

Influence of Substitution of Ligand at Donor and Acceptor Center on MMCT in Cyanide-Bridged Mixed-Valence System

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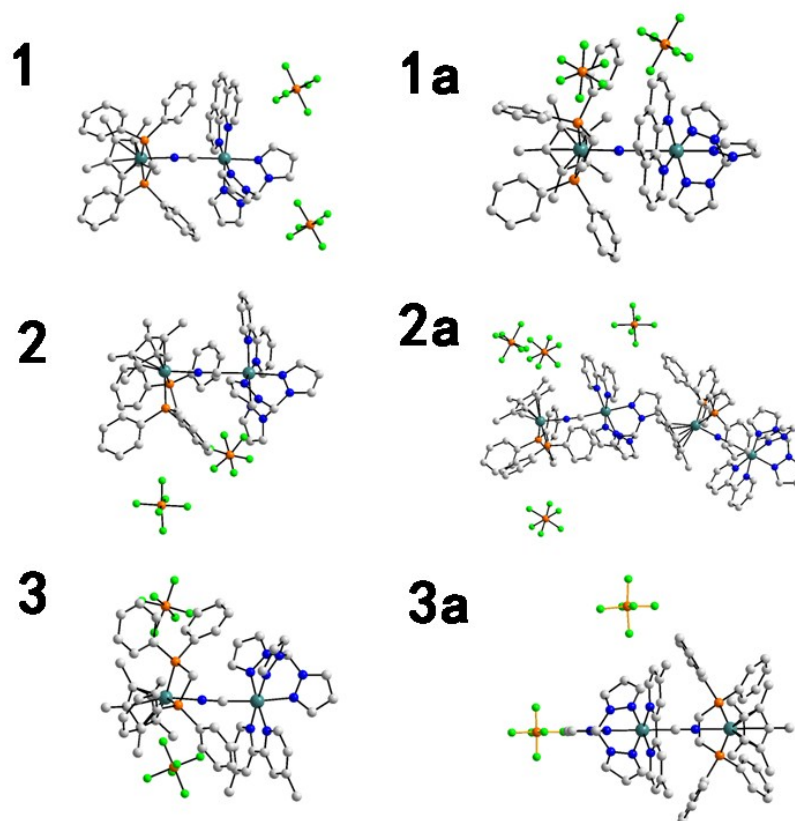


Figure S1 Molecular structures of complexes **1-3** and **1a-3a** (hydrogen atoms and solvent molecules have been removed for clarity). Ru, dark green; N, blue; P, orange; C, gray; F, light green.

Table S1. Crystallographic data of complexes **1-3** and **1a-3a**.

	1	2	3
Empirical formula	$C_{58}H_{55}F_{12}N_9P_4Ru_2$	$C_{57}H_{57}Cl_2F_{12}N_9OP_4$ Ru_2	$C_{58}H_{59}F_{12}N_9P_4Ru_2$
Formula weight	1432.13	1509.03	1436.16
Temperature (K)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
A (Å)	12.637(8)	13.517(2)	13.820(3)
B (Å)	26.812(15)	19.619(4)	19.400(4)

c (Å)	19.841(13)	27.456(4)	25.820(5)
Alpha (deg.)	90	90	90
Beta (deg.)	100.182(9)	112.215(6)	101.65(3)
Gamma (deg.)	90	90	90
Volume (Å ³)	6616(7)	6741(2)	6780(3)
Z	4	4	4
Calculated density (Mg/m ³)	1.438	1.487	1.407
Absorption coefficient (mm ⁻¹)	0.630	0.700	0.615
F(000)	2888	3040	2904
Theta range for data collection (deg.)	2.506 to 27.560	2.079 to 27.514	2.122 to 33.490
Reflections collected / unique	75792 / 14978 [R(int) = 0.0696]	91883 / 15393 [R(int) = 0.0645]	122165 / 24918 [R(int) = 0.0311]
Data / restraints / parameters	14978 / 12 / 771	15393 / 49 / 798	24918 / 1 / 773
Goodness-of-fit on F ²	1.094	1.110	1.090
Final R indices [I > 2sigma(I)]	R1 = 0.0866, wR2 = 0.2449	R1 = 0.0664, wR2 = 0.1912	R1 = 0.0562, wR2 = 0.1475
R indices (all data)	R1 = 0.1021, wR2 = 0.2699	R1 = 0.0769, wR2 = 0.2049	R1 = 0.0605, wR2 = 0.1518

	1a	2a	3a
Empirical formula	C ₅₉ H ₅₇ F ₁₂ N ₉ P ₄ Ru ₂	C ₂₃₁ H ₂₃₄ C ₁₆ F ₄₈ N ₃₆ P ₁₆ Ru ₈	C ₅₉ H ₆₁ F ₁₂ N ₉ P ₄ Ru ₂
Formula weight	1446.15	5943.31	1450.19
Temperature (K)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system,	Monoclinic,	Orthorhombic,	Orthorhombic,
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>Pna</i> 2 ₁	<i>Cmc</i> 2 ₁
a (Å)	14.377(7)	24.139(7)	14.330(4)
b (Å)	15.398(7)	28.614(8)	24.429(6)
c (Å)	28.270(14)	19.264(5)	19.346(8)

Alpha (deg.)	90	90	90
Beta (deg.)	94.152(6)	90	90
Gamma (deg.)	90	90	90
Volume (Å ³)	6242(5)	13306(6)	6772(4)
Z	4	2,	4
Calculated density (Mg/m ³)	1.539	1.483	1.422
Absorption coefficient (mm ⁻¹)	0.668	0.687	0.616
F(000)	2920	5996	2936
Theta range for data collection (deg.)	2.539 to 27.475	2.114 to 27.420	2.674 to 27.413
Reflections collected / unique	45554 / 14215 [R(int) = 0.1230]	103343 / 29820 [R(int) = 0.0742]	34227 / 7987 [R(int) = 0.0771]
Data / restraints / parameters	14215 / 0 / 780	29820 / 47 / 1594	7987 / 293 / 423
Goodness-of-fit on F ²	1.110	1.138	0.972
Final R indices [I > 2σ(I)]	R1 = 0.0806, wR2 = 0.1687	R1 = 0.0772, wR2 = 0.1839	R1 = 0.0811, wR2 = 0.2138
R indices (all data)	R1 = 0.1093, wR2 = 0.1854	R1 = 0.0912, wR2 = 0.1945	R1 = 0.0951, wR2 = 0.2346

$$R_1 = \frac{\sum(|F_0| - |F_c|)}{\sum|F_0|}$$

$$wR_2 = [\sum w(|F_0|^2 - |F_c|^2)^2 / \sum w|F_0|^2]^{1/2}$$

Table S2. Selected instances (Å) of complexes **1-3** and **1a-3a**.

