Electronic Supplementary Material (ESI) for Dalton Transactions

Solvent-dependent modulation of metal-metal electronic interactions in a dinuclear cyanoruthenate complex: a detailed electrochemical, spectroscopic and computational study
Supplementary information Calculations

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CONTENTS

S1. RU(III)/RU(III) COMPLEXES

Calculation of the structure of the doubly-oxidised Ru(III)/Ru(III) form of the complex in CH_2Cl_2 (Fig. 10) shows that the central ligand does not change its structure significantly upon oxidation of the metal atoms. The distance between the two pyridyl H^3 atoms increases by just 0.05Å upon this double oxidation. However, the $Ru(CN)_4^{2-}$ units undergo quite dramatic structural changes upon oxidation to $Ru(CN)_4^-$ according to the calculation. In particular, the axial CN^- units bend towards the equatorial CN^- units as is clear in Fig. 10, resulting in a trans C-Ru-C angle of 161°, compared to 180° in the Ru(II)/Ru(II) complex. The reason behind this counter-intuitive observation is somewhat unclear. If we use the Mulliken charges as a guide as to the changes in the charge distribution upon double oxidation, then it is clear that the partial charges on the nitrogen atoms of the ligand hardly change and that therefore the charge distribution on the ligand does not change significantly. The same observation can be made if one looks at the complete electrostatic potential. On the other hand, the cyanide nitrogens become significantly less negatively charged for the doubly-oxidized species. So, if we assume that the precise value of the trans C-Ru-C angle is caused by the repulsion between the nitrogen atoms of the central ligand as well as of the cyanides, then a change in the balance may well cause a deviation from octahedral geometry. Qualitatively, the change in C-Ru-C angle means a diminished interaction between those CN^- ligands and the Ru centre, which has an effect on the resulting IR spectrum. A similar structural distortion (decrease of the trans axial C-Ru-C angle) is calculated following double oxidation of the complex in a bare PCM water solvent. However, including the hydrogen-bonded water shell causes an additional change to the geometry of the complex upon double oxidation (Fig. 11): specifically, it shortens the distance between the two clashing pyridyl H^3 atoms on the bppz ligand, and it also results in distortion of one of the $Ru(CN)_4^-$ units quite significantly, with substantial compression of the trans C-Ru-C angle from 180°; the second $Ru(CN)_4^-$ unit however remains undistorted. This asymmetry is (again) very likely caused by our incomplete description of the solvation shell and a more complete solvation shell would therefore not show any asymmetry. However, even though the solvation shell is incomplete, this calculation shows that the $Ru(CN)_4^-$ units are quite flexible and will distort readily upon a change in the local environment. Interestingly, again for the mixed-valence Ru(II)-Ru(III) species no distortion was found as was also the case for CH_2Cl_2 solvation, suggesting again that the effects are very subtle and that the $Ru(CN)_4^-$ units are quite flexible and easy to distort.

S2. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{4-}$ IN DCM SOLVENT (PCM)

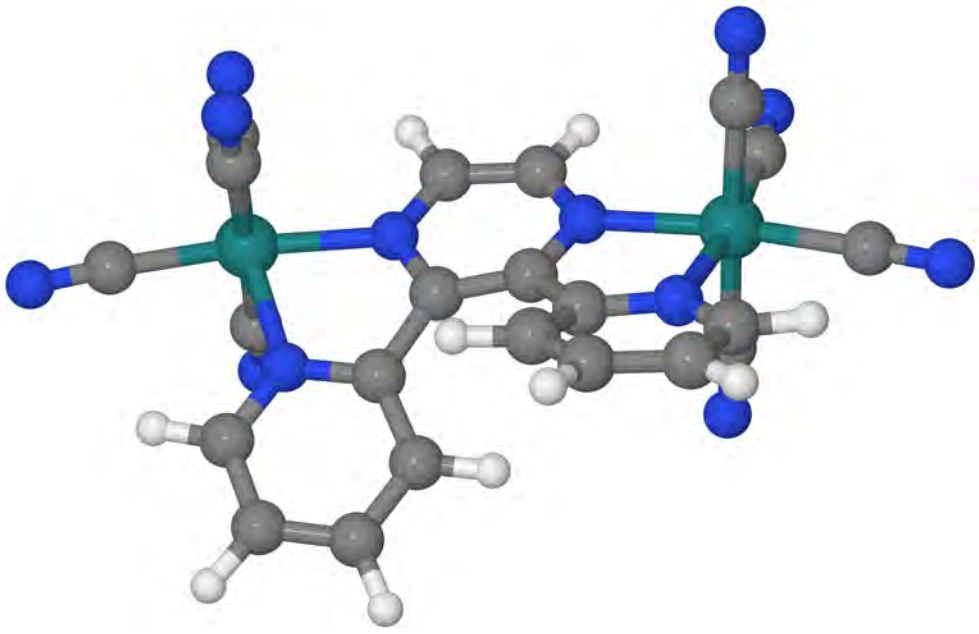


FIG. S1. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in DCM solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{4-}$
Charge	:	-4
Multiplicity	:	1
Energy	:	-1692.27657464 a.u.
Gibbs Energy	:	-1692.05804400 a.u.
Number of imaginary frequencies	:	0

S2.1. Cartesian Co-ordinates (XYZ format)

46

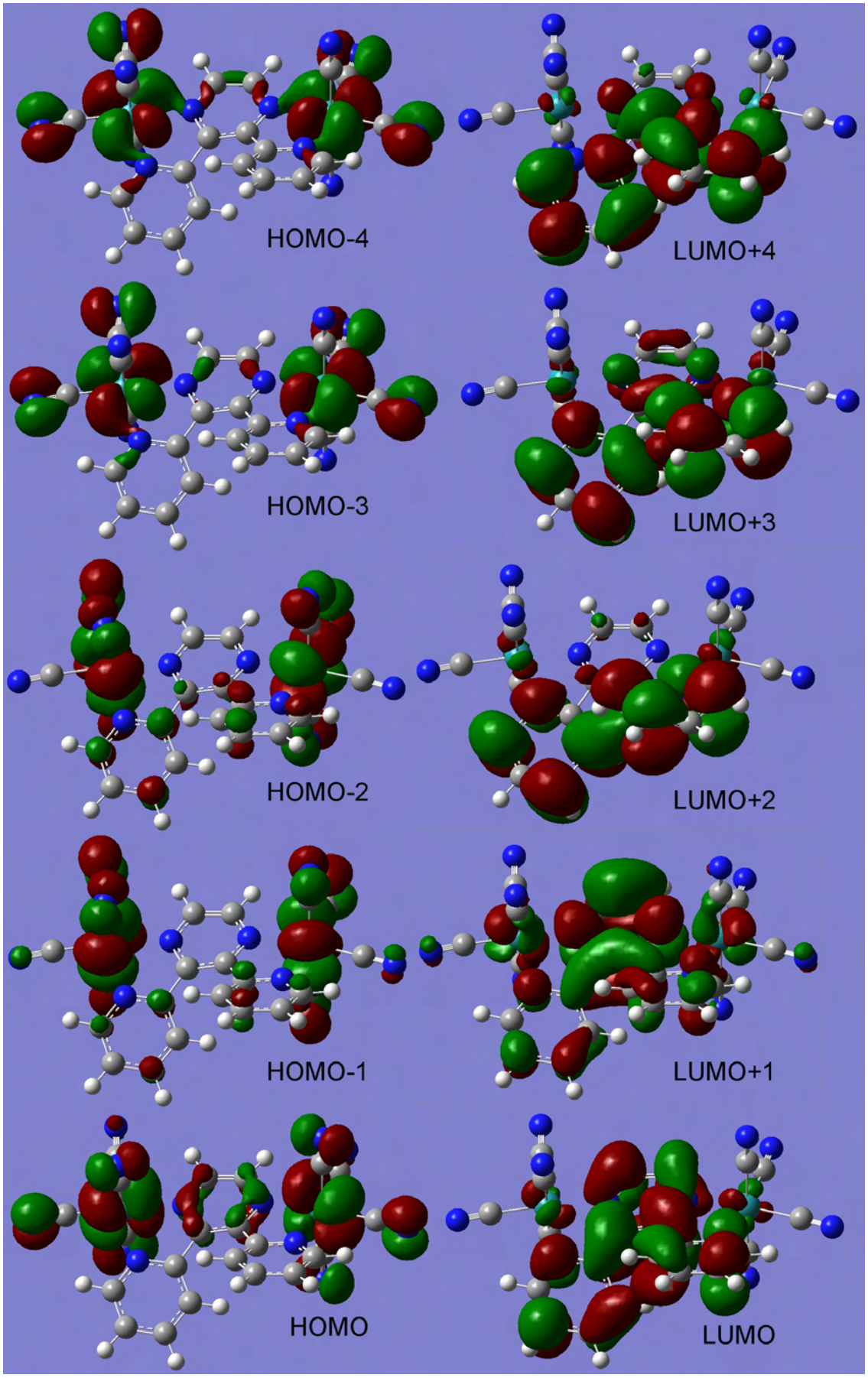
N	-1.38823783	-0.70782989	0.02417860
C	-3.82590437	-0.91586882	1.83375597
C	-0.69824648	0.46098521	0.10913201
C	-0.68973655	-1.85175633	-0.03585381
C	-5.45350409	-0.07582583	-0.36616823
C	-3.24554729	-0.11449600	-2.17988920
C	-3.83657169	-2.45720816	-0.57734913
N	-3.99562931	-1.11362302	2.97368217
C	0.69826669	0.46099547	-0.10920314
C	-1.52417207	1.61704063	0.51977926
C	0.68970752	-1.85177934	0.03524251
H	-1.26162839	-2.76598716	-0.11760040
N	-6.57256985	0.25567135	-0.46074760
N	-3.07987022	0.15452224	-3.30574894
N	-3.95299721	-3.59977126	-0.80454546
C	1.52422094	1.61713207	-0.51956445
N	1.38823295	-0.70785379	-0.02452096
C	-1.00560081	2.74394059	1.16768408
N	-2.86450648	1.45134735	0.37667593
H	1.26157904	-2.76604104	0.11678413
C	1.00568259	2.74419451	-1.16721284
N	2.86454940	1.45137954	-0.37647599
C	-1.86140490	3.74973440	1.59008074
H	0.05525500	2.81962991	1.35511887
C	-3.68661571	2.43919921	0.77170336
C	1.86151385	3.75007105	-1.58935821
H	-0.05516800	2.81994772	-1.35465038
C	3.68668485	2.43930864	-0.77125597
C	-3.22876072	3.60592246	1.36376274
H	-1.46814084	4.62277460	2.09627748
H	-4.74141407	2.25248575	0.61874700
C	3.22886276	3.60617971	-1.36304963
H	1.46827590	4.62323713	-2.09535789
H	4.74147654	2.25253892	-0.61832529
H	-3.93621898	4.36683702	1.66796172
H	3.93634105	4.36715174	-1.66705763
C	5.45350409	-0.07602173	0.36605179
C	3.83653140	-2.45742631	0.57660788
C	3.24551368	-0.11509806	2.17972064
C	3.82592773	-0.91549307	-1.83411098
N	6.57257748	0.25546581	0.46057570
N	3.95305920	-3.60003901	0.80350322
N	3.07914400	0.15379338	3.30550861
N	3.99638486	-1.11342406	-2.97389722
Ru	3.50995755	-0.52192569	0.16964628
Ru	-3.50996089	-0.52181298	-0.16991019

S2.2. TD-DFT

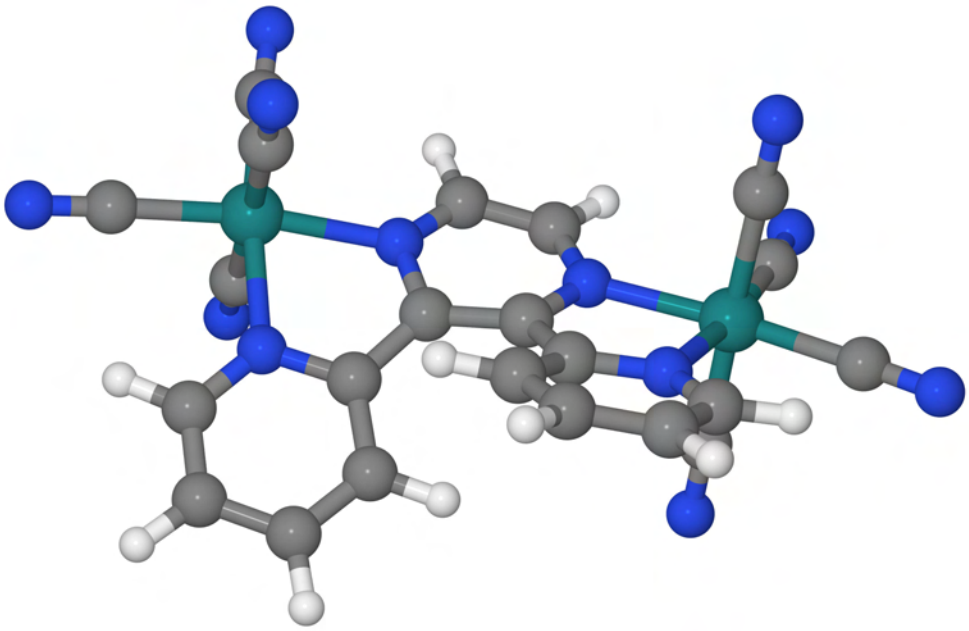
Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in DCM from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
7	16049	623.09	0.06	H-5→LUMO(14%), H-2→L+1(31%), H-1→LUMO(23%), HOMO→L+1(31%)
11	17853	560.12	0.29	H-2→L+1 (49%), HOMO→L+1 (43%)
16	23931	417.87	0.04	H-3→L+2 (39%), H-1→L+2 (38%)
17	24716	404.59	0.10	H-2→L+2 (84%)
19	27094	369.09	0.04	H-5→L+2 (46%), HOMO→L+3 (44%)
20	27259	366.86	0.04	H-1→L+3 (92%)
25	30094	332.29	0.07	H-6→LUMO (51%), HOMO→L+4 (44%)
26	30332	329.68	0.34	H-6→LUMO (44%), HOMO→L+4 (52%)
33	32442	308.24	0.13	H-6→L+1 (72%)
52	35466	281.96	0.05	H-17→LUMO (82%)
74	38428	260.23	0.05	H-6→L+2 (70%)
78	39359	254.07	0.08	H-22→LUMO (25%), H-19→LUMO (56%)
81	39697	251.91	0.06	H-22→LUMO (33%), H-20→LUMO (35%), H-19→LUMO (14%)
82	40031	249.81	0.05	H-7→L+2 (78%)
92	41177	242.85	0.07	H-24→LUMO (82%)

S2.3. Frontier orbitals



S3. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{4-}$ IN DCM SOLVENT (PCM) (^{3}A)



SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{4-,3}$
Charge	:	-4
Multiplicity	:	3
Energy	:	-1692.22558119 a.u.
Gibbs Energy	:	-1692.01263000 a.u.
Number of imaginary frequencies	:	0

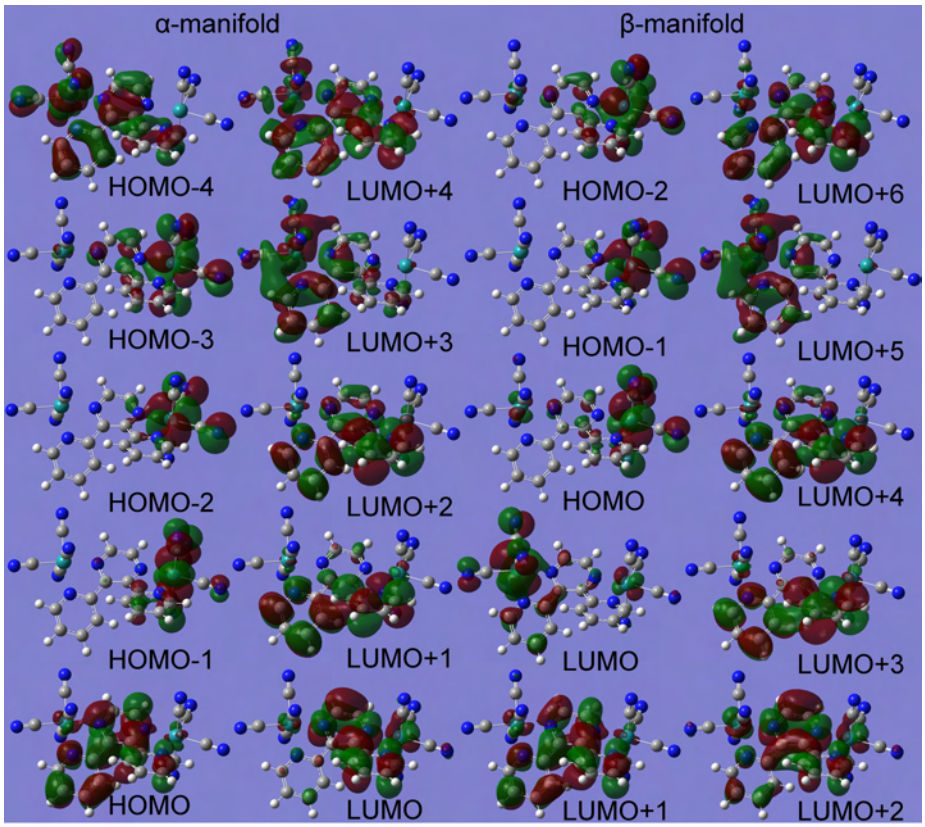
S3.1. Cartesian Co-ordinates (XYZ format)

