Electronic Supplementary Information

Synthesis, Characterization, Computational and DNA Interaction Studies of mono- and dinuclear Ru (II) complexes Containing terpyridine and *p*-cymene ligands

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Fig. S1 ^{1}H NMR spectra of the complexes **1-3** in $(CD_3)_2SO$.

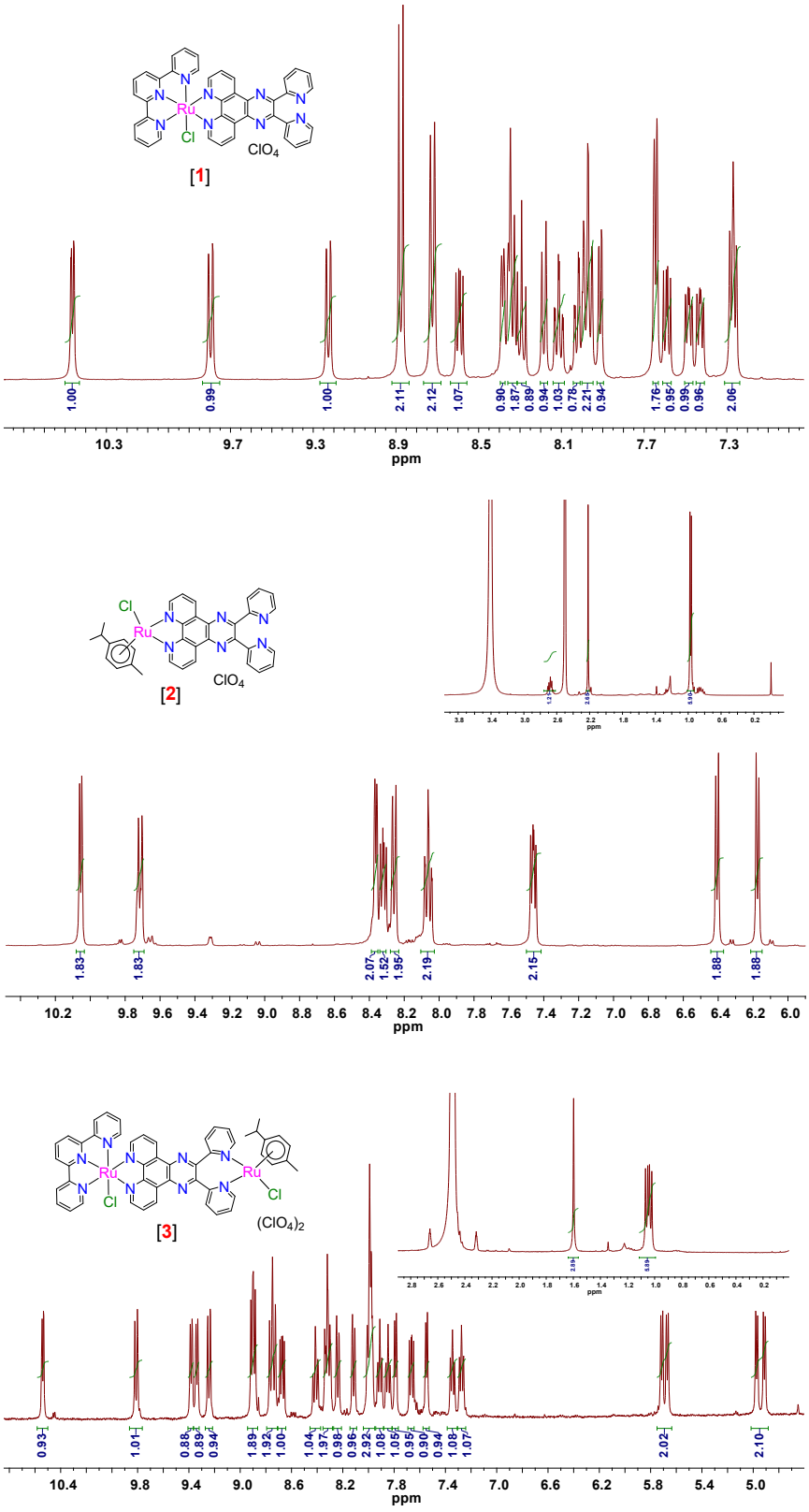

Fig. S2 ^{13}C NMR spectra of the complexes 1-3 in $(CD_3)_2SO$.

