Supplementary Information

Electronic Properties of Organodiruthenium Complexes Bridged by 2,3,5,6-Tetrakis(2-pyridyl)pyrazine.

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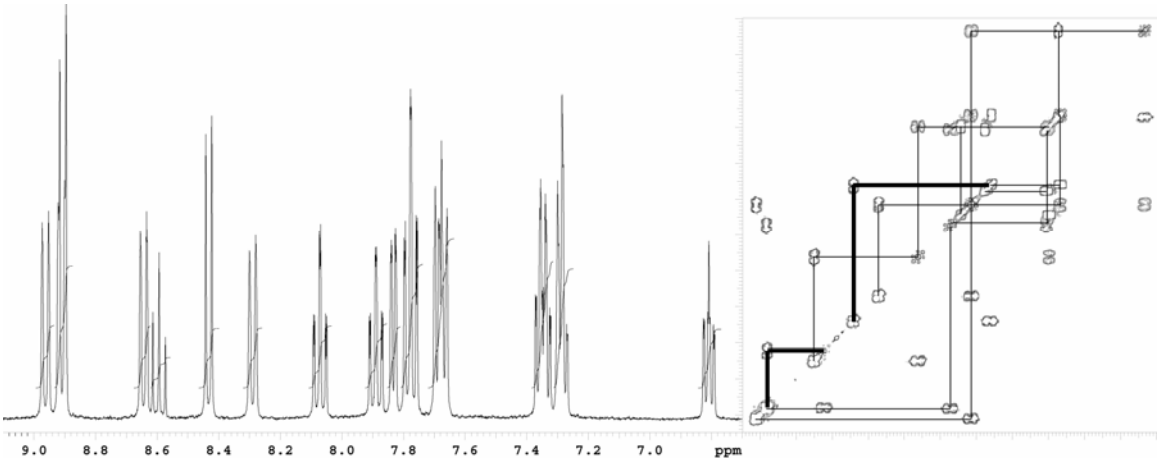

Figure S1. Aromatic region of the ^{1}H NMR spectrum (left) and ^{1}H-^{1}H COSY spectrum (right) of [**4a**]$^{3+}$ in CD_3CN. Correlations highlighted in the bottom part correspond to the tppz bridging ligand, correlation in the upper part to the tpy and H-N^C^N ligand. The bold lines connect signals assigned to the central phenyl (high field) and pyridine (low field) rings in the H-N^C^N and tpy ligands, respectively.

Table S1.1. Optimized geometry for [**3**]$^{4+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	2.568677	-0.05062	0.002076	H	9.374016	-0.05997	5.079655	N	-7.17305	-3.88095	-0.01599
C	1.335838	0.094117	2.313955	N	-5.66119	-0.20646	3.832549	H	-12.5836	-7.34545	0.13848
C	-1.33797	-0.19795	2.312063	C	-7.45678	-0.36395	5.661598	H	-9.46068	-10.8742	0.152657
N	-2.56791	-0.05179	-0.00127	C	-6.89522	-1.05443	8.149981	H	-4.80966	-9.83672	0.050042
C	-1.33523	0.095747	-2.31328	C	-4.39263	-1.7196	8.738236	H	-3.51066	-5.29157	-0.06434
C	1.339122	-0.19465	-2.31165	C	-2.5193	-1.49917	6.866944	H	-9.37444	0.036109	5.075655
C	3.129529	0.522184	4.439027	H	-8.38927	-1.13366	9.550913	N	10.14104	0.044628	0.000354
C	-3.13628	-0.60911	4.436263	H	-3.90477	-2.3875	10.61597	C	11.42401	-2.2032	-0.0304
C	-3.1302	0.524316	-4.43764	H	-0.60189	-2.0556	7.301215	C	14.07921	-2.20521	-0.04671
C	3.13872	-0.60261	-4.43555	Ru	-6.33614	-0.01293	0.000556	C	15.36873	0.123299	-0.01157
N	5.66381	-0.20436	-3.82935	Ru	6.336871	-0.01246	0.002251	C	14.01004	2.411851	0.029669
C	7.460853	-0.36284	-5.65701	N	-10.1399	0.045583	0.000465	C	11.35655	2.329731	0.025476
C	6.900733	-1.04717	-8.14732	C	-11.4235	-2.20197	0.027561	C	9.733146	-4.42467	-0.03678
C	4.397161	-1.70518	-8.73937	C	-14.0787	-2.20323	0.037745	H	15.12996	-3.96281	-0.08485
C	2.522769	-1.486	-6.86887	C	-15.3673	0.125668	0.000338	H	17.42072	0.154214	-0.0177
H	9.378844	0.031394	-5.06854	C	-14.008	2.413879	-0.03745	H	15.00695	4.200603	0.060946
H	8.396518	-1.12649	-9.54662	C	-11.3546	2.331107	-0.02764	C	9.601477	4.499793	0.033712
H	3.909637	-2.36677	-10.6194	C	-9.7336	-4.42395	0.03353	N	7.059057	3.879671	-0.01168
H	0.604966	-2.03864	-7.30567	H	-15.1306	-3.9602	0.07171	C	5.315603	5.765416	-0.0094
C	-2.50711	1.4037	-6.87094	H	-17.4194	0.157135	0.00094	C	5.976389	8.32229	0.052382
C	-4.3797	1.639216	-8.74136	H	-15.0051	4.202485	-0.07134	C	8.551815	8.973992	0.103615
C	-6.88741	0.995118	-8.15164	C	-9.59914	4.500697	-0.03405	C	10.3688	7.037634	0.090942
C	-7.4538	0.317218	-5.66104	N	-7.05705	3.879937	0.016208	H	3.356438	5.178509	-0.05283
N	-5.65946	0.152584	-3.83149	C	-5.31332	5.765446	0.018078	H	4.515744	9.761403	0.060501
H	-0.58543	1.942165	-7.3077	C	-5.97354	8.322514	-0.04572	H	9.1333	10.93949	0.152731
H	-3.8875	2.302184	-10.6198	C	-8.54872	8.974666	-0.10402	H	12.3612	7.507583	0.132732
H	-8.38146	1.082913	-9.55211	C	-10.366	7.038578	-0.09459	C	10.57612	-6.93827	-0.10106
H	-9.37449	-0.06431	-5.07274	H	-3.35447	5.177786	0.066532	C	8.817293	-8.92769	-0.11474
C	2.502798	1.398108	6.872403	H	-4.51247	9.761322	-0.05049	C	6.223645	-8.35323	-0.05583
C	4.373076	1.632903	8.744919	H	-9.12965	10.94026	-0.15609	C	5.485715	-5.81756	0.013913
C	6.882196	0.99297	8.156699	H	-12.3581	7.508812	-0.14195	N	7.172746	-3.88083	0.0155
C	7.452104	0.31873	5.66582	C	-10.5777	-6.9372	0.09235	H	12.5819	-7.34725	-0.14826
N	5.659555	0.153177	3.83442	C	-8.81981	-8.9274	0.101557	H	9.457349	-10.8746	-0.17106
H	0.579934	1.93352	7.307753	C	-6.22585	-8.35391	0.044838	H	4.806967	-9.83548	-0.06478
H	3.87781	2.291732	10.62388	C	-5.48677	-5.81835	-0.01774	H	3.509766	-5.29042	0.063011
H	8.374348	1.080077	9.559279								

Table S1.2. Orbital energies and Mulliken population on Ru for [**3**]$^{4+}$.