46

Ru	3.52760768	-0.62498778	0.23797096
Ru	-3.51085496	-0.60900766	-0.30645314
N	-1.38244784	-0.84060270	-0.01728112
C	-3.90472960	-1.22843695	1.63172686
C	-0.71449727	0.36636981	0.15575194
C	-0.67935872	-1.96060336	0.04302977
C	-5.46618223	-0.13736875	-0.45265213
C	-3.14755440	0.02055133	-2.25150800
C	-3.81476998	-2.51615500	-0.90024102
N	-4.12028599	-1.56078792	2.72760344
C	0.71915066	0.35451159	-0.03285140
C	-1.52312768	1.46115959	0.58317137
C	0.70248526	-1.95111847	0.24664663
H	-1.21787190	-2.89256263	-0.07142414
N	-6.58761692	0.17429727	-0.53064883
N	-2.95860791	0.39486989	-3.33909297
N	-3.95591068	-3.62294579	-1.23979592
C	1.52470911	1.47267580	-0.51069337
N	1.39669657	-0.80353314	0.14530860

C	-1.02298868	2.63468051	1.20957756
N	-2.89442229	1.30792284	0.45848879
H	1.26724660	-2.85901403	0.39791745
C	0.98506045	2.60737586	-1.14494777
N	2.87814236	1.31870830	-0.41334262
C	-1.88410950	3.62444544	1.62002742
H	0.03829971	2.72401285	1.39174700
C	-3.71717525	2.28703809	0.86531961
C	1.82542086	3.60113335	-1.61545455
H	-0.08366199	2.68416190	-1.28144324
C	3.68065310	2.29651880	-0.85867310
C	-3.27141118	3.47074032	1.42471004
H	-1.49361718	4.50851631	2.11160374
H	-4.77317715	2.09191346	0.72953075
C	3.20460415	3.45861983	-1.44911993
H	1.41273463	4.47166824	-2.11204076
H	4.74128771	2.11328340	-0.74155843
H	-3.97992778	4.23009777	1.72703469
H	3.90038681	4.21475363	-1.78988481
C	5.48811007	-0.19965069	0.27340353
C	3.87417388	-2.52104664	0.79357839
C	3.39526939	-0.04014026	2.21677279
C	3.70910501	-1.18009901	-1.74390912
N	6.61773062	0.11066268	0.27475846
N	4.02416039	-3.63845110	1.11129844
N	3.30942321	0.32187268	3.32590961
N	3.80597997	-1.47336876	-2.87218523

S3.2. Frontier orbitals



S4. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{3-}$ IN DCM SOLVENT (PCM)

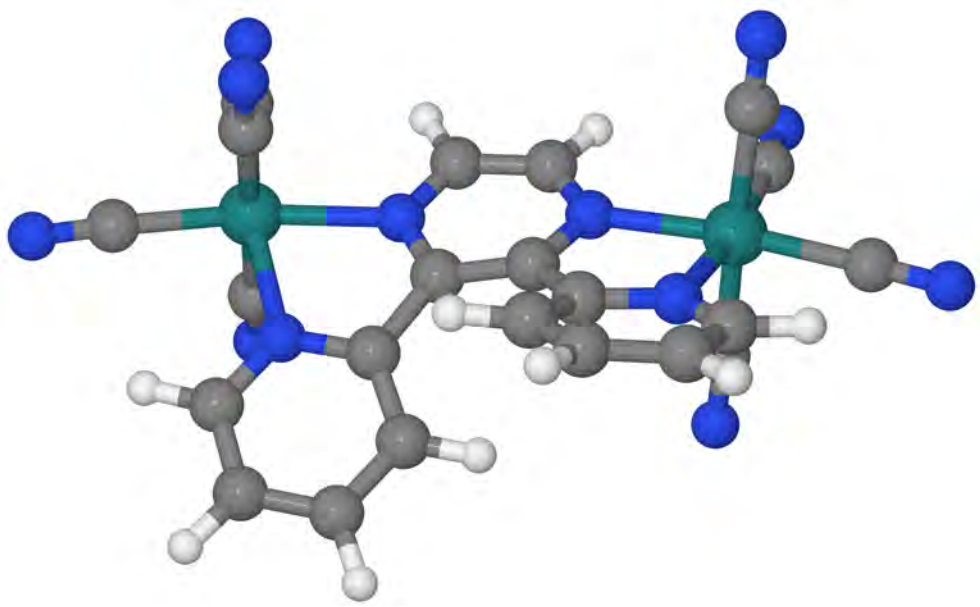


FIG. S2. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in DCM solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{3-,2}$
Charge	:	-3
Multiplicity	:	2
Energy	:	-1692.13477232 a.u.
Gibbs Energy	:	-1691.91901800 a.u.
Number of imaginary frequencies	:	0

S4.1. Cartesian Co-ordinates (XYZ format)

46

Ru	-3.47047663	-0.64565021	-0.18573524
Ru	3.47046304	-0.64553827	0.18582357
N	1.38508499	-0.82833141	-0.02562716
C	3.83132029	-1.02468514	-1.81602383
C	0.69339073	0.34771010	-0.11148576
C	0.68794411	-1.97733343	0.03326533
C	5.43684340	-0.25065690	0.40550584
C	3.23587489	-0.20178305	2.19631267
C	3.79354072	-2.58052468	0.60553664
N	4.02227926	-1.21062529	-2.95130539
C	-0.69338882	0.34767956	0.11173850
C	1.51857889	1.50807822	-0.51841074
C	-0.68785423	-1.97734499	-0.03286509
H	1.25880814	-2.89186597	0.11024007
N	6.56066370	0.04446699	0.51081640
N	3.08395600	0.08561268	3.31621861
N	3.91197610	-3.71757603	0.83987445
C	-1.51863599	1.50810266	0.51846880

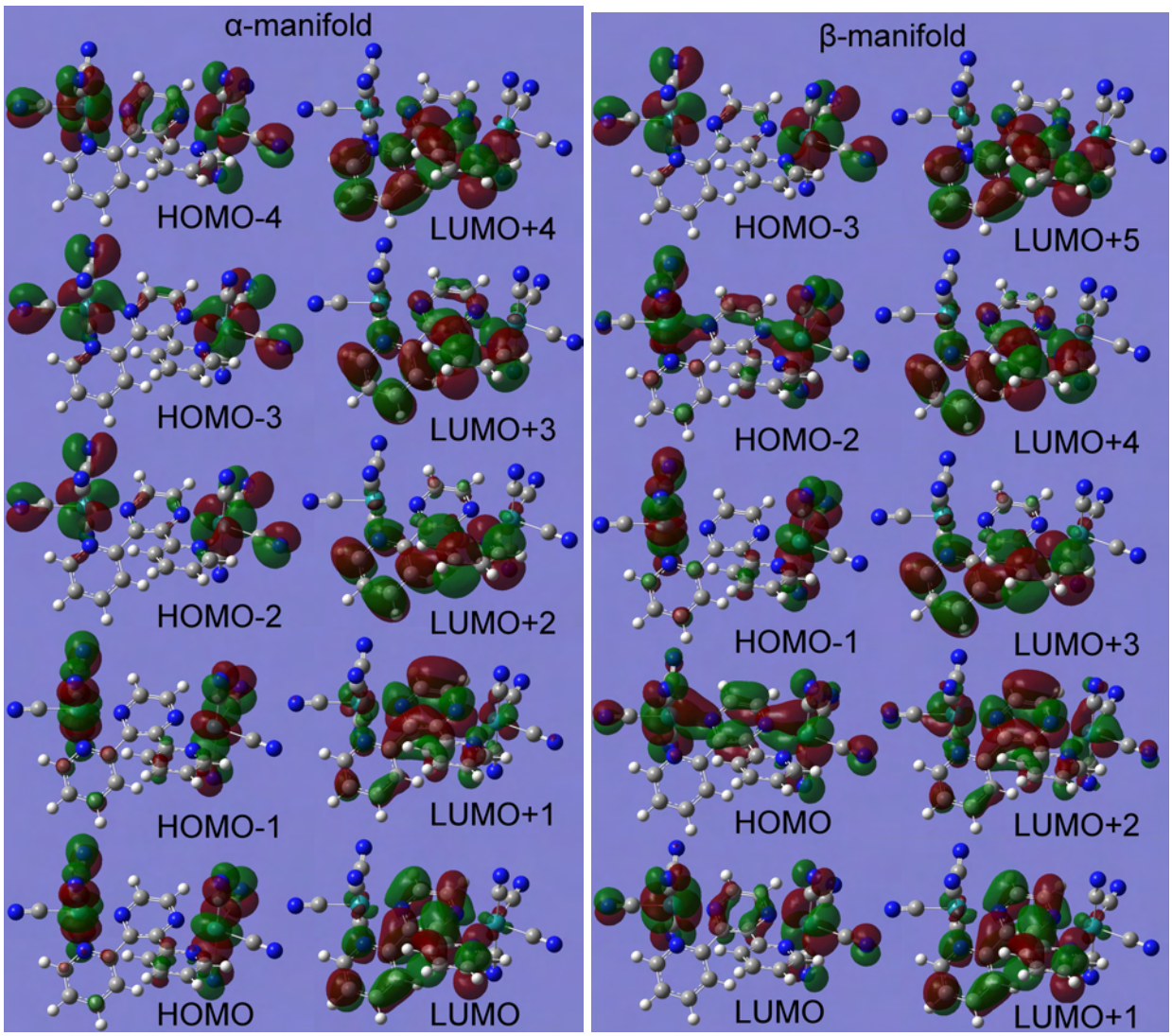
N	-1.38499618	-0.82836425	0.02601554
C	1.00373054	2.63206983	-1.16975987
N	2.85494804	1.35040152	-0.35866627
H	-1.25870192	-2.89189410	-0.10978606
C	-1.00386167	2.63214040	1.16978645
N	-2.85496855	1.35042250	0.35855082
C	1.86547947	3.64118743	-1.57667017
H	-0.05404601	2.70736337	-1.37321329
C	3.68258262	2.33488894	-0.73736721
C	-1.86567771	3.64129138	1.57648706
H	0.05388736	2.70746350	1.37337255
C	-3.68267298	2.33492708	0.73704886
C	3.22807217	3.50370383	-1.33216619
H	1.47675061	4.51439953	-2.08555698
H	4.73601103	2.15247297	-0.57158035
C	-3.22823453	3.50379395	1.33181012
H	-1.47701788	4.51455212	2.08534575
H	-4.73607397	2.15249443	0.57111752
H	3.93645835	4.26783609	-1.62415361
H	-3.93664217	4.26796436	1.62364459
C	-5.43661404	-0.25029209	-0.40599805
C	-3.79371738	-2.58064651	-0.60524893
C	-3.23550463	-0.20244575	-2.19627452
C	-3.83151889	-1.02447081	1.81617129
N	-6.56027651	0.04531057	-0.51166439
N	-3.91223860	-3.71768284	-0.83960289
N	-3.08340025	0.08457384	-3.31625009
N	-4.02249479	-1.21024632	2.95147610

S4.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in DCM from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
5	4159	2404.18	0.17	H-3(β)→LUMO(β) (14%), H-1(β)→LUMO(β) (15%), HOMO(β)⟶LUMO(β) (69%)
22	20833	480.00	0.04	H-3(α)⟶LUMO(α) (54%), H-3(α)⟶L+1(α) (12%), H-3(β)⟶L+1(β) (20%)
25	21357	468.23	0.09	H-2(α)⟶L+1(α) (33%), H-3(β)⟶L+2(β) (33%)
50	27701	360.99	0.05	HOMO(α)⟶L+2(α) (44%), H-1(β)⟶L+3(β) (24%)
59	29810	335.46	0.07	H-4(β)⟶ L+3(β) (53%)
60	29872	334.76	0.14	H-6(α)⟶LUMO(α) (18%), H-5(β)⟶L+1(β) (22%), H-4(β)⟶L+3(β) (19%), HOMO(β)⟶L+5(β) (17%)
61	29893	334.53	0.05	HOMO(β)⟶L+5(β) (55%)
82	31898	313.50	0.09	H-6(α)⟶L+1(α) (11%), H-6(β)⟶L+2(β) (22%), H-5(β)⟶L+2(β) (26%)

S4.3. Frontier orbitals



S5. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{2-}$ IN DCM SOLVENT (PCM)

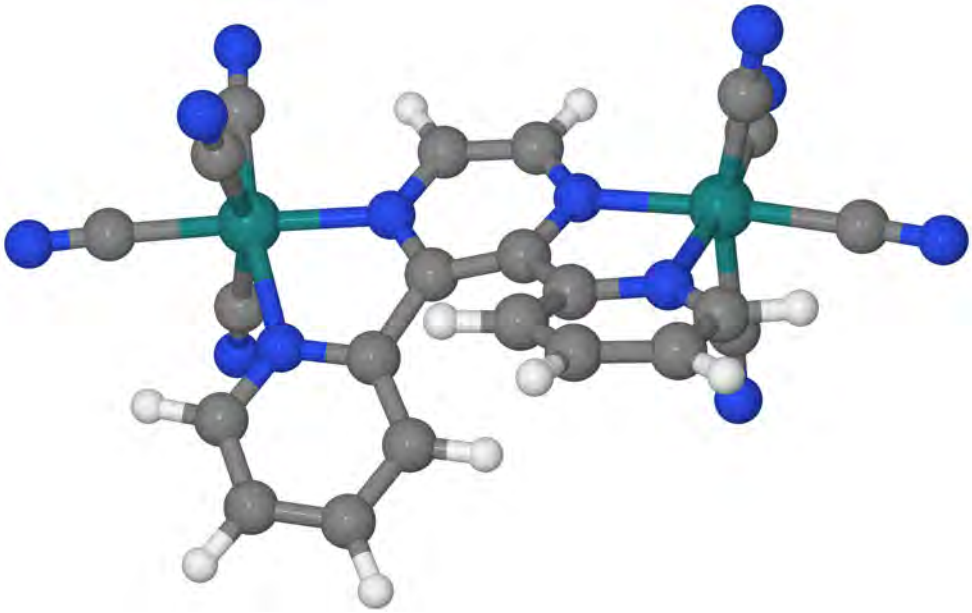


FIG. S3. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in DCM solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-1691.93276716 a.u.
Gibbs Energy	:	-1691.71815400 a.u.
Number of imaginary frequencies	:	0

S5.1. Cartesian Co-ordinates (XYZ format)

46

Ru	3.43199253	-0.56180805	0.13471180
Ru	-3.43258309	-0.56142807	-0.13557060
N	-1.38435805	-0.73408031	0.05298605
C	-4.01080132	-0.77809650	1.81453574
C	-0.68742710	0.44888902	0.12945856
C	-0.68598002	-1.88921511	-0.02043036
C	-5.42702341	-0.24469756	-0.39528301
C	-3.39034629	0.00907747	-2.10137820
C	-3.74085784	-2.49445558	-0.55289137
N	-4.31161976	-0.87037253	2.93626690
C	0.68718487	0.44880432	-0.13136633
C	-1.50480378	1.60875940	0.54624367
C	0.68525058	-1.88939393	0.01709012
H	-1.25605702	-2.80449414	-0.08344986
N	-6.55887890	-0.01367691	-0.52811766
N	-3.32885551	0.37049001	-3.20694566
N	-3.84556103	-3.63202572	-0.78458345
C	1.50479913	1.60878026	-0.54725367