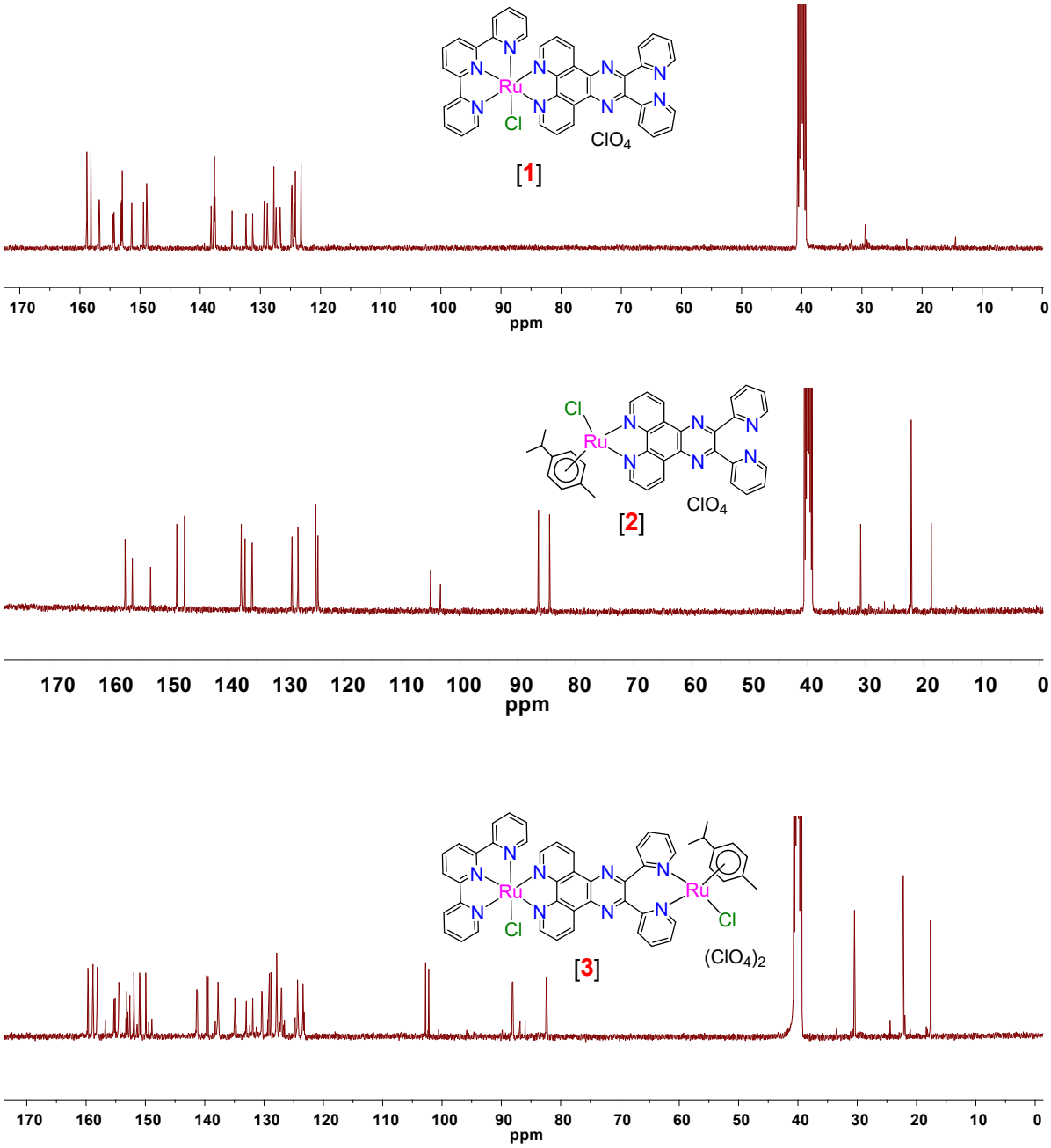

Table. TS1 Cartesian coordinates of DFT optimized $\mathbf{1}^{+}$ in the gas phase.

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	Ru	-2.84797	-0.374	0.284092
2	17	Cl	-4.33678	-1.90041	1.461426
3	7	N	-3.19457	1.05749	1.798808
4	7	N	-1.31052	0.77889	-0.59976
5	7	N	-4.44997	0.556653	-0.43826
6	7	N	-1.08788	-1.33357	1.025114
7	6	C	-3.98428	2.992786	3.648284
8	1	H	-4.29446	3.745789	4.365723
9	6	C	-2.87006	2.19108	3.89038
10	1	H	-2.28561	2.292276	4.798457
11	7	N	-3.18772	-1.47948	-1.48402
12	6	C	-2.51316	1.237637	2.941078
13	1	H	-1.6617	0.583507	3.089544
14	6	C	-4.70275	2.807806	2.469953
15	1	H	-5.57816	3.413758	2.266107
16	6	C	-4.29736	1.831266	1.557264
17	6	C	-5.01638	1.542502	0.299238
18	6	C	-0.04455	0.371432	-0.28459
19	6	C	0.076516	-0.76945	0.592163
20	6	C	-6.18743	2.157277	-0.15057
21	1	H	-6.65512	2.94899	0.422983
22	6	C	-4.28927	-1.05222	-2.17494
23	6	C	1.34267	-1.26248	0.96441
24	6	C	-1.4518	1.838267	-1.4067
25	1	H	-2.47035	2.131607	-1.63562
26	6	C	-1.02279	-2.39748	1.836589
27	1	H	-1.98118	-2.80126	2.148324
28	6	C	1.389843	-2.38526	1.810977
29	1	H	2.354969	-2.78634	2.099497
30	6	C	-5.01222	0.090737	-1.57993
31	6	C	2.533248	-0.60199	0.44836
32	6	C	1.103977	1.02436	-0.77648
33	6	C	-2.50348	-2.5384	-1.9445
34	1	H	-1.65382	-2.84634	-1.34606
35	6	C	-6.76339	1.724099	-1.34525
36	6	C	0.200601	-2.94742	2.246757
37	1	H	0.197443	-3.81255	2.901453
38	6	C	-0.36048	2.541347	-1.93101
39	1	H	-0.53896	3.39508	-2.57623
40	6	C	-4.69	-1.68929	-3.35159
41	1	H	-5.56434	-1.3404	-3.88907

42	6	C	-6.18326	0.678659	-2.06438
43	1	H	-6.64779	0.32253	-2.97647
44	6	C	2.41631	0.528527	-0.38457
45	6	C	-2.8557	-3.21661	-3.10794
46	1	H	-2.26903	-4.06891	-3.43327
47	6	C	0.9273	2.138608	-1.61545
48	1	H	1.801229	2.657865	-1.99203
49	6	C	-3.96824	-2.78146	-3.82608
50	1	H	-4.27475	-3.28582	-4.73691
51	1	H	-7.67493	2.188871	-1.70631
52	6	C	4.708265	0.738059	-0.44267
53	6	C	4.827216	-0.5037	0.276854
54	7	N	3.744209	-1.11304	0.743303
55	7	N	3.512956	1.194476	-0.79531
56	6	C	6.11905	-1.21898	0.459187
57	6	C	6.381544	-1.93795	1.631086
58	6	C	7.586147	-2.63157	1.726198
59	1	H	5.659701	-1.94119	2.440099
60	6	C	8.102607	-1.86615	-0.4869
61	6	C	8.468162	-2.59752	0.646904
62	1	H	7.831108	-3.18863	2.626024
63	1	H	8.758669	-1.82788	-1.35445
64	1	H	9.416316	-3.12529	0.676206
65	6	C	5.868993	1.618037	-0.74719
66	6	C	5.922453	2.348572	-1.93987
67	6	C	7.008082	3.196549	-2.14856
68	1	H	5.135626	2.242172	-2.67829
69	6	C	7.825569	2.540044	0.00795
70	6	C	7.982525	3.297344	-1.15641
71	1	H	7.091533	3.768008	-3.06864
72	1	H	8.558133	2.602827	0.810398
73	1	H	8.843852	3.947249	-1.27537
74	7	N	6.798781	1.713028	0.216194
75	7	N	6.959047	-1.18524	-0.58732

