2.5438)	0.0000	^{3}Metal+L→phen*(38.4%)[e]
			^{3}MLCT(57.1%)
^{1}ES1	473.14(2.6205)	0.0006	^{1}MLCT(99.5%)
^{3}ES8	472.68(2.6230)	0.0000	
^{3}ES9	472.08(2.6263)	0.0000	
^{1}ES2	471.61(2.6290)	0.0010	^{1}MLCT(97.6%)
^{1}ES3	470.6(2.6346)	0.0266	^{1}Metal+dppz-idzo→phen*+bpy*(97.0%)[f]
^{3}ES10	462.54(2.6805)	0.0000	
^{1}ES4	457.83(2.7081)	0.0011	
^{1}ES5	450.66(2.7512)	0.0892	
^{1}ES6	444.79(2.7875)	0.0027	
^{1}ES7	442.67(2.8008)	0.0012	
^{1}ES8	438.26(2.8290)	0.0194	
^{1}ES9	436.20(2.8424)	0.0143	
^{1}ES10	433.96(2.8571)	0.0013	

[a] ^{3}LLCT was considered as ^{3}dppz-idzo→dppz-idzo * transition in the context; [b] ^{3}MLCT was referring to ^{3}metal→phen* in the context; [c] ^{3}Metal→(Phen*+bpy*) was treated as ^{3}Metal→L*, for the excited orbitals contained both coligand and main ligand parts; [d] ^{3}Metal+dppz-idzo→bpy* meant the electron transition was originating from metal center and main ligand and transferred to the antibonding orbitals of bpy parts; [e] ^{3}Metal+L→phen* was a transition from all the complexes to the coligands; [f] ^{1}Metal+dppz-idzo→phen*+bpy* was a singlet transition from metal center and main ligand dppz-idzo and excited to coligands and bpy part.

Table S4 TD-DFT calculated energies, oscillator strengths (*f*), and natural transition orbital analysis results of the ten lowest-energy singlet and triplet excited states of [Ru(phen)$_2$dppz]$^{2+}$(1) in aqueous solution.

Excited State	λabs/nm(eV)	*f*	NTO Results
^{3}ES1	540.65(2.2932)	0.0000	^{3}metal→bpy*(16.3%)[a]
			^{3}LLCT (81.7%)[b]
^{3}ES2	510.21(2.4300)	0.0000	^{3}LLCT(12.9%)[c]
			^{3}metal→dppz*(83.6%)[d]
^{3}ES3	506.25(2.4491)	0.0000	^{3}MLCT(93.7%)[e]
^{3}ES4	500.34(2.4780)	0.0000	^{3}MLCT(28.2%)
			^{3}Metal→bpy*(66.9%)
^{3}ES5	500.08(2.4793)	0.0000	^{3}MLCT(21.2%)
			^{3}metal→phen*+bpy*(72.2%)
^{1}ES1	494.62(2.5066)	0.0001	^{1}metal→dppz*(99.9%)
^{3}ES6	481.87(2.5730)	0.0000	
^{3}ES7	478.50(2.5911)	0.0000	

^{3}ES8	476.38(2.6026)	0.0000	
^{3}ES9	472.59(2.6235)	0.0000	
^{3}ES10	470.42(2.6356)	0.0000	
^{1}ES2	465.17(2.6653)	0.0026	^{1}metal→L*(22.6%)
			^{1}metal→dppz*(76.8%)
^{1}ES3	465.06(2.6660)	0.0008	^{1}MLCT(83.9%)
			^{1}metal→dppz*(16.0%)
^{1}ES4	463.70(2.6738)	0.0382	^{1}MLCT(43.0%)
			^{1}metal→dppz*(56.8%)
^{1}ES5	462.39(2.6814)	0.0332	^{1}MLCT(42.5%)
			^{1}metal→dppz*(57.3%)
^{1}ES6	461.66(2.6856)	0.0008	
^{1}ES7	437.75(2.8323)	0.0005	
^{1}ES8	436.12(2.8429)	0.0182	
^{1}ES9	434.51(2.8534)	0.0156	
^{1}ES10	422.32(2.9358)	0.0194	

Table S5 TD-DFT calculated energies, oscillator strengths (*f*), and natural transition orbital analysis results of the ten lowest-energy singlet and triplet excited states of [Ru(phen)$_2$dppzi]$^{2+}$(2) in aqueous solution.

Excited State	λabs/nm(eV)	*f*	NTO Results
^{3}ES1	633.01(1.9587)	0.0000	^{3}LLCT(96.8%)
^{3}ES2	511.86(2.4222)	0.0000	^{3}metal→bpy*(92.5%)
^{3}ES3	507.91(2.4411)	0.0000	^{3}MLCT(94.1%)
^{3}ES4	501.35(2.4730)	0.0000	^{3}MLCT(20.0%)
			^{3}metal→phen *+bpy*(73.6%)
^{3}ES5	499.55(2.4819)	0.0000	^{3}MLCT(35.0%)
			^{3}metal→bpy*(59.3%)
^{1}ES1	491.06(2.5248)	0.0001	^{1}metal→dppzi*(99.8%)
^{3}ES6	482.02(2.5722)	0.0000	
^{3}ES7	478.81(2.5894)	0.0000	
^{3}ES8	478.48(2.5912)	0.0000	
^{3}ES9	474.69(2.6119)	0.0000	
^{3}ES10	467.91(2.6497)	0.0000	
^{1}ES2	466.75(2.6564)	0.0011	^{1}MLCT(99.6%)
^{1}ES3	464.82(2.6674)	0.0015	
^{1}ES4	461.96(2.6838)	0.0020	
^{1}ES5	460.87(2.6902)	0.0983	
^{1}ES6	458.85(2.7020)	0.0009	
^{1}ES7	440.23(2.8163)	0.0194	
^{1}ES8	438.39(2.8282)	0.0062	
^{1}ES9	435.95(2.8440)	0.0114	
^{1}ES10	434.66(2.8525)	0.0159	

Table S6 TD-DFT calculated energies, oscillator strengths (*f*), and natural transition orbital analysis results of the ten lowest-energy singlet and triplet excited states of [Ru(phen)$_2$dppz-idzo]$^{2+}$(3) in aqueous solution.

Excited State	λabs/nm(eV)	*f*	NTO Results
^{3}ES1	543.76(2.2801)	0.0000	^{3}metal→bpy*(9.1%)
			^{3}LLCT(89.3%)
^{3}ES2	508.79(2.4369)	0.0000	^{3}MLCT(94.2%)
^{3}ES3	506.52(2.4477)	0.0000	^{3}LLCT(5.3%)
			^{3}MLCT(14.2%)
			^{3}metal→phen*+bpy*(75.7%)
^{3}ES4	501.61(2.4717)	0.0000	^{3}MLCT (11.1%)
			^{3}metal→bpy*(16.6%)
			^{3}LLCT(69.1%)
^{3}ES5	499.23(2.4835)	0.0000	^{3}LLCT (5.1%)
			^{3}MLCT(6.6%)
			^{3} metal→phen*+bpy*(78.7%)
^{3}ES6	498.52(2.4871)	0.0000	^{3}MLCT(28.2%)
			^{3}metal→dppz-idzo*(68.3%)
^{3}ES7	480.80(2.5787)	0.0000	^{3}MLCT(38.7%)
			^{3}metal→bpy*(56.8%)
^{1}ES1	479.44(2.5860)	0.0000	^{1}metal→dppz-idzo*(99.8%)
^{3}ES8	479.10(2.5879)	0.0000	
^{1}ES2	467.57(2.6517)	0.0009	^{1}MLCT(99.7%)
^{1}ES3	465.65(2.6626)	0.0000	^{1}MLCT(99.5%)
^{3}ES9	462.15(2.6828)	0.0000	
^{3}ES10	458.46(2.7043)	0.0000	
^{1}ES4	450.41(2.7527)	0.0030	
^{1}ES5	446.38(2.7775)	0.2213	
^{1}ES6	444.80(2.7874)	0.0014	
^{1}ES7	439.17(2.8232)	0.0097	
^{1}ES8	435.78(2.8451)	0.0051	
^{1}ES9	425.94(2.91080	0.0643	
^{1}ES10	424.14(2.9232)	0.0076	

Table S7 Sum of the SOC integral between S_i (*i*=1-6) and ^{3}LLCT or ^{3}MLCT as well as the radiative rate constant (k_r), and the ratio of $(\Sigma\langle S_i|H_{SO}|^3MLCT\rangle)^2/(\Sigma\langle S_i|H_{SO}|^3LLCT\rangle)^2$ in gas phase and water solution.

Gas phase			
Complex	$\Sigma\langle S_i\|H_{SO}\|^3LLCT\rangle$ (cm^{-1})	$k_r(^3LLCT)^a$	
1	54.5	4.30E-04	
2	2.44	5.77E-05	
3	17.0	2.79E-01	
Complex	$\Sigma\langle S_i\|H_{SO}\|^3MLCT\rangle$ (cm^{-1})	$k_r(^3MLCT)$	$(\Sigma\langle S_i\|H_{SO}\|^3MLCT\rangle)^2/(\Sigma\langle S_i\|H_{SO}\|^3LLCT\rangle)^2$
1	667.5	2.00E+03	150
2	222.4	4.78E+03	8308
3	443.5	1.35E+03	680

Water			
Complex	$\Sigma\langle S_i\|H_{SO}\|^3LLCT\rangle$ (cm^{-1})	$k_r(^3LLCT)$	
1	439.5	1.75E+00	
2	39.4	4.24E-01	
3	176.0	2.00E+01	
Complex	$\Sigma\langle S_i\|H_{SO}\|^3MLCT\rangle$ (cm^{-1})	$k_r(^3MLCT)$	$(\Sigma\langle S_i\|H_{SO}\|^3MLCT\rangle)^2/(\Sigma\langle S_i\|H_{SO}\|^3LLCT\rangle)^2$
1	391.9	3.08E+03	0.80
2	329.3	8.95E+03	69.8
3	326.0	1.88E+04	3.43

a. The k_r was obtained from eq 1 and 2, at the optimized structures of ^{3}LLCT and ^{3}MLCT states.

1. Coordinates of optimized structure of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in gas phase at B3LYP//SDD/ 6-311G** level. E = -2149.32972436 Hartree.