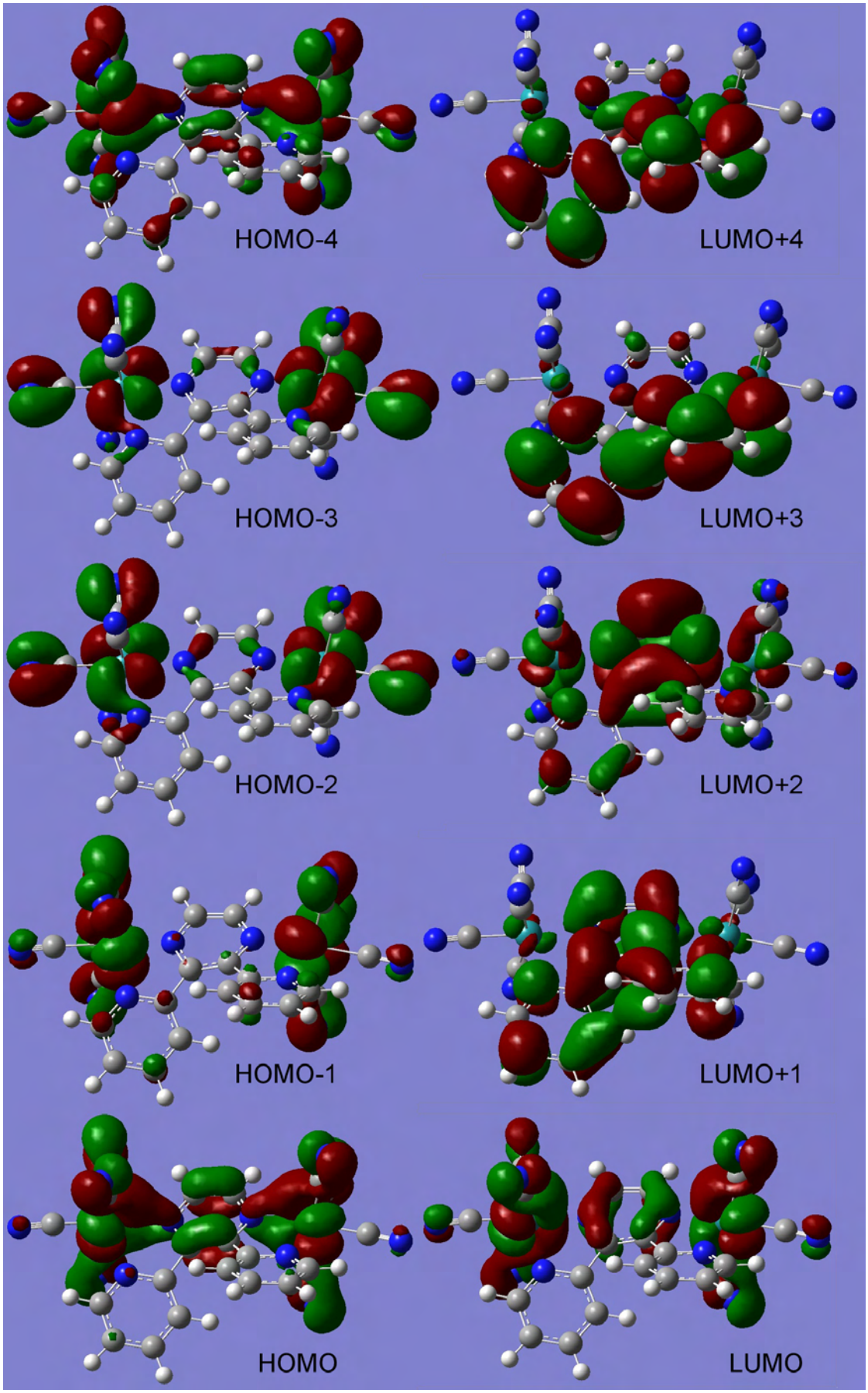
N	1.38388860	-0.73436642	-0.05557941
C	-0.98722899	2.73625350	1.18592179
N	-2.84085155	1.44773412	0.39844629
H	1.25508523	-2.80485654	0.07957818
C	0.98749161	2.73682833	-1.18612814
N	2.84080696	1.44750190	-0.39927793
C	-1.85251677	3.74303889	1.59470046
H	0.07175101	2.81937408	1.37977076
C	-3.67224717	2.42644191	0.77593631
C	1.85292721	3.74397755	-1.59371686
H	-0.07144862	2.82014561	-1.38012171
C	3.67236853	2.42642570	-0.77578449
C	-3.21543598	3.60056019	1.36123765
H	-1.46380639	4.62037230	2.09592271
H	-4.72622919	2.24069667	0.61872566
C	3.21577859	3.60113454	-1.36010742
H	1.46443141	4.62193298	-2.09401703
H	4.72630405	2.24051762	-0.61846948
H	-3.92368197	4.36389637	1.65436995
H	3.92421699	4.36470556	-1.65215600
C	5.42605829	-0.24497367	0.39826143
C	3.73956656	-2.49481702	0.55250823
C	3.38768125	0.00894231	2.10027623
C	4.01544857	-0.77652001	-1.81375146
N	6.55755949	-0.01387467	0.53373986
N	3.84383917	-3.63231540	0.78475064
N	3.32498431	0.37017205	3.20581985
N	4.32002687	-0.86777991	-2.93455172

S5.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in DCM from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
5	9853	1014.93	0.42	H-4→LUMO (35%), HOMO→LUMO (79%)
6	11592	862.67	0.05	H-5→LUMO (93%)
18	19362	516.47	0.05	H-13→LUMO (94%)
24	22556	443.34	0.06	H-20→LUMO (45%), H-1→L+2 (44%)
26	22751	439.55	0.08	H-21→LUMO (12%), H-20→LUMO (36%), H-1→L+2 (32%)
35	25132	397.89	0.05	H-24→LUMO (95%)
40	27974	357.48	0.04	H-30→LUMO (80%), H-29→LUMO (11%)
43	29652	337.24	0.36	H-31→LUMO (13%), H-5→L+1 (81%)
47	30461	328.29	0.09	H-5→L+2 (78%)
88	38570	259.27	0.12	H-17→L+2 (42%), H-16→L+1 (28%), H-4→L+4 (12%)
90	39133	255.54	0.07	H-38→LUMO (10%), H-18→L+1 (63%)
92	39806	251.22	0.09	H-17→L+1 (15%), H-5→L+3 (49%), H-1→L+5 (11%)

S5.3. Frontier orbitals



S6. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{4-}$ IN WATER SOLVENT (PCM)

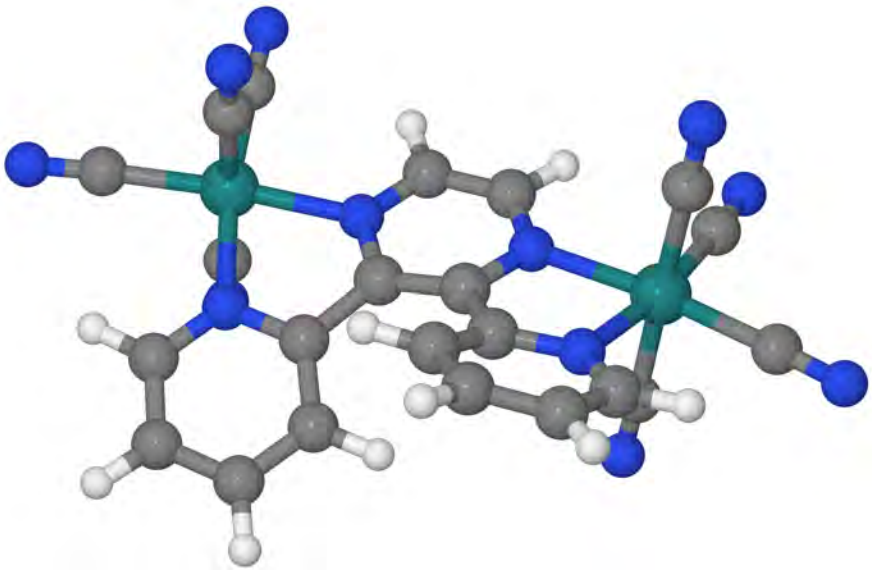


FIG. S4. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{4-}$
Charge	:	-4
Multiplicity	:	1
Energy	:	-1692.36220354 a.u.
Gibbs Energy	:	-1692.14523100 a.u.
Number of imaginary frequencies	:	0

S6.1. Cartesian Co-ordinates (XYZ format)

46

Ru	3.51472402	0.26889423	-0.47447965
Ru	-3.46115923	0.67077279	0.20698553
C	3.11248088	-0.26356274	-2.42842793
C	3.94712639	0.79719925	1.47362638
C	3.91451597	2.14253807	-1.05200267
C	5.42558670	-0.26843607	-0.74594313
N	1.41943443	0.57537293	-0.18775789
N	2.80797005	-1.62677598	0.26719433
N	2.86625648	-0.57699114	-3.52786446
N	4.17847729	1.08550763	2.58318543
N	4.09501123	3.25236416	-1.37956095
C	0.68136722	-0.54450208	0.03638161
C	0.77640176	1.74427700	-0.32321799
C	1.47360361	-1.70383751	0.50493479
C	3.60226226	-2.62029052	0.69944543
C	-0.72300833	-0.49125603	-0.11457188
C	-0.59611583	1.82259703	-0.19627936
C	0.94119442	-2.73792434	1.28180742
C	3.12561512	-3.70352697	1.42277515

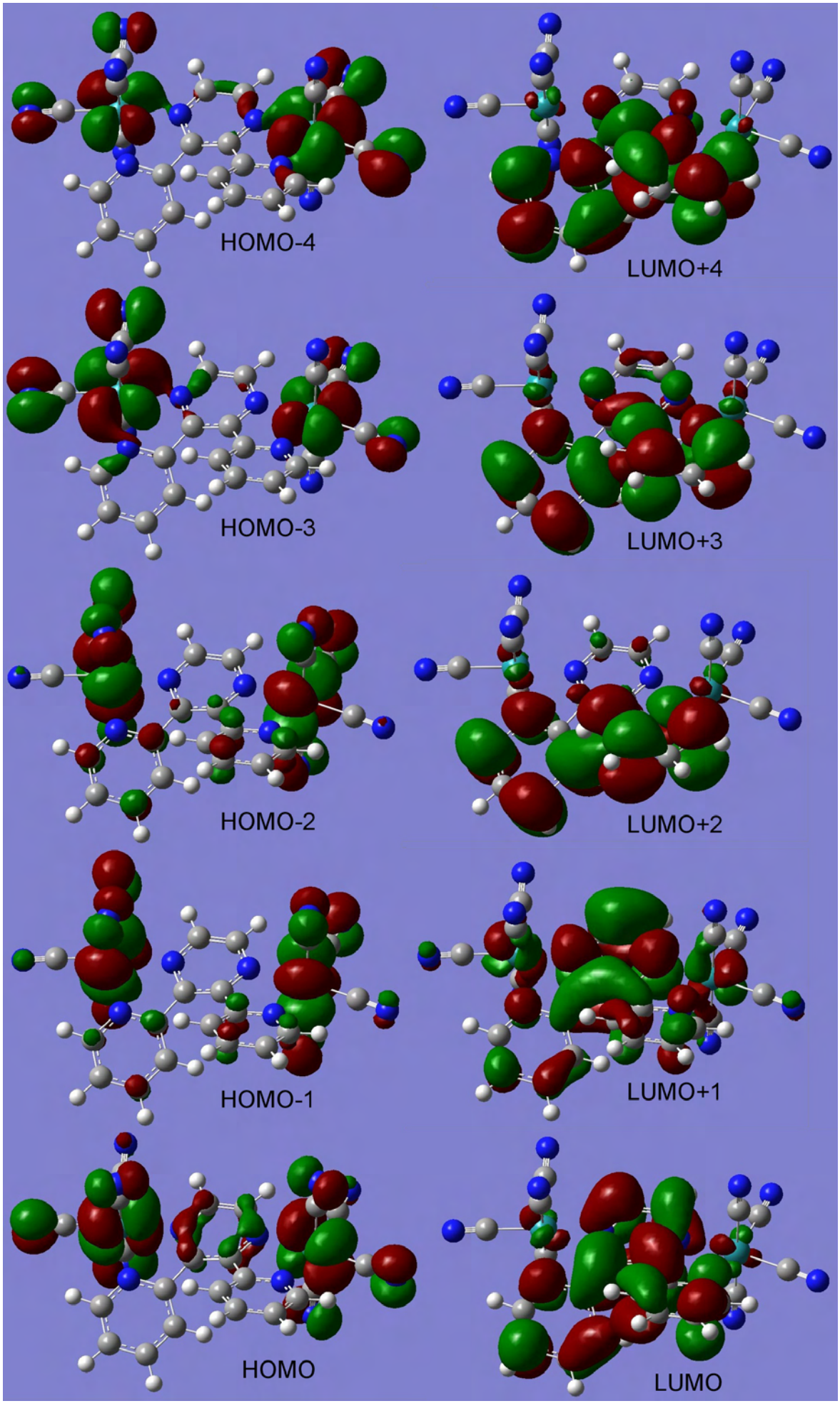
C	-1.62645614	-1.63745165	-0.36197171
N	-1.34886098	0.71596676	-0.11362654
C	1.77129459	-3.74933243	1.74293315
C	-1.20229363	-2.84599710	-0.92389143
N	-2.94510770	-1.38979852	-0.15509908
C	-2.12929940	-3.84266090	-1.19224584
C	-3.83451152	-2.36691880	-0.39816841
C	-3.09406972	0.48287502	2.23008776
C	-5.41191244	0.37928823	0.55812424
C	-3.85896325	0.85902637	-1.80984020
C	-3.67582464	2.64930797	0.41499776
C	-3.47002888	-3.60807419	-0.89866453
N	-2.86986065	0.36180913	3.37144613
N	-6.54477215	0.15946421	0.75649446
N	-4.07216644	0.95277256	-2.95592880
N	-3.74700952	3.81307626	0.52521944
N	6.53053999	-0.62900859	-0.88777661
H	1.38424146	2.61809754	-0.51212609
H	4.65311050	-2.51179457	0.46614805
H	-1.11609900	2.77029896	-0.18204647
H	-0.10841799	-2.74215555	1.53583515
H	3.81122732	-4.47444725	1.74987125
H	1.36799371	-4.55247450	2.34684610
H	-0.16028482	-2.99837422	-1.16311562
H	-1.81003857	-4.78047323	-1.62926292
H	-4.86800051	-2.11639810	-0.19914785
H	-4.22897577	-4.35814047	-1.07969725

S6.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
10	17378	575.44	0.04	H-5→LUMO (92%)
11	18376	544.19	0.29	H-2→L+1 (44%), HOMO→L+1 (46%)
14	25332	394.75	0.04	H-3→L+2 (20%), H-1→L+2 (57%), HOMO→L+3 (11%)
17	26182	381.95	0.09	H-2→L+2 (85%)
19	28589	349.78	0.05	H-5→L+2 (38%), H-2→L+3 (13%), HOMO→L+3 (43%)
24	30328	329.73	0.28	H-6→LUMO (90%)
26	31675	315.70	0.08	HOMO→L+4 (94%)
30	32288	309.71	0.12	H-7→LUMO (17%), H-6→L+1 (37%), H-1→L+4 (35%)
54	36676	272.66	0.06	H-17→LUMO (80%)
74	39092	255.81	0.06	H-6→L+2 (60%)
76	39422	253.66	0.16	H-19→LUMO (83%)
95	42076	237.67	0.08	H-24→LUMO (63%), H-8→L+2 (15%)

S6.3. Frontier orbitals



S7. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{3-}$ IN WATER SOLVENT (PCM)

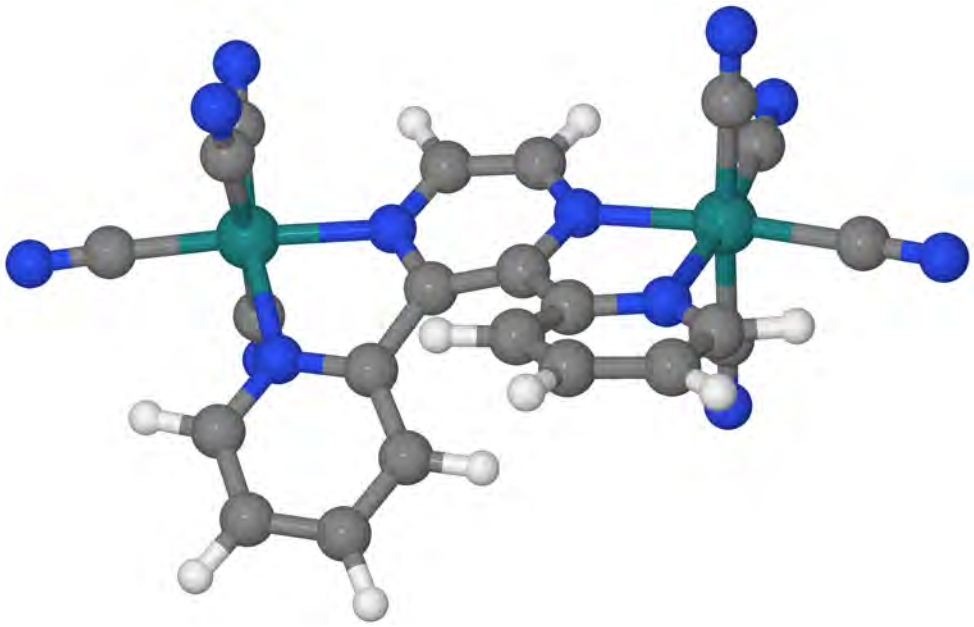


FIG. S5. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in water solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{3-,2}$
Charge	:	-3
Multiplicity	:	2
Energy	:	-1692.18761673 a.u.
Gibbs Energy	:	-1691.97340900 a.u.
Number of imaginary frequencies	:	0

S7.1. Cartesian Co-ordinates (XYZ format)

46

Ru	3.47037864	-0.53218716	0.14668459
Ru	-3.47036934	-0.53208399	-0.14694698
N	-1.38261998	-0.70429981	0.04442259
C	-3.80733848	-0.88054657	1.86446404
C	-0.69283563	0.47302949	0.11872641
C	-0.68803090	-1.85344338	-0.02251295
C	-5.44125986	-0.16105448	-0.36578122
C	-3.24994588	-0.13611068	-2.16665006
C	-3.80187273	-2.47213364	-0.53504962
N	-3.98725796	-1.06390405	3.00206804
C	0.69287622	0.47304410	-0.11878017
C	-1.51818299	1.63477886	0.52290368
C	0.68802834	-1.85346103	0.02193254
H	-1.25738358	-2.76932883	-0.08822269
N	-6.57334614	0.09704056	-0.47968784
N	-3.11200666	0.10207349	-3.29985309
N	-3.94369340	-3.61000705	-0.75337195