#	E (eV)	Ru[1]	p	d	Ru[2]	p	d
H-12	-16.8026	0.003822	0.0001	0.003722	0.005285	0.000099	0.005186
H-11	-16.7999	0.01185	2.1E-06	0.011848	0.010385	1.3E-06	0.010384
H-10	-16.5507	0.008523	0.000164	0.008358	0.009896	0.000171	0.009725
H-9	-16.5497	0.009045	-4.5E-05	0.00909	0.007688	-5E-05	0.007738
H-8	-15.8989	0.01068	-0.00021	0.011063	0.010681	-0.00021	0.011064
H-7	-15.6534	0.014132	0.000001	0.014126	0.014543	1.2E-06	0.014536
H-6	-15.6424	0.008002	-1.8E-05	0.008043	0.007578	-1.8E-05	0.00762
H-5	-15.4534	0.29666	0.006379	0.290281	0.29647	0.006374	0.290095
H-4	-14.9101	0.353517	0.002462	0.351055	0.364044	0.002537	0.361507
H-3	-14.8607	0.359352	0.002906	0.356447	0.349168	0.002827	0.346341
H-2	-14.7672	0.320224	-2.1E-05	0.320195	0.320094	-2.1E-05	0.320063
H-1	-14.6541	0.381272	0.004015	0.377257	0.381319	0.004014	0.377305
H	-14.6432	0.328737	8.9E-06	0.328835	0.328616	6.9E-06	0.328719
L	-12.2002	0.026924	0.000964	0.025914	0.026919	0.000957	0.025917
L+1	-12.0045	0.107437	0.000136	0.107302	0.10749	0.000134	0.107356
L+2	-11.1501	0.028031	0.002817	0.025215	0.028513	0.002852	0.02566
L+3	-11.1154	0.028748	0.001478	0.02727	0.02803	0.001427	0.026603
L+4	-11.0373	0.021274	0.00221	0.019064	0.02146	0.002219	0.01924
L+5	-10.8292	0.006903	-4.4E-06	0.006904	0.00759	-5.8E-06	0.007594
L+6	-10.8252	0.009753	0.000011	0.009747	0.009077	1.22E-05	0.009069
L+7	-10.3216	0.014617	0.001548	0.0115	0.014055	0.001557	0.010952
L+8	-10.2953	0.001773	0.000621	0.001148	0.00173	0.000629	0.001098
L+9	-10.265	0.008665	0.001343	0.007322	0.008716	0.001349	0.007367
L+10	-10.2505	0.019316	-0.00107	0.020321	0.019588	-0.00106	0.020584
L+11	-9.9531	0.011687	0.003965	0.007718	0.011829	0.004009	0.007815
L+12	-9.9397	0.004444	0.001728	0.002714	0.004307	0.001685	0.002618

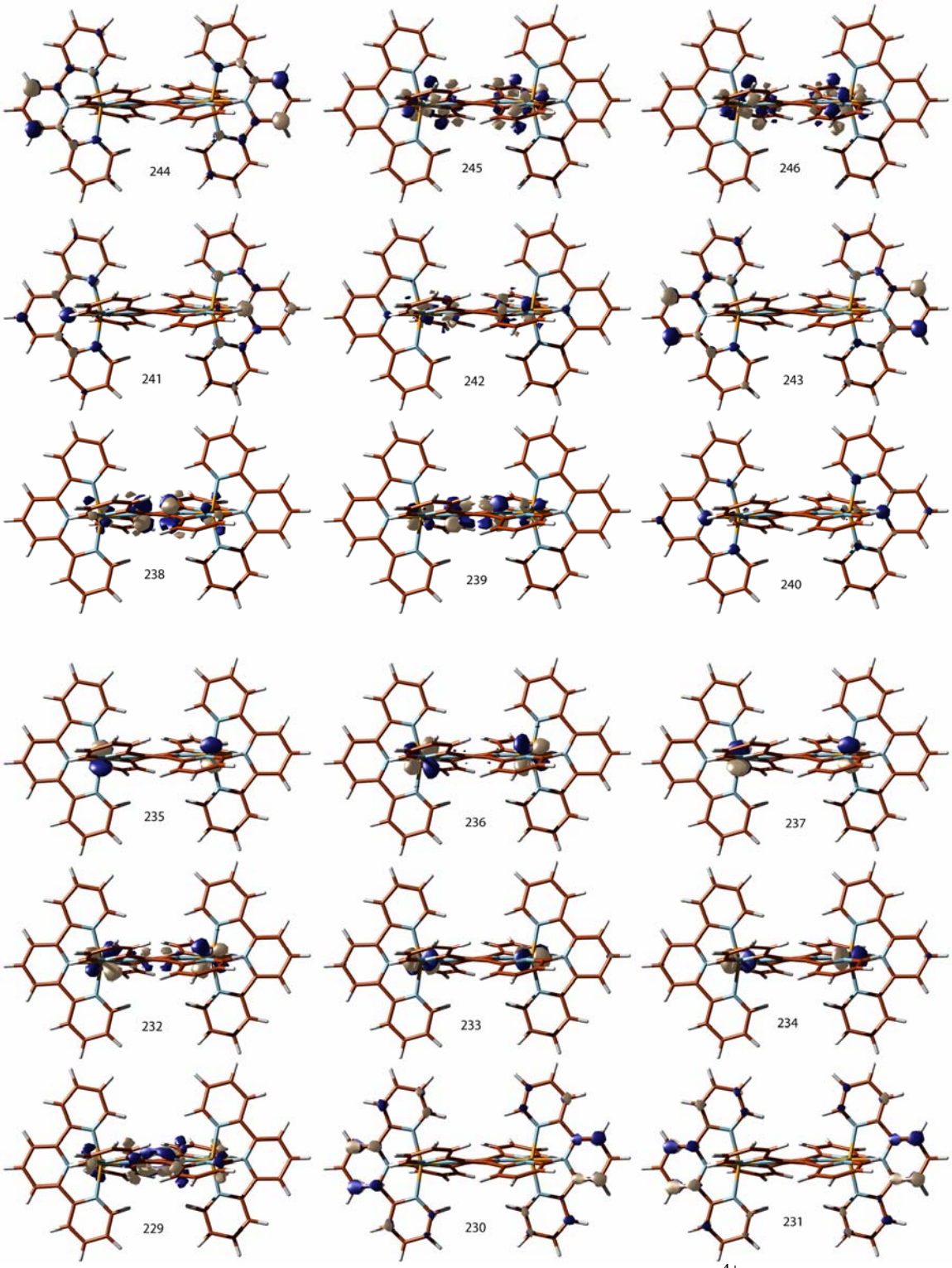

Figure S2 Isovalue (value = 0.05) plots of the frontier orbitals of $[\mathbf{3}]^{4+}$.

Table S1.3 Complete listing of electronic transitions for [**3**]$^{4+}$ calculated by TDDFT.

#	E (eV)	E (nm)	character	f	#	E (eV)	E (nm)	character	f
1	1.7331	715.39	H-1 →L (0.47436) H →L+1 (0.45865)	0.0040	26	3.1441	394.34	H-6 →L+1 (0.14886) H-4 →L+1 (-0.12544) H-4 →L+3 (0.10584) H-3 →L+2 (0.29947) H-3 →L+4 (0.54556) H-2 →L+5 (-0.10481) H →L+6 (-0.14168)	0.0022
2	1.7633	703.14	H-1 →L+1 (0.30492) H →L (0.63561)	0.0060	27	3.1834	389.47	H-4 →L+2 (0.35838) H-4 →L+4 (0.54555) H-3 →L+1 (-0.12204) H-3 →L+8 (0.11097) H-2 →L+6 (0.10202) H →L+5 (0.14521)	0.0000
3	1.7666	701.83	H-1 →L (-0.49571) H →L+1 (0.50352)	0.0147	28	3.2002	387.42	H-5 →L+5 (0.14535) H-3 →L+5 (0.18942) H-1 →L+6 (0.64316)	0.0001
4	1.8866	657.19	H-3 →L (0.11845) H-2 →L+1 (0.66194) H →L+4 (-0.10104)	0.0006	29	3.2016	387.25	H-5 →L+6 (0.14766) H-3 →L+6 (0.18029) H-1 →L+5 (0.64874)	0.0093
5	1.9178	646.49	H-5 →L+1 (0.11020) H-3 →L+1 (0.37923) H-2 →L (0.56973)	0.0000	30	3.2567	380.71	H-8 →L (0.55554) H-2 →L+5 (-0.18327) H →L+6 (-0.25753) H →L+7 (0.10261)	0.3992
6	1.9412	638.7	H-3 →L (0.68249) H-2 →L+1 (-0.11433)	0.0000	31	3.2606	380.25	H-2 →L+3 (0.54372) H →L+2 (-0.34756) H →L+4 (0.28007)	0.0002
7	1.9538	634.59	H-3 →L+1 (0.55612) H-2 →L (-0.37343)	0.0000	32	3.263	379.97	H-8 →L+1 (0.16636) H-2 →L+2 (-0.38469) H-2 →L+4 (0.37243) H →L+3 (0.41551)	0.0004
8	1.983	625.24	H-4 →L+1 (0.66073) H-3 →L+4 (0.11469) H-1 →L+1 (-0.10019)	0.0023	33	3.2802	377.98	H-4 →L+5 (-0.21499) H-4 →L+6 (-0.39093) H-3 →L+5 (0.39592) H-3 →L+6 (0.24572) H-1 →L+6 (-0.17212)	0.0115
9	1.9913	622.62	H-4 →L (0.69513)	0.0009	34	3.2806	377.94	H-4 →L+5 (-0.39563) H-4 →L+6 (0.22058) H-3 →L+5 (-0.23772) H-3 →L+6 (0.39887) H-1 →L+5 (-0.16865)	0.0243
10	2.3675	523.69	H-4 →L+1 (0.12269) H-4 →L+3 (-0.13143) H-3 →L+2 (0.11681) H-1 →L+1 (0.52656) H →L (-0.23278)	0.5685	35	3.344	370.77	H-4 →L+4 (-0.17940) H-3 →L+3 (-0.28570) H-2 →L+6 (0.21093) H-2 →L+14 (-0.10412) H →L+5 (0.45488) H →L+10 (-0.14868) H →L+13 (-0.11717)	0.0001
11	2.5416	487.81	H-5 →L (0.68269)	0.0018	36	3.3613	368.85	H-12 →L (0.11013) H-8 →L+1 (0.59462) H-2 →L+4 (-0.24201) H →L+8 (-0.16416)	0.1693
12	2.6756	463.39	H-2 →L+3 (0.42379) H →L+2 (0.50871) H →L+4 (-0.19701)	0.0164	37	3.3735	367.52	H-8 →L (0.31235) H-4 →L+3 (0.14662) H-3 →L+2 (-0.16678) H-3 →L+4 (0.21959) H-2 →L+5 (0.20207) H-1 →L+8 (0.12328) H →L+6 (0.36644) H →L+14 (-0.10418)	0.0025
13	2.6789	462.82	H-2 →L+2 (0.39536) H-2 →L+4 (-0.19059) H →L+3 (0.53475)	0.0009	38	3.4467	359.72	H-4 →L+2 (-0.16463) H-4 →L+3 (0.47592) H-4 →L+4 (0.13832) H-3 →L+2 (0.33506) H-3 →L+3 (-0.18558) H-3 →L+4 (-0.25626)	0.0000
14	2.7797	446.04	H-5 →L+3 (0.19275) H-1 →L+2 (0.63379)	0.0000	39	3.4478	359.6	H-4 →L+2 (0.36961) H-4 →L+3 (0.21826)	0.0000