	Ru-P1	Ru-P2		Ru-P1	Ru-P2		Ru-P1	Ru-P2
1	2.3062(19)	2.3104(15)	2	2.3024(12)	2.3205(13)	3	2.2920(9)	2.3130(8)
1a	2.3106(18)	2.2909(18)	2a	2.2953(11)	2.2954(10)	3a	2.2894(13)	2.2894(13)
	Ru-C(C≡N)	Ru-N(C≡N)		Ru-C(C≡N)	Ru-N(C≡N)		Ru-C(C≡N)	Ru-N(C≡N)
1	2.003(5)	2.067(4)	2	1.991(4)	2.064(3)	3	1.984(2)	2.063(2)
1a	2.008(6)	2.057(5)	2a	2.009(4)	2.078(3)	3a	2.012(6)	2.083(5)

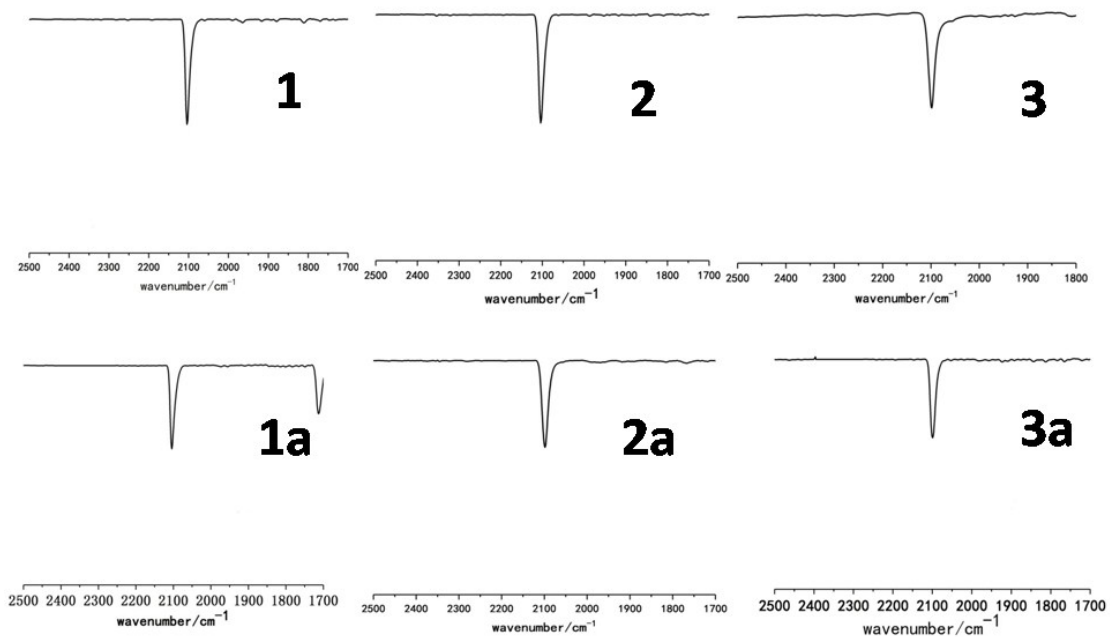


Figure S2. Stretching frequencies of complexes **1-3** and **1a-3a**.