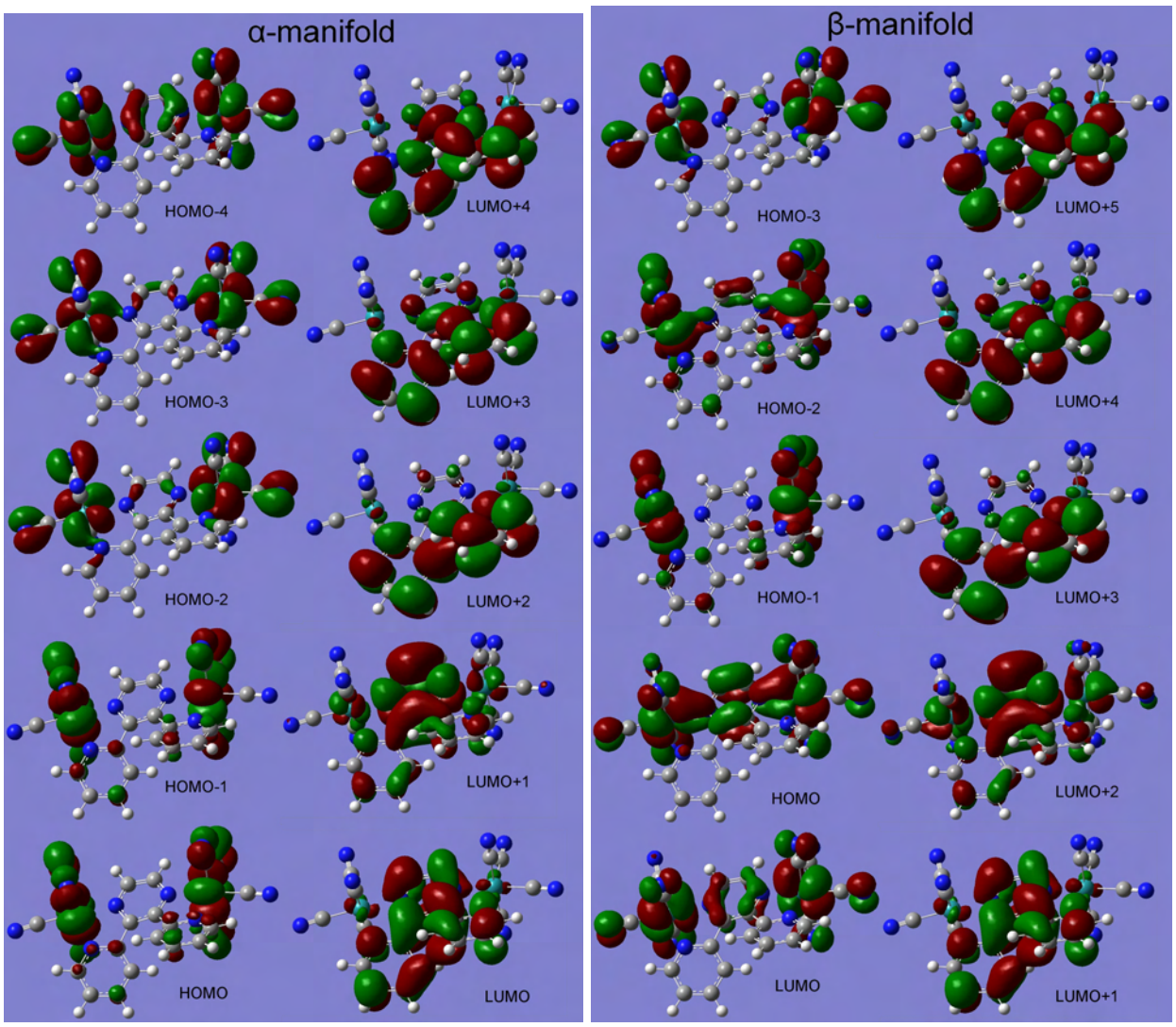
C	1.51824522	1.63486886	-0.52268857
N	1.38264370	-0.70431602	-0.04473400
C	-1.00334787	2.76320386	1.16499090
N	-2.85500598	1.47455668	0.36554053
H	1.25736368	-2.76937222	0.08743370
C	1.00343478	2.76344895	-1.16452527
N	2.85506439	1.47458005	-0.36535633
C	-1.86544681	3.77524281	1.56580353
H	0.05476107	2.84430861	1.36414123
C	-3.68208981	2.46182466	0.73706383
C	1.86555505	3.77555943	-1.56510913
H	-0.05467170	2.84461951	-1.36366284
C	3.68216848	2.46191573	-0.73665828
C	-3.22752142	3.63563323	1.32304215
H	-1.47651374	4.65333176	2.06551981
H	-4.73600817	2.28113103	0.57361859
C	3.22762704	3.63586473	-1.32237542
H	1.47664261	4.65376854	-2.06463027
H	4.73608208	2.28116155	-0.57324988
H	-3.93555784	4.40257406	1.60772514
H	3.93568063	4.40285349	-1.60688543
C	5.44126225	-0.16119809	0.36563268
C	3.80181098	-2.47233534	0.53433895
C	3.24992585	-0.13670427	2.16647863
C	3.80737638	-0.88021612	-1.86479306
N	6.57334566	0.09688459	0.47961569
N	3.94358850	-3.61026621	0.75240070
N	3.11197019	0.10120535	3.29973912
N	3.98731685	-1.06333053	-3.00243473

S7.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in water from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
5	4349	2299.39	0.07	H-3(β)→LUMO(β) (23%), H-1(β)→LUMO(β) (41%), HOMO(β)→LUMO(β) (33%)
20	19795	505.17	0.19	H-2(α)→L+1(α) (49%), H-1(β)→L+2(β) (20%)
53	28213	354.45	0.04	HOMO(α)→L+2(α) (45%), H-1(β)→L+3(β) (31%)
57	28853	346.58	0.07	H-4(α)→LUMO(α) (14%), H-3(α)→L+1(α) (17%), H-1(α)→L+2(α) (21%), H-5(β)→L+1(β) (23%)
61	29254	341.83	0.11	H-4(α)→LUMO(α) (13%), H-4(α)→L+1(α) (10%), H-3(α)→L+1(α) (34%), H-2(α)→L+2(α) (11%), H-5(β)→L+1(β) (12%)
67	30184	331.30	0.07	H-4(α)→L+1(α) (17%), H-3(α)→L+1(α) (10%), HOMO(α)→L+3(α) (18%), H-5(β)→L+2(β) (27%)
70	30797	324.71	0.04	HOMO(α)→L+3(α) (11%), H-31(β)→LUMO(β) (29%), H-1(β)→L+4(β) (12%)

S7.3. Frontier orbitals



S8. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{2-}$ IN WATER SOLVENT (PCM)

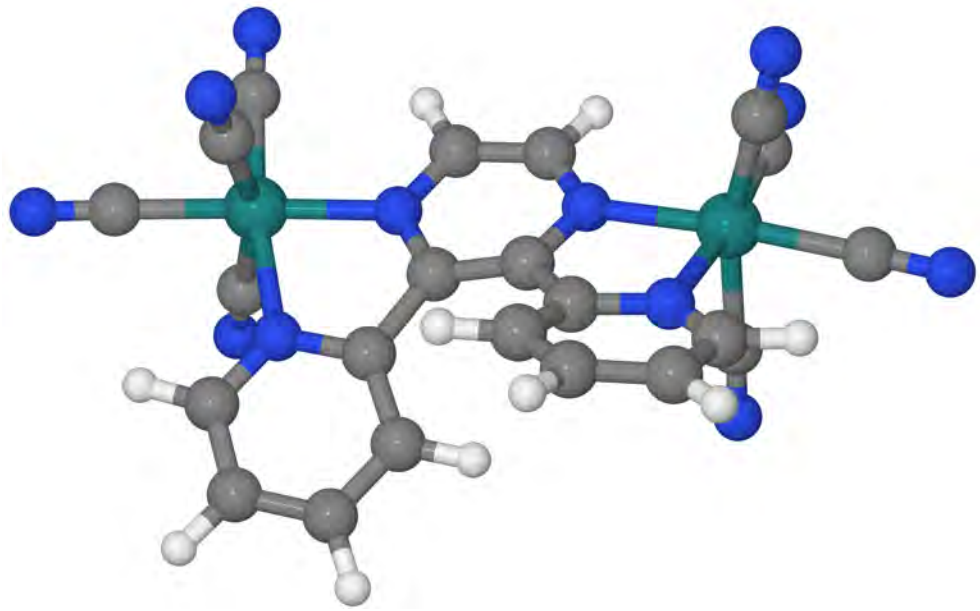


FIG. S6. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in water solvent (PCM)

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N
Formula	:	$C_{22}H_{10}N_{12}Ru_2^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-1691.96256836 a.u.
Gibbs Energy	:	-1691.74866400 a.u.
Number of imaginary frequencies	:	0

S8.1. Cartesian Co-ordinates (XYZ format)

46

Ru	3.42637801	-0.67235231	0.15811920
Ru	-3.42637801	-0.67233819	-0.15812699
N	-1.38303685	-0.83183283	0.04112585
C	-4.01377344	-0.89563805	1.78844941
C	-0.68923825	0.35294086	0.12317812
C	-0.68475664	-1.98768985	-0.02464486
C	-5.42493629	-0.37881142	-0.42785442
C	-3.39151025	-0.13478070	-2.13239288
C	-3.72914410	-2.61175871	-0.56270152
N	-4.33031225	-1.00620437	2.90416741
C	0.68924147	0.35293901	-0.12317707
C	-1.51510489	1.51156890	0.52532035
C	0.68475139	-1.98769224	0.02463523
H	-1.25263524	-2.90369654	-0.09012384
N	-6.56179762	-0.18209498	-0.57326961
N	-3.34929395	0.19194818	-3.24956393
N	-3.84776545	-3.74918842	-0.78794408
C	1.51511228	1.51156616	-0.52531344

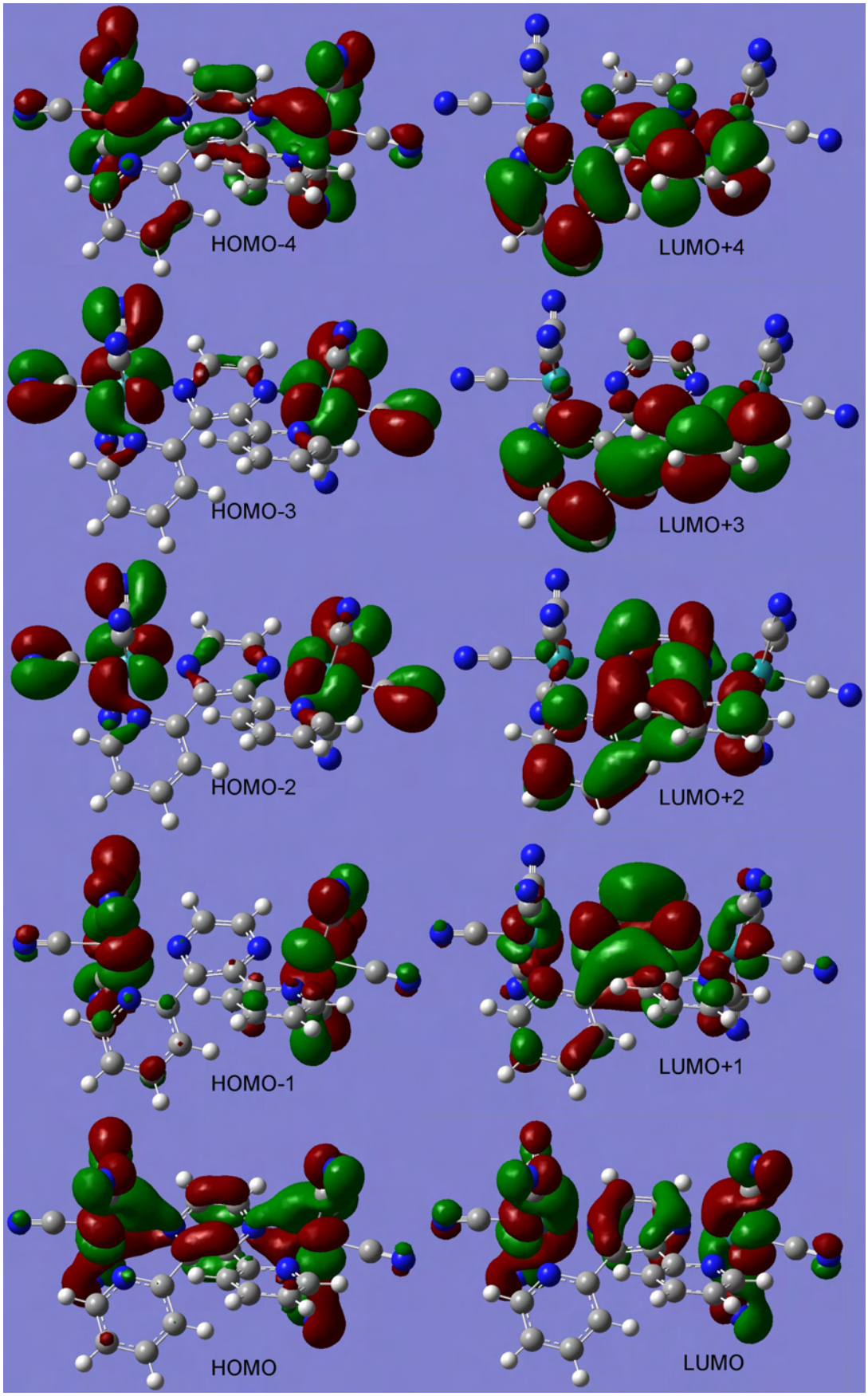
N	1.38303566	-0.83183759	-0.04113092
C	-1.00926077	2.64545274	1.16174185
N	-2.84970140	1.34372699	0.36347839
H	1.25262666	-2.90370131	0.09011071
C	1.00927222	2.64545608	-1.16172755
N	2.84970832	1.34371805	-0.36347395
C	-1.88235998	3.65336013	1.55193472
H	0.04706718	2.73630476	1.36558878
C	-3.68773198	2.32349658	0.72294307
C	1.88237536	3.65336251	-1.55191457
H	-0.04705529	2.73631382	-1.36557353
C	3.68774247	2.32348633	-0.72293293
C	-3.24137855	3.50452685	1.30328250
H	-1.50188386	4.53698921	2.04792929
H	-4.73977852	2.13619947	0.55602312
C	3.24139357	3.50452209	-1.30326438
H	1.50190246	4.53699636	-2.04790354
H	4.73978853	2.13618374	-0.55601519
H	-3.95522380	4.26884842	1.57931328
H	3.95524168	4.26884270	-1.57929087
C	5.42493868	-0.37883940	0.42784408
C	3.72913814	-2.61177564	0.56268281
C	3.39151788	-0.13479774	2.13238549
C	4.01376867	-0.89563692	-1.78846014
N	6.56180191	-0.18213142	0.57325828
N	3.84775591	-3.74920726	0.78791833
N	3.34930348	0.19193473	3.24955559
N	4.33030176	-1.00618958	-2.90418100

S8.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in water from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
3	7226	1383.90	0.08	H-5→LUMO (52%), H-1→LUMO (16%), HOMO→LUMO (30%)
5	8892	1124.67	0.08	H-6→LUMO (12%), H-5→LUMO (15%), H-3→LUMO (49%), HOMO→LUMO (17%)
6	10165	983.76	0.19	H-6→LUMO (11%), H-3→LUMO (49%), H-1→LUMO (13%), HOMO→LUMO (27%)
30	22446	445.52	0.08	H-2→L+1 (13%), H-1→L+2 (60%)
42	28311	353.22	0.15	H-33→LUMO (17%), H-3→L+1 (65%)
44	28729	348.08	0.05	H-36→LUMO (12%), H-34→LUMO (11%), H-33→LUMO (26%), H-3→L+1 (25%)
47	29239	342.01	0.04	H-38→LUMO (20%), H-37→LUMO (10%), H-6→L+1 (19%), H-5→L+1 (27%)
48	29539	338.53	0.23	H-3→L+2 (88%)
49	29779	335.81	0.05	H-6→L+1 (55%), H-5→L+1 (29%)
77	35827	279.12	0.05	H-12→L+1 (38%), H-10→L+2 (22%), H-1→L+4 (16%)
85	36926	270.81	0.04	H-13→L+1 (18%), H-1→L+5 (28%)

S8.3. Frontier orbitals



S9. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{4-}$ IN WATER SOLVENT (PCM) + 8 WATER