			H-1 →L+4 (-0.18820)					H-4 →L+4 (-0.31201) H-3 →L+2 (0.14347) H-3 →L+3 (0.41556) H-3 →L+4 (-0.11036)	
15	2.7925	443.99	H-5 →L+2 (0.17908) H-1 →L+3 (0.66301)	0.0008	40	3.5616	348.12	H-5 →L+2 (-0.11831) H-5 →L+4 (-0.13827) H-2 →L+5 (0.38035) H-2 →L+10 (-0.19197) H-2 →L+20 (0.18109) H →L+6 (-0.32897) H →L+7 (-0.27458) H →L+17 (-0.15006) H →L+21 (0.13493)	0.0180
16	2.9038	426.97	H-7 →L (-0.17662) H-5 →L+1 (0.44585) H-4 →L+2 (-0.13119) H-3 →L+3 (0.16835) H-1 →L+4 (-0.36373) H →L+10 (-0.12749)	0.0000	41	3.5842	345.92	H-2 →L+6 (0.58921) H →L+5 (-0.37473)	0.0000
17	2.9483	420.52	H-2 →L+1 (0.13629) H-2 →L+3 (-0.10928) H →L+2 (0.31497) H →L+4 (0.59415)	0.0002	42	3.5954	344.84	H-5 →L+2 (0.14914) H-5 →L+4 (0.15981) H-2 →L+5 (0.43750) H-2 →L+10 (0.17163) H-2 →L+20 (-0.16895) H →L+6 (-0.23377) H →L+7 (0.27342) H →L+17 (0.14040) H →L+21 (-0.12513)	0.0053
18	2.976	416.61	H-6 →L (0.61827) H-4 →L+3 (0.19033) H-3 →L+2 (-0.22102) H →L+6 (-0.11178)	0.0362	43	3.6175	342.74	H-2 →L+7 (0.26359) H-2 →L+17 (0.24311) H-2 →L+21 (-0.21743) H →L+10 (0.32894) H →L+15 (-0.12343) H →L+20 (-0.33841)	0.0000
19	2.9849	415.37	H-7 →L (0.58648) H-5 →L+1 (-0.11410) H-4 →L+2 (-0.10996) H-3 →L+3 (0.13609) H-1 →L+4 (-0.29481)	0.0000	44	3.6497	339.71	H-5 →L+10 (0.10777) H-4 →L+7 (-0.16226) H-3 →L+10 (0.23341) H-1 →L+7 (0.60437)	0.0010
20	2.9982	413.53	H-7 →L (0.18388) H-5 →L+1 (0.29007) H-4 →L+2 (-0.23643) H-3 →L+3 (0.21727) H-2 →L+6 (0.10611) H-1 →L+2 (0.17989) H-1 →L+4 (0.44071) H →L+5 (0.13278)	0.0000	45	3.663	338.47	H-5 →L+7 (0.10259) H-4 →L+10 (-0.19171) H-3 →L+7 (0.29148) H-1 →L+10 (0.54599)	0.0001
21	3.0091	412.03	H-6 →L (0.32740) H-4 →L+3 (-0.28899) H-3 →L+2 (0.37828) H-2 →L+5 (0.22037) H →L+6 (0.27981)	0.0039	46	3.6756	337.32	H-8 →L (-0.11080) H-5 →L+2 (-0.31047) H-5 →L+4 (-0.23952) H-2 →L+20 (-0.16458) H-1 →L+8 (0.45686) H →L+17 (0.14370) H →L+21 (-0.11803)	0.0939
22	3.0243	409.95	H-7 →L (0.29377) H-5 →L+1 (0.28411) H-4 →L+2 (0.26275) H-3 →L+3 (-0.26541) H-2 →L+6 (-0.24083) H-1 →L+4 (0.11398) H →L+5 (-0.29293)	0.0000	47	3.7204	333.26	H-4 →L+6 (0.16579) H-4 →L+7 (0.33986) H-3 →L+5 (0.18656) H-3 →L+10 (-0.32438) H-2 →L+9 (-0.14421) H-1 →L+7 (0.24354) H →L+8 (-0.27127)	0.0088
23	3.1052	399.28	H-8 →L+1 (-0.16771) H-6 →L+1 (0.42490) H-2 →L+2 (-0.32050) H-2 →L+4 (-0.39293) H →L+1 (-0.10697) H →L+3 (0.10829)	0.0160	48	3.7246	332.88	H-4 →L+5 (0.14562) H-4 →L+10 (-0.29972) H-3 →L+6 (0.11024) H-3 →L+7 (0.31647) H-2 →L+8 (0.21024) H-1 →L+10 (-0.22703) H →L+9 (0.34825)	0.0004
24	3.1362	395.34	H-7 →L+1 (0.69953)	0.0000	49	3.7508	330.56	H-11 →L (0.19720) H-4 →L+5 (-0.23637) H-4 →L+10 (0.13888)	0.0038

25	3.1398	394.89	H-8 →L+1 (0.13329) H-6 →L+1 (0.53686) H-3 →L+4 (-0.15838) H-2 →L+2 (0.25287) H-2 →L+4 (0.27225)	0.0173	50	3.7523	330.42	H-3 →L+6 (-0.21745) H-3 →L+7 (-0.13344) H-2 →L+8 (0.23648) H-1 →L+10 (0.22225) H →L+9 (0.40522) H-12 →L (0.22618) H-8 →L+1 (0.10655) H-4 →L+6 (0.26910) H-3 →L+5 (0.24831) H-2 →L+9 (0.23991) H-1 →L+7 (0.10479) H →L+8 (0.42539)	0.0723