Ru	1.15321677	-0.00013160	0.00002317
N	2.65670488	-1.06183951	-1.03608227
C	2.94451252	-2.27832449	-0.48194332
C	3.34061152	-0.68758394	-2.11864236
C	4.32848520	-1.48982418	-2.70693473
H	3.09284326	0.28018498	-2.53464427
C	4.62136550	-2.72162944	-2.16006870
H	4.84754747	-1.12855727	-3.58532736
H	5.37981816	-3.35891831	-2.59970415
N	1.28245014	-1.76343860	1.15295227
C	0.57912226	-2.10126799	2.23544096
C	2.20475704	-2.65661401	0.68136899
C	0.75267679	-3.32194551	2.90285986
H	-0.14482141	-1.37789951	2.58714562
C	2.44533880	-3.90570677	1.29558952
C	1.68399107	-4.22683096	2.43860228
H	0.14983913	-3.53566668	3.77604298
H	1.83516253	-5.17575788	2.93995629
N	2.65641514	1.06260284	1.03550461
C	2.94292893	2.27944254	0.48145820
C	3.34110326	0.68877161	2.11771877
C	4.32850688	1.49177031	2.70575823
H	3.09437183	-0.27928734	2.53366487
C	4.62008550	2.72392589	2.15899016
H	4.84822783	1.13080062	3.58388375
H	5.37815200	3.36180856	2.59842990
N	1.28068384	1.76347302	-1.15295603
C	2.20240835	2.65731635	-0.68151087
C	0.57673617	2.10086193	-2.23515038
C	2.44171574	3.90671923	-1.29560004
C	0.74900773	3.32181062	-2.90242385
H	-0.14665475	1.37689307	-2.58675899
C	1.67969945	4.22739817	-2.43830052
H	0.14570723	3.53516544	-3.77537564
H	1.82991323	5.17654405	-2.93952981
C	-1.60149454	-2.21773969	-2.65220124
C	-2.84109773	-1.83009425	-2.17673850
C	-2.90662817	-0.92962367	-1.10284048
C	-1.70021319	-0.46326878	-0.55547654
C	-0.44578202	-1.70639386	-2.05870721
C	-1.70028374	0.46218532	0.55600949
C	-2.90676541	0.92837966	1.10335578
C	-2.84136871	1.82870084	2.17739141
H	-3.76325601	2.19768179	2.60793037
C	-1.60183103	2.21631437	2.65303883
C	-0.44603841	1.70515899	2.05951779
H	-1.51078349	-2.91095202	-3.47863193
H	-3.76292630	-2.19918124	-2.60731120
H	0.53558834	-1.99063493	-2.41426109
H	-1.51122333	2.90935635	3.47962316
H	0.53528755	1.98940279	2.41519896
N	-0.48217967	0.84466049	1.03456163
N	-0.48204928	-0.84566032	-1.03393574
C	-4.17555731	-0.46370155	-0.54450533
C	-4.17562681	0.46242814	0.54489094
N	-5.30340307	-0.91511978	-1.07123112
N	-5.30354219	0.91379643	1.07151196
C	-6.46173566	-0.47039764	-0.54788643
C	-7.69896778	-0.92450996	-1.07514395
C	-6.46180694	0.46903695	0.54804651
H	-7.67833151	-1.62959038	-1.89648750
C	-7.69910902	0.92309736	1.07518507
H	-7.67858107	1.62817467	1.89653396
C	-8.87335762	-0.46483290	-0.53958130
C	-8.87342848	0.46338182	0.53950064
C	3.92066846	-3.15016980	-1.01333890
C	4.14720897	-4.41215779	-0.36957058
C	3.43983575	-4.77435751	0.73444106
H	4.89678271	-5.07645656	-0.78317411
H	3.61880792	-5.73095902	1.21099511
C	3.91854827	3.15204409	1.01261548
C	4.14375829	4.41434632	0.36900282
C	3.43566205	4.77614074	-0.73467663
H	4.89285156	5.07924355	0.78251480
H	3.61356101	5.73301800	-1.21107775
H	-9.82047779	0.80652890	0.93831062
H	-9.82035428	-0.80801234	-0.93848870

2. Coordinates of optimized structure of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in water at B3LYP//SDD/6-311G** level. E = -2149.50556892 Hartree.

Ru	1.14359096	-0.00012764	-0.00001521
N	2.64491047	-1.04895606	-1.04220211
C	2.94410865	-2.26222906	-0.48932608
C	3.31880051	-0.66719370	-2.12722345
C	4.31134883	-1.46164790	-2.71827305
H	3.06059886	0.29641505	-2.54456863
C	4.61793229	-2.68983090	-2.17249588
H	4.82128214	-1.09426006	-3.59881711
H	5.37979134	-3.32155689	-2.61325052
N	1.28020232	-1.76307648	1.14679971
C	0.58188033	-2.10347058	2.23057740
C	2.20964650	-2.64712000	0.67448842
C	0.76838315	-3.32218356	2.89801527
H	-0.14599441	-1.38721001	2.58642277
C	2.46240870	-3.89214272	1.28911007
C	1.70628861	-4.21896050	2.43340070
H	0.16930444	-3.53753952	3.77273763
H	1.86864069	-5.16569271	2.93445268
N	2.64460866	1.04957669	1.04168367
C	2.94267565	2.26318534	0.48892235
C	3.31915220	0.66816061	2.12642291
C	4.31127210	1.46327626	2.71729339
H	3.06182832	-0.29570942	2.54370458
C	4.61672285	2.69179051	2.17162951
H	4.82177572	1.09613148	3.59760714
H	5.37822984	3.32403321	2.61224726
N	1.27865483	1.76310253	-1.14684614
C	2.20755642	2.64774708	-0.67459604
C	0.57981950	2.10313927	-2.23038153
C	2.45918084	3.89309036	-1.28903786
C	0.76516005	3.32214887	-2.89761529
H	-0.14751803	1.38632874	-2.58621688
C	1.70246703	4.21956635	-2.43304127
H	0.16568652	3.53721257	-3.77213804
H	1.86392515	5.16654621	-2.93391904
C	-1.59822517	-2.19499976	-2.66883066
C	-2.83887760	-1.81369306	-2.19242901
C	-2.90759358	-0.92333546	-1.11200652
C	-1.70516016	-0.45959521	-0.55879128
C	-0.44532071	-1.68694167	-2.06937301
C	-1.70521117	0.45865917	0.55916612
C	-2.90769099	0.92228157	1.11237327
C	-2.83906651	1.81254692	2.19288045
H	-3.75479081	2.18257058	2.63342896
C	-1.59845852	2.19383580	2.66940370
C	-0.44549758	1.68589705	2.06994016
H	-1.50260995	-2.87942915	-3.50110796
H	-3.75456163	-2.18378570	-2.63300215
H	0.53597143	-1.96427042	-2.42806403
H	-1.50291454	2.87815755	3.50177726
H	0.53576111	1.96319327	2.42874658
N	-0.48714786	0.83519325	1.03741854
N	-0.48705620	-0.83606856	-1.03698212
C	-4.17690252	-0.46112145	-0.55002968
C	-4.17695181	0.46001917	0.55032983
N	-5.30600937	-0.90600985	-1.07718214
N	-5.30610711	0.90484144	1.07743518
C	-6.46569205	-0.46345575	-0.54881639
C	-7.70379769	-0.91306548	-1.07986007
C	-6.46574195	0.46221985	0.54901913
H	-7.68287571	-1.61153569	-1.90735954
C	-7.70389781	0.91174657	1.08001638
H	-7.68305452	1.61021843	1.90751631
C	-8.88101058	-0.45971814	-0.54286070
C	-8.88106069	0.45832123	0.54297274
C	3.92553204	-3.12429420	-1.02344327
C	4.16530822	-4.38331558	-0.37935228
C	3.46402178	-4.75125172	0.72681933
H	4.92031843	-5.03912042	-0.79587464
H	3.65148346	-5.70471770	1.20581756
C	3.92359825	3.12591986	1.02288885
C	4.16219094	4.38526386	0.37899625
C	3.46029012	4.75287655	-0.72689107
H	4.91684409	5.04154739	0.79541240
H	3.64688988	5.70656564	-1.20577742
H	-9.82701128	0.79930471	0.94636886
H	-9.82692365	-0.80075698	-0.94629822

3. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (dark state) = -2149.26149420 Hartree, $E(S_0)$= -2149.3155709Hartree.

Ru	1.16312317	-0.00000705	0.00000265
N	2.66393408	-1.06406420	-1.03652386
C	2.94956786	-2.28115343	-0.48273145
C	3.34792179	-0.69125755	-2.11949317
C	4.33396770	-1.49541332	-2.70820590
H	3.10156691	0.27690923	-2.53541330
C	4.62474619	-2.72781527	-2.16152915
H	4.85328702	-1.13517836	-3.58687096
H	5.38174474	-3.36658352	-2.60151521
N	1.28910058	-1.76282049	1.15230805
C	0.58403756	-2.09937351	2.23397320
C	2.20930653	-2.65801408	0.68070431
C	0.75467457	-3.32075800	2.90095840
H	-0.13874120	-1.37441013	2.58468377
C	2.44692184	-3.90779911	1.29453322
C	1.68439243	-4.22749415	2.43711883
H	0.15074120	-3.53355551	3.77360248
H	1.83331343	-5.17687195	2.93829048
N	2.66391313	1.06411667	1.03648989
C	2.94946491	2.28122675	0.48270132
C	3.34795028	0.69133773	2.11943772
C	4.33396699	1.49554231	2.70813232
H	3.10165957	-0.27684626	2.53535582
C	4.62466323	2.72796526	2.16145923
H	4.85332869	1.13532784	3.58678075
H	5.38163790	3.36677123	2.60143170
N	1.28898486	1.76281960	-1.15230400
C	2.20915374	2.65805809	-0.68071284
C	0.58388198	2.09934199	-2.23395169
C	2.44668727	3.90786112	-1.29453646
C	0.75443675	3.32074184	-2.90093033
H	-0.13886140	1.37433938	-2.58465380
C	1.68411462	4.22752470	-2.43710232
H	0.15047374	3.53351316	-3.77356023
H	1.83297311	5.17691512	-2.93826871
C	-1.61544907	-2.21274299	-2.64941521
C	-2.84790929	-1.82291812	-2.17128904
C	-2.90908291	-0.91728982	-1.09086906
C	-1.68712987	-0.45651765	-0.54880643
C	-0.44797503	-1.70484454	-2.05914209
C	-1.68713409	0.45644714	0.54884190
C	-2.90909168	0.91721012	1.09090207
C	-2.84792690	1.82283118	2.17132862
H	-3.77268056	2.18839836	2.59770456
C	-1.61547062	2.21265572	2.64946503
C	-0.44799157	1.70476847	2.05919186
H	-1.52888884	-2.90583112	-3.47633682
H	-3.77265944	-2.18849211	-2.59766675
H	0.52860723	-1.99615808	-2.42297435
H	-1.52891713	2.90573481	3.47639493
H	0.52858759	1.99608208	2.42303262
N	-0.47138832	0.84728631	1.03730995
N	-0.47138037	-0.84735094	-1.03726957
C	-4.15610479	-0.45329248	-0.53446019
C	-4.15610915	0.45320958	0.53448572
N	-5.32134075	-0.92735551	-1.08849830
N	-5.32134974	0.92726897	1.08851715
C	-6.46325641	-0.46714076	-0.54622842
C	-7.70648421	-0.90940575	-1.06000057
C	-6.46326096	0.46705183	0.54623969
H	-7.69032378	-1.61428161	-1.88249409
C	-7.70649305	0.90931432	1.06000337
H	-7.69033970	1.61418987	1.88249729
C	-8.95523732	-0.44502898	-0.51798064
C	-8.95524166	0.44493601	0.51797414
C	3.92369425	-3.15498921	-1.01458483
C	4.14762253	-4.41753070	-0.37093110
C	3.43957765	-4.77840909	0.73308833
H	4.89572399	-5.08339485	-0.78469220
H	3.61660237	-5.73550973	1.20938170
C	3.92355760	3.15511100	1.01453724
C	4.14740103	4.41767061	0.37088996
C	3.43930928	4.77852054	-0.73310865
H	4.89547664	5.08357146	0.78463870
H	3.61627012	5.73563494	-1.20939802
H	-9.88167185	0.80982393	0.94252767
H	-9.88166396	-0.80991778	-0.94254120

4. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in water at TD/B3LYP/ SDD/6-311G** level. E(T1) = -2149.43315568 Hartree, $E(S_0)$= -2149.4908531 Hartree.