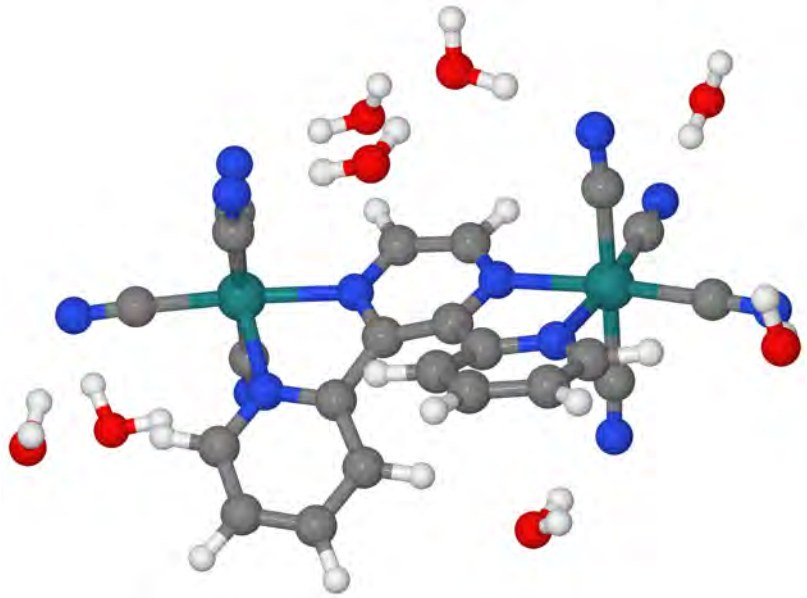


FIG. S7. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water solvent (PCM) with eight additional water molecules: Side-on view

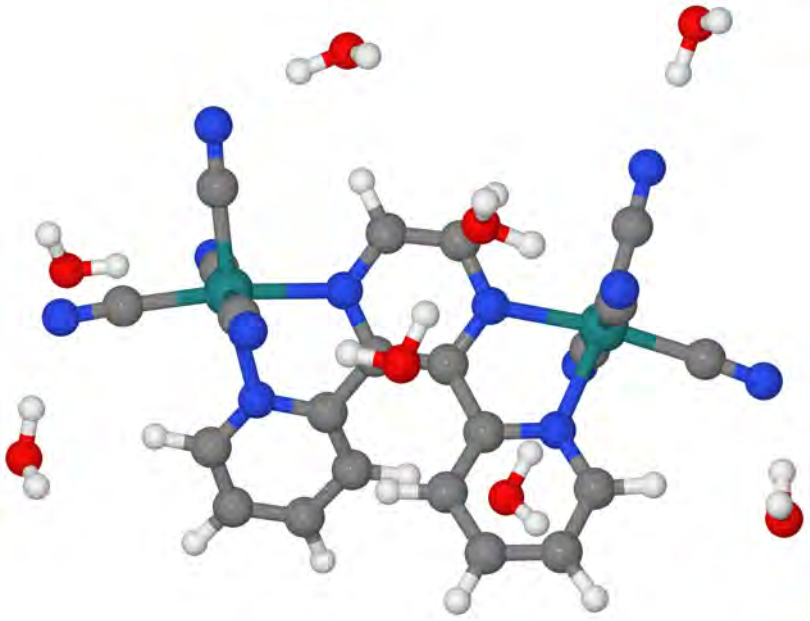


FIG. S8. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water solvent (PCM) with eight additional water molecules: Top view

SMILES	: c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N.O.O.O.O.O.O.O.O.O	
Formula	: $C_{22}H_{26}N_{12}O_8Ru_2^{4-}$	
Charge	:	-4
Multiplicity	:	1
Energy	:	-2304.10605105 a.u.
Gibbs Energy	:	-2303.73167400 a.u.
Number of imaginary frequencies	:	0

S9.1. Cartesian Co-ordinates (XYZ format)

70

Ru	3.54396105	0.12399373	-0.48078233
Ru	-3.43618703	0.78839278	-0.05909815
C	3.19295001	-1.14688873	-2.05876112
C	3.86353111	1.37712753	1.11451030
C	3.99875164	1.62139213	-1.72029507
C	5.44952011	-0.45768815	-0.44524845
N	1.44078624	0.51777345	-0.40753475
N	2.78195143	-1.36989534	0.88038558
N	2.94398570	-1.92015088	-2.90131164
N	3.97946239	2.10856533	2.02084899
N	4.22348547	2.51461124	-2.44211054
C	0.68241876	-0.45766202	0.15718256
C	0.82494861	1.57622623	-0.94645303
C	1.43334258	-1.38951087	1.03056812
C	3.53739524	-2.14250302	1.67892492
C	-0.71444470	-0.44422287	-0.04772352
C	-0.55048460	1.71243799	-0.88128054
C	0.83659065	-2.12317371	2.06009388
C	2.99736142	-2.93832040	2.67972064
C	-1.62413514	-1.60452223	0.07266521
N	-1.31837916	0.70363712	-0.45076558
C	1.62231898	-2.91039181	2.88896656
C	-1.19905627	-2.92064142	-0.13074386
N	-2.93550968	-1.30052412	0.24002700
C	-2.13079500	-3.94857955	-0.06363291
C	-3.82434559	-2.30314541	0.33122441
C	-2.95114708	1.25615871	1.88696837
C	-5.35571909	0.66604906	0.45170903
C	-3.91990948	0.31852955	-1.99996793
C	-3.65177464	2.71804047	-0.49250466
C	-3.46020937	-3.63744497	0.20415343
N	-2.62209916	1.50594401	2.98125839
N	-6.47904015	0.54122710	0.76159984
N	-4.21884871	0.04163945	-3.09710240
N	-3.72426462	3.85443807	-0.77042508
O	-7.22492218	-2.17516398	1.27251768
O	-1.33627510	4.94795895	-1.89529335
O	0.21979059	1.33574259	3.73452163
O	-7.09962559	-0.33417478	-3.07034111
O	1.62929332	-4.09150219	-1.42583501
O	1.54287207	3.51558948	2.48298383
O	5.05984449	4.98850822	-3.57973599
N	6.55438423	-0.84284770	-0.38021389
O	7.03130960	-2.49385071	1.90920103
H	1.44906628	2.32921791	-1.40644884
H	4.60725832	-2.10218453	1.52073622
H	-1.03552771	2.62852669	-1.19183505
H	-0.22796239	-2.06191063	2.22556567
H	3.65287971	-3.54084802	3.29510784
H	1.16785645	-3.48106241	3.68911886
H	-0.16621155	-3.14242721	-0.37501752
H	-1.82046258	-4.97356081	-0.22544147
H	-4.85611200	-2.02173829	0.49856967
H	-4.21777916	-4.40668535	0.28233933
H	-7.06967068	-1.22883689	1.07597315
H	-6.83567572	-2.28275919	2.14695168
H	-2.20807409	4.65224600	-1.56134689
H	-0.86373168	5.19212961	-1.09218204
H	-0.73076600	1.40555882	3.54053402

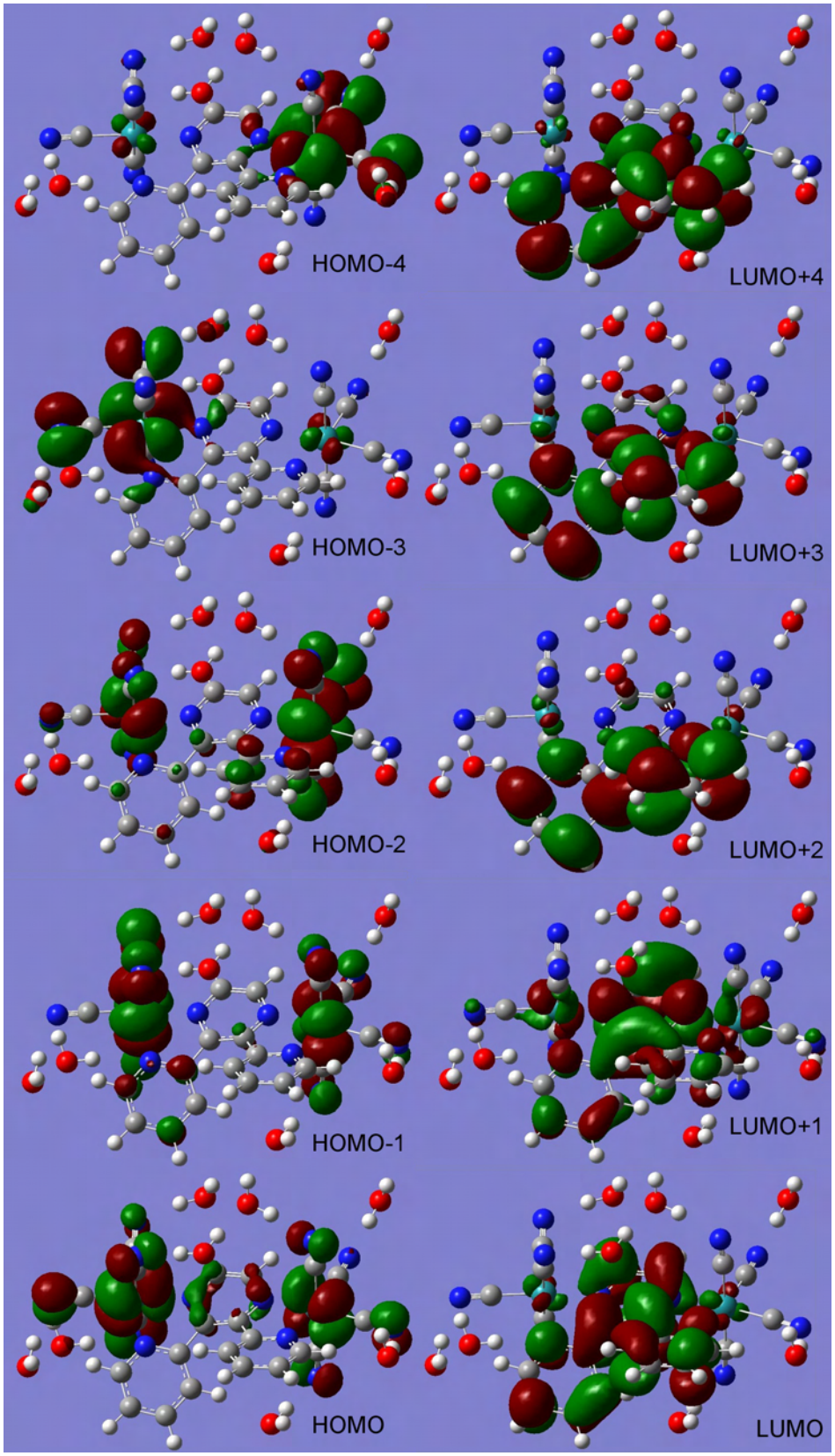
H	0.61643845	2.11845255	3.30994463
H	-6.13331699	-0.24160045	-3.16977215
H	-7.37692833	0.55032921	-2.81004834
H	2.04801869	-3.39354515	-1.96553981
H	2.27030921	-4.25450611	-0.72605759
H	2.42650628	3.10343742	2.37103295
H	1.68051195	4.24448061	3.09719563
H	4.75437641	4.12201023	-3.24359679
H	5.50880861	5.37320089	-2.82040501
H	6.95864105	-1.96579635	1.08820343
H	6.94834948	-1.83151555	2.60353708

S9.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in PCM water + 8 explicit waters from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
9	18829	531.09	0.08	H-5→LUMO (56%), H-4→L+1 (17%), H-2→L+1 (13%)
11	19594	510.37	0.20	H-5→LUMO (22%), H-2→L+1 (32%), HOMO→L+1 (34%)
14	27275	366.64	0.06	H-1→L+2 (73%), HOMO→L+3 (11%)
17	28037	356.67	0.06	H-3→L+2 (12%), H-2→L+2 (70%)
19	29937	334.03	0.27	H-6→LUMO (71%), HOMO→L+3 (14%)
24	31363	318.85	0.11	H-6→L+1 (66%), H-3→L+3 (11%)
28	33619	297.45	0.04	HOMO→L+4 (91%)
54	37954	263.47	0.04	H-18→LUMO (11%), H-17→LUMO (20%), H-16→LUMO (11%), H-14→LUMO (18%)
79	39689	251.96	0.04	H-25→LUMO (18%), H-24→LUMO (24%), H-16→L+1 (12%)
80	39791	251.31	0.08	H-22→LUMO (33%), H-6→L+2 (30%)

S9.3. Frontier orbitals



S10. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{4-}$ IN WATER SOLVENT (PCM) + 8 WATER (^{3}A)

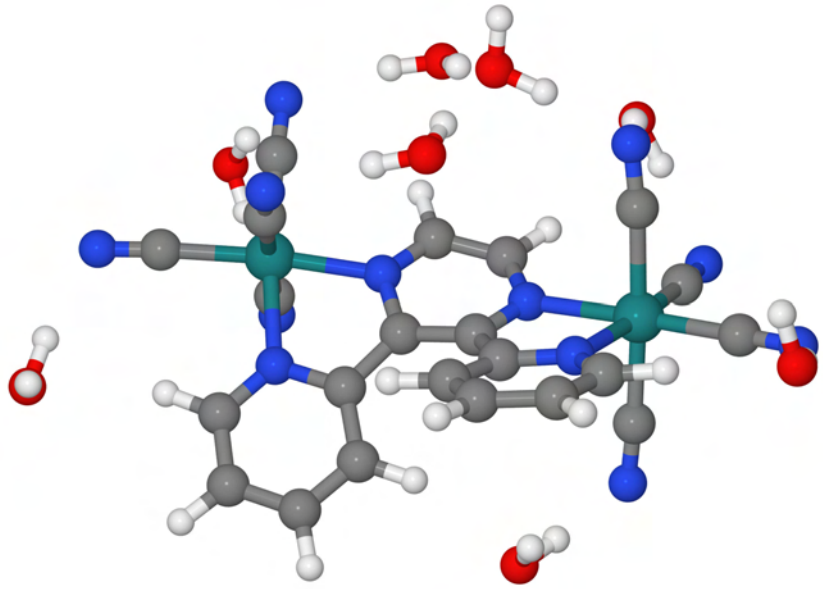


FIG. S9. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water solvent (PCM) with eight additional water molecules: Side-on view of triplet state

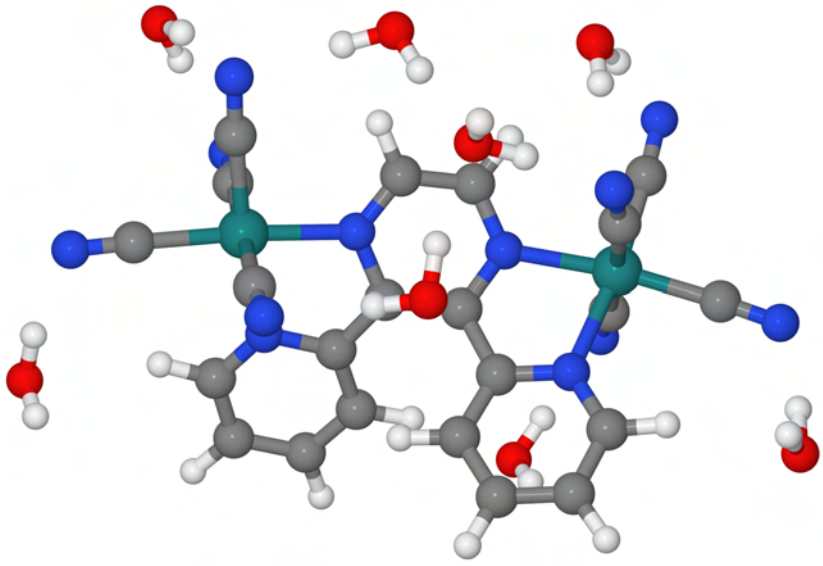


FIG. S10. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{4-}$ in water solvent (PCM) with eight additional water molecules: Top view of triplet state

SMILES	:	c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N.O.O.O.O.O.O.O.O	
Formula	:	$C_{22}H_{26}N_{12}O_8Ru_2^{4-,3}$	
Charge	:	-4	
Multiplicity	:	3	
Energy	:	-2304.05979105	a.u.
Gibbs Energy	:	-2303.68125400	a.u.
Number of imaginary frequencies	:	0	

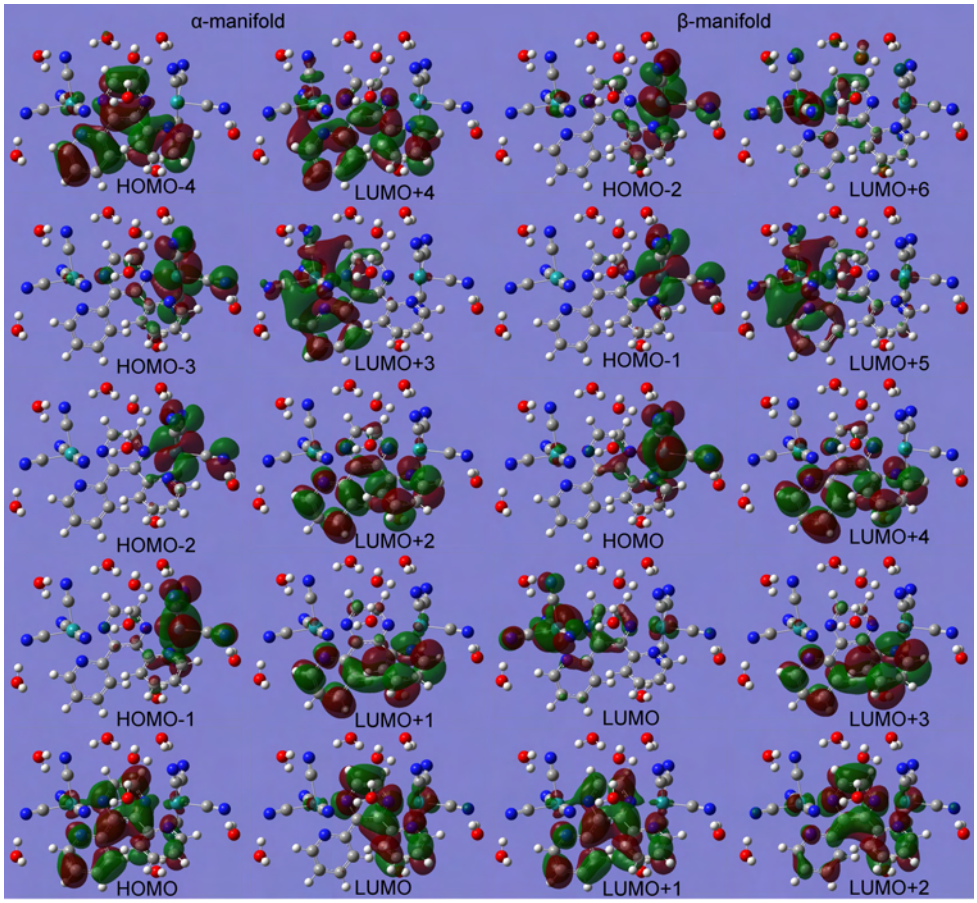
S10.1. Cartesian Co-ordinates (XYZ format)