Table. TS2 Cartesian coordinates of DFT optimized $\mathbf{2}^{+}$ in the gas phase.

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	Ru	-3.5898	-0.19298	-0.30513
2	17	Cl	-3.1151	-0.91576	-2.56005
3	7	N	-1.93469	-1.40369	0.208384
4	7	N	-1.96457	1.109676	-0.63106
5	6	C	-0.7256	-0.7986	0.066318
6	6	C	-0.74166	0.563999	-0.3913
7	6	C	0.458291	1.269424	-0.60222
8	6	C	-1.96885	-2.68986	0.568138
9	1	H	-2.94857	-3.14742	0.63481
10	6	C	-2.02595	2.350554	-1.12357
11	1	H	-3.01355	2.73357	-1.34943
12	6	C	0.370756	2.587844	-1.08203
13	1	H	1.282644	3.152569	-1.24029
14	6	C	1.720467	0.603228	-0.31389
15	6	C	0.490194	-1.46463	0.311169
16	6	C	-0.87895	3.121922	-1.35191
17	1	H	-0.98737	4.127526	-1.74349
18	6	C	-0.80467	-3.42339	0.83194
19	1	H	-0.88973	-4.46532	1.120856
20	6	C	1.737041	-0.73892	0.114075
21	6	C	0.432735	-2.8125	0.706515
22	1	H	1.357834	-3.34777	0.888672
23	6	C	4.038216	-0.7236	0.112897
24	6	C	4.01547	0.68972	-0.17225
25	7	N	2.865952	1.302485	-0.426
26	7	N	2.903287	-1.3868	0.296612
27	6	C	5.22567	1.552219	-0.10771
28	6	C	5.396805	2.617697	-0.99871
29	6	C	6.525516	3.422502	-0.85734

30	1	H	4.667485	2.796134	-1.78099
31	6	C	7.148089	2.071283	1.02401
32	6	C	7.422111	3.147065	0.174185
33	1	H	6.701337	4.248984	-1.53992
34	1	H	7.817479	1.834577	1.848772
35	1	H	8.312953	3.749242	0.322907
36	6	C	5.28725	-1.5308	0.123909
37	6	C	5.438455	-2.60847	1.004026
38	6	C	6.608624	-3.36155	0.93215
39	1	H	4.660548	-2.83676	1.723989
40	6	C	7.310272	-1.94158	-0.86903
41	6	C	7.56676	-3.02471	-0.02292
42	1	H	6.768656	-4.1962	1.608655
43	1	H	8.028063	-1.65776	-1.63614
44	1	H	8.491275	-3.58578	-0.11661
45	7	N	6.20173	-1.20171	-0.80186
46	7	N	6.079831	1.282172	0.891868
47	6	C	-4.66345	0.730966	1.560509
48	6	C	-4.80394	-0.67994	1.5414
49	6	C	-5.41707	-1.37679	0.453479
50	6	C	-5.85459	-0.68567	-0.6952
51	6	C	-5.62429	0.728379	-0.7429
52	6	C	-5.05064	1.404703	0.357778
53	6	C	-6.48082	-1.3945	-1.86018
54	1	H	-5.93654	-1.1671	-2.78177
55	1	H	-6.47877	-2.47775	-1.71881
56	1	H	-7.51918	-1.06094	-1.97808
57	6	C	-4.15024	1.454801	2.805099
58	1	H	-4.89376	1.238836	3.587119
59	6	C	-2.79605	0.908791	3.296865
60	1	H	-2.52589	1.384472	4.245044

61	1	H	-2.81513	-0.17239	3.466775
62	1	H	-2.00505	1.124632	2.570044
63	6	C	-4.08872	2.981224	2.649364
64	1	H	-5.05988	3.410676	2.380506
65	1	H	-3.78471	3.433466	3.598116
66	1	H	-3.35244	3.282182	1.893853
67	1	H	-5.87904	1.279491	-1.64126
68	1	H	-4.88171	2.471921	0.273092
69	1	H	-5.52182	-2.4555	0.498983
70	1	H	-4.45173	-1.25868	2.389542

Table. TS3 Cartesian coordinates of DFT optimized $\mathbf{3}^{2+}$ in the gas phase.