Table S2.1. Optimized geometry for [**4a**]$^{3+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	-2.56444	-0.01543	0.000874	H	-9.36397	0.83416	-5.07186	N	7.282439	-3.88443	0.278549
C	-1.33453	0.127202	-2.30041	N	5.650854	-0.56854	-3.78951	H	12.63876	-7.4258	0.155352
C	1.327022	-0.23452	-2.30695	C	7.423085	-1.1047	-5.5827	H	9.475454	-10.915	0.307759
N	2.570361	-0.01975	-0.00227	C	6.795031	-2.06283	-7.95906	H	4.830808	-9.80123	0.47934
C	1.329418	0.178583	2.305704	C	4.23752	-2.53477	-8.51815	H	3.593671	-5.26204	0.447253
C	-1.33305	-0.17686	2.299839	C	2.394076	-1.91115	-6.72272	H	9.367011	-0.78837	-5.03721
C	-3.09702	0.735302	-4.39765	H	8.28447	-2.48268	-9.30256	N	-10.1582	0.048834	-0.00271
C	3.097889	-0.84923	-4.37909	H	3.693213	-3.38087	-10.3053	C	-11.4289	-2.20856	-0.06385
C	3.099938	0.788423	4.379172	H	0.425994	-2.31307	-7.11744	C	-14.084	-2.23398	-0.05731
C	-3.09954	-0.78405	4.395157	Ru	6.388878	0.010818	-0.00738	C	-15.3935	0.080772	-0.02084
N	-5.64932	-0.52081	3.823117	Ru	-6.37444	0.019302	0.004317	C	-14.0555	2.380028	0.021314
C	-7.40986	-1.05766	5.61841	C	10.15785	0.043666	-0.00085	C	-11.4001	2.323202	0.045102
C	-6.76942	-1.99058	8.005347	C	11.50782	-2.25718	0.101447	C	-9.73301	-4.41844	-0.15074
C	-4.20911	-2.43394	8.553786	C	14.17774	-2.24661	0.101456	H	-15.1271	-3.99747	-0.09153
C	-2.37504	-1.81312	6.739035	C	15.47536	0.077738	0.013454	H	-17.4454	0.091822	-0.02574
H	-9.36425	-0.75732	5.09532	C	14.14727	2.386194	-0.07527	H	-15.0793	4.155153	0.046337
H	-8.24696	-2.40714	9.362174	C	11.47597	2.364365	-0.08777	C	-9.67197	4.509919	0.134735
H	-3.6431	-3.2462	10.35021	C	9.843732	-4.46447	0.209682	N	-7.12041	3.917226	0.243442
H	-0.39929	-2.17449	7.128907	H	15.26119	-3.9912	0.175923	C	-5.40994	5.83392	0.346676
C	2.39235	1.785944	6.749202	H	17.52694	0.08807	0.013491	C	-6.11772	8.381156	0.315124
C	4.232922	2.381939	8.556722	H	15.21021	4.143606	-0.14311	C	-8.6991	8.999498	0.181359
C	6.794722	1.96292	7.976123	C	9.77681	4.548042	-0.19563	C	-10.4825	7.037097	0.098731
C	7.426508	1.084454	5.570869	N	7.22599	3.919764	-0.28594	H	-3.43861	5.29016	0.43982
N	5.654463	0.56033	3.774366	C	5.472861	5.802724	-0.39248	H	-4.67929	9.839857	0.39018
H	0.420715	2.151097	7.159149	C	6.119691	8.356711	-0.38586	H	-9.31574	10.95512	0.141702
H	3.682128	3.162479	10.3712	C	8.696494	9.02272	-0.27356	H	-12.4816	7.475317	0.001243
H	8.284114	2.360916	9.326056	C	10.51674	7.106957	-0.18529	C	-10.5885	-6.92994	-0.13273
H	9.372088	0.819186	5.005281	H	3.512189	5.215653	-0.46978	C	-8.84083	-8.92337	-0.20819
C	-2.36162	1.699421	-6.76467	H	4.652157	9.783024	-0.46395	C	-6.24851	-8.34929	-0.32221
C	-4.18785	2.309605	-8.59013	H	9.272447	10.99113	-0.25278	C	-5.49522	-5.8148	-0.34219
C	-6.75503	1.935385	-8.02304	H	12.50955	7.577347	-0.0952	N	-7.17212	-3.86788	-0.24186
C	-7.40585	1.075216	-5.61185	C	10.63543	-7.00585	0.223876	H	-12.596	-7.3293	-0.05815
N	-5.64951	0.53405	-3.81367	C	8.857496	-8.95927	0.311091	H	-9.49075	-10.8681	-0.18017
H	-0.38067	2.011071	-7.16725	C	6.267393	-8.34397	0.400875	H	-4.83559	-9.83291	-0.39243
H	-3.60939	3.05892	-10.4094	C	5.567801	-5.80349	0.385885	H	-3.51344	-5.30899	-0.42624
H	-8.22851	2.346756	-9.38564								

Table S2.2. Orbital energies and Mulliken population on Ru for [**4a**]$^{3+}$.

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-14.2592	0.005322	-0.00035	0.005674	0.000122	2.66E-05	9.56E-05
H-11	-13.8382	1.32E-05	3.1E-06	7.1E-06	0.019216	6.1E-06	0.019185
H-10	-13.6936	0.015429	0.00087	0.014559	7.98E-05	6.4E-06	7.35E-05
H-9	-13.5595	0.014704	-0.00155	0.014424	0.014757	-0.00039	0.015312
H-8	-13.4606	0.16331	0.007528	0.129194	0.004578	0.000345	0.004067
H-7	-13.0862	0.061297	0.00268	0.058617	0.592494	0.0082	0.584293
H-6	-12.9483	0.345906	0.00689	0.339014	0.011677	0.000143	0.011533
H-5	-12.791	0.003601	0.000106	0.003495	0.704959	0.007424	0.697534
H-4	-12.6685	0.01125	0.000113	0.011128	0.648438	-0.00013	0.648554
H-3	-12.3338	0.186618	2.36E-05	0.186566	0.011284	1.08E-05	0.011302
H-2	-11.9437	0.529675	0.011524	0.51815	0.136586	0.000421	0.136165
H-1	-11.8427	0.472809	-0.00012	0.473001	0.004794	0.000032	0.004779
H	-11.4821	0.403448	0.00088	0.402567	0.001557	6.7E-06	0.001551
L	-9.8413	0.043625	0.001261	0.042635	0.023748	0.000645	0.023113
L+1	-9.5488	0.132332	-2.6E-05	0.132357	0.07917	0.001246	0.077924
L+2	-9.2709	0.007272	1.83E-05	0.007254	0.071343	0.00279	0.068553
L+3	-9.05	0.000155	1.21E-05	0.000144	0.019514	1.78E-05	0.01952
L+4	-8.7372	0.074806	0.000639	0.074168	0.008434	0.002165	0.00627
L+5	-8.3162	0.001105	0.000675	7.54E-05	0.013999	0.001386	0.012402
L+6	-8.2059	0.003776	0.00149	0.002285	0.01104	0.001867	0.009172
L+7	-8.1274	0.000319	0.000171	0.000148	0.011324	0.004826	0.006498
L+8	-8.0125	0.002154	0.001017	0.00027	0.060171	-0.00045	0.060598
L+9	-7.8363	0.007275	0.002562	0.004712	0.004724	0.000878	0.003844
L+10	-7.7749	0.038741	-0.00035	0.039545	0.005716	0.00164	0.002065
L+11	-7.6545	0.025325	8E-07	0.025412	0.000378	0.00015	0.000116
L+12	-7.5728	0.049592	0.009764	0.03983	6.89E-05	-8.2E-06	7.55E-05