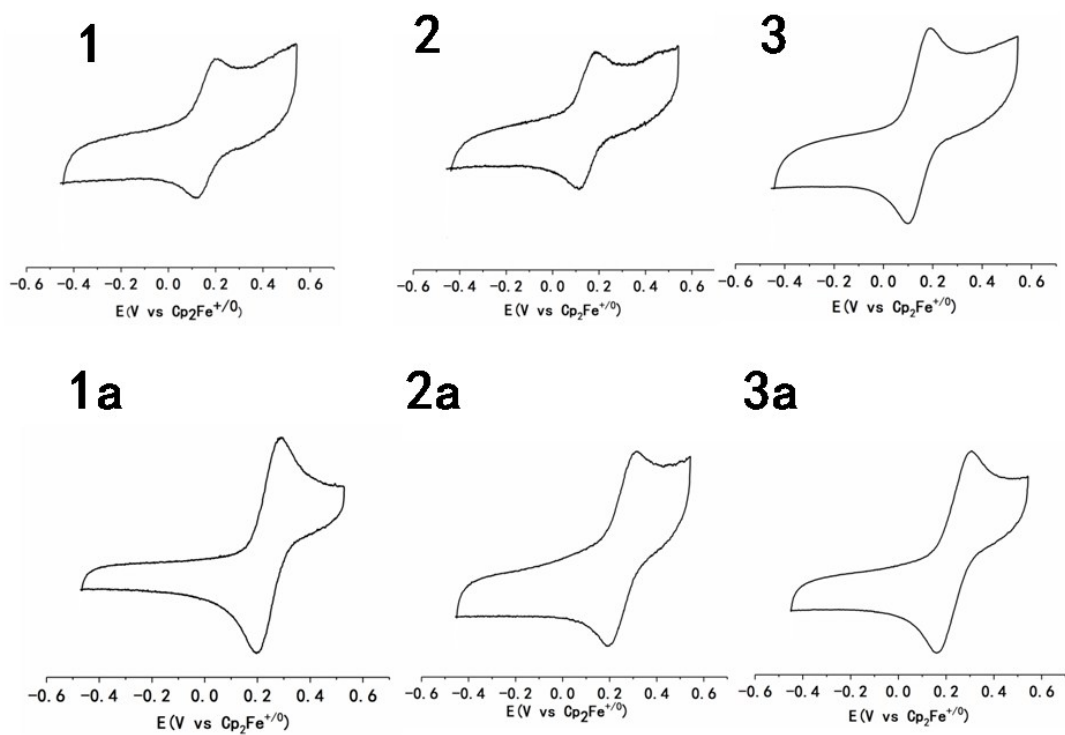
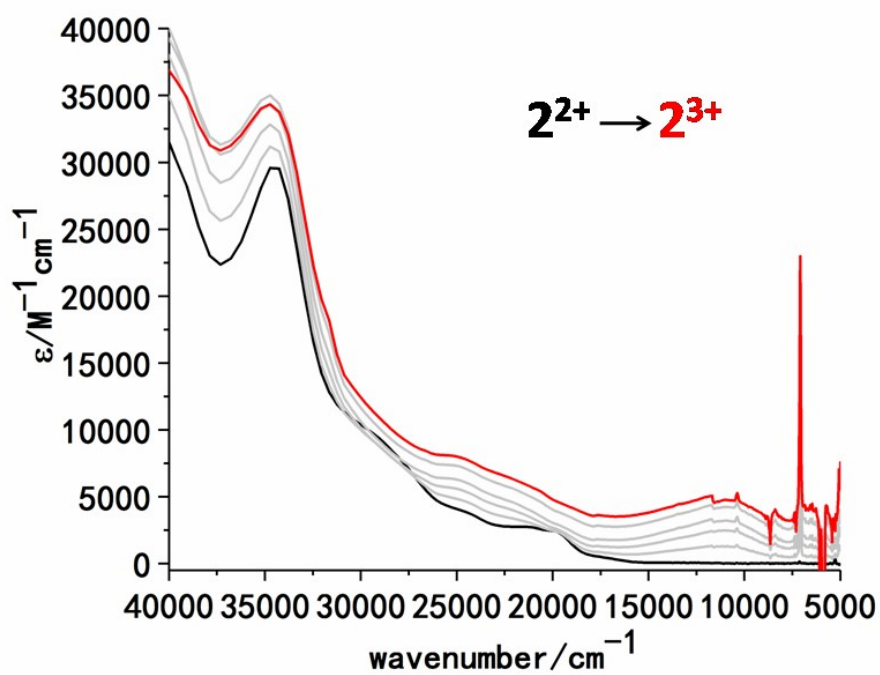
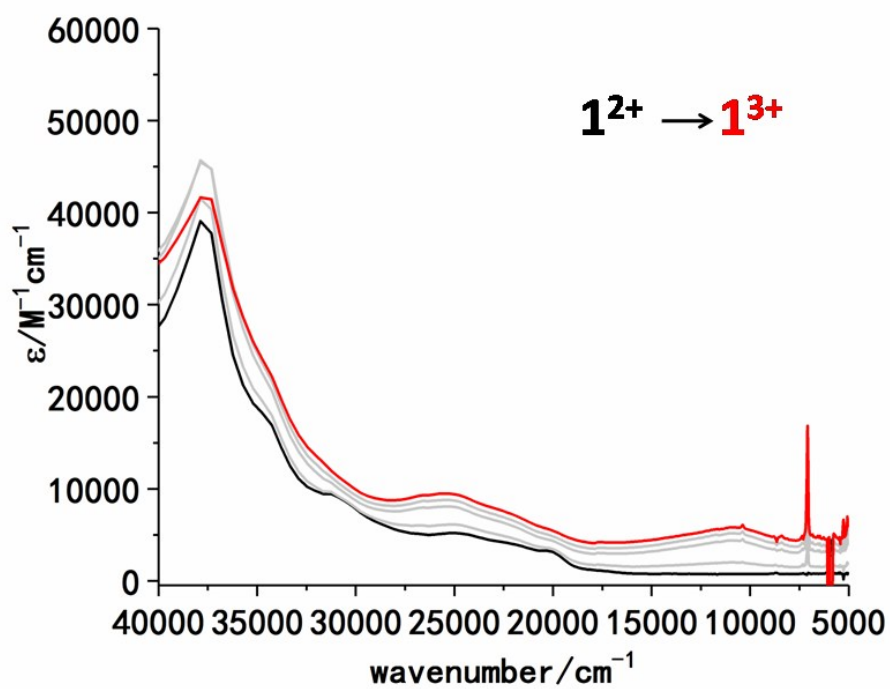
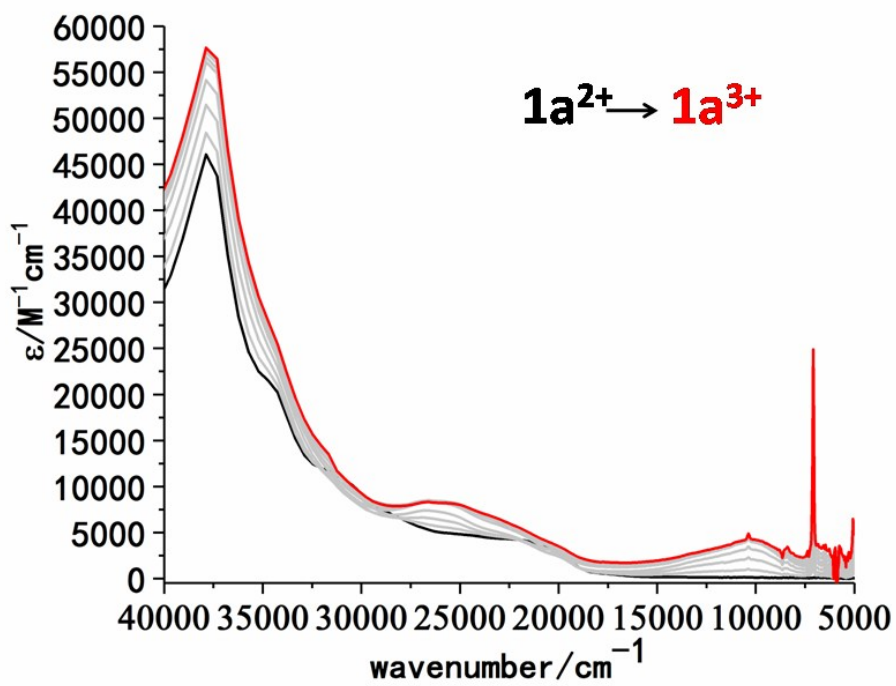
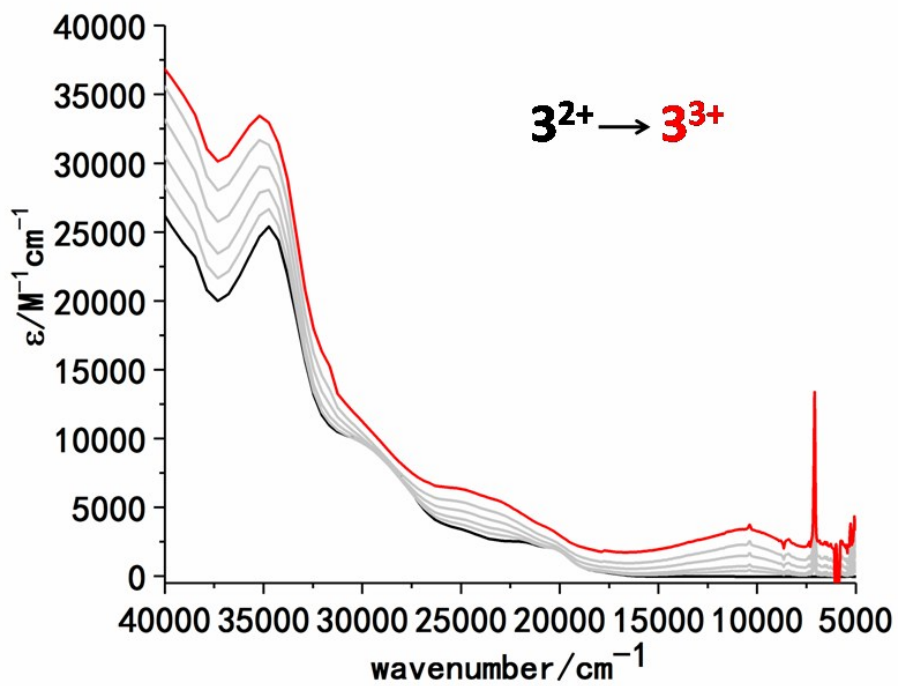


Figure S3. Cyclic voltammograms (vs $\text{Cp}_2\text{Fe}^{+/0}$) for complexes **1-3** and **1a-3a** in 0.10 M acetonitrile solution of Bu_4NPF_6 at a scan rate of 100 mV s^{-1} .