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	Ru	4.980986	0.096796	-0.38212
2	6	C	6.791824	1.95904	0.902762
3	6	C	7.27376	-0.32303	1.340293
4	6	C	7.89661	2.360468	1.658027
5	6	C	8.387647	0.035211	2.103866
6	6	C	8.688461	1.387483	2.268322
7	1	H	8.150688	3.409092	1.758505
8	1	H	9.022809	-0.72074	2.550375
9	1	H	9.552368	1.682347	2.85477
10	6	C	6.84117	-1.69656	1.008842
11	6	C	7.508609	-2.84095	1.451267
12	6	C	7.061441	-4.0986	1.054454
13	1	H	8.378897	-2.75129	2.091088
14	6	C	5.324096	-3.00822	-0.18493
15	6	0	5.950317	-4.18445	0.217444
16	1	H	7.578486	-4.993	1.386954
17	1	H	4.465448	-3.02428	-0.84638
18	1	H	5.574781	-5.14134	-0.12859
19	6	C	5.8829	2.83957	0.139753
20	6	C	6.014205	4.229423	0.097721
21	6	C	5.14106	4.982617	-0.683
22	1	H	6.799771	4.720021	0.660759
23	6	C	4.066519	2.938205	-1.32276
24	6	C	4.150378	4.324941	-1.40989
25	1	H	5.240332	6.062426	-0.72771
26	1	H	3.321184	2.382387	-1.87998
27	1	H	3.456202	4.868485	-2.04157
28	17	Cl	6.526874	0.062295	-2.25432
29	6	C	2.185831	-0.31471	0.494811

30	6	C	3.462273	0.305747	2.331207
31	6	C	2.14615	-0.59579	-0.92198
32	6	C	1.018207	-0.40022	1.280135
33	6	C	2.347116	0.244679	3.17444
34	1	H	4.438889	0.580521	2.713807
35	6	C	0.942838	-0.96301	-1.55656
36	6	C	-0.23166	-0.77784	0.63245
37	6	C	1.112635	-0.10836	2.65157
38	1	H	2.464153	0.478022	4.227354
39	6	C	0.974006	-1.21727	-2.93946
40	6	C	-0.26796	-1.05369	-0.75345
41	6	C	3.336945	-0.73131	-2.9144
42	1	H	0.223558	-0.15965	3.269319
43	6	C	2.17942	-1.1005	-3.61402
44	1	H	0.058479	-1.49414	-3.44971
45	1	H	4.304515	-0.62403	-3.39595
46	1	H	2.244641	-1.28783	-4.68056
47	6	C	-2.49574	-1.16164	0.776622
48	6	C	-2.53115	-1.44898	-0.62261
49	7	N	-1.41651	-1.43336	-1.34069
50	7	N	-1.34571	-0.88566	1.376976
51	7	N	3.325667	-0.4821	-1.59649
52	7	N	3.398455	0.036571	1.019222
53	7	N	6.49462	0.64182	0.795443
54	7	N	5.741849	-1.79203	0.199489
55	7	N	4.897687	2.204467	-0.56641
56	6	C	-3.72617	-1.95842	-1.35737
57	6	C	-3.52443	-3.10777	-2.13764
58	6	C	-4.58263	-3.69957	-2.81273
59	1	H	-2.52509	-3.52135	-2.19005
60	6	C	-5.97393	-1.97793	-1.91221

61	6	C	-5.84509	-3.12525	-2.68051
62	1	H	-4.43039	-4.59207	-3.41144
63	1	H	-6.94402	-1.51926	-1.79299
64	1	H	-6.72086	-3.54934	-3.15976
65	6	C	-3.65379	-1.3142	1.704399
66	6	C	-3.41834	-2.06153	2.868625
67	6	C	-4.44737	-2.32058	3.763484
68	1	H	-2.41756	-2.43719	3.041375
69	6	C	-5.87632	-1.07797	2.306222
70	6	C	-5.7151	-1.82847	3.461983
71	1	H	-4.26926	-2.90474	4.660863
72	1	H	-6.84726	-0.68855	2.045403
73	1	H	-6.57005	-2.01538	4.102727
74	7	N	-4.94633	-1.37006	-1.27311
75	7	N	-4.87758	-0.78816	1.442822
76	44	Ru	-5.44537	0.502201	-0.23924
77	17	Cl	-3.18492	1.407914	-0.41605
78	6	C	-7.64877	1.34458	0.619153
79	6	C	-7.80424	0.698342	-0.62397
80	6	C	-7.03371	1.095622	-1.76141
81	6	C	-6.11417	2.164497	-1.7082
82	6	C	-5.87638	2.722044	-0.4127
83	6	C	-6.589	2.300195	0.727151
84	1	H	-8.55957	-0.0747	-0.73387
85	1	H	-7.18356	0.586115	-2.70842
86	1	H	-5.0871	3.454879	-0.29481
87	1	H	-6.35634	2.750934	1.68375
88	6	C	-8.63319	1.081522	1.749361
89	1	H	-8.82067	-0.00142	1.787213
90	6	C	-8.17387	1.56104	3.134779
91	1	H	-8.11657	2.654231	3.179206

92	1	H	-8.90323	1.248418	3.887921
93	1	H	-7.19824	1.158065	3.425908
94	6	C	-9.97979	1.754623	1.375392
95	1	H	-10.3789	1.376748	0.429171
96	1	H	-10.7173	1.554639	2.158926
97	1	H	-9.86336	2.840438	1.289605
98	6	C	-5.38338	2.667932	-2.92074
99	1	H	-5.47013	1.9695	-3.75756
100	1	H	-5.80738	3.628953	-3.23733
101	1	H	-4.32334	2.818252	-2.69717

Fig. S3 DFT optimized geometry of the complexes $\mathbf{1}^{+}$ and $\mathbf{2}^{+}$ in the gas phase.