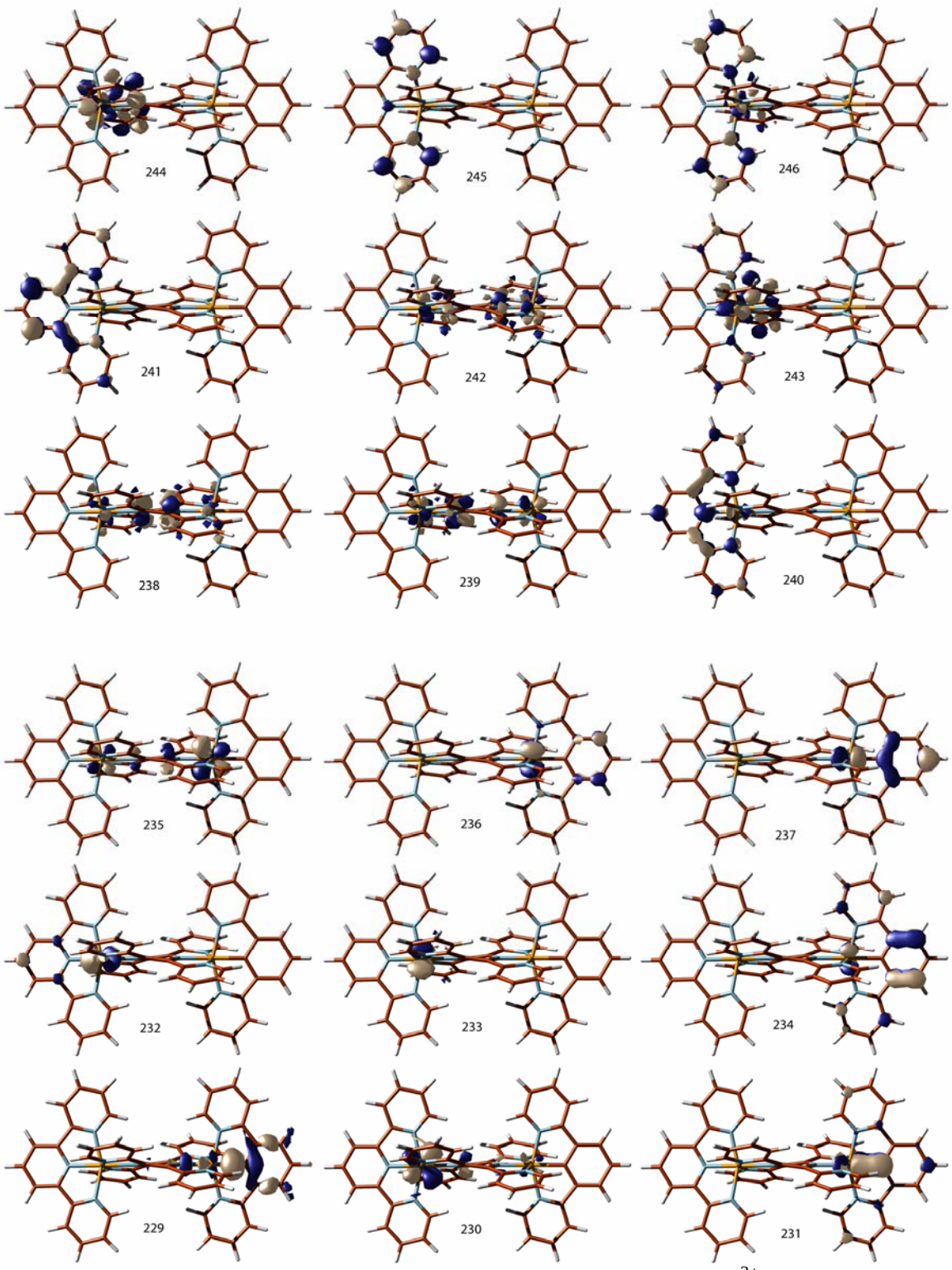

Figure S3. Isovalue (value = 0.05) plots of the frontier orbitals of [**4a**]$^{3+}$.

Table S2.3 Complete listing of electronic transitions for [**4a**]$^{3+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	1.007	1231.2	H →L (0.69379)	0.0001	26	2.7734	447.05	H-5 →L+2 (0.51308) H-4 →L+3 (0.41515) H-3 →L+3 (0.11653)	0.0080
2	1.177	1053.38	H →L+1 (0.64207) H →L+4 (0.18038)	0.0003	27	2.7763	446.59	H-4 →L+2 (-0.16824) H-3 →L+2 (0.67228)	0.0001
3	1.379	899.09	H-2 →L (0.58115) H-1 →L (-0.10187) H-1 →L+1 (0.25161) H-1 →L+4 (0.10185)	0.0081	28	2.8109	441.09	H →L+5 (0.69449)	0.0001
4	1.3858	894.69	H-3 →L (0.10723) H-2 →L+1 (0.25372) H-1 →L (0.63688)	0.0056	29	2.8772	430.92	H →L+6 (0.67242) H →L+9 (0.13362)	0.0053
5	1.4962	828.67	H-3 →L+1 (0.15278) H-2 →L (-0.32943) H-1 →L+1 (0.57489) H-1 →L+4 (0.13776)	0.0056	30	2.9013	427.34	H-8 →L (-0.14411) H-7 →L+1 (0.51925) H-7 →L+2 (-0.16931) H-5 →L+2 (0.10654) H-4 →L+3 (-0.27109) H-3 →L+3 (-0.11832) H →L+6 (0.11191)	0.0572
6	1.8935	654.79	H →L+1 (-0.14293) H →L+2 (0.67425) H →L+4 (0.12887)	0.0005	31	2.9693	417.56	H-5 →L+3 (0.68085)	0.0283
7	1.9489	636.18	H-3 →L (0.58199) H-2 →L+1 (0.30797) H-1 →L (-0.19823)	0.0287	32	2.9737	416.94	H →L+9 (0.20890) H →L+10 (0.63307) H →L+11 (0.11356)	0.0003
8	2.0974	591.14	H-7 →L+2 (0.12311) H-4 →L (-0.24996) H-3 →L (0.25288) H-2 →L+1 (-0.27639) H-2 →L+2 (0.47776) H →L+4 (0.13628)	0.0204	33	2.9856	415.27	H →L+6 (-0.12870) H →L+7 (-0.11875) H →L+9 (0.63680) H →L+10 (-0.20831)	0.0020
9	2.1174	585.54	H-4 →L (0.11692) H →L+1 (-0.18042) H →L+2 (-0.17342) H →L+4 (0.62528)	0.0047	34	2.9916	414.44	H-9 →L (0.15543) H-8 →L (0.60112) H-7 →L+2 (-0.28032)	0.0210
10	2.1558	575.13	H →L+3 (0.70455)	0.0000	35	3.0061	412.45	H-9 →L (0.10222) H-8 →L (0.24806) H-7 →L+2 (0.51327) H-5 →L+2 (0.14112) H-3 →L+3 (-0.27688) H-2 →L+2 (-0.14662)	0.0007
11	2.1652	572.61	H-7 →L+2 (0.12451) H-5 →L+1 (0.13637) H-4 →L (0.38745) H-3 →L (-0.18021) H-2 →L+1 (0.17055) H-2 →L+2 (0.44263) H-2 →L+4 (-0.11813)	0.0277	36	3.0232	410.1	H-7 →L+1 (0.14434) H-7 →L+2 (0.23364) H-4 →L+3 (-0.12731) H-3 →L+3 (0.61729)	0.0002
12	2.2045	562.4	H-5 →L (-0.25613) H-4 →L+1 (-0.40284) H-4 →L+2 (0.10431) H-1 →L+2 (0.45247) H-1 →L+4 (0.12010)	0.0031	37	3.0499	406.52	H →L+7 (0.69409) H →L+9 (0.11123)	0.0000
13	2.2169	559.28	H-4 →L+1 (0.27896) H-3 →L+1 (0.50088) H-1 →L+1 (-0.21505) H-1 →L+2 (0.30924)	0.0030	38	3.0811	402.41	H-3 →L+1 (-0.10536) H-3 →L+4 (0.67265) H-1 →L+4 (-0.12511)	0.0017
14	2.2402	553.46	H-5 →L (0.63546) H-4 →L+1 (-0.12283) H-3 →L+1 (-0.13705) H-1 →L+2 (0.22559)	0.0008	39	3.1028	399.59	H-2 →L+5 (0.68819)	0.0002
15	2.2669	546.94	H-5 →L+2 (-0.12692) H-4 →L (0.46794) H-3 →L (0.17787) H-2 →L+1 (-0.34128) H-2 →L+2 (-0.10487)	0.3763	40	3.1275	396.43	H-7 →L+1 (0.10750) H-5 →L+2 (-0.17931) H-4 →L+3 (0.26085) H-1 →L+5 (0.54431)	0.0502
16	2.2733	545.4	H-5 →L (-0.10507)	0.0004	41	3.1288	396.26	H-8 →L+1 (0.35288)	0.0360

			H-4 →L+1 (0.43186) H-3 →L+1 (-0.37908) H-1 →L+1 (0.10031) H-1 →L+2 (0.32604)					H →L+8 (0.36629) H →L+11 (0.41193)	
17	2.3462	528.45	H-5 →L+1 (0.67180) H-2 →L+2 (-0.11553)	0.0124	42	3.1401	394.85	H-8 →L+1 (-0.30704) H →L+8 (0.58213) H →L+11 (-0.18515)	0.0058
18	2.4436	507.38	H-7 →L+3 (0.12315) H-2 →L+3 (0.67925)	0.0002	43	3.1618	392.14	H-8 →L+1 (-0.44688) H-8 →L+4 (-0.11452) H →L+10 (-0.10114) H →L+11 (0.44357)	0.0389
19	2.4765	500.65	H-7 →L (0.13681) H-4 →L+2 (0.58785) H-3 →L+2 (0.14315) H-1 →L+4 (-0.22676)	0.0149	44	3.1736	390.67	H-7 →L+1 (-0.20108) H-5 →L+2 (0.22006) H-4 →L+3 (-0.29846) H-4 →L+8 (-0.15443) H-2 →L+6 (0.27195) H-1 →L+5 (0.39200)	0.0050
20	2.492	497.52	H-1 →L+3 (0.69876)	0.0001	45	3.1815	389.7	H-9 →L (-0.26672) H-7 →L+1 (0.11176) H-5 →L+2 (-0.10974) H-4 →L+3 (0.15117) H-2 →L+6 (0.56292) H-1 →L+5 (-0.12139)	0.0140
21	2.4933	497.28	H-7 →L (-0.19959) H-6 →L (0.62831) H-1 →L+4 (-0.18981)	0.0012	46	3.2124	385.95	H-9 →L+1 (0.13780) H-1 →L+6 (0.67066)	0.0051
22	2.513	493.37	H-7 →L (0.21011) H-6 →L (0.23943) H-4 →L+2 (0.19606) H-3 →L+1 (-0.11484) H-1 →L+1 (-0.10491) H-1 →L+2 (-0.13494) H-1 →L+4 (0.53050)	0.0204	47	3.2235	384.62	H-9 →L (0.14788) H-1 →L+10 (-0.13270) H-1 →L+11 (-0.10694) H →L+12 (0.63075)	0.0145
23	2.539	488.31	H-7 →L (0.59802) H-6 →L (0.14679) H-4 →L+1 (-0.12049) H-4 →L+2 (-0.18705) H-1 →L+4 (-0.17034)	0.0109	48	3.3091	374.67	H-9 →L (0.47281) H-8 →L (-0.14258) H-2 →L+6 (0.25493) H-2 →L+7 (0.12143) H-2 →L+9 (-0.25282) H-1 →L+10 (-0.10796) H →L+12 (-0.16296)	0.1964
24	2.6369	470.19	H-2 →L+4 (0.63078) H-1 →L+10 (0.13997)	0.0653	49	3.3234	373.07	H-7 →L+3 (0.58386) H-2 →L+3 (-0.12816) H-2 →L+8 (-0.29542)	0.0002
25	2.7264	454.76	H-6 →L+1 (0.65757) H-6 →L+4 (0.14676) H →L+4 (-0.10111)	0.0028	50	3.343	370.87	H-7 →L+7 (0.10729) H-2 →L+7 (0.68249)	0.0045