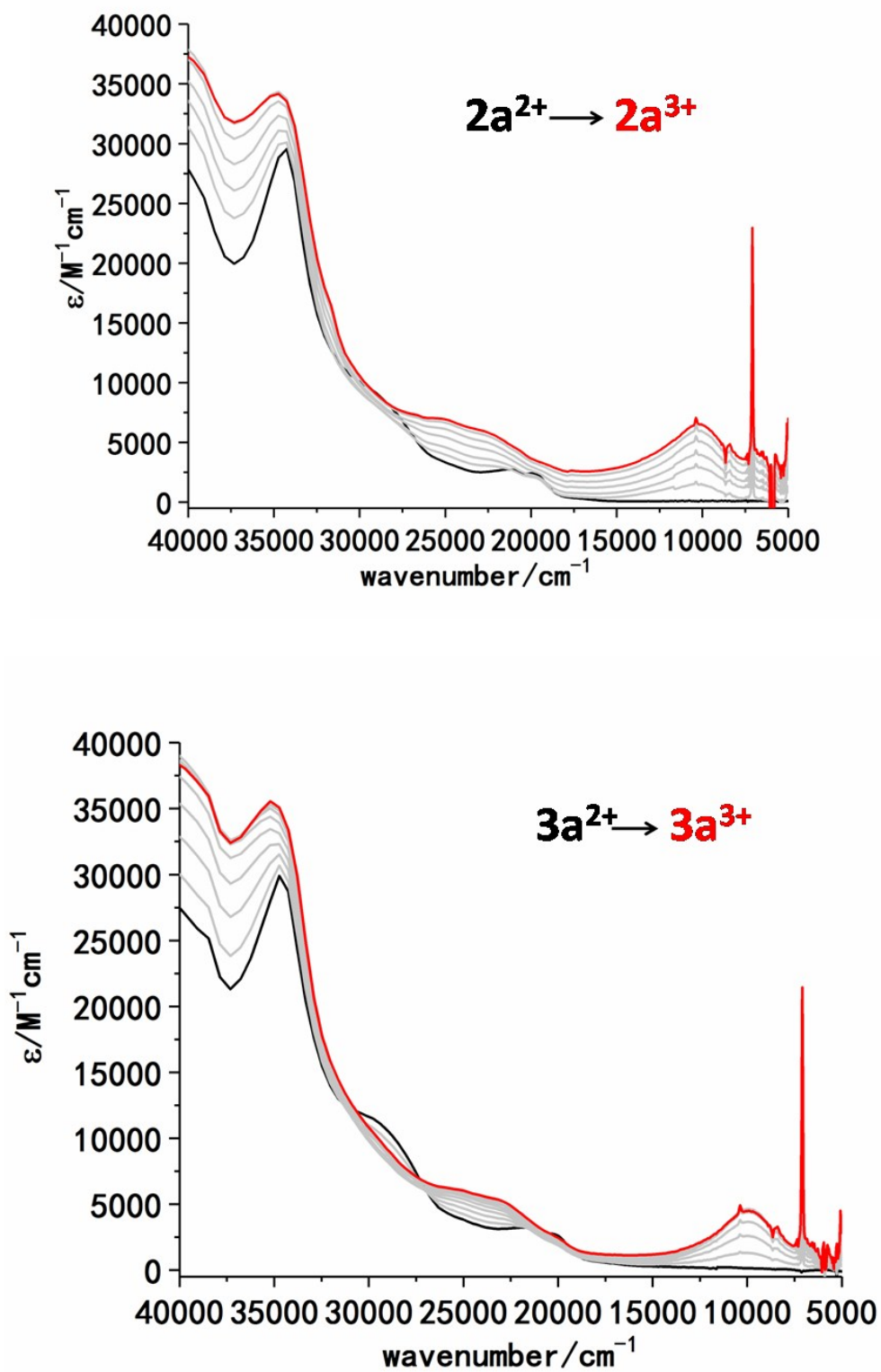


Figure S4. UV-Vis-NIR absorption spectra of complexes **1-3** and **1a-3a** were oxidized slowly by addition of ammonium ceric nitrate in the dichloromethane.

Table S3. Mulliken spin densities of mixed-valence species.

	Ru1	Ru2
1³⁺	0.039458	0.844889
2³⁺	0.057586	0.828997
3³⁺	0.066070	0.820681
1a³⁺	0.062427	0.820157
2a³⁺	0.062986	0.819070
3a³⁺	0.071993	0.808535

Optimized crystallographic coordinatesComplex **1³⁺**

Ru	-2.044446	-0.336414	1.058279
Ru	3.056088	0.334820	-0.011241
P	-3.057904	1.539413	-0.320718
P	-2.807930	-1.255699	-1.161207
N	2.705089	1.394060	-1.806070
N	-0.087146	-0.073911	0.408717
N	3.724565	3.283473	0.225285
N	3.559157	-0.769778	1.718581
N	5.141733	0.763443	-0.357744
C	-0.152791	4.539763	-0.481974
H	0.754800	4.801408	0.055007
N	3.001968	2.273776	0.857735
N	3.366726	-1.575833	-0.838053
C	-2.047484	3.044089	-0.809387
C	2.466164	2.853353	1.954882
H	1.833101	2.282563	2.616324
N	5.474997	2.024292	-0.837394
C	-3.203810	0.461380	-1.882970
H	-2.416500	0.757003	-2.581716
H	-4.166237	0.508598	-2.397035
N	3.454895	2.544218	-2.044494
C	6.839081	2.138810	-1.027195
H	7.300855	3.044102	-1.394256
C	3.709156	-2.534035	0.097627
C	-1.615810	-2.070319	-2.347802

C	1.093446	0.046625	0.255361
C	-1.691314	-1.864458	2.795599
C	-3.741282	-0.729598	2.592358
C	3.801584	-2.106766	1.462383
C	4.326661	-2.531436	3.802215
H	4.625291	-3.198951	4.605639
C	3.093914	3.126512	-3.243932
H	3.563514	4.026067	-3.614961
C	6.312490	0.097875	-0.254620
H	6.338271	-0.920841	0.099881
C	-0.848143	3.361495	-0.144620
H	-0.462846	2.705504	0.630320
C	3.719924	-0.323744	2.981765
H	3.564723	0.733122	3.155513
C	3.363473	-1.924489	-2.139929
H	3.116200	-1.152689	-2.856940
C	-1.725945	-1.833980	-3.736414
H	-2.454106	-1.126977	-4.126807
C	-0.695447	-3.025939	-1.870411
H	-0.604936	-3.215335	-0.803726
C	4.190396	-3.028242	2.475327
C	1.876391	1.278277	-2.866225
H	1.165359	0.467574	-2.913525
C	7.400190	0.919100	-0.663183
H	8.445858	0.655364	-0.686224
C	3.645508	4.465631	0.933156
H	4.149070	5.366822	0.613937
C	-0.922442	-2.553447	-4.640505
H	-1.025219	-2.381760	-5.708346
C	-2.543960	3.899733	-1.819613
H	-3.485001	3.682149	-2.319441
C	0.094835	-3.755646	-2.778617
H	0.776239	-4.516645	-2.408825
C	-0.644529	5.391590	-1.487846
H	-0.118602	6.310186	-1.734474
C	-1.504139	-0.514892	3.293461
C	-3.078759	1.540308	3.754084
H	-2.244240	2.243589	3.659777
H	-3.292238	1.432282	4.827739
H	-3.962949	1.988040	3.294849
C	4.412571	3.001016	-1.038192
H	4.864614	3.930529	-1.393909
C	3.682977	-3.234517	-2.572644
H	3.679449	-3.451527	-3.635164

C	2.089881	2.336097	-3.793059
H	1.581396	2.497978	-4.730266
C	-2.765921	0.191660	3.168940
C	4.005466	-4.215940	-1.636754
H	4.258079	-5.224678	-1.951622
C	4.384325	-4.805252	0.792023
H	4.613529	-5.832311	0.521131
C	-5.225558	-0.489558	2.529906
H	-5.474735	0.504850	2.147798
H	-5.650817	-0.565437	3.541112
H	-5.732939	-1.233231	1.910805
C	4.025628	-3.875585	-0.254545
C	4.098065	-1.177408	4.046659
H	4.217183	-0.759696	5.040647
C	4.459246	-4.398973	2.105144
H	4.745924	-5.101977	2.882472
C	-0.670727	-2.966094	2.844720
H	-0.862191	-3.737714	2.092280
H	-0.698749	-3.460697	3.826773
H	0.345522	-2.586026	2.696761
C	-3.076117	-2.002737	2.388086
C	-4.743128	2.296658	0.019873
C	2.846775	4.220472	2.046428
H	2.581152	4.924815	2.819123
C	-4.806860	3.322780	0.992484
H	-3.906686	3.659124	1.501843
C	-5.915706	1.925567	-0.671420
H	-5.903915	1.170175	-1.450742
C	-4.374517	-2.276551	-1.343746
C	-1.838319	5.065596	-2.162893
H	-2.228625	5.725442	-2.932574
C	-0.263831	0.011675	3.957713
H	-0.245710	-0.298234	5.012492
H	-0.232295	1.106299	3.942585
H	0.645790	-0.374255	3.485642
C	-5.610589	-1.756022	-0.899106
H	-5.669188	-0.773046	-0.442735
C	-3.741349	-3.287920	1.989953
H	-4.570421	-3.132677	1.296306
H	-4.154412	-3.768432	2.889477
H	-3.043350	-3.998062	1.536349
C	-0.017925	-3.522735	-4.163110
H	0.573755	-4.103024	-4.866152
C	-4.327058	-3.567518	-1.913192