Ru	1.15363871	-0.00000367	-0.00000064
N	2.65227725	-1.05240883	-1.04252979
C	2.94861988	-2.26625904	-0.48952369
C	3.32627639	-0.67295267	-2.12825510
C	4.31639458	-1.47019879	-2.71966595
H	3.07012085	0.29112131	-2.54584460
C	4.62018646	-2.69898510	-2.17361376
H	4.82670179	-1.10454930	-3.60072835
H	5.38010127	-3.33285749	-2.61465866
N	1.28749250	-1.76190703	1.14763487
C	0.58844106	-2.10000207	2.23164617
C	2.21400030	-2.64876462	0.67501846
C	0.77168719	-3.31917196	2.89920241
H	-0.13712820	-1.38123128	2.58715269
C	2.46354825	-3.89435841	1.28981490
C	1.70694137	-4.21873586	2.43447712
H	0.17227091	-3.53279409	3.77413319
H	1.86673667	-5.16583567	2.93568510
N	2.65226802	1.05242785	1.04251471
C	2.94857577	2.26628803	0.48951161
C	3.32628667	0.67298275	2.12823168
C	4.31639191	1.47024923	2.71963667
H	3.07015788	-0.29109906	2.54581947
C	4.62014912	2.69904530	2.17358735
H	4.82671678	1.10460767	3.60069210
H	5.38005360	3.33293337	2.61462749
N	1.28744455	1.76190644	-1.14763548
C	2.21393575	2.64878314	-0.67502145
C	0.58837727	2.09999066	-2.23163940
C	2.46344839	3.89438660	-1.28981249
C	0.77158723	3.31916969	-2.89918921
H	-0.13717529	1.38120306	-2.58714576
C	1.70682296	4.21875347	-2.43446573
H	0.17215843	3.53278248	-3.77411367
H	1.86659028	5.16586084	-2.93566847
C	-1.61263187	-2.19400908	-2.66151964
C	-2.84616607	-1.81060432	-2.18444669
C	-2.91194100	-0.91232232	-1.09806719
C	-1.69209049	-0.45356183	-0.55118255
C	-0.44661485	-1.68839560	-2.06653774
C	-1.69209204	0.45353518	0.55119270
C	-2.91194409	0.91229231	1.09807662
C	-2.84617209	1.81057140	2.18445887
H	-3.76469485	2.17812349	2.62035197
C	-1.61263933	2.19397519	2.66153595
C	-0.44662047	1.68836482	2.06655445
H	-1.52062461	-2.88001522	-3.49306590
H	-3.76468754	-2.17815856	-2.62034066
H	0.52950350	-1.97390527	-2.43370647
H	-1.52063420	2.87997765	3.49308547
H	0.52949669	1.97387254	2.43372789
N	-0.47531172	0.83920289	1.03913540
N	-0.47530886	-0.83922832	-1.03912277
C	-4.15471863	-0.44919873	-0.53651937
C	-4.15472008	0.44916675	0.53652703
N	-5.32651631	-0.92032191	-1.09462672
N	-5.32651959	0.92028694	1.09463364
C	-6.47101166	-0.46424800	-0.55087432
C	-7.70951106	-0.90224647	-1.06840726
C	-6.47101319	0.46420964	0.55088069
H	-7.69709836	-1.60042892	-1.89632337
C	-7.70951434	0.90220384	1.06841348
H	-7.69710423	1.60038652	1.89632945
C	-8.95697900	-0.44101461	-0.52170196
C	-8.95698054	0.44096755	0.52170813
C	3.92738236	-3.13119926	-1.02397341
C	4.16410541	-4.39068585	-0.37958932
C	3.46247653	-4.75639327	0.72712006
H	4.91705446	-5.04872328	-0.79634919
H	3.64764342	-5.71027639	1.20619400
C	3.92732285	3.13124889	1.02395641
C	4.16400978	4.39074486	0.37957784
C	3.46236144	4.75644220	-0.72712251
H	4.91694713	5.04879771	0.79633451
H	3.64750127	5.71033243	-1.20619260
H	-9.88365176	0.80215044	0.94894575
H	-9.88364891	-0.80220119	-0.94893929

5. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (^{3}MLCT)= -2149.24889238 Hartree, E(S_0)= -2149.3188521 Hartree.

Ru	1.18731566	-0.00088080	0.00164724
N	2.54760096	-1.08328268	-1.01209711
C	2.78674688	-2.35812371	-0.46035898
C	3.33029538	-0.70241619	-2.10395968
C	4.25131150	-1.53307005	-2.66671962
H	3.14543678	0.28755894	-2.49418803
C	4.46432674	-2.84659437	-2.14482366
H	4.81908521	-1.18950467	-3.52169134
H	5.18987771	-3.50973290	-2.59648870
N	1.19633735	-1.75371421	1.19402513
C	0.48256735	-2.05789588	2.27521479
C	2.06278259	-2.70468956	0.68378466
C	0.57612879	-3.29406205	2.92910133
H	-0.18766096	-1.29153853	2.64571016
C	2.21885903	-3.98613570	1.30138512
C	1.44769748	-4.25722260	2.44140544
H	-0.02979945	-3.47510426	3.80647732
H	1.53916250	-5.21765192	2.93589723
N	2.69242021	1.01341546	1.05684850
C	3.03563735	2.21300934	0.49761264
C	3.33925748	0.60300321	2.14955175
C	4.35042421	1.36511573	2.74894151
H	3.04501179	-0.35687431	2.55220081
C	4.70098153	2.58251313	2.20130289
H	4.84480990	0.98447763	3.63311079
H	5.48142184	3.18613620	2.65040086
N	1.39387915	1.75460893	-1.17330627
C	2.33891016	2.61152980	-0.68441207
C	0.73089960	2.10555183	-2.27358500
C	2.64663145	3.84402319	-1.30096394
C	0.97027287	3.31350652	-2.94637762
H	-0.00963973	1.40572183	-2.63923868
C	1.92583271	4.18325635	-2.46596331
H	0.40066832	3.54260827	-3.83767415
H	2.12894442	5.11938588	-2.97309691
C	-1.60419077	-2.26714906	-2.56531090
C	-2.84099219	-1.84812748	-2.11139905
C	-2.90499573	-0.90220627	-1.07620384
C	-1.69698546	-0.42415856	-0.54473148
C	-0.44385917	-1.74409943	-1.98996365
C	-1.69243385	0.54456408	0.52880350
C	-2.89668308	1.04139198	1.05305155
C	-2.82489271	1.98352959	2.09077396
H	-3.74529222	2.37514863	2.50468300
C	-1.58449036	2.38329776	2.55354405
C	-0.43136195	1.84190316	1.98192059
H	-1.51634804	-2.99569889	-3.36089285
H	-3.76447323	-2.22754256	-2.52969832
H	0.53879611	-2.04957814	-2.32149081
H	-1.49106246	3.10770647	3.35231451
H	0.55089359	2.13500276	2.32852993
N	-0.47642718	0.94008216	0.99492705
N	-0.48491921	-0.84019228	-1.00448156
C	-4.17156170	-0.40387014	-0.54164094
C	-4.16734043	0.56352151	0.51069337
N	-5.30149840	-0.86565799	-1.05455259
N	-5.29237014	1.04354727	1.01780350
C	-6.45737740	-0.39248604	-0.55151393
C	-7.69677207	-0.85618525	-1.06464118
C	-6.45277711	0.58773255	0.50963402
H	-7.68029364	-1.59132760	-1.85921414
C	-7.68748495	1.06979755	1.01729523
H	-7.66368981	1.80429564	1.81230686
C	-8.86849660	-0.36821008	-0.54849711
C	-8.86388360	0.59888053	0.49618976
C	3.72426059	-3.25853936	-1.01400355
C	3.87615923	-4.53624140	-0.38727459
C	3.15122639	-4.89080019	0.72170892
H	4.59132578	-5.23209837	-0.81031489
H	3.28676603	-5.86607840	1.17422944
C	4.03970895	3.04207144	1.04191550
C	4.33444967	4.28876979	0.39640229
C	3.66508262	4.67350906	-0.72422099
H	5.10574709	4.92133310	0.81942984
H	3.89662988	5.61718882	-1.20374197
H	-9.80925346	0.96290845	0.88013450
H	-9.81734067	-0.71880223	-0.93634607

6. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppz]^{2+}$ (Complex **1**) in water at TD/B3LYP/ SDD/6-311G** level. E(^{3}MLCT) = -2149.42424996 Hartree E(S_0)= -2149.4941082 Hartree.