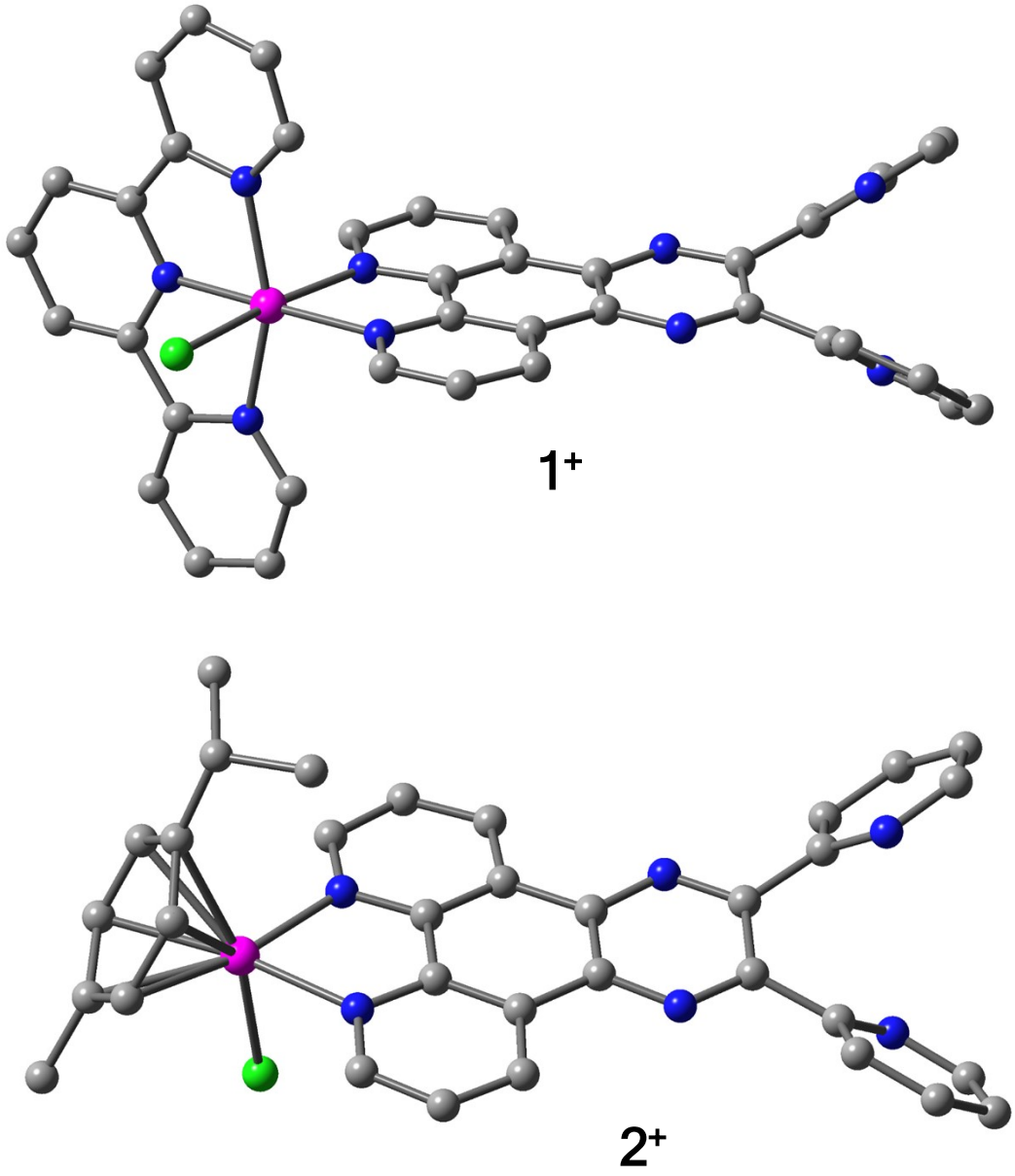

Fig. S4 DFT optimized frontier orbitals of complex $\mathbf{1}^{+}$ in the gas phase.