70

Ru	-3.40102863	0.38491538	0.17997688
C	-3.64164996	2.32394886	0.67568457
C	-5.35520172	0.08113923	0.62278450
N	-3.72670603	3.46109509	0.92622340
C	-3.92558980	0.82881135	-1.77457547
C	-2.87322187	-0.07331362	2.13232660
N	-6.47697878	-0.14244646	0.84964454
N	-4.23283529	1.12672770	-2.85884738
N	-2.52462363	-0.29992378	3.22082376
N	-1.36733890	0.53149599	-0.35387468
C	-0.67021555	1.61636209	-0.66895777
C	-0.72495413	-0.71089268	-0.41476193
C	0.67481792	1.53863502	-1.01410711
H	-1.15991378	2.57810497	-0.59929901
C	0.72149086	-0.68351340	-0.32003695
C	-1.56908929	-1.83606899	-0.60699534
N	1.37171686	0.40667117	-0.75782561
H	1.23630548	2.41420960	-1.30007207
C	1.54785812	-1.65728247	0.39550686
C	-1.12507784	-3.09604001	-1.09166396
N	-2.91785336	-1.63529730	-0.36693159
C	1.01824093	-2.68714881	1.19103515
N	2.89442182	-1.43572402	0.36345983
C	-2.02768683	-4.12009096	-1.25895250
H	-0.08739386	-3.23375988	-1.37090278
C	-3.77797222	-2.65504670	-0.52644628
C	1.86806381	-3.50930715	1.91302681
H	-0.05044144	-2.82172251	1.25419414
C	3.70852423	-2.24433088	1.05858862
C	-3.38538885	-3.91270709	-0.95022178
H	-1.69292152	-5.07620764	-1.64487445
H	-4.81792068	-2.44892097	-0.30401358
C	3.24322128	-3.29616737	1.83669996
H	1.46234095	-4.30053902	2.53199053
H	4.76776266	-2.02896643	0.99838579
H	-4.12131071	-4.69817781	-1.05840731
H	3.94680405	-3.91499376	2.37832642
Ru	3.50112224	0.26605538	-0.82327884
C	5.46908712	-0.05339123	-0.69371039
C	3.80041838	1.84702015	-2.00725675
C	3.50450420	1.55045033	0.77678728
C	3.37926316	-0.97274899	-2.45838165
N	6.61150503	-0.28570294	-0.57023060
N	3.91992235	2.79856181	-2.68130589
N	3.37052846	2.35887909	1.61515629
N	3.24253488	-1.72460163	-3.34463644
O	1.87137842	-4.14278841	-2.51096106
H	2.27627683	-4.27907228	-1.64825785
H	2.31890965	-3.34312391	-2.85127187
O	7.23036671	-2.10980701	1.54233956
H	6.97396564	-1.56631374	2.29498029
H	7.11188602	-1.50465226	0.78181189
O	-7.24862432	-2.89848018	0.28702956
H	-6.86266518	-3.32832909	1.05783105
H	-7.11319160	-1.95140672	0.46973658
O	-0.90446204	4.62706614	0.81898177
H	-0.33941215	4.08494949	1.39705968
H	-1.80428898	4.29965305	0.96769291
O	2.64618278	4.54560137	-0.59740555

H	2.85336971	3.95631862	0.14287432
H	3.06176353	4.08647346	-1.34777367
O	0.83829564	3.14985919	2.59854388
H	0.96680671	3.71100402	3.37198997
H	1.74609172	2.94252419	2.27410650
O	0.38418081	0.46777061	3.54642510
H	-0.55118227	0.22013699	3.49753809
H	0.41773739	1.38753808	3.23188591
O	-5.55386782	3.73887849	-1.66160297
H	-5.00978470	3.78454161	-0.86283332
H	-5.17073631	2.98973441	-2.13989091

S10.2. Frontier orbitals



S11. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{3-}$ IN WATER SOLVENT (PCM) + 8 WATER

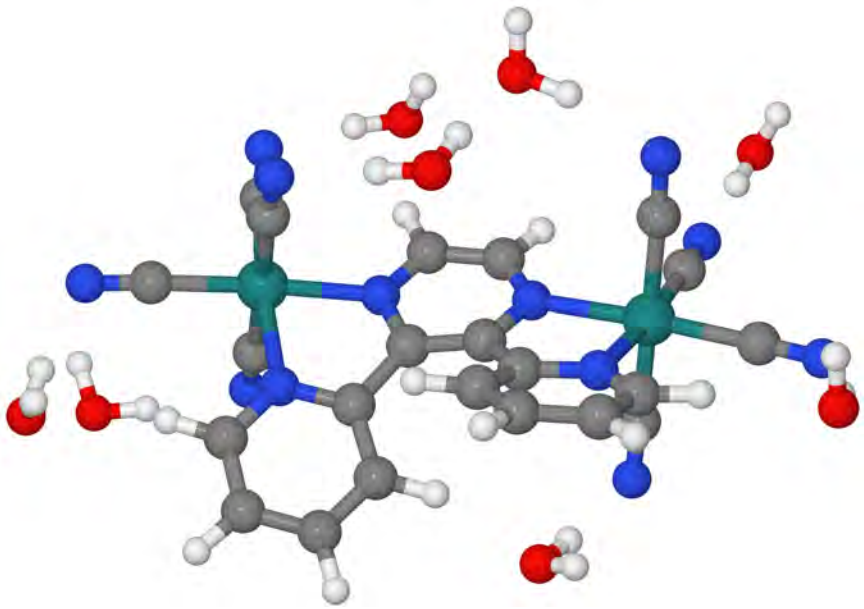


FIG. S11. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in water solvent (PCM) with eight additional water molecules: Side-on view

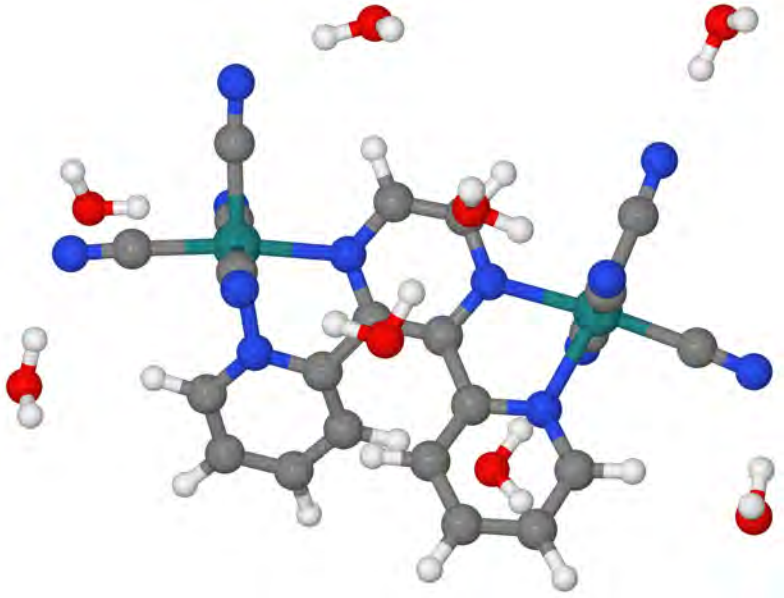


FIG. S12. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in water solvent (PCM) with eight additional water molecules: Top view

SMILES	: c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N.O.O.O.O.O.O.O.O.O	
Formula	: $C_{22}H_{26}N_{12}O_8Ru_2^{3-,2}$	
Charge	: -3	
Multiplicity	: 2	
Energy	: -2303.92073604	a.u.
Gibbs Energy	: -2303.55247700	a.u.
Number of imaginary frequencies	: 0	

S11.1. Cartesian Co-ordinates (XYZ format)

70

Ru	3.50219440	0.28964677	-0.44150546
Ru	-3.43389010	0.65814400	0.27523965
C	3.18081832	-0.40918887	-2.36097598
C	3.82674885	0.93070847	1.50000405
C	3.96384907	2.12824774	-1.11534858
C	5.45223236	-0.15431359	-0.64201158
N	1.40354204	0.59228784	-0.20436282
N	2.80465961	-1.60048020	0.31790215
N	2.96335006	-0.86438739	-3.41107249
N	3.94152832	1.31935799	2.59171391
N	4.19187450	3.20378566	-1.49731171
C	0.67452985	-0.53561181	0.00151858
C	0.77109313	1.76405525	-0.33836058
C	1.46044159	-1.69429028	0.48417613
C	3.59852457	-2.58520508	0.76708841
C	-0.72498268	-0.47883531	-0.16125053
C	-0.60181361	1.84385443	-0.20288068
C	0.90651298	-2.75181675	1.20580208
C	3.09618402	-3.69197726	1.43800831
C	-1.62112665	-1.62352312	-0.42595991
N	-1.34862030	0.73258507	-0.12652859
C	1.73010635	-3.76233006	1.68292344
C	-1.19153261	-2.79192734	-1.06044614
N	-2.93157363	-1.40483141	-0.15186967
C	-2.11838031	-3.79177856	-1.32831788
C	-3.81474257	-2.38671136	-0.38928697
C	-2.96895051	0.42658615	2.27016449
C	-5.35860157	0.36316583	0.72503823
C	-3.95036793	0.87751877	-1.70511007
C	-3.66151142	2.62191463	0.52831990
C	-3.44479156	-3.59969163	-0.95747989
N	-2.65708566	0.27797845	3.38641548
N	-6.47857857	0.13769913	0.97791153
N	-4.27238464	0.98960310	-2.82325196
N	-3.74087024	3.78301454	0.65445435
O	-7.20534515	-2.60942316	0.53343493
O	-1.35482585	5.19163752	-0.06564980
O	0.22090843	-0.17944868	3.88043404
O	-7.15343285	0.55177546	-2.91653013
O	1.56813526	-3.43022585	-2.69784069
O	1.45518124	2.37641406	3.66717410
O	5.01821852	5.95212555	-1.93062401
N	6.57190084	-0.46526888	-0.72828251
O	7.03500748	-2.95971560	0.73474467
H	1.37472904	2.64129496	-0.52130091
H	4.66310692	-2.47443295	0.60447037
H	-1.10091197	2.80320692	-0.17209925
H	-0.15217426	-2.77610517	1.41098523
H	3.77582741	-4.45982885	1.78272653
H	1.30757987	-4.58569765	2.24465275
H	-0.16199538	-2.91305828	-1.37835824
H	-1.80532455	-4.70139599	-1.82563281
H	-4.84597301	-2.18694329	-0.12776498
H	-4.19743538	-4.35776424	-1.13160682
H	-7.06573105	-1.65251172	0.67577571
H	-6.83128881	-3.00584221	1.32765687
H	-2.23092985	4.81868887	0.15914117
H	-0.88873285	5.18606710	0.77746642
H	-0.73794657	-0.05383599	3.78330231

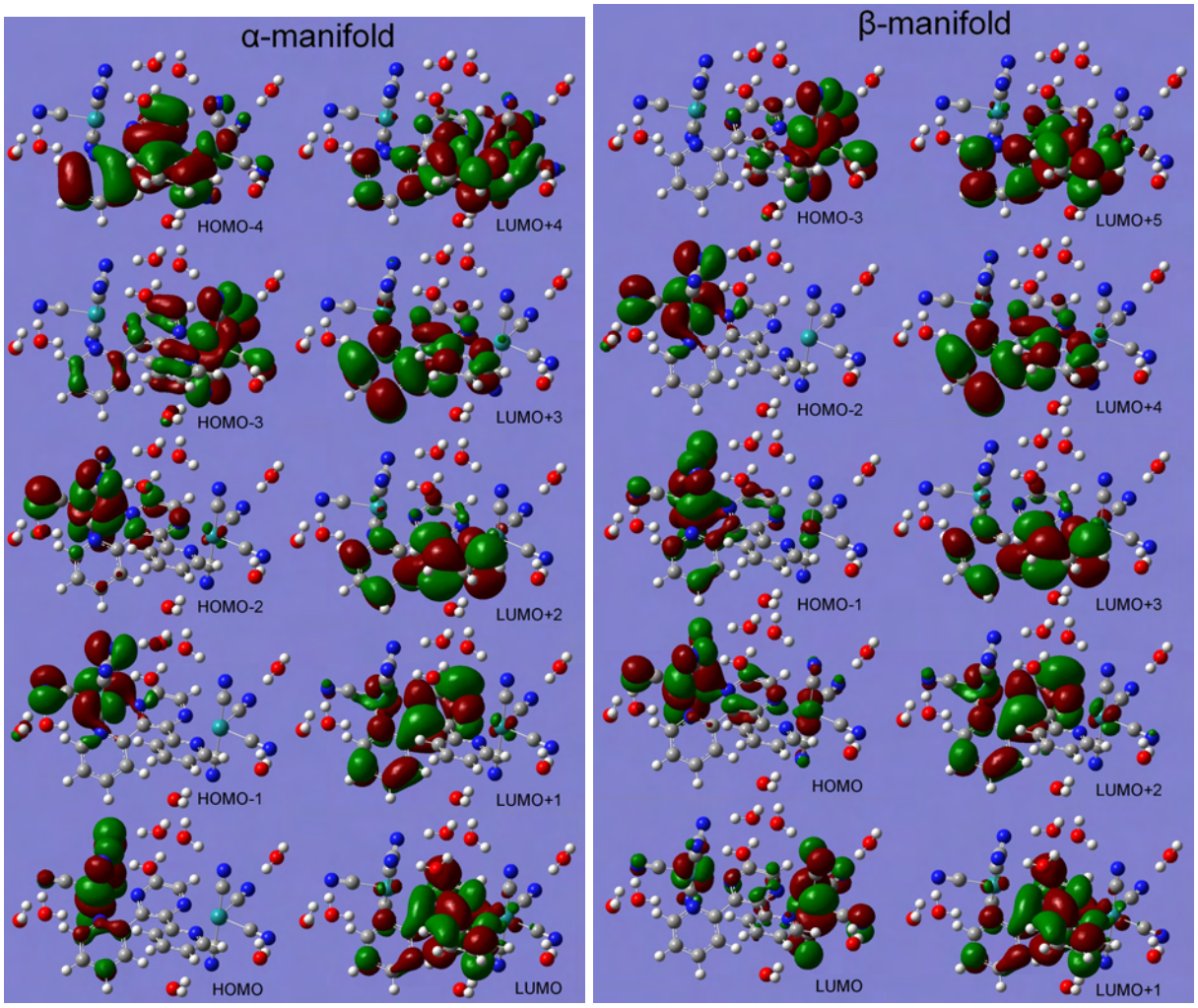
H	0.59019649	0.72052044	3.82621574
H	-6.19254017	0.69718277	-2.99159837
H	-7.44511080	1.29662728	-2.38064647
H	1.98865223	-2.61802101	-3.02578068
H	2.27816939	-3.88902330	-2.23637772
H	2.35442328	2.09030080	3.42187738
H	1.55172026	2.79856825	4.52761221
H	4.71895742	5.02939892	-1.84653664
H	5.49717045	6.10522556	-1.10993826
H	7.01764059	-2.15786839	0.18378419
H	7.03516388	-2.61235356	1.63341069

S11.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{3-}$ in PCM water + 8 explicit waters from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
5	4349	2299.39	0.07	H-3(β)→LUMO(β) (23%), H-1(β)→LUMO(β) (41%), HOMO(β)→LUMO(β) (33%)
20	19795	505.17	0.19	H-2(α)→L+1(α) (49%), H-1(β)→L+2(β) (20%)
53	28213	354.45	0.04	HOMO(α)→L+2(α) (45%), H-1(β)→L+3(β) (31%)
57	28853	346.58	0.07	H-4(α)→LUMO(α) (14%), H-3(α)→L+1(α) (17%), H-1(α)→L+2(α) (21%), H-5(β)→L+1(β) (23%)
61	29254	341.83	0.11	H-4(α)→LUMO(α) (13%), H-4(α)→L+1(α) (10%), H-3(α)→L+1(α) (34%), H-2(α)→L+2(α) (11%), H-5(β)→L+1(β) (12%)
67	30184	331.30	0.07	H-4(α)→L+1(α) (17%), H-3(α)→L+1(α) (10%), HOMO(α)→L+3(α) (18%), H-5(β)→L+2(β) (27%)
70	30797	324.71	0.04	HOMO(α)→L+3(α) (11%), H-31(β)→LUMO(β) (29%), H-1(β)→L+4(β) (12%)