Ru	1.19044205	-0.00820018	0.00138603
N	2.55934494	-1.06138516	-1.01276186
C	2.82323649	-2.33395667	-0.46606151
C	3.32912845	-0.66350054	-2.10984689
C	4.26248665	-1.47749988	-2.67582175
H	3.12187614	0.32219164	-2.49795932
C	4.50379453	-2.78880244	-2.15728551
H	4.81838283	-1.12037689	-3.53318595
H	5.23976535	-3.43878500	-2.61128005
N	1.22848266	-1.75770695	1.19017774
C	0.52518329	-2.06791795	2.27361701
C	2.10867426	-2.69429211	0.67934659
C	0.64162868	-3.30411480	2.92869528
H	-0.15335720	-1.31200388	2.64767622
C	2.28910626	-3.97086321	1.29771284
C	1.52561491	-4.25336752	2.44134718
H	0.04093944	-3.48999044	3.80836626
H	1.63548868	-5.21141421	2.93643523
N	2.67186587	1.03494768	1.05499074
C	2.99466133	2.23603171	0.48910370
C	3.31279613	0.64516660	2.15714073
C	4.30416846	1.43151645	2.75766285
H	3.02897404	-0.31224588	2.57112396
C	4.63794513	2.64865497	2.20163915
H	4.79249045	1.06815918	3.65149864
H	5.40088947	3.27244304	2.65170787
N	1.36023242	1.74362829	-1.17721093
C	2.29157199	2.61681846	-0.69384531
C	0.68431839	2.07772811	-2.27354822
C	2.57498339	3.85115453	-1.31437866
C	0.90050045	3.28829946	-2.94917913
H	-0.04644711	1.36688590	-2.63451722
C	1.84337571	4.17447457	-2.47652338
H	0.32078220	3.50359749	-3.83654016
H	2.02889208	5.11274504	-2.98514916
C	-1.58917989	-2.26013782	-2.58184712
C	-2.82715848	-1.84924487	-2.12572145
C	-2.89591153	-0.91788553	-1.07991884
C	-1.69304359	-0.44375337	-0.53886312
C	-0.43359838	-1.74142195	-1.99631359
C	-1.69028359	0.51526906	0.54432377
C	-2.89147213	1.00356788	1.07646745
C	-2.81876278	1.93247728	2.12424510
H	-3.73397582	2.32201910	2.54897618
C	-1.57902161	2.32765126	2.58917070
C	-0.42685064	1.79582692	2.00826155
H	-1.49582623	-2.97593605	-3.38720229
H	-3.74417755	-2.22783287	-2.55641629
H	0.54969392	-2.03647560	-2.33329969
H	-1.48198924	3.04140985	3.39587244
H	0.55378446	2.08608265	2.35815456
N	-0.47599601	0.90854451	1.00977203
N	-0.48148240	-0.85229018	-0.99888444
C	-4.16399321	-0.42608342	-0.54151361
C	-4.16177058	0.52967428	0.52746501
N	-5.29345961	-0.87894981	-1.06058391
N	-5.28894823	0.99966396	1.03612484
C	-6.45157910	-0.41048595	-0.55247357
C	-7.69071680	-0.86601499	-1.07585286
C	-6.44928004	0.54917002	0.51702777
H	-7.67179506	-1.58952420	-1.88148710
C	-7.68606004	1.02420383	1.02848767
H	-7.66346205	1.74743057	1.83428896
C	-8.86622786	-0.38683615	-0.55833419
C	-8.86390276	0.56365312	0.49953129
C	3.77460507	-3.21621153	-1.02410375
C	3.95060126	-4.49047641	-0.39728925
C	3.23540585	-4.85797178	0.71553358
H	4.67685002	-5.17331345	-0.82314034
H	3.38953431	-5.82996501	1.16926635
C	3.97864547	3.08620762	1.03344371
C	4.25310861	4.33350839	0.38145835
C	3.57876830	4.70031927	-0.74212145
H	5.01136854	4.98039013	0.80513499
H	3.79073983	5.64506408	-1.22760714
H	-9.80902385	0.92403839	0.88759512
H	-9.81310228	-0.73216139	-0.95569546

7. Coordinates of optimized structure of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in gas phase at B3LYP//SDD/ 6-311G** level. E = -2296.9859821 Hartree.

Ru	1.68201771	0.00055700	0.00141433
N	3.18429313	-1.07359866	-1.02345892
C	3.46834495	-2.28589411	-0.45840820
C	3.87013913	-0.71086807	-2.10870775
C	4.85635218	-1.52092911	-2.68895630
H	3.62502262	0.25370762	-2.53360782
C	5.14533920	-2.74870293	-2.13104984
H	5.37701924	-1.16894228	-3.57016718
H	5.90222851	-3.39203099	-2.56454055
N	1.80625746	-1.75195186	1.17015273
C	1.09973474	-2.07867446	2.25388596
C	2.72624509	-2.65199092	0.70731889
C	1.26812194	-3.29456017	2.93133766
H	0.37735734	-1.34999624	2.59762528
C	2.96182143	-3.89675379	1.33208341
C	2.19739915	-4.20615473	2.47622008
H	0.66264316	-3.49948520	3.80479369
H	2.34444299	-5.15159086	2.98533242
N	3.18663761	1.07209624	1.02593388
C	3.47479793	2.28249084	0.45885554
C	3.87173810	0.70851515	2.11136006
C	4.86121087	1.51588025	2.68984533
H	3.62352243	-0.25471570	2.53755423
C	5.15444012	2.74169132	2.12982006
H	5.38126160	1.16324808	3.57116456
H	5.91414653	3.38277394	2.56170985
N	1.81042256	1.75175910	-1.16844934
C	2.73374835	2.64927772	-0.70735975
C	1.10513295	2.07886821	-2.25290764
C	2.97406020	3.89183269	-1.33469446
C	1.27821899	3.29270897	-2.93288399
H	0.38022649	1.35211963	-2.59540290
C	2.21093804	4.20170088	-2.47959496
H	0.67380070	3.49787539	-3.80702667
H	2.36184787	5.14534729	-2.99089709
C	-1.07221040	-2.23656226	-2.63275712
C	-2.31143775	-1.84453432	-2.16044185
C	-2.37780723	-0.93506814	-1.09368706
C	-1.17055791	-0.46516031	-0.55059483
C	0.08416394	-1.72138196	-2.04357392
C	-1.17079924	0.46978803	0.55288024
C	-2.37820888	0.94101691	1.09633788
C	-2.30984575	1.85043885	2.16273408
H	-3.23147561	2.22338618	2.59026225
C	-1.07019063	2.24171261	2.63487956
C	0.08540011	1.72533823	2.04563589
H	-0.98207374	-2.93650416	-3.45360263
H	-3.23374530	-2.21645263	-2.58761476
H	1.06546464	-2.00902015	-2.39645698
H	-0.97909654	2.94177610	3.45550721
H	1.06714796	2.01199318	2.39811764
N	0.04728989	0.85612898	1.02809209
N	0.04722466	-0.85246940	-1.02583827
C	-3.64595026	-0.46478753	-0.53984827
C	-3.64724397	0.47161208	0.54281318
N	-4.77144521	-0.91970751	-1.06257760
N	-4.77438924	0.92602724	1.06450925
C	-5.93829247	-0.47771117	-0.55121508
C	-7.15178644	-0.95297795	-1.09443307
C	-5.93946899	0.48170108	0.54994101
H	-7.13986217	-1.66396403	-1.90951402
C	-7.15563467	0.95560821	1.09128025
H	-7.13045986	1.66658789	1.90677164
C	-8.32708726	-0.48303599	-0.55588899
C	-8.31262675	0.46836928	0.53245712
C	-10.36687928	-0.07971775	-0.09521745
H	-11.44800475	-0.07292397	-0.08758635
N	-9.63170884	-0.78641029	-0.90283025
N	-9.64418408	0.69508256	0.79156840
H	-10.02836946	1.30900508	1.49339175
C	4.44242982	-3.16517495	-0.98132626
C	4.66432531	-4.42231976	-0.32656014
C	3.95434845	-4.77311761	0.77945432
H	5.41227959	-5.09246630	-0.73362797
H	4.12961429	-5.72637899	1.26402636
C	4.45246306	3.15895698	0.97981051
C	4.67902989	4.41397666	0.32255573
C	3.97014756	4.76537381	-0.78398123
H	5.42988183	5.08189234	0.72796000
H	4.14923260	5.71687126	-1.27062793

8. Coordinates of optimized structure of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in water at B3LYP//SDD/6-311G** level. E = -2297.16548598 Hartree.

Ru	1.67176247	0.00031783	0.00011272
N	3.17413503	-1.05840353	-1.03067319
C	3.47281550	-2.26631745	-0.46601114
C	3.84960865	-0.68664310	-2.11825115
C	4.84321756	-1.48639534	-2.70029374
H	3.59180072	0.27297693	-2.54492454
C	5.14934309	-2.70930556	-2.14246650
H	5.35446338	-1.12734802	-3.58351372
H	5.91198288	-3.34491339	-2.57623788
N	1.80631171	-1.75218261	1.16273004
C	1.10582003	-2.08274459	2.24815126
C	2.73657138	-2.64047676	0.70024131
C	1.29105629	-3.29535886	2.92697413
H	0.37734445	-1.36312645	2.59578493
C	2.98847971	-3.87977974	1.32681569
C	2.23008705	-4.19621715	2.47251831
H	0.69021985	-3.50292439	3.80238738
H	2.39143455	-5.13830300	2.98262229
N	3.17266227	1.05911183	1.03302796
C	3.47236929	2.26685522	0.46853724
C	3.84667446	0.68736519	2.12151539
C	4.83975516	1.48695895	2.70467556
H	3.58810563	-0.27214270	2.54798487
C	5.14688741	2.70970539	2.14704118
H	5.34981403	1.12790969	3.58858273
H	5.90915136	3.34518783	2.58166051
N	1.80790425	1.75279471	-1.16231547
C	2.73773091	2.64097756	-0.69873718
C	1.10879195	2.08338148	-2.24862581
C	2.99069307	3.88013872	-1.32516893
C	1.29512052	3.29588398	-2.92735177
H	0.38059823	1.36387465	-2.59709631
C	2.23380613	4.19658246	-2.47186552
H	0.69541738	3.50346585	-3.80353856
H	2.39603289	5.13854506	-2.98191736
C	-1.06642977	-2.21651777	-2.65296594
C	-2.30759769	-1.83171654	-2.18038425
C	-2.37862799	-0.93275857	-1.10725397
C	-1.17626020	-0.46439826	-0.55719578
C	0.08597586	-1.70360397	-2.05688115
C	-1.17737801	0.46350172	0.55337883
C	-2.38076042	0.93115398	1.10213525
C	-2.31164275	1.83045580	2.17509788
H	-3.22773764	2.20377259	2.61219821
C	-1.07132632	2.21648261	2.64894653
C	0.08204504	1.70420482	2.05427762
H	-0.97025004	-2.90760424	-3.47973112
H	-3.22287752	-2.20571147	-2.61862123
H	1.06772336	-1.98350244	-2.41225382
H	-0.97656861	2.90793017	3.47556702
H	1.06320151	1.98496058	2.41062937
N	0.04025224	0.84469149	1.02891007
N	0.04227561	-0.84453092	-1.03129265
C	-3.64903293	-0.46683889	-0.54989900
C	-3.65027335	0.46411299	0.54375205
N	-4.77565513	-0.91540845	-1.07260810
N	-4.77772379	0.91181612	1.06599350
C	-5.94454628	-0.47511462	-0.55508132
C	-7.15968695	-0.94567779	-1.10118164
C	-5.94517600	0.46985781	0.54719232
H	-7.14169445	-1.65036540	-1.92241401
C	-7.16082225	0.93993022	1.09399562
H	-7.14169164	1.64414169	1.91542349
C	-8.33700991	-0.48063417	-0.55864730
C	-8.31934751	0.45850581	0.53375703
C	-10.37821474	-0.06910503	-0.07886085
H	-11.45847093	-0.05476017	-0.06129533
N	-9.65040049	-0.77733513	-0.90253800
N	-9.65097549	0.68830037	0.80201907
H	-10.02861701	1.29829258	1.51163819
C	4.45538509	-3.13313290	-0.99041890
C	4.69459947	-4.38586066	-0.33396556
C	3.99149146	-4.74367386	0.77439522
H	5.45065632	-5.04526159	-0.74286372
H	4.17864105	-5.69252493	1.26257331
C	4.45448976	3.13351917	0.99404784
C	4.69485017	4.38607306	0.33767600
C	3.99321539	4.74387932	-0.77162133
H	5.45057774	5.04534180	0.74739461
H	4.18120669	5.69259928	-1.25973304

9. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (DS) = -2296.92778812 Hartree, $E(S_0)$= -2296.9766116 Hartree.