H	-3.390975	-3.988172	-2.266704
C	-6.028473	3.957130	1.275734
H	-6.064683	4.752196	2.015189
C	-7.199806	3.577233	0.589986
H	-8.142594	4.072187	0.804056
C	-7.137694	2.566898	-0.386983
H	-8.031923	2.284261	-0.935331
C	-6.788931	-2.509526	-1.043123
H	-7.737927	-2.097636	-0.710486
C	-5.509129	-4.321235	-2.047923
H	-5.466088	-5.310744	-2.494083
C	-6.741511	-3.795490	-1.617677
H	-7.652089	-4.376841	-1.730076

Complex 2³⁺

Ru	1.962642	-0.209314	1.145952
Ru	-3.139984	0.036923	-0.049812
P	2.730698	1.609573	-0.409245
P	2.674077	-1.226027	-1.047416
N	-3.978547	2.275182	-1.927951
N	-3.124760	2.007915	-0.857397
N	-2.965205	-0.486039	-2.106244
N	-3.487505	0.490124	1.964279
N	-5.263160	0.085289	-0.417972
N	0.014855	-0.039603	0.458448
N	-3.363031	-1.870154	0.782317
N	-3.819390	0.144362	-3.011843
N	-5.714005	0.638887	-1.608761
C	0.863986	-3.574896	-3.976803
H	0.957486	-3.710905	-5.050736
C	-2.488323	3.173458	-0.609208
H	-1.732911	3.233328	0.158766
C	-2.932212	4.192710	-1.496204
H	-2.605299	5.219033	-1.524646
C	2.612438	0.460948	-1.932931
H	3.373442	0.632271	-2.697496
H	1.616963	0.567483	-2.375172
C	-3.873098	3.593170	-2.325350
H	-4.457023	4.000561	-3.138072
C	0.833376	4.830148	-2.259140

H	0.689874	5.194402	-3.272683
C	6.591705	-2.012534	-2.351843
H	7.381450	-1.493348	-2.887451
C	0.430718	5.615481	-1.161269
H	-0.013336	6.593914	-1.325805
C	-1.162562	0.002613	0.247336
C	-3.643458	-0.591253	2.803328
C	5.559248	1.409845	-0.104926
H	5.378404	0.358567	0.088752
C	1.686279	3.123793	-0.733929
C	1.521389	-2.413869	-1.931212
C	4.345568	-2.010648	-1.394340
C	4.743616	3.654604	-0.606536
H	3.937258	4.352087	-0.806537
C	3.673844	-0.868177	2.580595
C	-6.375828	-0.319985	0.233058
H	-6.309325	-0.792965	1.200446
C	4.484404	2.286157	-0.371649
C	-4.735801	1.183004	-2.540035
H	-5.271477	1.583008	-3.404798
C	-7.090904	0.578643	-1.695225
H	-7.637087	0.958854	-2.546476
C	-3.616031	1.745407	2.471410
H	-3.517153	2.562383	1.769501
C	-3.571468	-4.278029	0.683776
H	-3.588102	-5.177438	0.077469
C	6.772518	-3.347940	-1.948056
H	7.703257	-3.863039	-2.167488
C	6.067970	4.132874	-0.586451
H	6.259544	5.186240	-0.770018
C	-2.524368	-1.196104	-4.231886
H	-2.076137	-1.730008	-5.054418
C	1.833780	0.334094	3.414157
C	6.880103	1.891003	-0.093665
H	7.702537	1.208169	0.102537
C	-3.561919	-0.272738	-4.302836
H	-4.119202	0.096151	-5.151912
C	-3.765333	-4.333517	2.076704
H	-3.925460	-5.283087	2.577693
C	-3.371549	-3.031357	0.075144
H	-3.229281	-2.947266	-0.993939
C	-3.575737	-1.910114	2.142391
C	2.543972	-1.787791	2.698021
C	1.462999	3.588396	-2.047545

H	1.805787	3.017991	-2.907293
C	5.384182	-1.341879	-2.074710
H	5.279493	-0.312907	-2.403450
C	7.138423	3.255351	-0.333221
H	8.158487	3.628399	-0.320086
C	-2.181839	-1.293236	-2.854555
H	-1.413768	-1.892308	-2.390884
C	-7.541683	-0.031669	-0.528769
H	-8.565697	-0.240020	-0.261421
C	0.667726	-3.250347	-1.183295
H	0.591508	-3.128460	-0.106075
C	1.012267	1.422634	4.045827
H	1.327558	2.418811	3.718856
H	1.126911	1.394084	5.139427
H	-0.054483	1.310417	3.824970
C	4.107769	1.634501	3.255527
H	4.915914	1.708391	2.524037
H	4.573449	1.561624	4.249575
H	3.542305	2.571044	3.233462
C	-3.883581	1.984677	3.826288
H	-3.988468	3.003783	4.182860
C	-0.070599	-4.261229	-1.830861
H	-0.694716	-4.932653	-1.246695
C	-3.768603	-3.135210	2.808422
H	-3.937998	-3.160078	3.878647
C	3.233641	0.432414	3.036699
C	-3.905242	-0.410457	4.174860
H	-4.032591	-1.265268	4.829007
C	5.098807	-1.287875	2.335501
H	5.207239	-1.943464	1.465517
H	5.466555	-1.846393	3.208273
H	5.761073	-0.428743	2.205619
C	1.415393	-1.042028	3.224217
C	5.735140	-4.019291	-1.269905
H	5.862474	-5.055620	-0.969959
C	4.526582	-3.356644	-0.996349
H	3.723140	-3.905429	-0.510291
C	-4.024259	0.887601	4.696666
H	-4.236074	1.038588	5.750511
C	1.258692	3.901007	0.365105
H	1.440838	3.561699	1.382336
C	0.637087	5.145993	0.151632
H	0.346208	5.758155	1.001239
C	1.616830	-2.576580	-3.331319

H	2.295197	-1.960978	-3.917862
C	2.623633	-3.281290	2.543543
H	1.667946	-3.724182	2.244122
H	2.903714	-3.736728	3.504790
H	3.386095	-3.574891	1.817109
C	0.027725	-4.426961	-3.226088
H	-0.521724	-5.222679	-3.721748
C	0.093624	-1.621964	3.639097
H	-0.721617	-0.902901	3.514268
H	0.129819	-1.901657	4.701993
H	-0.152537	-2.525262	3.072076

Complex 3^{3+}

C	-3.337970	-2.822855	-0.488689
H	-3.097800	-2.665521	-1.531860
C	-3.641708	-4.099152	-0.004478
H	-3.637401	-4.942314	-0.688528
C	-3.969792	-4.281999	1.359711
C	-3.972396	-3.128250	2.172037
H	-4.231397	-3.223153	3.220859
C	-3.668229	-1.864972	1.634746
C	-3.721672	-0.603379	2.404314
C	-4.072839	-0.524635	3.764142
H	-4.290240	-1.429476	4.321085
C	-4.169416	0.721730	4.418089
C	-3.891138	1.871184	3.640985
H	-3.958973	2.862997	4.077514
C	-3.538502	1.739156	2.294528
H	-3.339247	2.610866	1.685695
C	-4.335661	-5.640177	1.909171
H	-4.214875	-5.688869	2.995920
H	-3.729685	-6.434378	1.459310
H	-5.386007	-5.874013	1.685489
C	-4.582226	0.830904	5.866404
H	-3.986350	1.580988	6.398795
H	-4.485681	-0.122854	6.394246
H	-5.632359	1.145178	5.943696
C	-4.400196	1.651455	-2.814607
H	-4.870761	2.143542	-3.669690
C	-3.179921	0.302612	-4.629500
H	-3.675733	0.762053	-5.472457