S11.3. Frontier orbitals



S12. $[(RU(CN)_4)_2(\mu\text{-DPPZ})]^{2-}$ IN WATER SOLVENT (PCM) + 8 WATER

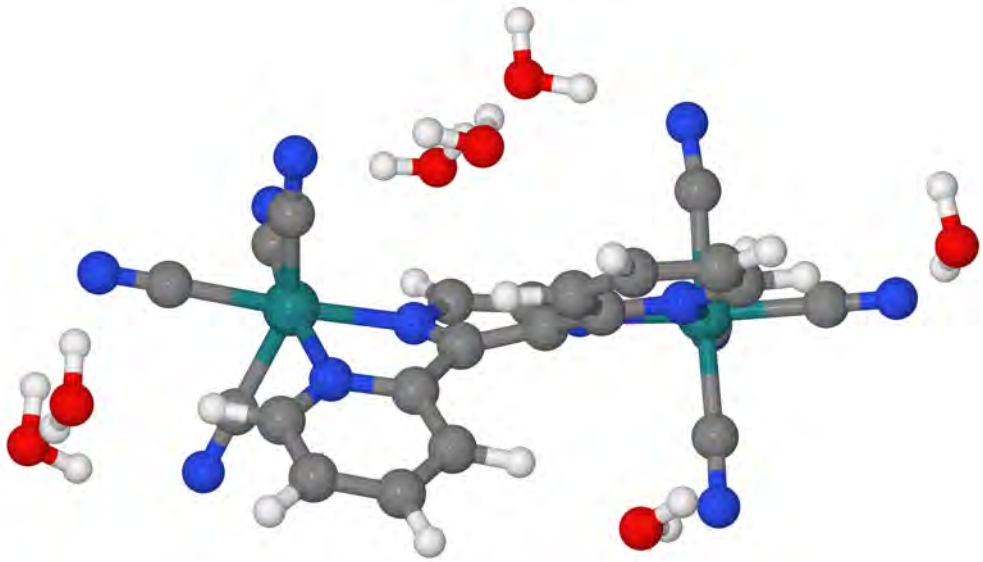


FIG. S13. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with eight additional water molecules: Side-on view

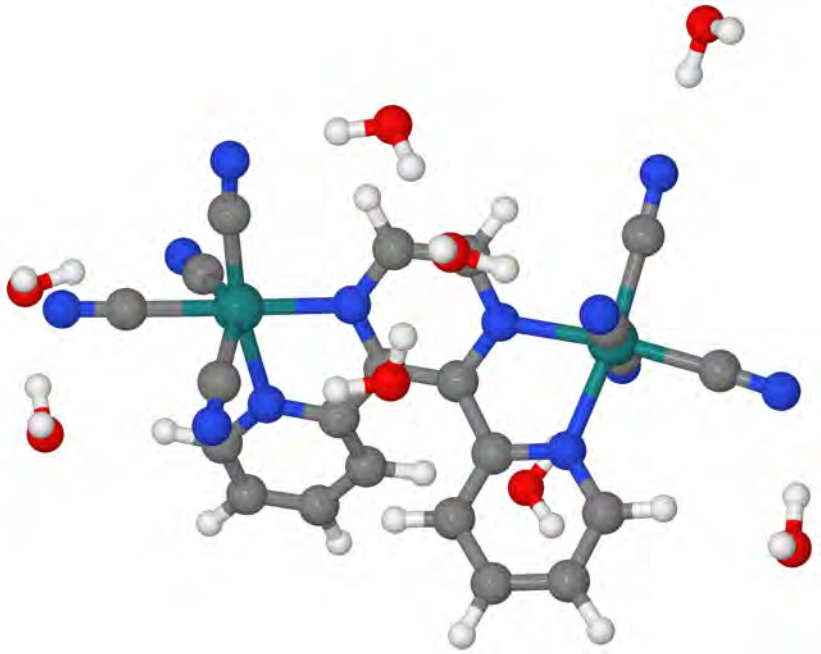


FIG. S14. structure of $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with eight additional water molecules: Top view

SMILES	: c1cc[n+]2c(c1)C3=C4c5cccc[n+]5[Ru](N4C=CN3[Ru]2(C#N)(C#N)(C#N)C#N)(C#N)(C#N)(C#N)C#N.O.O.O.O.O.O.O.O.O	
Formula	: $C_{22}H_{26}N_{12}O_8Ru_2^{2-}$	
Charge	:	-2
Multiplicity	:	1
Energy	:	-2303.70232040 a.u.
Gibbs Energy	:	-2303.31940700 a.u.
Number of imaginary frequencies	:	1

S12.1. Cartesian Co-ordinates (XYZ format)

70

Ru	3.53327727	0.25709298	-0.45693731
Ru	-3.27754545	0.67509162	0.19729769
C	3.46762586	-0.65621930	-2.29888248
C	3.67120600	1.16701794	1.39378893
C	3.94577599	2.03484988	-1.28970575
C	5.50354671	-0.14963208	-0.36810115
N	1.48372579	0.51676536	-0.37684077
N	2.84051204	-1.59845543	0.40294084
N	3.37577248	-1.22901332	-3.31145334
N	3.63668013	1.74145448	2.40823865
N	4.14735174	3.07630563	-1.77270794
C	0.73478734	-0.60167396	-0.13343218
C	0.86307108	1.70412171	-0.50243229
C	1.49121642	-1.73755956	0.43414491
C	3.61203456	-2.53920603	0.96551055
C	-0.65279418	-0.52945590	-0.32997045
C	-0.49665946	1.80655861	-0.34778276
C	0.89662933	-2.79791880	1.11948967
C	3.07875538	-3.64743781	1.61218226
C	-1.56817377	-1.64450812	-0.62174708
N	-1.26010787	0.69642377	-0.28675935
C	1.69781089	-3.76701450	1.70771921
C	-1.16219199	-2.82951593	-1.23453367
N	-2.87948942	-1.38657010	-0.38762370
C	-2.12112594	-3.79398727	-1.52734280
C	-3.79896426	-2.32346368	-0.65348619
C	-3.23935103	-0.11337103	2.03875518
C	-5.24020624	0.71167171	0.78365117
C	-4.31705856	0.68839705	-1.52212703
C	-3.32217360	2.61421967	0.69904655
C	-3.45050406	-3.55118680	-1.20798707
N	-3.13535452	-0.55602747	3.10953283
N	-6.36241627	0.74113500	1.08074939
N	-4.92027044	0.68096620	-2.51673746
N	-3.23359656	3.73285937	1.01269615
O	-7.05448008	-2.17284226	-0.10211486
O	-0.25974044	4.60723591	1.17519891
O	0.00113110	0.36753747	2.73219585
O	-7.76345587	0.16661721	-1.55363107
O	1.67446220	-3.57383919	-2.61130905
O	1.10867393	2.94325209	3.08473825
O	4.87688303	5.84173632	-2.10694051
N	6.63132763	-0.43673953	-0.27986392
O	7.06269836	-2.82225609	1.32704294
H	1.47897732	2.57210016	-0.68116313
H	4.68315458	-2.39301538	0.91264158
H	-0.97321689	2.77048683	-0.27226108
H	-0.17602497	-2.86001015	1.21460044
H	3.74377799	-4.37934208	2.05117488
H	1.24574471	-4.59371376	2.24071813
H	-0.12514739	-2.99073553	-1.51220250
H	-1.82599628	-4.71870899	-2.00708818
H	-4.83565664	-2.08727837	-0.43769151
H	-4.22491932	-4.27933884	-1.40907323
H	-7.33561134	-1.47322226	-0.72310776
H	-6.91350603	-1.67873895	0.71430212
H	-1.20564675	4.47415686	1.32764709
H	0.18520473	4.05318308	1.84088337
H	-0.89473647	0.26428494	3.07296181

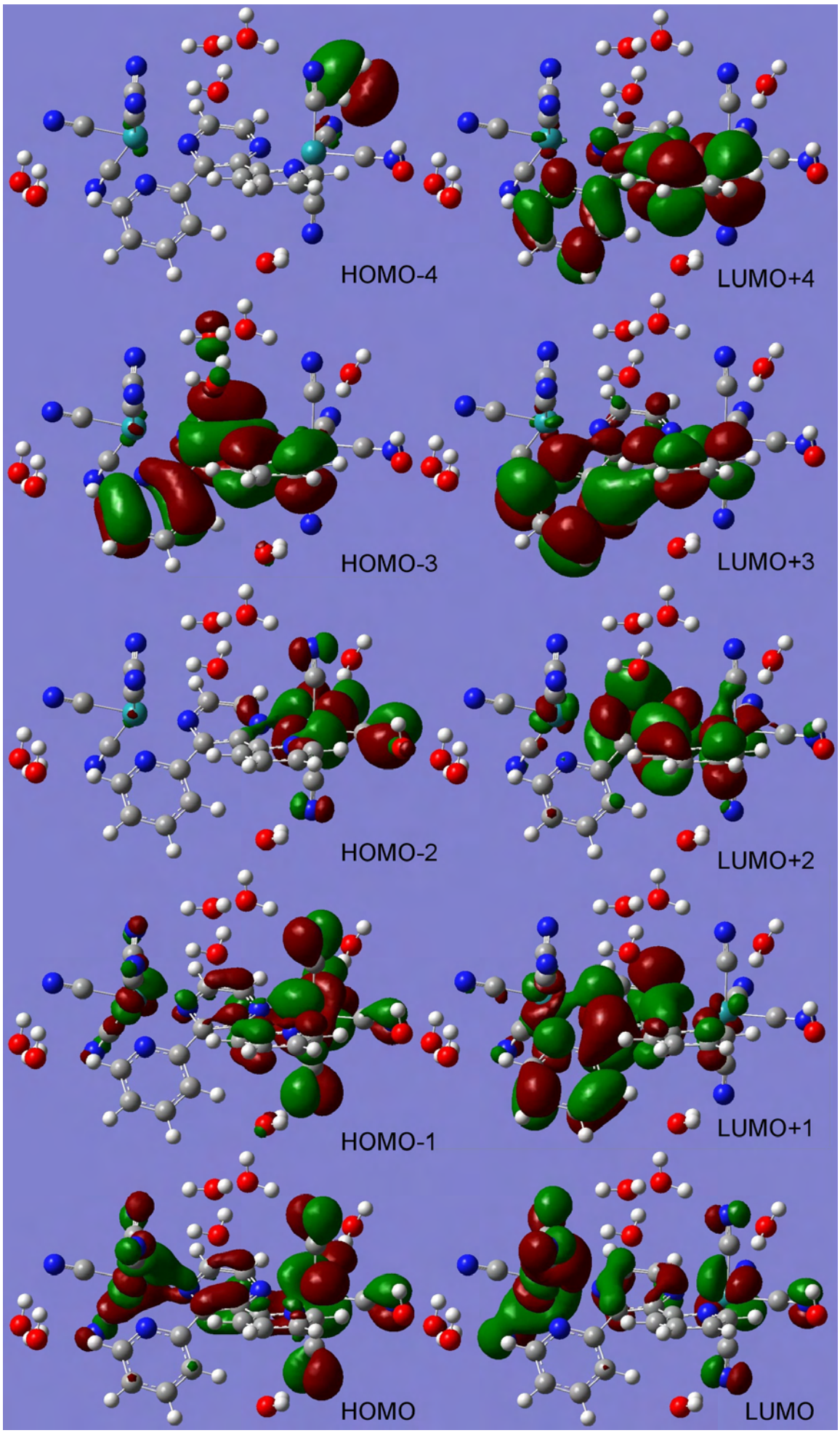
H	0.25450060	1.28823566	2.92872667
H	-6.99841022	0.36327818	-2.11519122
H	-7.55728006	0.63529849	-0.73013020
H	2.22312951	-2.83302975	-2.92361641
H	2.26384282	-4.07327652	-2.03613353
H	2.02743268	2.64846539	2.90775919
H	1.11610532	3.29492712	3.98227048
H	4.61305380	4.90387249	-2.06137729
H	5.40461016	5.96168947	-1.31107152
H	7.05391693	-2.04785514	0.73602068
H	6.94155359	-2.43482018	2.20075417

S12.2. TD-DFT

Detailed breakdown of transitions for $[(Ru(CN)_4)_2(\mu\text{-dppz})]^{2-}$ in PCM water + 8 explicit waters from a TD-DFT calculation for all transitions with $f > 0.04$.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs
3	7226	1383.90	0.08	H-5→LUMO (52%), H-1→LUMO (16%), HOMO→LUMO (30%)
5	8892	1124.67	0.08	H-6→LUMO (12%), H-5→LUMO (15%), H-3→LUMO (49%), HOMO→LUMO (17%)
6	10165	983.76	0.19	H-6→LUMO (11%), H-3→LUMO (49%), H-1→LUMO (13%), HOMO→LUMO (27%)
30	22446	445.52	0.08	H-2→L+1 (13%), H-1→L+2 (60%)
42	28311	353.22	0.15	H-33→LUMO (17%), H-3→L+1 (65%)
44	28729	348.08	0.05	H-36→LUMO (12%), H-34→LUMO (11%), H-33→LUMO (26%), H-3→L+1 (25%)
47	29239	342.01	0.04	H-38→LUMO (20%), H-37→LUMO (10%), H-6→L+1 (19%), H-5→L+1 (27%)
48	29539	338.53	0.23	H-3→L+2 (88%)
49	29779	335.81	0.05	H-6→L+1 (55%), H-5→L+1 (29%)
77	35827	279.12	0.05	H-12→L+1 (38%), H-10→L+2 (22%), H-1→L+4 (16%)
85	36926	270.81	0.04	H-13→L+1 (18%), H-1→L+5 (28%)

S12.3. Frontier orbitals



S13. $[RU(CN)_4(\mu\text{-DPPZ})]^{2-}$ IN DCM SOLVENT (PCM) (^{1}A)

FIG. S15. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in DCM solvent (PCM): Singlet ground state

SMILES	: c1ccnc(c1)c2c-3[n+](ccn2)[Ru]([n+]4c3cccc4)(C#N)(C#N)(C#N)C#N	
Formula	: $C_{18}H_{10}N_8Ru^{2-}$	
Charge	: -2	
Multiplicity	: 1	
Energy	: -1225.49330380	a.u.
Gibbs Energy	: -1225.29878600	a.u.
Number of imaginary frequencies	: 0	

S13.1. Cartesian Co-ordinates (XYZ format)

37

N	-1.42372847	-0.73264933	-0.07042614
C	-3.61185908	-0.90839207	2.00881958
C	-0.70438915	0.42133045	0.02339069
C	-0.76057988	-1.87502003	-0.30341664
C	-5.49415922	-0.09725918	-0.02227386
C	-3.47748709	-0.16085309	-2.05747080
C	-3.91160393	-2.47818351	-0.37610364
N	-3.62175822	-1.08970273	3.16379786
C	0.67291790	0.39875701	-0.28393492
C	-1.48468828	1.59934223	0.45734656
C	0.61554706	-1.87860024	-0.45598555
H	-1.35751760	-2.77401853	-0.37645572
N	-6.61965561	0.22336625	-0.01270085
N	-3.39838290	0.08490856	-3.19782281
N	-4.05540419	-3.62232041	-0.57842910
C	1.50568247	1.62386823	-0.51334178
N	1.32810938	-0.74984717	-0.48526356
C	-0.91810733	2.77403378	0.96496570
N	-2.83376431	1.43817961	0.42216134
H	1.15171826	-2.81107831	-0.59595072
C	1.21610165	2.47522330	-1.58374453
N	2.55851340	1.80215609	0.29653320
C	-1.73993027	3.81449795	1.37463999
H	0.15223795	2.86515141	1.06333745
C	-3.62202621	2.45458579	0.80893910
C	2.05531406	3.55837679	-1.82030046
H	0.35797501	2.28436947	-2.21633434
C	3.35141420	2.85360360	0.06097790
C	-3.11983991	3.65985250	1.27605164
H	-1.30793619	4.72471857	1.77223337
H	-4.68549252	2.26548219	0.74817723
C	3.14615703	3.75712156	-0.97890353
H	1.86136150	4.23152018	-2.64718080
H	4.19229031	2.97684741	0.73747033
H	-3.80201316	4.44472790	1.57690263

H	3.82559872	4.58820391	-1.12283814
Ru	-3.53380418	-0.54165477	-0.02483408

S14. $[RU(CN)_4(\mu\text{-DPPZ})]^{2-}$ IN DCM SOLVENT (PCM) (^{3}A)

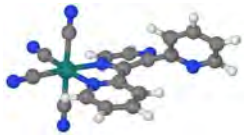


FIG. S16. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in DCM solvent (PCM): Triplet ground state