Ru	1.69382264	0.00093604	0.00130433
N	3.19591955	-1.07408863	-1.02169861
C	3.47820814	-2.28669713	-0.45654957
C	3.88290665	-0.71227623	-2.10649010
C	4.86872689	-1.52342401	-2.68584818
H	3.63892285	0.25247124	-2.53167339
C	5.15601811	-2.75149239	-2.12767461
H	5.39042399	-1.17205754	-3.56669460
H	5.91255720	-3.39565852	-2.56051633
N	1.81507717	-1.75060931	1.16980444
C	1.10565088	-2.07660808	2.25176201
C	2.73441458	-2.65190784	0.70834672
C	1.27137102	-3.29293539	2.92919266
H	0.38322144	-1.34703229	2.59338047
C	2.96735133	-3.89703309	1.33317066
C	2.20051986	-4.20556518	2.47590837
H	0.66381469	-3.49735474	3.80131328
H	2.34551967	-5.15122811	2.98517777
N	3.19324357	1.07595538	1.02867622
C	3.47938595	2.28712095	0.46231065
C	3.87689554	0.71441327	2.11565469
C	4.86298959	1.52445203	2.69612058
H	3.63012857	-0.24939504	2.54140174
C	5.15417167	2.75104237	2.13669549
H	5.38206918	1.17328083	3.57859282
H	5.91121547	3.39419661	2.57016270
N	1.81977454	1.75146645	-1.16781065
C	2.73953287	2.65179855	-0.70528976
C	1.11417160	2.07671659	-2.25253578
C	2.97695050	3.89516157	-1.33192500
C	1.28448970	3.29137443	-2.93186536
H	0.39147276	1.34782158	-2.59506723
C	2.21423144	4.20294133	-2.47764019
H	0.68017692	3.49510934	-3.80640515
H	2.36298524	5.14711101	-2.98860068
C	-1.07679394	-2.23558470	-2.63374384
C	-2.31010574	-1.84244838	-2.15999912
C	-2.37426489	-0.92829518	-1.08786497
C	-1.15404614	-0.46211534	-0.54835866
C	0.08954700	-1.72213116	-2.04613917
C	-1.15721148	0.46081766	0.54113801
C	-2.38031462	0.92569179	1.07794072
C	-2.31974792	1.84042521	2.14957068
H	-3.24579437	2.20849378	2.57106158
C	-1.08840152	2.23643854	2.62641083
C	0.07982404	1.72429495	2.04200484
H	-0.98903354	-2.93544009	-3.45482285
H	-3.23414484	-2.21234758	-2.58447037
H	1.06701482	-2.01563086	-2.40574465
H	-1.00356466	2.93706410	3.44711613
H	1.05605494	2.01948098	2.40371757
N	0.05734154	0.85751444	1.02795951
N	0.06275732	-0.85639634	-1.03161443
C	-3.62475076	-0.46097845	-0.53716579
C	-3.62922009	0.45669285	0.52543166
N	-4.78248654	-0.93650759	-1.08248287
N	-4.79163712	0.93041783	1.06920343
C	-5.93363068	-0.47950603	-0.55296223
C	-7.15867310	-0.94859484	-1.08705435
C	-5.93570479	0.47251723	0.53961981
H	-7.15151550	-1.66041214	-1.90233974
C	-7.17192507	0.94296089	1.07652358
H	-7.13991149	1.65479756	1.89182279
C	-8.38592108	-0.46778833	-0.53548273
C	-8.36446178	0.45619001	0.51977991
C	-10.42706272	-0.06714201	-0.07658813
H	-11.50606979	-0.06693309	-0.07561949
N	-9.66126074	-0.77980882	-0.89086567
N	-9.69437326	0.69297550	0.79116853
H	-10.06864393	1.31113027	1.49693237
C	4.45168757	-3.16712251	-0.97857644
C	4.67126885	-4.42453782	-0.32350283
C	3.95954061	-4.77450767	0.78164612
H	5.41884102	-5.09561129	-0.72974754
H	4.13303934	-5.72805135	1.26630882
C	4.45347826	3.16633497	0.98525123
C	4.67760364	4.42201133	0.32836761
C	3.96962700	4.77145281	-0.77936834
H	5.42578393	5.09207782	0.73516416
H	4.14678577	5.72355366	-1.26555030

10. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in water at TD/B3LYP/ SDD/6-311G** level. E(DS) = -2297.10340980 Hartree, $E(S_0)$= -2297.1545113 Hartree.

Ru	1.68364071	0.00057736	0.00003421
N	3.18485418	-1.06043192	-1.02938366
C	3.48102752	-2.26882424	-0.46434404
C	3.86108973	-0.69067231	-2.11714511
C	4.85313522	-1.49265367	-2.69879122
H	3.60516218	0.26931655	-2.54418569
C	5.15678537	-2.71596266	-2.14044621
H	5.36517303	-1.13498481	-3.58212005
H	5.91819315	-3.35328313	-2.57386418
N	1.81550917	-1.75046732	1.16388106
C	1.11372274	-2.07922104	2.24896363
C	2.74393749	-2.64100780	0.70198316
C	1.29607678	-3.29205150	2.92823263
H	0.38665820	-1.35763341	2.59551776
C	2.99296117	-3.88059235	1.32901870
C	2.23344480	-4.19506372	2.47452451
H	0.69432937	-3.49813152	3.80338135
H	2.39255824	-5.13733942	2.98499116
N	3.18007897	1.06293256	1.03510358
C	3.47769319	2.27133857	0.47083617
C	3.85277905	0.69367271	2.12522230
C	4.84252791	1.49615444	2.71007202
H	3.59581930	-0.26637150	2.55151837
C	5.14754738	2.71950352	2.15256184
H	5.35173367	1.13882769	3.59517841
H	5.90722145	3.35721867	2.58844239
N	1.81819465	1.75183481	-1.16317538
C	2.74449281	2.64295408	-0.69811525
C	1.11976167	2.08019684	-2.25054801
C	2.99496148	3.88262884	-1.32439973
C	1.30367382	3.29314232	-2.92919368
H	0.39425759	1.35819028	-2.59953550
C	2.23910576	4.19663610	-2.47245329
H	0.70470024	3.49889337	-3.80632143
H	2.39947336	5.13894765	-2.98246096
C	-1.07364251	-2.21669368	-2.64957933
C	-2.30886091	-1.83037871	-2.17677264
C	-2.37748107	-0.92474866	-1.09843799
C	-1.16074313	-0.46082612	-0.55359831
C	0.08987557	-1.70589443	-2.05669565
C	-1.16379293	0.45664660	0.54272042
C	-2.38390685	0.91828160	1.08388789
C	-2.32059539	1.82498545	2.16227973
H	-3.24041261	2.19476939	2.59370764
C	-1.08790289	2.21449691	2.63853158
C	0.07855386	1.70570776	2.04949853
H	-0.98019307	-2.90894480	-3.47581743
H	-3.22630130	-2.20231264	-2.61148782
H	1.06737363	-1.99288476	-2.41894529
H	-0.99838224	2.90754339	3.46452540
H	1.05429110	1.99509479	2.41460220
N	0.05117575	0.84755649	1.02866358
N	0.05704905	-0.84870372	-1.03548015
C	-3.62451842	-0.45809187	-0.54142925
C	-3.62708866	0.44903850	0.52441576
N	-4.79118587	-0.93041425	-1.09116169
N	-4.79872874	0.91995246	1.07364314
C	-5.94126253	-0.47877452	-0.56008418
C	-7.16611021	-0.94266134	-1.09721779
C	-5.94174434	0.46710856	0.54347893
H	-7.15356172	-1.64730967	-1.91870158
C	-7.17427637	0.93180065	1.08443427
H	-7.15511290	1.63630212	1.90578889
C	-8.39650081	-0.46662863	-0.54056279
C	-8.37354463	0.44475232	0.51919043
C	-10.43831779	-0.06068031	-0.06538744
H	-11.51638260	-0.04990663	-0.05102151
N	-9.68175662	-0.77124081	-0.89263376
N	-9.69524619	0.68536653	0.80098315
H	-10.05904254	1.30003462	1.51598850
C	4.46182136	-3.13785206	-0.98831620
C	4.69831068	-4.39086230	-0.33132111
C	3.99428769	-4.74680541	0.77705119
H	5.45304857	-5.05200472	-0.73987518
H	4.17937559	-5.69589843	1.26556213
C	4.45631507	3.14089988	0.99800567
C	4.69447151	4.39391250	0.34161071
C	3.99399919	4.74939191	-0.76915843
H	5.44755074	5.05544165	0.75259001
H	4.18025213	5.69851125	-1.25717631

11. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (^{3}MLCT)= -2296.90578966 Hartree, $E(S_0)$= -2296.9753792 Hartree.

Ru	1.71394326	-0.00102058	-0.00004924
N	3.21563906	-1.03171004	-1.04507513
C	3.55186135	-2.22817325	-0.47511472
C	3.86534024	-0.63424740	-2.14079373
C	4.87280156	-1.40697383	-2.73267408
H	3.57596510	0.32354740	-2.55189649
C	5.21634524	-2.62149614	-2.17411321
H	5.36970125	-1.03694905	-3.61991986
H	5.99368060	-3.23328445	-2.61750283
N	1.91065211	-1.74664244	1.18974046
C	1.24329683	-2.08496510	2.29123308
C	2.85159957	-2.61280426	0.70936832
C	1.47455271	-3.28885790	2.97400659
H	0.50575712	-1.37797854	2.64896681
C	3.15122645	-3.84198793	1.33638310
C	2.42624344	-4.16775632	2.50254009
H	0.90156952	-3.50782963	3.86566455
H	2.62284462	-5.10103777	3.01741627
N	3.08235273	1.08471690	1.00332221
C	3.32680722	2.35248785	0.43842245
C	3.86525298	0.71039441	2.09565400
C	4.79255363	1.54133069	2.64861002
H	3.67598615	-0.27477011	2.49614677
C	5.01113789	2.84808252	2.11356333
H	5.36037736	1.20270491	3.50549729
H	5.74152505	3.51163335	2.55683503
N	1.73017542	1.74072445	-1.20769908
C	2.60247760	2.69186601	-0.70777941
C	1.01523481	2.03834174	-2.29001703
C	2.76393839	3.96635316	-1.33785680
C	1.11394288	3.26762099	-2.95551292
H	0.34005806	1.27196684	-2.65124075
C	1.99203229	4.23070467	-2.47858159
H	0.50706643	3.44368305	-3.83323269
H	2.08777794	5.18587894	-2.98236213
C	-1.06419153	-2.39298520	-2.53231317
C	-2.30286985	-1.98276537	-2.07462267
C	-2.37233338	-1.03114437	-1.04478870
C	-1.16539064	-0.53635186	-0.52393993
C	0.09159638	-1.85329182	-1.96423770
C	-1.16666581	0.44122336	0.54117661
C	-2.37384526	0.92957180	1.06775453
C	-2.30319402	1.88366214	2.09529273
H	-3.22493260	2.27115069	2.50983761
C	-1.06470612	2.30025955	2.54657293
C	0.09354215	1.76718225	1.97640567
H	-0.97388597	-3.12482145	-3.32468124
H	-3.22507104	-2.37288897	-2.48597818
H	1.07272438	-2.15471035	-2.30669214
H	-0.97362506	3.03489726	3.33618403
H	1.07769036	2.07039651	2.30537053
N	0.04704626	0.85544758	0.99836090
N	0.04901040	-0.94250284	-0.98530625
C	-3.64020737	-0.54300754	-0.50856035
C	-3.64225543	0.43412402	0.53702887
N	-4.76472145	-1.02108715	-1.01272278
N	-4.76977436	0.90456821	1.04332712
C	-5.93183052	-0.56279505	-0.51791780
C	-7.14447125	-1.06046586	-1.04234612
C	-5.93412546	0.43804978	0.54764177
H	-7.13189869	-1.80102708	-1.83061450
C	-7.15066681	0.92867861	1.07210839
H	-7.12686494	1.66989949	1.86019679
C	-8.32015943	-0.57307219	-0.52059975
C	-8.30693137	0.41842400	0.53227561
C	-10.35997558	-0.15674930	-0.07379912
H	-11.44111926	-0.15169766	-0.06615110
N	-9.62372053	-0.89132959	-0.85531036
N	-9.63819464	0.65190047	0.78322960
H	-10.02350426	1.29122941	1.46157543
C	4.55180247	-3.06741771	-1.01137342
C	4.83879512	-4.31021857	-0.35496172
C	4.16578814	-4.68186493	0.76790125
H	5.60691045	-4.95074008	-0.77176042
H	4.39123483	-5.62294929	1.25536288
C	4.27082359	3.25312992	0.98127670
C	4.42814132	4.52419921	0.34152766
C	3.70280223	4.87172533	-0.76868157
H	5.14811683	5.22011856	0.75626891
H	3.84245740	5.84176419	-1.23113991

12. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppzi]^{2+}$ (Complex **2**) in water at TD/B3LYP/ SDD/6-311G** level. E(^{3}MLCT) = -2297.08440107 Hartree $E(S_0)$= -2297.1540739 Hartree.

Ru	1.71732411	0.00678793	-0.00054733
N	3.19810533	-1.04947854	-1.04281634
C	3.51721076	-2.24596514	-0.46534306
C	3.84164654	-0.67122305	-2.14742155
C	4.83240278	-1.46517182	-2.73891336
H	3.56049859	0.28301091	-2.57047901
C	5.16262836	-2.67777959	-2.17098974
H	5.32316408	-1.11126440	-3.63518781
H	5.92510770	-3.30721400	-2.61392566
N	1.88109980	-1.73473544	1.19369759
C	1.20221473	-2.05737848	2.29154390
C	2.81116257	-2.61440191	0.71985432
C	1.41397898	-3.26253871	2.97821061
H	0.47268356	-1.34126742	2.64445380
C	3.09056197	-3.84377542	1.35196638
C	2.35568625	-4.15509330	2.51533347
H	0.83189846	-3.46872564	3.86619444
H	2.53768748	-5.08932830	3.03263488
N	3.08862443	1.06558441	1.00551243
C	3.35717621	2.33183006	0.44651178
C	3.85727098	0.67540911	2.10583995
C	4.79383575	1.49130294	2.66393286
H	3.64658494	-0.30578828	2.50347588
C	5.03968718	2.79667074	2.13296948
H	5.34866195	1.14024928	3.52450008
H	5.77809501	3.44829959	2.58063821
N	1.76100084	1.74540259	-1.20493079
C	2.64416483	2.68376558	-0.70252212
C	1.05882063	2.04784038	-2.29127856
C	2.82913818	3.95374055	-1.33296311
C	1.17948853	3.27739131	-2.95784354
H	0.37789626	1.29059264	-2.65821695
C	2.06683826	4.22811086	-2.47924028
H	0.57957562	3.45710701	-3.83932530
H	2.18020055	5.18100739	-2.98342105
C	-1.05295756	-2.34471023	-2.57066467
C	-2.29237559	-1.94112315	-2.11186321
C	-2.36545137	-1.00235463	-1.07284947
C	-1.16323147	-0.51327624	-0.54312830
C	0.09992520	-1.81147183	-1.99265536
C	-1.16492386	0.45560581	0.53167111
C	-2.36757614	0.93843989	1.06639046
C	-2.29605099	1.87900254	2.10378205
H	-3.21251604	2.26457400	2.52950714
C	-1.05738993	2.29003079	2.55829517
C	0.09739693	1.76245921	1.97947642
H	-0.95683231	-3.06639302	-3.37046155
H	-3.20803323	-2.33166160	-2.53480589
H	1.08041278	-2.10820690	-2.33746076
H	-0.96308188	3.01287399	3.35727974
H	1.08132104	2.05713584	2.31490136
N	0.04722411	0.86442493	0.98997987
N	0.05074875	-0.91462805	-1.00264561
C	-3.63565185	-0.51962220	-0.53087218
C	-3.63695597	0.44663493	0.53043807
N	-4.76151683	-0.98897858	-1.03635866
N	-4.76375670	0.90739891	1.04220470
C	-5.93002555	-0.53587032	-0.53039254
C	-7.14486776	-1.02752483	-1.05792667
C	-5.93080418	0.44432625	0.54216167
H	-7.12685521	-1.75767368	-1.85650984
C	-7.14628300	0.92675369	1.07789804
H	-7.12737803	1.65674368	1.87642422
C	-8.32188502	-0.54970880	-0.52635808
C	-8.30442932	0.42350549	0.53652878
C	-10.36261983	-0.13089900	-0.05292868
H	-11.44283379	-0.11986528	-0.03233663
N	-9.63475324	-0.86158993	-0.85671691
N	-9.63557315	0.65655564	0.80153027
H	-10.01345392	1.28739801	1.49266153
C	4.50032457	-3.10322296	-1.00003749
C	4.77097455	-4.34506380	-0.33612164
C	4.09369768	-4.70020242	0.78942698
H	5.52864048	-4.99742531	-0.75239302
H	4.30284720	-5.64092443	1.28383639
C	4.31192997	3.21586011	0.99603614
C	4.49265169	4.48351586	0.35688553
C	3.77882292	4.84297827	-0.75917791
H	5.22155644	5.16760575	0.77616329
H	3.93652279	5.81000074	-1.22223096

13. Coordinates of optimized structure of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in gas phase at B3LYP//SDD/ 6-311G** level. E = -2372.26643113 Hartree.

Ru	1.91082172	-0.00000492	0.00000110
N	3.41444348	-1.07354754	-1.02380083
C	3.70153297	-2.28385731	-0.45592297
C	4.09964026	-0.71157266	-2.10971218
C	5.08811349	-1.52040065	-2.68787130
H	3.85236885	0.25155603	-2.53669622
C	5.38026035	-2.74611105	-2.12702143
H	5.60820244	-1.16902249	-3.56968240
H	6.13916889	-3.38831654	-2.55867548
N	2.03770738	-1.75038789	1.17108766
C	1.33178016	-2.07639174	2.25545610
C	2.96022676	-2.64912413	0.71062328
C	1.50371294	-3.28997768	2.93618317
H	0.60709521	-1.34896652	2.59700324
C	3.19929255	-3.89158124	1.33867835
C	2.43577187	-4.20007661	2.48367518
H	0.89883929	-3.49426719	3.81022654
H	2.58568982	-5.14361289	2.99549585
N	3.41444930	1.07350555	1.02382782
C	3.70157336	2.28380963	0.45595539
C	4.09962001	0.71151630	2.10975088
C	5.08810019	1.52032359	2.68792702
H	3.85232097	-0.25160703	2.53673105
C	5.38028236	2.74602786	2.12708219
H	5.60816651	1.16893449	3.56974712
H	6.13919683	3.38821749	2.55874946
N	2.03776403	1.75037588	-1.17108369
C	2.96029421	2.64909265	-0.71060309
C	1.33186264	2.07639439	-2.25546429
C	3.19939650	3.89154504	-1.33865348
C	1.50383186	3.28997720	-2.93618784
H	0.60716963	1.34898322	-2.59702419
C	2.43590171	4.20005678	-2.48366323
H	0.89897779	3.49427935	-3.81024179
H	2.58584816	5.14359013	-2.99548099
C	-0.84557265	-2.24166413	-2.63021708
C	-2.08403132	-1.84908476	-2.15783702
C	-2.15078928	-0.93772589	-1.09174398
C	-0.94154439	-0.46725387	-0.55021984
C	0.31200205	-1.72562257	-2.04243540
C	-0.94154325	0.46731779	0.55016595
C	-2.15078678	0.93782119	1.09166588
C	-2.08402653	1.84917300	2.15776477
H	-3.00622465	2.22203036	2.58411223
C	-0.84556713	2.24171715	2.63017223
C	0.31200596	1.72564619	2.04241316
H	-0.75575173	-2.94278787	-3.45009886
H	-3.00623057	-2.22191982	-2.58420152
H	1.29285018	-2.01434231	-2.39587242
H	-0.75574446	2.94283471	3.45005909
H	1.29285442	2.01433703	2.39587283
N	0.27623053	0.85566976	1.02642107
N	0.27622888	-0.85564135	-1.02644733
C	-3.41574723	-0.46663872	-0.53776581
C	-3.41574590	0.46676945	0.53766009
N	-4.54908247	-0.92427511	-1.06088731
N	-4.54907972	0.92444011	1.06075466
C	-5.70632370	-0.47972716	-0.54810715
C	-6.93125092	-0.95386153	-1.08593143
C	-5.70632222	0.47996655	0.54791275
H	-6.90847355	-1.66719648	-1.89897389
C	-6.93124854	0.95386767	1.08594456
H	-6.90846947	1.66695929	1.89920035
C	-8.09377200	-0.47832821	-0.54385392
C	-8.09377084	0.47849499	0.54372873
C	-10.27615708	0.00064849	-0.00055795
N	-9.40959161	0.73161564	0.83160022
H	-9.76645805	1.35480174	1.53975401
C	4.67816015	-3.16173747	-0.97648924
C	4.90350865	-4.41657289	-0.31845437
C	4.19439918	-4.76652689	0.78841059
H	5.65352959	-5.08559633	-0.72360323
H	4.37249816	-5.71795777	1.27557445
C	4.67821010	3.16166928	0.97653839
C	4.90359576	4.41650033	0.31850800
C	4.19451216	4.76646971	-0.78836868
H	5.65362384	5.08550790	0.72366979
H	4.37263919	5.71789713	-1.27552907
N	-9.40959319	-0.73193958	-0.83129110
H	-9.76646049	-1.35609152	-1.53859345
O	-11.47250614	-0.00031809	0.00029387

14. Coordinates of optimized structure of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in water at B3LYP//SDD/6-311G** level. E = -2372.44912082 Hartree.