C	-2.178995	-0.661624	-4.581826
H	-1.702093	-1.141215	-5.421500
C	-1.918546	-0.885701	-3.201125
H	-1.196690	-1.547337	-2.748613
C	-6.820172	1.075361	-2.153442
H	-7.302143	1.546043	-2.998189
C	-7.358972	0.390171	-1.068722
H	-8.403601	0.202764	-0.876176
C	-6.249797	-0.007205	-0.271804
H	-6.254520	-0.560628	0.654152
C	-3.474164	4.000609	-2.343184
H	-3.996623	4.497137	-3.148086
C	-2.566513	4.492358	-1.412492
H	-2.209022	5.505482	-1.330559
C	-2.205733	3.384605	-0.596391
H	-1.495444	3.350748	0.215128
C	-1.040740	0.090639	0.052564
C	1.721964	-0.107723	3.412702
C	1.276360	-1.428415	3.010284
C	2.417057	-2.143246	2.469305
C	3.580866	-1.262800	2.555106
C	3.147857	-0.016041	3.149477
C	0.885654	0.920722	4.120476
H	1.279103	1.932954	3.985140
H	0.878764	0.721461	5.202230
H	-0.154220	0.907896	3.776888
C	-0.091206	-2.002133	3.247257
H	-0.872593	-1.242368	3.151301
H	-0.148775	-2.411768	4.266178
H	-0.317588	-2.817839	2.553494
C	2.462074	-3.605971	2.123206
H	1.513162	-3.968511	1.714100
H	2.668506	-4.193139	3.030144
H	3.257811	-3.832524	1.408134
C	5.005495	-1.707652	2.354679
H	5.163658	-2.213570	1.396710
H	5.277213	-2.421403	3.145435
H	5.707348	-0.873302	2.425467
C	4.037584	1.114629	3.583242
H	4.907547	1.239359	2.934755
H	4.411886	0.908249	4.596839
H	3.506790	2.070814	3.624340
C	2.867333	0.657659	-1.819789
H	1.900865	0.853144	-2.294322

H	3.673794	0.887611	-2.519795
C	4.701232	2.223766	0.050174
C	5.727784	1.301852	0.351709
H	5.507730	0.247060	0.468742
C	7.055729	1.740632	0.495918
H	7.840580	1.022663	0.718962
C	7.369286	3.106744	0.354843
H	8.394282	3.446857	0.471465
C	6.346889	4.029197	0.065279
H	6.580645	5.084500	-0.042819
C	5.016542	3.594162	-0.087087
H	4.248138	4.326399	-0.310257
C	1.952403	3.188972	-0.372486
C	1.481841	3.854907	0.780498
H	1.594974	3.401502	1.762515
C	0.903606	5.133950	0.672180
H	0.578536	5.658021	1.567029
C	0.784370	5.749996	-0.589916
H	0.374370	6.753598	-0.668883
C	1.229558	5.076615	-1.744278
H	1.152972	5.552697	-2.717963
C	1.814592	3.800112	-1.637067
H	2.188943	3.314983	-2.535251
C	4.505857	-1.902285	-1.468206
C	4.626371	-3.298904	-1.271841
H	3.773070	-3.891564	-0.949801
C	5.843311	-3.948616	-1.539171
H	5.924485	-5.022432	-1.395915
C	6.950001	-3.213377	-2.009667
H	7.887652	-3.717506	-2.225187
C	6.830336	-1.826337	-2.212240
H	7.674841	-1.255446	-2.587716
C	5.614507	-1.169087	-1.940110
H	5.557794	-0.098607	-2.109122
C	1.708637	-2.178289	-2.205512
C	0.796625	-3.062134	-1.592800
H	0.663837	-3.046145	-0.514284
C	0.073978	-3.983092	-2.377364
H	-0.598417	-4.690291	-1.898445
C	0.248035	-4.012346	-3.774771
H	-0.289994	-4.739224	-4.377205
C	1.144322	-3.113657	-4.389382
H	1.295901	-3.145403	-5.464848
C	1.880909	-2.204586	-3.607269

H	2.605639	-1.553423	-4.090742
N	-3.341824	-1.719362	0.305799
N	-3.444669	0.531287	1.676028
N	-3.496323	0.619846	-3.323134
N	-2.716526	-0.115648	-2.429943
N	-5.449340	1.071618	-1.987523
N	-5.088002	0.404269	-0.825014
N	-3.641112	2.657202	-2.071480
N	-2.860544	2.268041	-0.982942
N	0.119813	-0.025128	0.324691
P	2.934026	1.612213	-0.163280
P	2.830521	-1.120414	-1.138057
Ru	-2.989630	0.237571	-0.348126
Ru	2.005860	-0.351743	1.107314

Complex **1a**³⁺

C	2.958101	2.834025	1.217291
H	3.119422	3.190494	0.208670
C	2.848585	3.748146	2.293161
H	2.920273	4.810647	2.088840
C	2.660877	3.273944	3.590583
H	2.583356	3.961316	4.428315
C	2.591791	1.869503	3.811976
C	2.440929	1.272148	5.119166
H	2.349542	1.925132	5.982908
C	2.436401	-0.095508	5.276895
H	2.342096	-0.534072	6.266644
C	2.580409	-0.975799	4.139893
C	2.640152	-2.394099	4.244114
H	2.563529	-2.871608	5.216963
C	2.816585	-3.152680	3.087975
H	2.881375	-4.234185	3.130909
C	2.924749	-2.508969	1.831429
H	3.073501	-3.086649	0.928836
C	2.707572	1.017845	2.678178
C	2.699783	-0.405586	2.841877
C	5.382996	-0.290554	-2.208874
H	6.166557	-0.385555	-2.965056
C	4.700194	1.775287	-3.582194
H	5.498775	1.709002	-4.307064
C	3.649856	2.681532	-3.473078

H	3.447999	3.514295	-4.128281
C	2.912913	2.284804	-2.322903
H	2.020528	2.721708	-1.902595
C	4.642809	-2.589564	-3.094911
H	5.438291	-2.702501	-3.817437
C	3.571329	-3.423329	-2.789863
H	3.344980	-4.373420	-3.247634
C	2.851662	-2.767413	-1.752682
H	1.951011	-3.079412	-1.246842
C	7.358571	-0.127552	-0.567355
H	8.145345	-0.220083	-1.302224
C	7.423330	0.028478	0.813471
H	8.315546	0.087125	1.416804
C	6.074190	0.094585	1.260153
H	5.707249	0.213203	2.267864
C	1.114855	-0.046740	-0.415425
C	-1.992830	-1.100098	-3.352026
C	-3.288693	-1.371985	-2.760646
C	-3.953809	-0.099587	-2.520865
C	-3.079517	0.952970	-3.025512
C	-1.863750	0.332995	-3.512984
C	-1.021377	-2.116107	-3.884981
H	0.019609	-1.819262	-3.713418
H	-1.153483	-2.218895	-4.972059
H	-1.180124	-3.108684	-3.453081
C	-3.919280	-2.728872	-2.627914
H	-3.184672	-3.520729	-2.451162
H	-4.438573	-2.971859	-3.566779
H	-4.661961	-2.768467	-1.828605
C	-5.398078	0.079593	-2.137346
H	-5.776183	-0.772407	-1.567741
H	-6.015101	0.169449	-3.043108
H	-5.560144	0.982601	-1.540139
C	-3.477486	2.384721	-3.256105
H	-4.369835	2.651202	-2.686691
H	-3.724210	2.519465	-4.319263
H	-2.682486	3.098448	-3.017370
C	-0.737078	1.029390	-4.224005
H	-0.740392	2.107676	-4.036998
H	-0.839543	0.891748	-5.310209
H	0.241051	0.627230	-3.936904
C	-1.827014	0.870267	2.103240
H	-0.740263	0.839402	1.981253
H	-2.055951	1.523144	2.953399