SMILES	: c1ccnc(c1)c2c-3[n+](ccn2)[Ru]([n+]4c3cccc4)(C#N)(C#N)(C#N)C#N	
Formula	: $C_{18}H_{10}N_8Ru^{2-,3}$	
Charge	: -2	
Multiplicity	: 3	
Energy	: -1225.44200073	a.u.
Gibbs Energy	: -1225.25280000	a.u.
Number of imaginary frequencies	: 0	

S14.1. Cartesian Co-ordinates (XYZ format)

37

N	-1.40911555	-0.75262517	-0.05176865
C	-3.57688951	-1.08643675	1.91971087
C	-0.69326693	0.44089678	0.10617692
C	-0.71951902	-1.89409101	-0.15747423
C	-5.50992918	-0.10857039	-0.04301418
C	-3.43400168	0.07278612	-2.07223368
C	-3.99816394	-2.40322590	-0.63234568
N	-3.58979964	-1.39233875	3.04386926
C	0.72068620	0.38645911	-0.15220886
C	-1.45492482	1.57617772	0.51061577
C	0.66055113	-1.91033769	-0.17230175
H	-1.29974711	-2.80384231	-0.25311705
N	-6.64143038	0.17054668	-0.00421345
N	-3.36003137	0.41433018	-3.18371367
N	-4.22266722	-3.50121951	-0.95368981
C	1.53255379	1.60308421	-0.47176629
N	1.37777758	-0.75113523	-0.24712099
C	-0.91403371	2.80040026	0.99456567
N	-2.83485770	1.43072605	0.48186350
H	1.21089590	-2.84158134	-0.22368757
C	1.15578711	2.43677449	-1.53319538
N	2.64910436	1.80923080	0.24463096
C	-1.74125123	3.83298731	1.36171401
H	0.15502895	2.90384841	1.10374272
C	-3.62562418	2.45736599	0.84071606
C	1.96920300	3.51144838	-1.86695802
H	0.24614052	2.23223281	-2.08426261
C	3.41652179	2.85550761	-0.08329014
C	-3.14079428	3.67748117	1.26734734
H	-1.31612289	4.75603580	1.73970020
H	-4.68953180	2.26565790	0.78053534
C	3.12770128	3.73285437	-1.12437797
H	1.70604014	4.16282272	-2.69256282
H	4.30848551	2.99837327	0.52095914
H	-3.82506204	4.46946335	1.54061091

H	3.79065990	4.56099892	-1.34371269
Ru	-3.52356195	-0.51244086	-0.07771044

S15. $[RU(CN)_4(\mu\text{-DPPZ})]^{2-}$ IN WATER SOLVENT (PCM) (^{1}A)

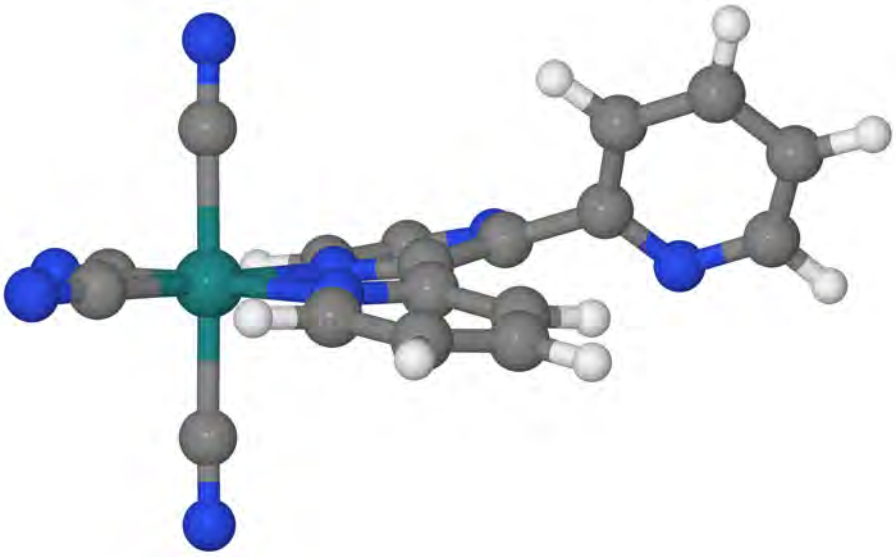


FIG. S17. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in water solvent (PCM): Singlet ground state

SMILES	: c1ccnc(c1)c2c-3[n+](ccn2)[Ru]([n+]4c3cccc4)(C#N)(C#N)(C#N)C#N	
Formula	: $C_{18}H_{10}N_8Ru^{2-}$	
Charge	: -2	
Multiplicity	: 1	
Energy	: -1225.52773050	a.u.
Gibbs Energy	: -1225.33381300	a.u.
Number of imaginary frequencies	: 0	

S15.1. Cartesian Co-ordinates (XYZ format)

37

N	-1.41977489	-0.73008865	-0.09428260
C	-3.57239103	-0.91474032	2.01655912
C	-0.70516717	0.42520520	0.00287226
C	-0.75735080	-1.86961329	-0.33659926
C	-5.49987459	-0.12706889	0.03736796
C	-3.53893042	-0.18816176	-2.04796624
C	-3.92839408	-2.48520637	-0.35076138
N	-3.57597017	-1.10946751	3.16972756
C	0.67343587	0.40659273	-0.30280763
C	-1.48841703	1.60299373	0.43795875
C	0.61939472	-1.87190926	-0.49025196
H	-1.35056496	-2.77054954	-0.41185203
N	-6.63296986	0.16500853	0.07830390
N	-3.51748824	0.02909842	-3.19689226
N	-4.10269833	-3.62666392	-0.54714435
C	1.51257777	1.63149750	-0.51240987
N	1.32775378	-0.74185652	-0.50949717
C	-0.92235756	2.78072858	0.93776911
N	-2.83738637	1.44144785	0.40499684
H	1.15673864	-2.80256319	-0.63594609

C	1.24505544	2.49210858	-1.58008194
N	2.55161381	1.79755783	0.31794578
C	-1.74430013	3.82485795	1.33937216
H	0.14755532	2.87481785	1.03449309
C	-3.62507272	2.46219683	0.78012925
C	2.09277892	3.57455373	-1.79144967
H	0.39827427	2.31170607	-2.23076344
C	3.35224771	2.84869289	0.10716629
C	-3.12342501	3.67167020	1.23828268
H	-1.31198978	4.73769665	1.72976899
H	-4.68914461	2.27652359	0.71958649
C	3.16808677	3.76204467	-0.92833775
H	1.91671121	4.25604057	-2.61525345
H	4.18087196	2.96361661	0.79957092
H	-3.80508804	4.46030426	1.52960324
H	3.85205698	4.59236097	-1.05200076
Ru	-3.53958654	-0.55078745	-0.01514351

S16. $[RU(CN)_4(\mu\text{-DPPZ})]^{2-}$ IN WATER SOLVENT (PCM) + 4 WATER (^{1}A)

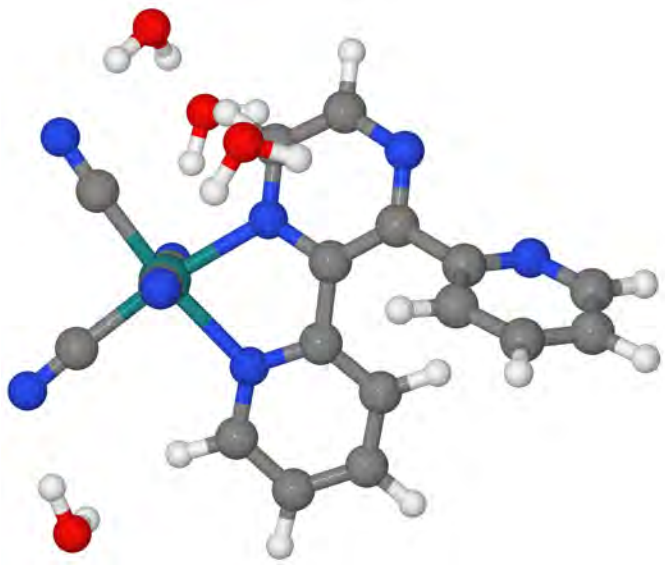


FIG. S18. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with four additional water molecules: Singlet ground state. Side-on View

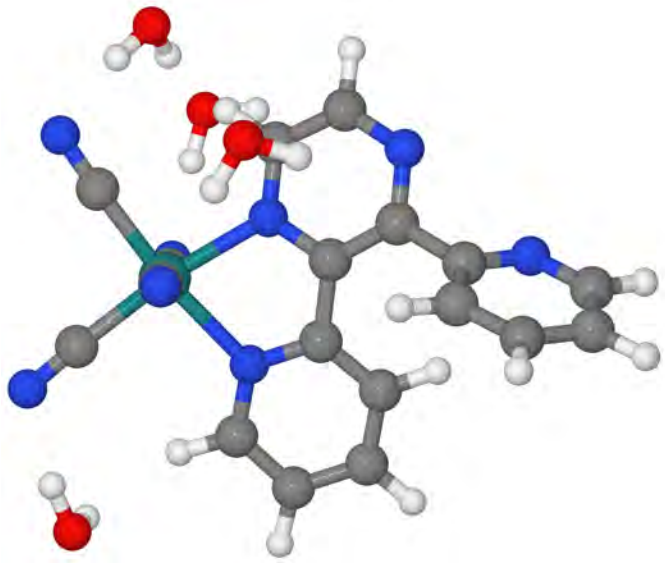


FIG. S19. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with four additional water molecules: Singlet ground state. Top View

SMILES	:	c1ccnc(c1)c2c-3[n+](ccn2)[Ru]([n+]4c3cccc4)(C#N)(C#N)(C#N)C#N.O.O.O.O
Formula	:	$C_{18}H_{18}N_8O_4Ru^{2-}$
Charge	:	-2
Multiplicity	:	1
Energy	:	-1531.40336507 a.u.
Gibbs Energy	:	-1531.12629600 a.u.
Number of imaginary frequencies	:	0

S16.1. Cartesian Co-ordinates (XYZ format)

49

N	-1.94740093	-0.71808791	-0.20575617
C	-4.35940599	-0.99653834	1.52988899
C	-1.21542466	0.42151463	-0.08285351
C	-1.30045724	-1.88675475	-0.29209110
C	-5.98281813	0.07817419	-0.59237999
C	-3.74810696	0.07573768	-2.38932276
C	-4.49085236	-2.30218267	-0.97859496
N	-4.47585487	-1.38088167	2.62967181
C	0.18269274	0.35927793	-0.27027518
C	-1.99149549	1.62610054	0.29011276
C	0.08729352	-1.92478812	-0.29167473
H	-1.89207506	-2.79179573	-0.34297952
N	-7.09689665	0.43509811	-0.66108626
N	-3.51412845	0.35232949	-3.50230408
N	-4.69116068	-3.41351891	-1.29150963
C	1.05190563	1.55365098	-0.51639336
N	0.82191908	-0.81457770	-0.33535710
C	-1.41437995	2.78350568	0.82257062
N	-3.34081817	1.50432444	0.19054854
H	0.61156130	-2.87404203	-0.30014297
C	0.82672560	2.35933232	-1.63591933
N	2.07207513	1.74729574	0.33122289
C	-2.22363806	3.84658289	1.19949293
H	-0.34706929	2.84638691	0.96446002
C	-4.11732388	2.53975821	0.54932880
C	1.69757402	3.41575503	-1.88200498
H	-0.00346078	2.15266967	-2.30020833
C	2.89502215	2.77300382	0.08593292
C	-3.60032511	3.72903919	1.04444551
H	-1.78326249	4.74462748	1.61446548
H	-5.18583536	2.40150237	0.44796559
C	2.75267744	3.63272309	-1.00122154
H	1.55519140	4.05381012	-2.74603629
H	3.70742440	2.91239071	0.79286808
H	-4.27377081	4.53066111	1.31904066
H	3.45357418	4.44451523	-1.15035105
Ru	-4.06441021	-0.43415603	-0.42310590
H	-1.92603970	-0.72035789	-3.92208219
O	-1.12042201	-1.26007545	-4.02666521
H	-0.42926964	-0.70438904	-3.65237641
H	-3.40521622	-4.55393887	-0.32034260
O	-2.70179439	-4.97926044	0.20170151
H	-2.80134654	-4.58755970	1.08982670
H	-7.53966331	2.07940292	0.15886720
O	-7.62768602	2.91026855	0.66911054
H	-7.52222109	2.61764884	1.58068514
H	-3.46392274	-2.99600434	2.78099036
O	-2.87294292	-3.77779865	2.78894305
H	-1.99918115	-3.40627694	2.95273948

S17. $[RU(CN)_4(\mu\text{-DPPZ})]^{2-}$ IN WATER SOLVENT (PCM) + 4 WATER (^{3}A)

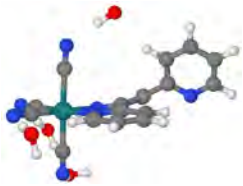


FIG. S20. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with four additional water molecules: Triplet excited state. Side-on View

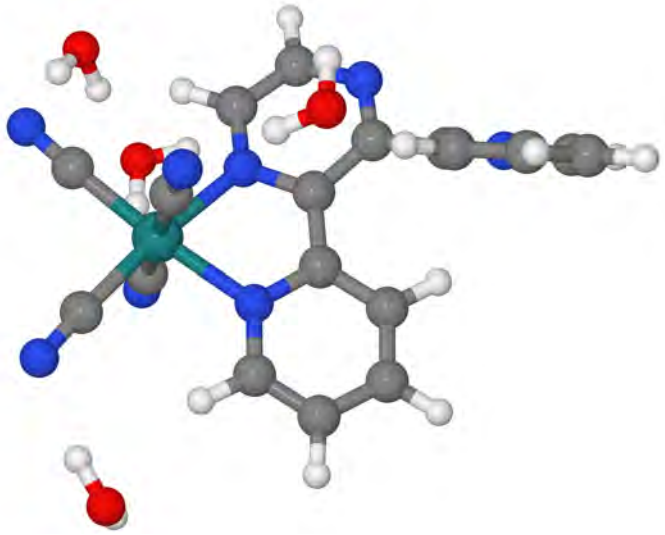


FIG. S21. structure of $[Ru(CN)_4(\mu\text{-dppz})]^{2-}$ in water solvent (PCM) with four additional water molecules: Triplet excited state. Top View

SMILES	:	c1ccnc(c1)c2c-3[n+](ccn2)[Ru]([n+]4c3cccc4)(C#N)(C#N)(C#N)C#N.O.O.O.O
Formula	:	$C_{18}H_{18}N_8O_4Ru^{2-,3}$
Charge	:	-2
Multiplicity	:	3
Energy	:	-1531.34163228 a.u.
Gibbs Energy	:	-1531.07113800 a.u.
Number of imaginary frequencies	:	0

S17.1. Cartesian Co-ordinates (XYZ format)

49

N	0.12099194	-1.14050376	-0.30597094
C	2.47553182	-0.10555397	-1.66551626
C	-1.07806802	-0.43633613	-0.49249241
C	0.10919257	-2.47071004	-0.49681720
C	3.22052550	1.38658237	0.76959640
C	0.98290855	0.17847224	2.19297814
C	3.02307439	-1.40905941	0.80723619
N	2.86604118	-0.29441357	-2.74705100
C	-2.28352499	-1.21395969	-0.56556666
C	-0.95474285	0.97973424	-0.60868335

C	-1.05592787	-3.14515710	-0.78404111
H	1.05220604	-2.99768853	-0.41183653
N	4.03231382	2.18100524	1.03510177
N	0.49429604	0.23007877	3.24891853
N	3.72440720	-2.29935861	1.08226192
C	-3.64241290	-0.62281954	-0.33597413
N	-2.27269840	-2.51922297	-0.73755962
C	-1.97240424	1.85826623	-1.07221520
N	0.28950387	1.51327825	-0.29905054
H	-1.05284011	-4.21224737	-0.96807706
C	-3.94829178	-0.02895632	0.89420682
N	-4.54170847	-0.75241661	-1.32433128
C	-1.74343526	3.20925975	-1.15844297
H	-2.92082405	1.45338309	-1.38992143
C	0.49028248	2.84393716	-0.38374844
C	-5.23889208	0.44410029	1.10302246
H	-3.20330453	0.04040738	1.67931855
C	-5.77655649	-0.28172445	-1.10867751
C	-0.48493654	3.73024416	-0.79010010
H	-2.52366638	3.86652851	-1.52446949
H	1.47875333	3.19799995	-0.11981301
C	-6.17614651	0.32291707	0.07972502
H	-5.50766897	0.89669639	2.05072975
H	-6.47947645	-0.39447328	-1.92938876
H	-0.26744616	4.78872108	-0.83847630
H	-7.19097900	0.68286800	0.19637766
Ru	1.75724018	0.07808194	0.27045697
H	-1.35568440	0.16924237	3.78865194
O	-2.30905819	0.06372824	3.96447158
H	-2.45219398	-0.88355255	3.86668873
H	3.28623128	-3.86008263	-0.16846952
O	2.95291686	-4.51744318	-0.79901689
H	2.92625666	-4.04013491	-1.64931333
H	3.68996239	4.03439760	0.54032421
O	3.39045238	4.87998199	0.16013744
H	3.50334358	4.74567795	-0.78699809
H	2.84644175	-2.20358515	-3.19410419
O	2.71499634	-3.16389179	-3.30127931
H	1.78071034	-3.24688840	-3.52304363

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