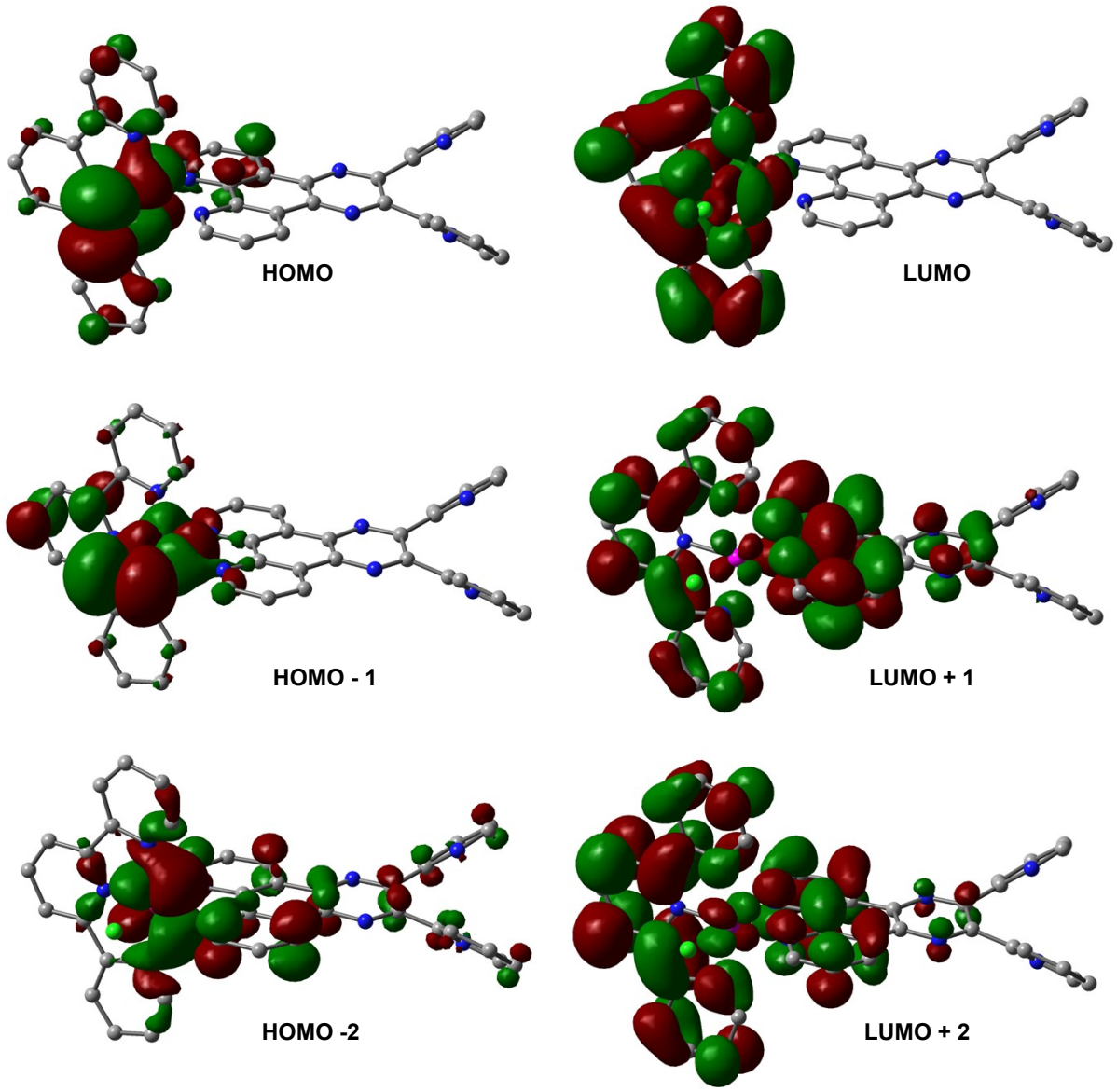

Fig. S5 DFT optimized frontier orbitals of complex $\mathbf{2}^{+}$ in the gas phase.

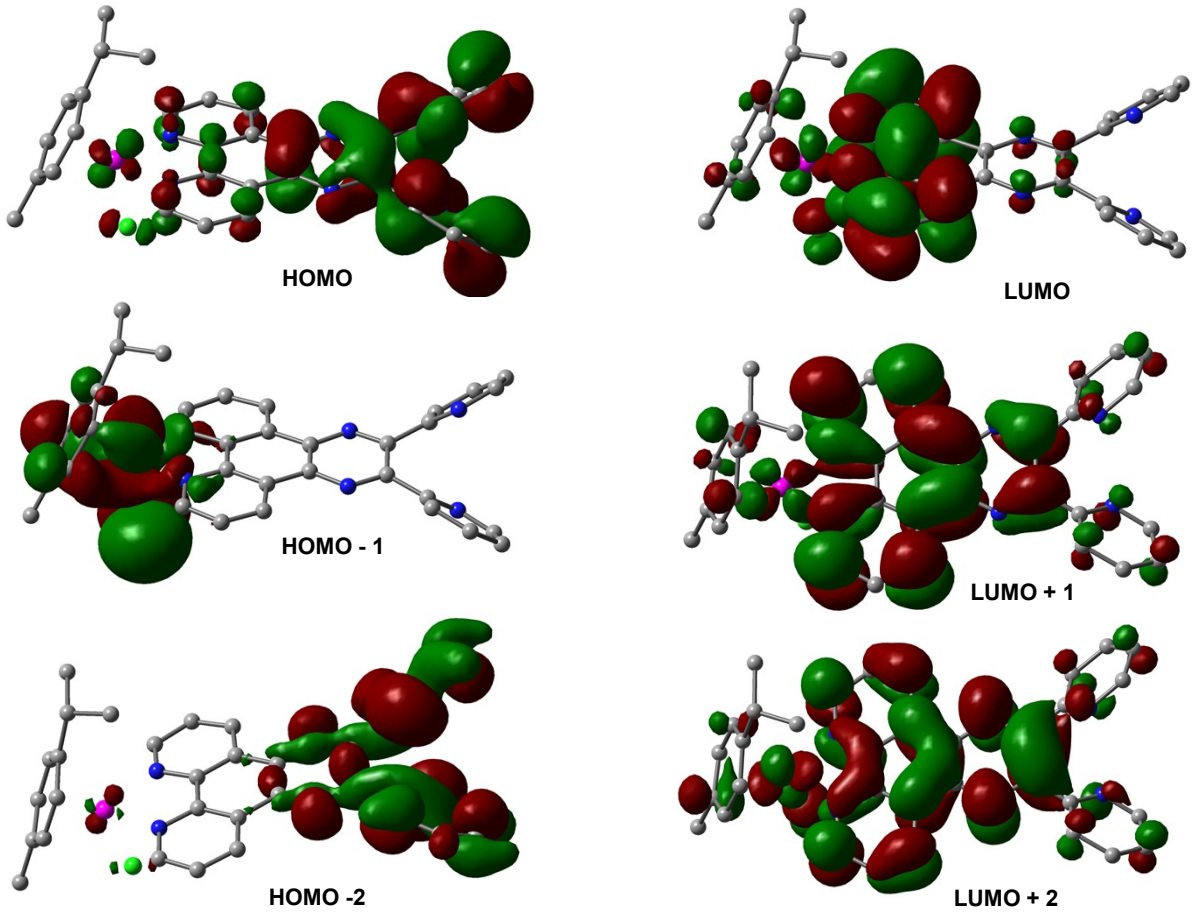

Table. TS4 Composition of frontier orbitals of DFT optimized $\mathbf{1}^{+}$ in the gas phase.

Orbitals	**Energy (eV)**	**phpy**	**tpy**	**Cl_{tpy}**	**Ru_{tpy}**
H-10	-9.381	57.1	40	1.1	1.8
H-9	-9.358	45.9	50.8	1.8	1.5
H-8	-9.055	3.3	13.3	60.6	22.8
H-7	-8.95	99.8	0	0.2	0
H-6	-8.919	2.1	18.6	58.4	20.8
H-5	-8.818	99.1	0.1	0	0.7
H-4	-8.627	100	0	0	0
H-3	-8.356	91.1	0.9	0.1	7.9
H-2	-8.105	22.1	7.7	0.1	70.1
H-1	-7.726	2.3	11.8	33	52.9
HOMO	-7.599	5.4	8.3	31.1	55.2
LUMO	-4.667	0.6	89.9	1	8.5
L+1	-4.604	66.9	31.2	0.1	1.8
L+2	-4.525	29	66.9	0.2	3.9
L+3	-4.416	98.3	1.2	0	0.4
L+4	-4.293	97.6	0.7	0	1.6
L+5	-3.553	0	99	0	0.9
L+6	-3.492	3	93.6	0	3.3
L+7	-3.124	98.5	0.7	0	0.8
L+8	-2.789	0.1	98.1	0	1.8
L+9	-2.702	96.1	1.4	0	2.5
L+10	-2.594	10.3	12.9	12.5	64.3

Table. TS5 Composition of frontier orbitals of DFT optimized $\mathbf{2}^{+}$ in the gas phase.