Table S3.1. Optimized geometry for [**4b**]$^{3+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
Ru	-5.30371	0.009236	0.17285	N	-6.30681	-3.86063	0.059555	H	-8.39728	0.470867	-4.83989
Ru	7.426664	-0.0429	-0.08861	C	-8.88528	-4.36491	0.078398	H	1.642399	2.125235	7.180344
N	8.277295	-3.90785	0.196491	C	-9.74713	-6.8827	0.141304	H	4.958365	2.999599	10.38625
C	10.84549	-4.42173	0.145835	C	-8.01888	-8.88362	0.188958	H	9.518133	2.069964	9.309877
C	11.73303	-6.92235	0.192109	C	-5.41031	-8.34595	0.153584	H	10.53225	0.596774	4.945046
C	10.00991	-8.93715	0.284646	C	-4.64259	-5.82594	0.082026	H	-7.06923	-1.74096	9.677937
C	7.4094	-8.39742	0.345894	C	-2.11793	0.546175	-4.3098	H	-2.50009	-2.76979	10.62443
C	6.624554	-5.87352	0.307839	C	-1.4605	1.420211	-6.74175	H	0.716488	-2.09808	7.275462
C	12.50585	-2.18465	0.012209	C	-3.33293	1.874181	-8.55698	H	-14.3159	-3.66441	-0.18094
N	11.20086	0.049066	-0.13229	C	-5.87779	1.445553	-7.91755	C	-17.1452	0.639315	-0.26664
C	12.39566	2.345275	-0.25695	C	-6.46332	0.716573	-5.45114	H	-13.9655	4.416147	0.071551
C	15.04664	2.449755	-0.23249	N	-4.65941	0.335419	-3.64995	H	-2.24818	5.166168	0.483563
C	16.42228	0.179102	-0.08532	C	4.092535	-0.93038	-4.40175	H	-3.28044	9.770638	0.418311
C	15.1587	-2.15727	0.035577	N	6.644728	-0.58924	-3.88942	H	-7.86749	11.08158	0.253034
N	8.088066	3.857977	-0.42704	C	8.377838	-1.03076	-5.73504	H	-11.1869	7.737674	0.180415
C	10.6281	4.497561	-0.40514	C	7.711647	-1.93713	-8.12485	H	-11.7619	-7.2539	0.171675
C	11.39116	7.037728	-0.50599	C	5.159325	-2.48656	-8.60653	H	-8.68419	-10.8225	0.258183
C	9.570979	8.96342	-0.63254	C	3.352057	-1.97993	-6.73061	H	-4.01439	-9.84608	0.184222
C	7.000244	8.295554	-0.67534	C	-10.4793	-2.09985	0.068357	H	-2.65573	-5.33161	0.053979
C	6.341669	5.737897	-0.57693	C	-9.04874	0.153643	0.172934	H	-8.20869	-0.37517	5.302774
N	3.628879	-0.11063	-0.00419	C	-10.2793	2.522363	0.18208	H	16.23303	-3.89589	0.155472
C	2.446531	0.10901	2.31735	C	-12.928	2.645015	0.073318	H	18.47145	0.23043	-0.06109
C	-0.21719	-0.22823	2.382806	C	-14.3418	0.388205	-0.06768	H	16.03552	4.240129	-0.3238
N	-1.4978	-0.09561	0.09295	C	-13.1366	-1.99095	-0.0607	H	4.382326	5.149342	-0.60462
C	-0.30543	0.022441	-2.24512	C	-8.52114	4.654119	0.264164	H	5.535656	9.725393	-0.7806
C	2.356639	-0.3305	-2.27688	N	-5.99126	3.959586	0.337558	H	10.14719	10.93007	-0.69664
C	4.259221	0.725699	4.372226	C	-4.19304	5.802997	0.407978	H	13.38216	7.516926	-0.47941
C	3.599619	1.720169	6.749599	C	-4.77874	8.372969	0.374839	H	13.7452	-7.30045	0.142539
C	5.474629	2.236166	8.554778	C	-7.3404	9.099552	0.286206	H	10.68273	-10.8739	0.30465
C	8.014409	1.748874	7.955878	C	-9.20413	7.225951	0.242201	H	6.017303	-9.89992	0.417984
C	8.595005	0.899768	5.523535	H	10.33125	-0.67712	-5.24575	H	4.638517	-5.38403	0.352221
N	6.793933	0.453525	3.745077	H	9.162172	-2.2524	-9.53693	O	-18.2653	2.701713	-0.16214
C	-1.96343	-0.70277	4.516184	H	4.581238	-3.29115	-10.4017	O	-18.3067	-1.65071	-0.62063
N	-4.51864	-0.37856	3.964065	H	1.386419	-2.43462	-7.06668	C	-21.0949	-1.68709	-0.92676
C	-6.26349	-0.71271	5.830855	H	0.497717	1.794298	-7.19911	H	-21.4816	-2.9855	-2.47982
C	-5.60819	-1.50217	8.261509	H	-2.82129	2.550943	-10.4235	H	-21.9208	-2.38559	0.831123

Table S3.2. Orbital energies and Mulliken population on Ru for [**4b**]$^{3+}$.

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-13.6378	0.013207	-0.00163	0.050343	7.99E-05	-0.00052	0.008451
H-11	-13.6022	0.058322	0.006906	0.090744	0.007663	0.000523	0.009198
H-10	-13.5469	0.116523	0.002824	0.061814	0.01	0.008102	0.579433
H-9	-13.1176	0.064648	0.006735	0.347856	0.587535	9.97E-05	0.008819
H-8	-13.0006	0.354778	7.87E-05	0.002697	0.008919	0.007057	0.699422
H-7	-12.8134	0.002776	4.09E-05	0.013837	0.706479	-4.6E-05	0.292185
H-6	-12.6867	0.013882	0.000109	0.002929	0.292129	-3.4E-05	0.354139
H-5	-12.6745	0.003073	8.3E-06	0.170672	0.354109	1.26E-05	0.012065
H-4	-12.3665	0.170646	0.000216	0.004066	0.012052	-8E-07	0.001002
H-3	-12.2479	0.00436	0.010807	0.516601	0.000998	0.000421	0.139339
H-2	-11.9836	0.52741	0.000218	0.48353	0.13976	4.31E-05	0.008125
H-1	-11.8776	0.483717	0.001024	0.390032	0.008157	0.000004	0.001274
H	-11.5343	0.391059	0.001306	0.041873	0.001278	0.000772	0.022882
L	-9.8699	0.042963	-4.8E-05	0.134469	0.023681	0.001456	0.078241
L+1	-9.5811	0.134416	2.33E-05	0.004377	0.079698	0.002941	0.068871
L+2	-9.285	0.004401	1.31E-05	0.000193	0.071812	2.7E-06	0.019412
L+3	-9.0599	0.000206	0.000755	0.070928	0.019398	0.002167	0.005384
L+4	-8.7706	0.07168	0.000621	0.000055	0.007553	0.001036	0.012548
L+5	-8.3328	0.000988	0.001559	0.002133	0.014237	0.002051	0.008849
L+6	-8.2357	0.003695	0.000192	0.000181	0.010916	0.004876	0.006422
L+7	-8.1428	0.000378	0.000816	0.000258	0.011303	-0.00061	0.061135
L+8	-8.0254	0.001848	0.00258	0.004051	0.060424	0.00102	0.003786
L+9	-7.8629	0.006669	-0.00089	0.041153	0.004806	0.00139	0.002502
L+10	-7.8021	0.039932	-9.7E-06	0.024112	0.006126	0.00013	0.000124
L+11	-7.6606	0.024043	0.010623	0.042817	0.000323	4.57E-05	0.000052
L+12	-7.6063	0.053416	-0.00163	0.050343	0.000121	-0.00052	0.008451