C	-2.387308	-0.545600	2.338814
H	-3.370078	-0.519034	2.816561
H	-1.717768	-1.104058	3.000385
C	-1.441537	3.228998	0.277554
C	-0.666601	3.421726	-0.883686
H	-0.617278	2.637889	-1.634199
C	0.022716	4.634631	-1.081146
H	0.578124	4.803765	-2.001358
C	-0.044473	5.653604	-0.112088
H	0.465820	6.598948	-0.276297
C	-0.804513	5.456368	1.058199
H	-0.875120	6.245756	1.801401
C	-1.508251	4.253463	1.249055
H	-2.130651	4.139317	2.133088
C	-4.154602	2.389265	0.933609
C	-4.707817	3.377471	0.086511
H	-4.160213	3.728687	-0.782606
C	-5.948631	3.963640	0.390010
H	-6.357157	4.729486	-0.263380
C	-6.651953	3.575680	1.547515
H	-7.607809	4.033411	1.785318
C	-6.097551	2.608028	2.405477
H	-6.620848	2.321364	3.313495
C	-4.856496	2.015664	2.101103
H	-4.449113	1.293146	2.801165
C	-4.315067	-2.312624	0.902063
C	-5.421406	-1.453382	1.092377
H	-5.294232	-0.374810	1.110391
C	-6.713008	-1.985467	1.252681
H	-7.555631	-1.316996	1.406803
C	-6.915823	-3.379304	1.211849
H	-7.913439	-3.790036	1.338057
C	-5.818587	-4.236388	1.006208
H	-5.966938	-5.312018	0.971795
C	-4.522352	-3.708593	0.850562
H	-3.692763	-4.392123	0.701078
C	-1.464774	-3.054171	0.910207
C	-1.374402	-3.735492	2.145260
H	-1.913437	-3.379445	3.019851
C	-0.625711	-4.922577	2.248348
H	-0.584298	-5.451470	3.196594
C	0.027936	-5.448260	1.116194
H	0.573088	-6.385672	1.187882
C	-0.057431	-4.770499	-0.115164

H	0.415529	-5.194188	-0.998493
C	-0.795528	-3.574754	-0.215845
H	-0.865094	-3.060057	-1.169167
N	2.880807	1.499860	1.394258
N	2.861953	-1.168762	1.700757
N	4.578256	0.889244	-2.530600
N	3.472293	1.200479	-1.742522
N	4.549767	-1.493175	-2.261188
N	3.441461	-1.597335	-1.423207
N	6.019052	-0.150830	-0.905710
N	5.217178	-0.013755	0.221829
N	-0.055226	-0.066993	-0.662454
P	-2.470248	1.669427	0.500906
P	-2.596091	-1.565477	0.722997
Ru	3.077691	-0.021094	-0.052547
Ru	-2.060210	-0.094839	-1.219230

Complex **2a**³⁺

C	3.628956	2.526043	1.528117
H	3.489304	3.022288	0.577202
C	3.921978	3.256235	2.688017
H	4.012414	4.335995	2.636080
C	4.108168	2.565087	3.899699
H	4.337171	3.100964	4.815486
C	4.013834	1.164164	3.901328
H	4.179259	0.616101	4.821630
C	3.731162	0.481609	2.702985
C	3.706126	-0.989674	2.577301
C	3.960840	-1.874913	3.641934
H	4.141245	-1.497328	4.641745
C	4.007824	-3.257613	3.402102
H	4.215857	-3.948637	4.212964
C	3.801864	-3.726401	2.091275
H	3.856279	-4.784102	1.856653
C	3.537434	-2.800493	1.072854
H	3.381841	-3.122804	0.052162
C	4.525139	0.210791	-2.997511
H	4.995574	0.285356	-3.981361
C	6.950762	0.095614	-2.145242
H	7.430825	0.169393	-3.110478
C	7.494757	-0.020622	-0.869899

H	8.541945	-0.059475	-0.614161
C	6.386856	-0.076707	0.020379
H	6.396163	-0.166351	1.095614
C	3.494682	2.476587	-3.636148
H	3.995051	2.569807	-4.589327
C	2.573568	3.310172	-3.010797
H	2.181371	4.240626	-3.389181
C	2.261437	2.685927	-1.771392
H	1.572721	3.013475	-1.008122
C	3.408271	-1.873025	-4.005635
H	3.906079	-1.824054	-4.963446
C	2.452946	-2.762622	-3.525295
H	2.025230	-3.599624	-4.053479
C	2.163790	-2.344938	-2.196608
H	1.462574	-2.767775	-1.494098
C	1.165623	-0.013293	0.240529
C	-1.770221	0.469491	3.340034
C	-1.916789	-0.966688	3.229226
C	-3.224808	-1.243833	2.668349
C	-3.878992	0.026668	2.393062
C	-2.986502	1.086658	2.850788
C	-0.626431	1.178125	4.010329
H	0.341735	0.744061	3.736031
H	-0.609385	2.245749	3.771258
H	-0.725042	1.094436	5.102432
C	-0.949194	-1.979053	3.775570
H	0.092496	-1.690714	3.594184
H	-1.078041	-2.064593	4.864597
H	-1.113760	-2.976887	3.358288
C	-3.869284	-2.598397	2.596364
H	-4.652744	-2.648388	1.838156
H	-3.149416	-3.399222	2.398845
H	-4.340584	-2.817952	3.565883
C	-5.322945	0.206094	2.009395
H	-5.697245	-0.641283	1.429931
H	-5.943337	0.287183	2.913605
H	-5.483803	1.113030	1.418334
C	-3.361046	2.530868	3.040935
H	-4.277132	2.783810	2.503997
H	-3.556462	2.711086	4.107911
H	-2.571985	3.226059	2.736363
C	-1.823783	0.806685	-2.291506
H	-2.057867	1.430282	-3.161980
H	-0.735775	0.771252	-2.182973

C	-2.397732	-0.612806	-2.467990
H	-1.742252	-1.200779	-3.118168
H	-3.387373	-0.595757	-2.931725
C	-1.410850	3.225623	-0.543187
C	-0.601043	3.432499	0.592308
H	-0.533520	2.663196	1.355385
C	0.110590	4.639117	0.744184
H	0.705286	4.807679	1.638702
C	0.026335	5.640187	-0.243017
H	0.556694	6.580074	-0.116259
C	-0.772882	5.430508	-1.385445
H	-0.856587	6.206482	-2.141341
C	-1.495475	4.232047	-1.532404
H	-2.142895	4.106695	-2.396592
C	-4.132963	2.371965	-1.149109
C	-4.684759	3.373336	-0.316842
H	-4.134973	3.738532	0.544986
C	-5.927025	3.953159	-0.626241
H	-6.334650	4.729253	0.015524
C	-6.633310	3.545121	-1.775041
H	-7.590441	3.997716	-2.017483
C	-6.080203	2.564297	-2.618769
H	-6.605522	2.262649	-3.520729
C	-4.837480	1.978395	-2.308510
H	-4.430446	1.246436	-2.999075
C	-1.457187	-3.066618	-0.974560
C	-0.688130	-3.500547	0.124071
H	-0.683137	-2.923573	1.043047
C	0.067470	-4.687085	0.038619
H	0.631609	-5.031399	0.901678
C	0.065988	-5.443647	-1.149342
H	0.628261	-6.371589	-1.208473
C	-0.691350	-5.006028	-2.255286
H	-0.715652	-5.596232	-3.167276
C	-1.453920	-3.826552	-2.167561
H	-2.067901	-3.533457	-3.015850
C	-4.305125	-2.325185	-0.936014
C	-4.514131	-3.710568	-0.757285
H	-3.684785	-4.378036	-0.546291
C	-5.810493	-4.249588	-0.863436
H	-5.959493	-5.317633	-0.732093
C	-6.907464	-3.413524	-1.144001
H	-7.905592	-3.832943	-1.231549
C	-6.703446	-2.029501	-1.311534