Ru	1.90135714	0.00000442	-0.00000256
N	3.40262830	-1.06077655	-1.03018363
C	3.70161875	-2.26775383	-0.46358677
C	4.07746873	-0.69109381	-2.11887639
C	5.07064452	-1.49196050	-2.70011290
H	3.81948112	0.26780202	-2.54708914
C	5.37704231	-2.71390772	-2.14031045
H	5.58137612	-1.13450020	-3.58428109
H	6.13935844	-3.35034578	-2.57343184
N	2.03632858	-1.75037105	1.16535856
C	1.33630730	-2.07902511	2.25166596
C	2.96611650	-2.63972634	0.70384541
C	1.52164885	-3.29054366	2.93241626
H	0.60818133	-1.35859225	2.59836685
C	3.21815275	-3.87796614	1.33241971
C	2.46032009	-4.19234815	2.47905465
H	0.92117896	-3.49651230	3.80846689
H	2.62177564	-5.13358012	2.99070534
N	3.40262227	1.06079333	1.03017910
C	3.70160513	2.26777304	0.46358343
C	4.07746422	0.69111429	2.11887222
C	5.07063436	1.49198702	2.70011003
H	3.81948237	-0.26778336	2.54708435
C	5.37702464	2.71393658	2.14030859
H	5.58136760	1.13452953	3.58427839
H	6.13933627	3.35037930	2.57343102
N	2.03631939	1.75038107	-1.16536367
C	2.96610123	2.63974190	-0.70384896
C	1.33629762	2.07903106	-2.25167187
C	3.21813010	3.87798377	-1.33242209
C	1.52163189	3.29055134	-2.93242111
H	0.60817728	1.35859321	-2.59837420
C	2.46029652	4.19236176	-2.47905759
H	0.92116180	3.49651656	-3.80847240
H	2.62174636	5.13359523	-2.99070735
C	-0.84203964	-2.22015431	-2.64669249
C	-2.08194409	-1.83366425	-2.17359733
C	-2.15139088	-0.93224868	-1.10140223
C	-0.94687930	-0.46418884	-0.55377467
C	0.31234109	-1.70716068	-2.05285860
C	-0.94688088	0.46419053	0.55376706
C	-2.15139397	0.93224819	1.10139300
C	-2.08195036	1.83366252	2.17358934
H	-2.99799228	2.20771000	2.61015468
C	-0.84204733	2.22015354	2.64668737
C	0.31233515	1.70716211	2.05285492
H	-0.74727801	-2.91280702	-3.47234220
H	-2.99798472	-2.20771361	-2.61016377
H	1.29317613	-1.98899502	-2.40937025
H	-0.74728809	2.91280518	3.47233823
H	1.29316916	1.98899706	2.40936895
N	0.27113606	0.84663518	1.02922213
N	0.27113906	-0.84663232	-1.02922709
C	-3.41788855	-0.46395114	-0.54308522
C	-3.41788999	0.46394914	0.54307369
N	-4.55155765	-0.91469909	-1.06634288
N	-4.55156032	0.91469710	1.06632851
C	-5.71129056	-0.47266437	-0.54896087
C	-6.93666451	-0.94350988	-1.09288261
C	-5.71129188	0.47267342	0.54893414
H	-6.91909355	-1.64958281	-1.91231515
C	-6.93666700	0.94345939	1.09290444
H	-6.91909805	1.64947345	1.91238768
C	-8.09673376	-0.47114656	-0.54500283
C	-8.09673497	0.47113537	0.54498838
C	-10.27066883	0.00012324	-0.00012065
N	-9.42063400	0.72170600	0.83480133
H	-9.76806337	1.34270475	1.54936713
C	4.68376018	-3.13557991	-0.98707804
C	4.92325418	-4.38716220	-0.32849191
C	4.22076931	-4.74293941	0.78090169
H	5.67903276	-5.04735217	-0.73665084
H	4.40812269	-5.69094946	1.27064356
C	4.68374051	3.13560514	0.98707609
C	4.92322682	4.38718959	0.32849133
C	4.22074056	4.74296316	-0.78090256
H	5.67900069	5.04738416	0.73665154
H	4.40808828	5.69097486	-1.27064344
N	-9.42063231	-0.72183857	-0.83471318
H	-9.76806040	-1.34307682	-1.54907149
O	-11.48231190	-0.00011730	0.00008619

15. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (dark state) = -2372.19213950 Hartree, $E(S_0)$= -2372.2580907 Hartree.

Ru	1.92398064	0.00000000	0.00000114
N	3.42526256	-1.07572571	-1.02413791
C	3.71051960	-2.28646660	-0.45648567
C	4.11032192	-0.71506932	-2.11051720
C	5.09710756	-1.52562340	-2.68909640
H	3.86416990	0.24834715	-2.53747901
C	5.38746007	-2.75179453	-2.12834504
H	5.61728153	-1.17521645	-3.57122632
H	6.14495349	-3.39537063	-2.56040086
N	2.04854327	-1.74969945	1.17091258
C	1.34143150	-2.07425566	2.25483660
C	2.96898437	-2.65031399	0.71030310
C	1.51073643	-3.28845803	2.93520445
H	0.61828870	-1.34508358	2.59582543
C	3.20545040	-3.89332436	1.33804202
C	2.44106359	-4.20036283	2.48283878
H	0.90522388	-3.49171029	3.80902293
H	2.58898933	-5.14426145	2.99454151
N	3.42526124	1.07573435	1.02413298
C	3.71050931	2.28647644	0.45647877
C	4.11032723	0.71508226	2.11050949
C	5.09711104	1.52564196	2.68908394
H	3.86418224	-0.24833535	2.53747281
C	5.38745451	2.75181432	2.12833061
H	5.61729079	1.17523829	3.57121177
H	6.14494634	3.39539475	2.56038275
N	2.04852849	1.74969958	-1.17091169
C	2.96896695	2.65031921	-0.71030686
C	1.34141005	2.07425160	-2.25483261
C	3.20542356	3.89333054	-1.33804747
C	1.51070555	3.28845448	-2.93520189
H	0.61826936	1.34507572	-2.59581780
C	2.44102995	4.20036441	-2.48284092
H	0.90518790	3.49170315	-3.80901766
H	2.58894833	5.14426359	-2.99454474
C	-0.85438384	-2.24074514	-2.62595177
C	-2.08609933	-1.84584199	-2.15161292
C	-2.14961448	-0.92851994	-1.08054197
C	-0.92535479	-0.46144743	-0.54287564
C	0.31419070	-1.72628232	-2.04074565
C	-0.92535483	0.46143518	0.54288791
C	-2.14961469	0.92850401	1.08055681
C	-2.08609974	1.84582613	2.15162770
H	-3.01056708	2.21634053	2.57434371
C	-0.85438432	2.24073235	2.62596416
C	0.31419052	1.72627349	2.04075509
H	-0.76777473	-2.94248388	-3.44550855
H	-3.01056670	-2.21635859	-2.57432697
H	1.29070817	-2.02162103	-2.40156296
H	-0.76777549	2.94247143	3.44552069
H	1.29070791	2.02161557	2.40156981
N	0.29043674	0.85852626	1.02853611
N	0.29043676	-0.85853478	-1.02852687
C	-3.39670508	-0.46035638	-0.53070958
C	-3.39670503	0.46033887	0.53072491
N	-4.55980542	-0.93800087	-1.07547692
N	-4.55980567	0.93798473	1.07548965
C	-5.70652781	-0.47440163	-0.54145622
C	-6.93986312	-0.94152420	-1.07089768
C	-5.70652807	0.47438367	0.54146831
H	-6.91740421	-1.65556898	-1.88436062
C	-6.93986254	0.94151724	1.07089878
H	-6.91740510	1.65557346	1.88435175
C	-8.14708698	-0.46188745	-0.52440311
C	-8.14708746	0.46187431	0.52440678
C	-10.33506351	-0.00002718	0.00001926
N	-9.46016015	0.73012278	0.82865381
H	-9.81038273	1.35583431	1.53846434
C	4.68522001	-3.16615509	-0.97749438
C	4.90832476	-4.42143782	-0.31951781
C	4.19878683	-4.77010112	0.78746054
H	5.65693284	-5.09187767	-0.72490326
H	4.37511512	-5.72194263	1.27444321
C	4.68520724	3.16617046	0.97748277
C	4.90830240	4.42145403	0.31950454
C	4.19875774	4.77011291	-0.78747089
H	5.65690865	5.09189812	0.72488636
H	4.37507873	5.72195512	-1.27445483
N	-9.46016095	-0.73010302	-0.82867897
H	-9.81038331	-1.35579302	-1.53850844
O	-11.53272243	0.00001455	-0.00001576

16. Optimized coordinates of first triplet state/ dark state of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in water at TD/B3LYP/ SDD/6-311G** level. E(T1) = -2372.37383325 Hartree, $E(S_0)$= -2372.4392885 Hartree.

Ru	1.91377368	0.00000083	-0.00000083
N	3.41295445	-1.06308134	-1.03086490
C	3.71024249	-2.27035142	-0.46408308
C	4.08737089	-0.69507769	-2.12031087
C	5.07872742	-1.49786141	-2.70203820
H	3.83058299	0.26409979	-2.54865347
C	5.38350436	-2.72008495	-2.14195288
H	5.58934944	-1.14164991	-3.58676971
H	6.14441039	-3.35799198	-2.57539009
N	2.04724930	-1.74948707	1.16596716
C	1.34692008	-2.07654672	2.25250106
C	2.97507686	-2.64062597	0.70408078
C	1.53037871	-3.28827426	2.93342500
H	0.62027983	-1.35444520	2.59888271
C	3.22519509	-3.87912824	1.33280041
C	2.46731307	-4.19182816	2.47987949
H	0.92986304	-3.49306812	3.80971647
H	2.62730218	-5.13324189	2.99166253
N	3.41295407	1.06308063	1.03086615
C	3.71024592	2.27034970	0.46408419
C	4.08736682	0.69507642	2.12031422
C	5.07872345	1.49785859	2.70204353
H	3.83057583	-0.26410020	2.54865693
C	5.38350452	2.72008092	2.14195783
H	5.58934240	1.14164680	3.58677668
H	6.14441092	3.35798660	2.57539637
N	2.04725527	1.74948769	-1.16596939
C	2.97508390	2.64062488	-0.70408174
C	1.34693004	2.07654750	-2.25250578
C	3.22520683	3.87912576	-1.33280221
C	1.53039352	3.28827371	-2.93343080
H	0.62028933	1.35444703	-2.59888854
C	2.46732866	4.19182605	-2.47988375
H	0.92988097	3.49306772	-3.80972439
H	2.62732150	5.13323868	-2.99166765
C	-0.85263577	-2.22053082	-2.63967641
C	-2.08594153	-1.83222729	-2.16620346
C	-2.15272869	-0.92293405	-1.08857151
C	-0.93165020	-0.45876749	-0.54628406
C	0.31395214	-1.70916720	-2.04969837
C	-0.93164990	0.45877005	0.54628348
C	-2.15272809	0.92293446	1.08857362
C	-2.08594010	1.83222837	2.16620496
H	-3.00455868	2.20410064	2.59836642
C	-0.85263394	2.22053470	2.63967461
C	0.31395357	1.70917218	2.04969483
H	-0.76081015	-2.91478916	-3.46440734
H	-3.00456045	-2.20410187	-2.59836226
H	1.29007468	-1.99861319	-2.41377663
H	-0.76080770	2.91479311	3.46440542
H	1.29007638	1.99861876	2.41377193
N	0.28492030	0.84987466	1.03081679
N	0.28491961	-0.84987038	-1.03081975
C	-3.39591294	-0.45530869	-0.53270731
C	-3.39591280	0.45530280	0.53271559
N	-4.56546926	-0.93014768	-1.08296476
N	-4.56546910	0.93013678	1.08297769
C	-5.71449415	-0.47169143	-0.54748087
C	-6.94215959	-0.93454910	-1.08207137
C	-5.71449420	0.47165457	0.54751638
H	-6.92863721	-1.64067934	-1.90190216
C	-6.94215986	0.93458052	1.08204784
H	-6.92863684	1.64082283	1.90178222
C	-8.14933276	-0.45478277	-0.52574424
C	-8.14933302	0.45470971	0.52581024
C	-10.32592816	-0.00033470	0.00028923
N	-9.46788799	0.71921439	0.83152176
H	-9.80707902	1.34289054	1.54826366
C	4.69042284	-3.14010330	-0.98799998
C	4.92821073	-4.39189233	-0.32915860
C	4.22589463	-4.74607616	0.78085913
H	5.68251681	-5.05355679	-0.73765950
H	4.41189521	-5.69428593	1.27072897
C	4.69042691	3.14009978	0.98800276
C	4.92821944	4.39188754	0.32916070
C	4.22590711	4.74607182	-0.78085931
H	5.68252613	5.05355056	0.73766280
H	4.41191152	5.69428048	-1.27072982
N	-9.46788699	-0.71905053	-0.83166276
H	-9.80707616	-1.34226190	-1.54880949
O	-11.54080609	0.00008876	-0.00007777

17. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in gas phase at TD/B3LYP/ SDD/6-311G** level. E (^{3}MLCT)= -2372.18622852 Hartree, E(S_0)= -2372.255753 Hartree.

Ru	1.94341284	0.00204429	0.00075061
N	3.31078863	-1.08557454	-1.00061969
C	3.55409936	-2.35314526	-0.43490139
C	4.09411990	-0.71293104	-2.09381931
C	5.02052838	-1.54514744	-2.64584193
H	3.90552128	0.27186943	-2.49541702
C	5.23815149	-2.85169814	-2.10963773
H	5.58854647	-1.20788663	-3.50315350
H	5.96785654	-3.51633078	-2.55236875
N	1.95796794	-1.73869140	1.21043661
C	1.24253762	-2.03467928	2.29258598
C	2.82940153	-2.69105584	0.71141820
C	1.33972930	-3.26371808	2.95915585
H	0.56804560	-1.26726312	2.65290145
C	2.98947568	-3.96527527	1.34251976
C	2.21686164	-4.22792975	2.48326592
H	0.73234730	-3.43853881	3.83676944
H	2.31148809	-5.18286225	2.98773510
N	3.44508276	1.03414619	1.04519201
C	3.78295993	2.22874284	0.47257345
C	4.09399089	0.63834295	2.14175494
C	5.10250530	1.41102556	2.73208295
H	3.80334433	-0.31823288	2.55484037
C	5.44775288	2.62367939	2.17080995
H	5.59896898	1.04221716	3.62007974
H	6.22602624	3.23533348	2.61274746
N	2.14182796	1.74533096	-1.19178466
C	3.08362332	2.61142229	-0.71317587
C	1.47552289	2.08164480	-2.29450917
C	3.38538192	3.83846428	-1.34324177
C	1.70890276	3.28340848	-2.98033593
H	0.73737496	1.37455706	-2.65075952
C	2.66160191	4.16215170	-2.51071298
H	1.13691530	3.50073741	-3.87303850
H	2.86002085	5.09364805	-3.02812478
C	-0.83815003	-2.30064055	-2.54291155
C	-2.07558875	-1.88394649	-2.09091236
C	-2.14514200	-0.92833122	-1.06337407
C	-0.93636638	-0.43991564	-0.53887457
C	0.32183012	-1.76712618	-1.97432963
C	-0.93601407	0.53694302	0.52313007
C	-2.14543655	1.03052793	1.04308483
C	-2.07626707	1.98404448	2.07222056
H	-2.99864767	2.37367530	2.48331081
C	-0.83876676	2.39653268	2.52933991
C	0.31869481	1.85756497	1.96205782
H	-0.74787107	-3.03588918	-3.33204512
H	-2.99767276	-2.27185285	-2.50420052
H	1.30522662	-2.07133171	-2.30474936
H	-0.74930524	3.12957022	3.32067715
H	1.29910273	2.16124709	2.30474064
N	0.27803465	0.94588333	0.98495872
N	0.27726610	-0.85523293	-0.99751482
C	-3.40983416	-0.43272252	-0.53177721
C	-3.40981705	0.54012742	0.50755342
N	-4.54332446	-0.90699778	-1.03976480
N	-4.54268703	1.01882893	1.01325818
C	-5.70031452	-0.44223055	-0.54497054
C	-6.92506389	-0.93283240	-1.06681733
C	-5.69999400	0.55692430	0.51726738
H	-6.90312674	-1.67444014	-1.85407940
C	-6.92432002	1.05028194	1.03797236
H	-6.90157297	1.79141966	1.82566369
C	-8.08752221	-0.43740701	-0.54190254
C	-8.08714528	0.55686998	0.51242995
C	-10.26903536	0.06122705	-0.01528435
N	-9.40203427	0.82089335	0.79064881
H	-9.75868470	1.46791418	1.47737666
C	4.49721362	-3.25511351	-0.97685848
C	4.65328720	-4.52570741	-0.33617129
C	3.92743482	-4.87189393	0.77432430
H	5.37265475	-5.22262154	-0.75030189
H	4.06615363	-5.84177789	1.23737738
C	4.78396346	3.06785493	1.00697372
C	5.07304346	4.30859646	0.34750366
C	4.40102503	4.67832455	-0.77653274
H	5.84209482	4.94894333	0.76284059
H	4.62817434	5.61771117	-1.26648045
N	-9.40253831	-0.69944468	-0.82094221
H	-9.75963738	-1.34714011	-1.50683847
O	-11.46492043	0.06198232	-0.01555008

18. Optimized coordinates of first bright triplet state of $[Ru(phen)_2dppz\text{-}idzo]^{2+}$ (Complex **3**) in water at TD/B3LYP/ SDD/6-311G** level. E(^{3}MLCT) = -2372.36815507 Hartree E(S_0)= -2372.4377589 Hartree.

Ru	1.94648189	0.00585730	-0.00078317
N	3.42592419	-1.05435975	-1.04122168
C	3.74317130	-2.25031842	-0.46168859
C	4.07017077	-0.67889134	-2.14635992
C	5.05989211	-1.47525228	-2.73632645
H	3.79044182	0.27507684	-2.57097163
C	5.38825484	-2.68740703	-2.16628637
H	5.55137685	-1.12361272	-3.63309567
H	6.14992606	-3.31865273	-2.60803143
N	2.10777700	-1.73370733	1.19636971
C	1.42814905	-2.05342793	2.29460849
C	3.03644600	-2.61566845	0.72406793
C	1.63779532	-3.25784094	2.98321131
H	0.69981083	-1.33539802	2.64610161
C	3.31379122	-3.84445102	1.35825087
C	2.57817088	-4.15268472	2.52195506
H	1.05522060	-3.46169174	3.87141387
H	2.75852039	-5.08636713	3.04084239
N	3.31980262	1.06465368	1.00286711
C	3.58858130	2.33012992	0.44228848
C	4.08825863	0.67565967	2.10340692
C	5.02497371	1.49198905	2.66071160
H	3.87761385	-0.30517077	2.50203342
C	5.27112844	2.79663529	2.12813482
H	5.57973048	1.14181376	3.52167658
H	6.00972414	3.44859099	2.57503992
N	1.99183191	1.74227104	-1.20807903
C	2.87560151	2.68085818	-0.70706079
C	1.28955943	2.04360601	-2.29470028
C	3.06094957	3.94994907	-1.33915349
C	1.41072806	3.27215678	-2.96289032
H	0.60816986	1.28615386	-2.66037051
C	2.29864480	4.22315395	-2.48559772
H	0.81076883	3.45105317	-3.84450965
H	2.41232345	5.17535536	-2.99102433
C	-0.83005919	-2.34682602	-2.56447182
C	-2.06793418	-1.93994993	-2.10585854
C	-2.13886568	-0.99817588	-1.06834877
C	-0.93410720	-0.51045601	-0.54088372
C	0.32518046	-1.81462017	-1.98851679
C	-0.93410653	0.45935169	0.53015590
C	-2.13769382	0.94426771	1.06282565
C	-2.06523588	1.88757979	2.09875852
H	-2.98142275	2.27514984	2.52323628
C	-0.82677873	2.29801010	2.55281902
C	0.32874407	1.76801758	1.97585072
H	-0.73589050	-3.07050549	-3.36272092
H	-2.98461874	-2.32968626	-2.52728280
H	1.30455391	-2.11463822	-2.33378156
H	-0.73209863	3.02247223	3.35032221
H	1.31248421	2.06290084	2.31174328
N	0.27862318	0.86838996	0.98877340
N	0.27906268	-0.91580409	-1.00101666
C	-3.40479254	-0.51150988	-0.52626982
C	-3.40425999	0.45219125	0.52695384
N	-4.53801784	-0.98239395	-1.03233061
N	-4.53707301	0.91744328	1.03915186
C	-5.69711628	-0.52616846	-0.52714227
C	-6.92233042	-1.01721723	-1.05234880
C	-5.69664405	0.45501786	0.54059068
H	-6.90514227	-1.74911141	-1.84871355
C	-6.92150469	0.93905935	1.07309804
H	-6.90376434	1.67121746	1.86920614
C	-8.08203813	-0.53097915	-0.51599383
C	-8.08163501	0.44569899	0.54410381
C	-10.25530501	-0.04959266	0.02118993
N	-9.40464073	0.70111685	0.82994402
H	-9.75177714	1.34322840	1.52583320
C	4.72510597	-3.10995069	-0.99478220
C	4.99374226	-4.35109652	-0.32874087
C	4.31571389	-4.70334313	0.79727150
H	5.75046740	-5.00533361	-0.74378864
H	4.52336576	-5.64356995	1.29324530
C	4.54364955	3.21457468	0.99078022
C	4.72473093	4.48144974	0.34994570
C	4.01105333	4.83963615	-0.76649049
H	5.45380926	5.16587506	0.76838631
H	4.16905432	5.80600900	-1.23080875
N	-9.40522542	-0.79470113	-0.79329908
H	-9.75277670	-1.43950131	-1.48649217
O	-11.46652580	-0.05359107	0.02530700