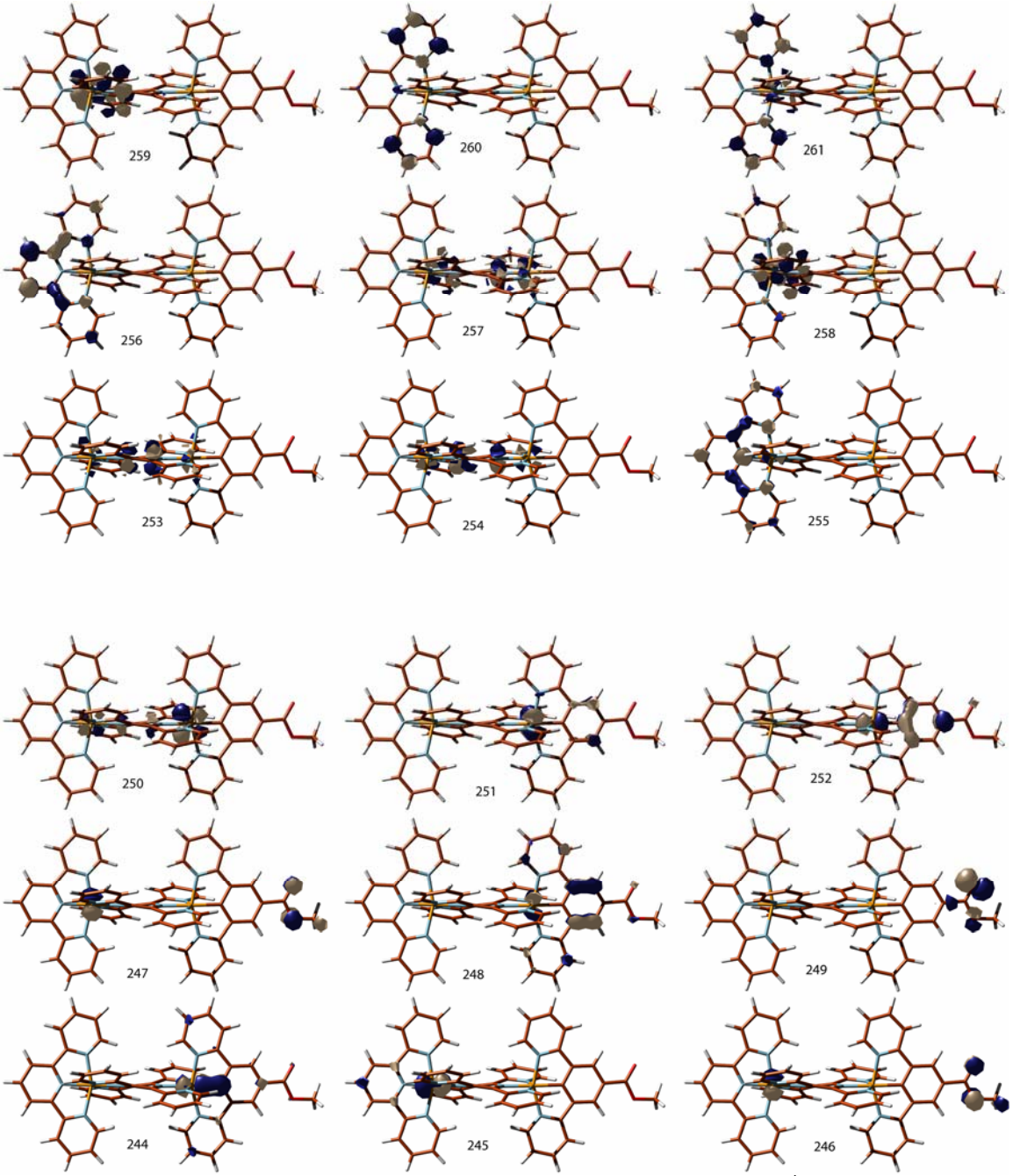

Figure S4. Isovalue (value = 0.05) plots of the frontier orbitals of [**4b**]$^{4+}$.

Table S3.3 Complete listing of electronic transitions for [**4b**]$^{3+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	1.043	1188.75	252 →253 (0.69378)	0.0002	16	2.2576	549.18	245 →255 (0.12042) 246 →253 (-0.31971) 247 →253 (-0.28218) 248 →253 (-0.18532) 250 →254 (0.34981) 251 →255 (0.14651)	0.3898
2	1.208	1026.37	252 →254 (0.64645) 252 →257 (0.17564)	0.0003	17	2.2778	544.31	246 →254 (-0.25297) 247 →254 (-0.16131) 248 →254 (0.41816) 250 →254 (-0.10864) 250 →255 (0.12288) 251 →255 (0.38667)	0.0258
3	1.3741	902.33	250 →253 (-0.36036) 250 →254 (0.13366) 251 →253 (0.49297) 251 →254 (-0.22481)	0.0067	18	2.3357	530.81	245 →254 (0.67048) 250 →255 (-0.12842)	0.0083
4	1.4041	882.99	250 →253 (0.44853) 250 →254 (0.22212) 251 →253 (0.41543) 251 →254 (0.16245)	0.0068	19	2.3798	520.99	249 →254 (0.70134)	0.0026
5	1.4972	828.11	248 →254 (0.14509) 250 →253 (-0.34958) 251 →254 (0.56328) 251 →257 (0.13059)	0.0062	20	2.4622	503.55	243 →256 (0.11870) 246 →255 (0.10021) 250 →256 (0.61295) 251 →256 (-0.26594)	0.0003
6	1.9406	638.89	252 →254 (0.11399) 252 →255 (0.67961) 252 →257 (-0.11771)	0.0009	21	2.4772	500.5	243 →253 (-0.13407) 246 →255 (0.43764) 247 →255 (0.38977) 248 →255 (0.13559) 250 →256 (-0.12794) 251 →255 (-0.11209) 251 →257 (0.20874)	0.0149
7	1.9614	632.11	247 →253 (0.12014) 248 →253 (0.57171) 250 →254 (0.30595) 251 →253 (-0.19196)	0.0333	22	2.5029	495.37	243 →253 (0.19906) 244 →253 (0.43583) 246 →253 (-0.26090) 247 →253 (0.30035) 251 →256 (0.10889) 251 →257 (0.26703)	0.0042
8	2.0878	593.86	249 →253 (0.70529)	0.0001	23	2.5108	493.81	243 →253 (0.17279) 244 →253 (-0.17309) 246 →253 (0.21868) 246 →255 (-0.10875) 247 →253 (-0.25218) 251 →255 (0.10392) 251 →256 (0.23105) 251 →257 (0.44182)	0.0147
9	2.11	587.61	243 →254 (0.10184) 243 →255 (0.10477) 246 →253 (0.27953) 247 →253 (0.21318) 248 →253 (-0.28413) 250 →254 (0.26379) 250 →255 (0.39200) 250 →257 (-0.10179) 251 →255 (-0.11203)	0.0258	24	2.5227	491.48	250 →256 (0.27602) 251 →256 (0.58668) 251 →257 (-0.21287)	0.0028
10	2.1431	578.52	246 →253 (-0.10539) 250 →255 (0.14282) 252 →254 (-0.18263) 252 →255 (0.12886) 252 →257 (0.61229)	0.0035	25	2.5334	489.39	243 →253 (0.47829) 244 →253 (0.22360) 246 →253 (0.20191) 246 →255 (0.13577) 247 →253 (-0.23286)	0.0107