H	-7.545573	-1.377190	-1.525700
C	-5.411107	-1.485859	-1.202635
H	-5.285088	-0.413615	-1.321839
N	3.522453	1.170471	1.528513
N	3.478000	-1.461973	1.303629
N	5.577603	0.105959	-1.995650
N	5.220422	-0.000475	-0.657297
N	3.714717	1.410514	-2.786951
N	2.953333	1.533750	-1.624183
N	3.669771	-0.975856	-2.989541
N	2.901751	-1.263349	-1.861301
N	-0.004705	-0.027171	0.487703
P	-2.445800	1.663450	-0.710609
P	-2.584343	-1.571349	-0.812634
Ru	3.125342	-0.004774	-0.156696
Ru	-2.006746	-0.036287	1.065685

Complex **3a**³⁺

Ru	2.977034	0.010356	-0.500270
Ru	-2.046859	-0.037681	1.056336
P	-2.638653	1.648425	-0.681545
N	3.446115	1.253768	1.118067
N	3.399850	1.334965	-3.210214
N	2.694882	1.487256	-2.015770
N	5.330177	0.101878	-2.467322
N	5.043804	0.039070	-1.109669
N	-0.104118	-0.036506	0.328054
C	3.519907	2.611048	1.072386
H	3.303563	3.074938	0.119378
C	3.872452	3.383473	2.183195
H	3.929833	4.463154	2.082927
C	4.167884	2.759027	3.418180
C	4.095792	1.350450	3.449797
H	4.332319	0.831697	4.372255
C	3.749425	0.617775	2.300329
C	4.575772	3.562365	4.630019
H	3.958420	4.460933	4.742731
H	5.616738	3.900869	4.534123
H	4.504103	2.978551	5.552771
C	4.225491	0.144963	-3.416310
H	4.643854	0.190914	-4.425103

C	3.112160	2.361241	-4.087895
H	3.561190	2.426786	-5.068522
C	2.203921	3.198662	-3.449087
H	1.771041	4.104572	-3.842576
C	1.969517	2.617241	-2.172104
H	1.312546	2.959830	-1.387892
C	6.693724	0.114179	-2.687168
H	7.122125	0.160557	-3.678014
C	7.304064	0.057829	-1.437976
H	8.363491	0.050225	-1.235437
C	6.244053	0.012700	-0.490361
H	6.308556	-0.035905	0.585524
C	1.048938	-0.018144	0.006666
C	-1.587315	0.427823	3.294151
C	-2.820210	1.095498	2.927269
C	-3.795002	0.072557	2.560516
C	-0.357495	1.088989	3.851439
H	-0.364114	1.022734	4.949250
H	-0.313343	2.151644	3.593593
H	0.561912	0.607524	3.499741
C	-3.115021	2.553381	3.154441
H	-3.164827	2.745288	4.235894
H	-4.083097	2.837936	2.737725
H	-2.348450	3.218527	2.743961
C	-5.263483	0.309031	2.329830
H	-5.778091	0.423337	3.294935
H	-5.450928	1.216775	1.748801
C	-2.130467	0.791586	-2.303045
H	-2.429977	1.412815	-3.154898
H	-1.036972	0.762599	-2.274498
C	-1.613616	3.225686	-0.607309
C	-0.645443	3.413544	0.400954
H	-0.448264	2.624468	1.120431
C	0.066488	4.626963	0.480369
H	0.786775	4.778126	1.280677
C	-0.173013	5.653332	-0.453607
H	0.361633	6.596512	-0.380949
C	-1.129460	5.462074	-1.471295
H	-1.329743	6.254630	-2.186938
C	-1.853449	4.257716	-1.543449
H	-2.618421	4.144512	-2.307415
C	-4.364839	2.330511	-0.991021
C	-4.885155	3.295842	-0.098228
H	-4.293361	3.645283	0.742251

C	-6.153945	3.859476	-0.316979
H	-6.537222	4.608297	0.370578
C	-6.919706	3.469450	-1.433618
H	-7.897739	3.909300	-1.606082
C	-6.400765	2.522161	-2.335200
H	-6.974345	2.232766	-3.211410
C	-5.130658	1.953996	-2.116350
H	-4.753926	1.246328	-2.847987
P	-2.766667	-1.582504	-0.762694
N	3.442683	-1.380482	0.993625
N	3.399382	-1.058052	-3.319312
N	2.692969	-1.315944	-2.144262
C	3.506780	-2.727949	0.822132
H	3.287906	-3.099819	-0.169955
C	3.850440	-3.603106	1.857257
H	3.898952	-4.669194	1.657522
C	4.146628	-3.098345	3.145377
C	4.082876	-1.698168	3.308117
H	4.318410	-1.269600	4.276102
C	3.745616	-0.859365	2.231126
C	4.548682	-4.011606	4.278713
H	3.980793	-4.948449	4.262834
H	5.611122	-4.280336	4.195983
H	4.406464	-3.539454	5.255854
C	3.106485	-1.997945	-4.287349
H	3.555424	-1.975815	-5.269944
C	2.194159	-2.885772	-3.727437
H	1.757350	-3.749549	-4.202317
C	1.961702	-2.422645	-2.402570
H	1.303728	-2.831531	-1.651710
C	-1.800057	-1.001338	3.193709
C	-3.166342	-1.222508	2.761677
C	-0.822874	-2.052555	3.641075
H	-0.822394	-2.115047	4.739167
H	-1.084438	-3.046672	3.267097
H	0.201892	-1.819251	3.329024
C	-3.867786	-2.550131	2.732305
H	-4.274245	-2.759369	3.732964
H	-4.706442	-2.561661	2.033718
H	-3.198047	-3.377130	2.475880
H	-5.734940	-0.526692	1.806635
C	-2.709320	-0.631619	-2.431759
H	-3.731725	-0.620413	-2.818728
H	-2.101212	-1.218850	-3.127115

C	-1.657785	-3.079135	-1.004527
C	-0.810927	-3.507791	0.037443
H	-0.736990	-2.922939	0.948073
C	-0.064562	-4.695522	-0.095953
H	0.561460	-5.035208	0.725346
C	-0.151610	-5.457834	-1.277144
H	0.404836	-6.386340	-1.371907
C	-0.984451	-5.023641	-2.328690
H	-1.072620	-5.616389	-3.235063
C	-1.738552	-3.843173	-2.191873
H	-2.408801	-3.552008	-2.997170
C	-4.496289	-2.323165	-0.740203
C	-4.705297	-3.712849	-0.603968
H	-3.868393	-4.396937	-0.506548
C	-6.013786	-4.233390	-0.604096
H	-6.164606	-5.304798	-0.506448
C	-7.120934	-3.374536	-0.736374
H	-8.128652	-3.779898	-0.743577
C	-6.915126	-1.985840	-0.859249
H	-7.765005	-1.316097	-0.958272
C	-5.610661	-1.460785	-0.854342
H	-5.478516	-0.385518	-0.934643