Orbitals	**Energy (eV)**	***p*-cym**	**phpy**	**Cl**	**Ru**
H-10	-9.897	1.8	72.1	4.2	21.9
H-9	-9.803	0.2	97.4	1.7	0.7
H-8	-9.621	0.3	98.8	0.7	0.3
H-7	-9.519	0.8	95.8	0.4	3
H-6	-9.369	16	13.3	33.4	37.4
H-5	-9.12	0	100	0	0
H-4	-8.974	0.2	93.5	4.3	2
H-3	-8.803	6.6	15.4	39.9	38.1
H-2	-8.775	0.1	98.7	0.5	0.6
H-1	-8.603	12.4	4.3	46.4	36.9
HOMO	-8.487	0.4	97.4	0.8	1.4
LUMO	-5.026	2.7	93.4	1.5	2.4
L+1	-4.804	3.8	93.6	0.1	2.6
L+2	-4.626	3.4	89.3	2.3	5
L+3	-4.538	22.3	18.4	12.9	46.4
L+4	-4.258	31	21.2	0.6	47.2
L+5	-3.483	52.6	25.6	0.1	21.7
L+6	-3.399	69.1	14.7	1.7	14.5
L+7	-3.341	24.8	68.1	0.2	6.9
L+8	-3.06	2.5	95.5	0.2	1.8
L+9	-2.57	0.3	99.3	0	0.4
L+10	-2.497	0.1	99.9	0	0.1

Table. TS6 Composition of frontier orbitals of DFT optimized $\mathbf{3}^{2+}$ in the gas phase.

Orbitals	**Energy (eV)**	***p*-cym**	**phpy**	**tpy**	**$Cl_{p\text{-cym}}$**	**Cl_{tpy}**	**$Ru_{p\text{-cym}}$**	**Ru_{tpy}**
H-10	-11.155	4.4	39.6	0.5	8.2	0.1	46.5	0.8
H-9	-11.037	0	9.7	4.4	0	67.8	0.1	18
H-8	-10.894	12	46.9	0.7	14.2	0	25.2	1
H-7	-10.637	0.1	1.2	88.9	0.1	4.8	0.3	4.7
H-6	-10.411	0	3	14.5	0	59.1	0	23.4
H-5	-10.373	8.3	13.7	0.1	36.7	0.1	40.7	0.4
H-4	-10.299	8.3	6.3	0	37.2	0	48.2	0.1
H-3	-10.257	0	1.6	23.2	0	54.2	0	21
H-2	-9.539	0	13.7	8.7	0.1	0.1	0	77.4
H-1	-9.088	0	2.4	10.8	0	34.7	0	52
HOMO	-8.975	0	5.3	7.7	0	33.2	0	53.8
LUMO	-6.717	8.5	74.9	0.1	3.3	0	13.2	0
L+1	-6.579	17.8	53.5	0	2.1	0	26.5	0.1
L+2	-6.518	7.9	73.8	0	3.2	0	14.8	0.2
L+3	-6.261	19.6	18.1	0.1	8.9	0	53.1	0.2
L+4	-6.149	0.7	89.6	2.2	0.3	0.2	1.6	5.4
L+5	-5.953	0	0.6	90.8	0	0.9	0	7.7
L+6	-5.86	14.3	81.2	0.2	0.4	0	3.7	0.2
L+7	-5.802	0	1.1	96.8	0	0	0	2
L+8	-5.721	2	95.4	0.3	0.1	0	2	0.3
L+9	-5.283	2.2	96.6	0.3	0.1	0	0.7	0.2
L+10	-5.193	6.1	92.4	0.5	0	0	0.7	0.2

Table TS7. TD-DFT data for complex $\mathbf{1}^{+}$ in the gas phase.

Sl. No.	λ (nm) DFT	λ (nm) Expt.	Energy (eV)	f value	Transition	Character
1	547	509	2.2655	0.0281	H-1->LUMO (23%), HOMO->L+1 (22%), HOMO->L+2 (49%)	dπ(Ru/Cl) → π*(tpy) dπ(Ru/Cl) → π*(tpy/phpy) dπ(Ru/Cl) → π*(tpy/phpy)
2	510	509	2.4283	0.0202	H-1->L+1 (23%), H-1->L+2 (68%)	dπ(Ru/Cl) → π*(tpy/phpy) dπ(Ru/Cl) → π*(tpy/phpy)
3	497	509	2.4922	0.0828	H-1->LUMO (52%), HOMO->L+2 (32%)	dπ(Ru/Cl) → π*(tpy) dπ(Ru/Cl) → π*(tpy/phpy)
4	448	509	2.7653	0.0131	H-2->L+1 (43%), H-2->L+2 (48%)	dπ(Ru)/π(phpy) → π*(tpy/phpy) dπ(Ru)/π(phpy) → π*(tpy/phpy)
5	428	509	2.8960	0.15	H-2->L+1 (38%), H-2->L+2 (34%)	dπ(Ru)/π(phpy) → π*(tpy/phpy) dπ(Ru)/π(phpy) → π*(tpy/phpy)
6	400	509	3.0939	0.0217	H-2->L+3 (92%)	dπ(Ru)/π(phpy) → π*(phpy)
7	377	353	3.2873	0.0179	H-3->L+1 (43%), H-2->L+4 (32%)	π(phpy) → π*(tpy/phpy) dπ(Ru)/π(phpy) → π*(phpy)
8	374	353	3.3088	0.0629	H-3->L+1 (34%), H-2->L+4 (45%)	π(phpy) → π*(tpy/phpy) dπ(Ru)/π(phpy) → π*(phpy)
9	372	353	3.3317	0.0287	HOMO->L+5 (92%)	dπ(Ru/Cl) → π*(tpy)
10	351	353	3.5284	0.0235	H-3->L+2 (41%)	π(phpy) → π*(tpy/phpy)

Table TS8. TD-DFT data for complex $\mathbf{2}^{+}$ in the gas phase.

λ (nm) DFT	λ (nm) Expt.	Energy (eV)	f value	Transition	Character
415		2.98	0.102	HOMO->LUMO (78%)	π(phpy) → π*(phpy)
385	340, 263	3.22	0.024	H-1->L+1 (58%)	dπ(Ru/Cl) → π*(phpy)
384		3.23	0.034	HOMO->L+1 (63%)	π(phpy) → π*(phpy)
377		3.28	0.034	H-2->LUMO (61%), HOMO->L+1 (23%)	π(phpy) → π*(phpy) π(phpy) → π*(phpy)
376		3.29	0.081	HOMO->L+2 (71%)	π(phpy) → π*(phpy)
367		3.37	0.052	H-2->L+1 (73%),	π(phpy) → π*(phpy)
360		3.44	0.01	H-2->L+2 (25%), H-1->L+2 (50%)	π(phpy) → π*(phpy) dπ(Ru/Cl) → π*(phpy)
356		3.48	0.041	H-6->LUMO (28%), H-4->LUMO (38%)	dπ(Ru/Cl) → π*(phpy) π(phpy) → π*(phpy)
338		3.67	0.015	H-5->LUMO (55%), H-4->L+1 (30%)	π(phpy) → π*(phpy) π(phpy) → π*(phpy)
335		3.70	0.014	H-4->L+2 (64%)	π(phpy) → π*(phpy)
326		3.80	0.290	H-5->L+1 (58%)	π(phpy) → π*(phpy)
322		3.85	0.022	H-8->L+2 (20%), H-5->L+2 (50%)	π(phpy) → π*(phpy) π(phpy) → π*(phpy)
320		3.87	0.011	HOMO->L+4 (88%)	π(phpy) → dπ(Ru)/ π*(*p*-cym/phpy)
314		3.95	0.011	H-6->L+1 (75%)	dπ(Ru/Cl) → π*(phpy)
307		4.03	0.011	H-8->L+1 (40%)	π(phpy) → π*(phpy)
307		4.04	0.032	H-8->L+1 (17%), H-1->L+6 (21%)	π(phpy) → π*(phpy) dπ(Ru/Cl) → π*(*p*-cym)
306		4.05	0.035	H-1->L+6 (31%)	dπ(Ru/Cl) → π*(*p*-cym)
305		4.07	0.030	H-7->LUMO (44%),	π(phpy) → π*(phpy)

Table TS9. TD-DFT data for complex $\mathbf{3}^{2+}$ in the gas phase.

Sl. No.	λ (nm) DFT	λ (nm) Expt.	Energy (eV)	f value	Transition	Character
1	613	511	2.0238	0.0124	HOMO->L+4 (87%)	dπ(^{1st}Ru/Cl) → π*(phpy)
2	552	511	2.2463	0.0302	H-2->L+1 (82%)	dπ(^{1st}Ru)/ π(phpy/tpy) → dπ(^{2nd}Ru)/π*(phpy/*p*-cym)
3	516	511	2.4037	0.0125	H-2->L+2 (82%)	dπ(^{1st}Ru)/ π(phpy/tpy) → dπ(^{2nd}Ru)/π*(phpy/*p*-cym)
4	485	511	2.5590	0.1028	H-1->L+6 (30%), HOMO->L+8 (39%)	dπ(^{1st}Ru/Cl) → π*(phpy/*p*-cym) dπ(^{1st}Ru/Cl) → π*(phpy)
5	484	511	2.5641	0.0316	H-1->L+8 (85%)	dπ(^{1st}Ru/Cl) → π*(phpy)
6	451	511	2.7475	0.0127	H-3->L+1 (80%)	dπ(^{1st}Ru/Cl)/π(tpy) → dπ(^{2nd}Ru)/π*(phpy/*p*-cym)
7	441	511	2.8101	0.041	H-2->L+4 (30%), HOMO->L+5 (31%), HOMO->L+7 (26%)	dπ(^{1st}Ru)/ π(phpy/tpy) → π*(phpy) dπ(^{1st}Ru/Cl) → dπ(^{1st}Ru)/π*(tpy) dπ(^{1st}Ru/Cl) → π*(tpy)
8	434	361	2.8564	0.0478	H-2->L+4 (23%), HOMO->L+7 (56%)	dπ(^{1st}Ru)/ π(phpy/tpy) → π*(phpy) dπ(^{1st}Ru/Cl) → π*(tpy)
9	429	361	2.8871	0.0121	H-2->L+3 (82%)	dπ(^{1st}Ru)/ π(phpy/tpy) → dπ(^{2nd}Ru)/π*(phpy/*p*-cym)
10	403	361	3.0757	0.0322	H-7->L+1 (51%)	dπ(^{1st}Ru/Cl)/π(tpy)→ dπ(^{2nd}Ru)/π*(phpy/*p*-cym)

Fig. S6 Emission spectra of the complexes **1-3** recorded in phosphate buffer (pH 7.4). The spectra were recorded by excitation at 510 nm for **1** and **3** and 360 nm for complex **2**.