								247 →255 (0.12050) 251 →257 (-0.20313)	
11	2.1636	573.05	243 →255 (0.13355) 245 →254 (0.13049) 246 →253 (-0.25629) 247 →253 (-0.21001) 248 →253 (0.13932) 250 →254 (-0.11308) 250 →255 (0.46569) 251 →255 (-0.14400) 252 →257 (-0.19634)	0.0105	26	2.5495	486.32	243 →253 (-0.37143) 244 →253 (0.45569) 246 →253 (0.22361) 247 →253 (-0.27349)	0.0017
12	2.1978	564.13	245 →253 (-0.22359) 246 →254 (0.37447) 247 →254 (0.35149) 248 →254 (0.24217) 251 →255 (0.14749) 252 →256 (0.24927)	0.0053	27	2.6386	469.88	250 →257 (0.63334) 251 →263 (0.13681)	0.0718
13	2.2022	563.01	245 →253 (0.10723) 246 →254 (-0.13866) 247 →254 (-0.13132) 252 →256 (0.65555)	0.0015	28	2.7414	452.27	244 →254 (0.62925) 244 →257 (0.13898) 246 →254 (-0.13584) 247 →254 (0.15395) 252 →257 (-0.10340)	0.0018
14	2.2299	556	245 →253 (0.48830) 247 →254 (0.11605) 248 →254 (0.35256) 251 →254 (-0.14971) 251 →255 (-0.24535)	0.0013	29	2.7676	447.98	249 →255 (0.69616)	0.0002
15	2.2426	552.86	245 →253 (0.42588) 246 →254 (0.13654) 248 →254 (-0.22811) 250 →255 (0.13401) 251 →254 (0.14908) 251 →255 (0.40940) 251 →257 (-0.10594)	0.0052	30	2.7788	446.18	245 →255 (0.50506) 246 →256 (-0.31357) 247 →256 (-0.28053) 248 →256 (-0.10793)	0.0066

Table S4.1. Optimized geometry for [**5a**]$^{2+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	2.562395	-0.05139	0.002071	H	9.387477	0.025291	5.087468	N	-7.29056	-3.9023	-0.03477
C	1.336033	0.096569	2.310722	N	-5.68761	-0.24947	3.810131	H	-12.6321	-7.47411	0.134789
C	-1.33884	-0.20262	2.308864	C	-7.46612	-0.42739	5.667081	H	-9.44063	-10.9413	0.155099
N	-2.56238	-0.05217	-0.00087	C	-6.87396	-1.12619	8.140231	H	-4.80228	-9.81012	0.027212
C	-1.33628	0.099173	-2.30947	C	-4.36121	-1.77904	8.708074	H	-3.60413	-5.25121	-0.10111
C	1.33899	-0.19899	-2.30807	C	-2.50996	-1.53544	6.829889	H	-9.38802	-0.03919	5.090126
C	3.14323	0.542449	4.411098	H	-8.35828	-1.22034	9.550708	C	10.15223	0.042984	-0.00072
C	-3.15107	-0.63214	4.408388	H	-3.85559	-2.46706	10.57105	C	11.51572	-2.26198	-0.0165
C	-3.14464	0.546533	-4.40868	H	-0.58347	-2.08702	7.232216	C	14.18474	-2.22109	-0.02437
C	3.151937	-0.62586	-4.40766	Ru	-6.41831	-0.0118	0.001561	C	15.45746	0.120408	-0.00998
N	5.688545	-0.2463	-3.80749	Ru	6.418428	-0.0119	0.001236	C	14.11677	2.423536	0.009035
C	7.468154	-0.42385	-5.66344	C	-10.152	0.044565	0.001477	C	11.44779	2.386747	0.010557
C	6.876916	-1.11832	-8.13794	C	-11.5165	-2.25981	0.013456	C	9.85426	-4.48421	-0.02456
C	4.363669	-1.76659	-8.70867	C	-14.1855	-2.2178	0.016623	H	15.29896	-3.9476	-0.03945
C	2.511471	-1.52408	-6.8313	C	-15.4574	0.124201	0.000314	H	17.50876	0.150476	-0.01376
H	9.390105	-0.03875	-5.08451	C	-14.1155	2.426724	-0.01592	H	15.17996	4.181926	0.019494
H	8.362296	-1.21251	-9.54726	C	-11.4466	2.388838	-0.01217	C	9.72368	4.56038	0.020383
H	3.858476	-2.45055	-10.5732	C	-9.85589	-4.48272	0.020595	N	7.176643	3.9054	-0.03101
H	0.584724	-2.07282	-7.23614	H	-15.3004	-3.94392	0.028997	C	5.401403	5.767724	-0.03318
C	-2.49561	1.434105	-6.83409	H	-17.5087	0.15529	0.00016	C	6.007431	8.331878	0.037302
C	-4.3454	1.690989	-8.7119	H	-15.1778	4.185653	-0.02901	C	8.576933	9.026637	0.10052
C	-6.8644	1.065843	-8.14084	C	-9.72156	4.561801	-0.01965	C	10.42418	7.131467	0.085743
C	-7.46299	0.386331	-5.66395	N	-7.17484	3.905915	0.036006	H	3.453258	5.145046	-0.08991
N	-5.68569	0.198973	-3.80711	C	-5.39892	5.767606	0.041308	H	4.516473	9.738317	0.038351
H	-0.56402	1.963788	-7.24014	C	-6.00386	8.331966	-0.0309	H	9.120268	11.00431	0.157324
H	-3.83378	2.367728	-10.5774	C	-8.57298	9.027603	-0.09964	H	12.41052	7.633072	0.131158
H	-8.3484	1.169852	-9.55087	C	-10.4209	7.133111	-0.0875	C	10.629	-7.03388	-0.09534
H	-9.38885	0.024881	-5.08286	H	-3.45108	5.144332	0.101864	C	8.836777	-8.98122	-0.10921
C	2.492209	1.427391	6.836958	H	-4.51236	9.737858	-0.02912	C	6.248357	-8.36071	-0.03824
C	4.340994	1.684609	8.715704	H	-9.1154	11.00547	-0.15851	C	5.567857	-5.81549	0.038103
C	6.860887	1.062491	8.145054	H	-12.407	7.635489	-0.13712	N	7.289226	-3.90288	0.033657
C	7.461074	0.384802	5.667974	C	-10.6316	-7.03222	0.086301	H	12.6293	-7.47636	-0.14604
N	5.684674	0.19683	3.810237	C	-8.84013	-8.98028	0.097456	H	9.436532	-10.9424	-0.17116
H	0.559787	1.954489	7.242624	C	-6.25144	-8.36062	0.02946	H	4.798623	-9.80965	-0.0381
H	3.827864	2.359219	10.58155	C	-5.5699	-5.81553	-0.04133	H	3.602362	-5.25045	0.10034
H	8.344263	1.167184	9.555744								

Table S4.2. Orbital energies and Mulliken population on Ru for [**5a**]$^{2+}$.

#	E (eV)	Ru[1]	p	d	Ru[2]	p	d
H-12	-11.5308	0.067797	-0.00995	0.063472	0.068096	-0.00999	0.063753
H-11	-11.4527	0.08114	0.011561	0.059495	0.080755	0.011491	0.059225
H-10	-11.31	0.014299	0.000558	0.012749	0.014316	0.000558	0.012762
H-9	-11.0289	0.144806	0.003114	0.141692	0.143632	0.003083	0.140549
H-8	-11.0145	0.138587	0.003837	0.134751	0.139742	0.003864	0.135879
H-7	-10.514	0.046991	0.000033	0.046939	0.047097	3.28E-05	0.047045
H-6	-10.4861	0.028165	-5E-07	0.028188	0.028084	-4E-07	0.028106
H-5	-10.3342	0.287866	0.007957	0.279909	0.287831	0.007951	0.27988
H-4	-9.8527	0.281956	-5.5E-05	0.28194	0.282402	-5.4E-05	0.282385
H-3	-9.7044	0.316301	1.39E-05	0.316402	0.315858	1.41E-05	0.315959
H-2	-9.5519	0.3444	0.00455	0.33985	0.344193	0.004546	0.339647
H-1	-9.4511	0.230875	0.000962	0.229913	0.243698	0.001019	0.242678
H	-9.4494	0.27482	0.002451	0.272369	0.262205	0.002397	0.259808
L	-7.5416	0.038369	0.001188	0.03732	0.03835	0.001185	0.037305
L+1	-7.1343	0.124217	-0.00041	0.124623	0.124251	-0.00041	0.124659
L+2	-6.5181	0.031744	0.00179	0.029954	0.031746	0.001788	0.029958
L+3	-5.8651	0.003896	-9E-05	0.004003	0.00392	-8.8E-05	0.004026
L+4	-5.8502	0.011678	0.000012	0.011678	0.0117	1.21E-05	0.011701
L+5	-5.8252	0.01616	0.002448	0.01263	0.015841	0.002391	0.01239
L+6	-5.8205	0.011187	0.002799	0.007963	0.011251	0.002822	0.008003
L+7	-5.7932	0.012144	0.003606	0.008538	0.012207	0.003617	0.008588
L+8	-5.7215	0.029436	-0.00062	0.030011	0.029356	-0.00063	0.029939
L+9	-5.7152	0.025231	0.00345	0.021777	0.025471	0.003479	0.021988
L+10	-5.6935	0.021841	0.002565	0.019275	0.021726	0.002553	0.019171
L+11	-5.2773	0.018167	-0.0018	0.019577	0.01815	-0.0018	0.019568
L+12	-5.1876	0.019766	0.000245	0.019159	0.019777	0.000247	0.019167

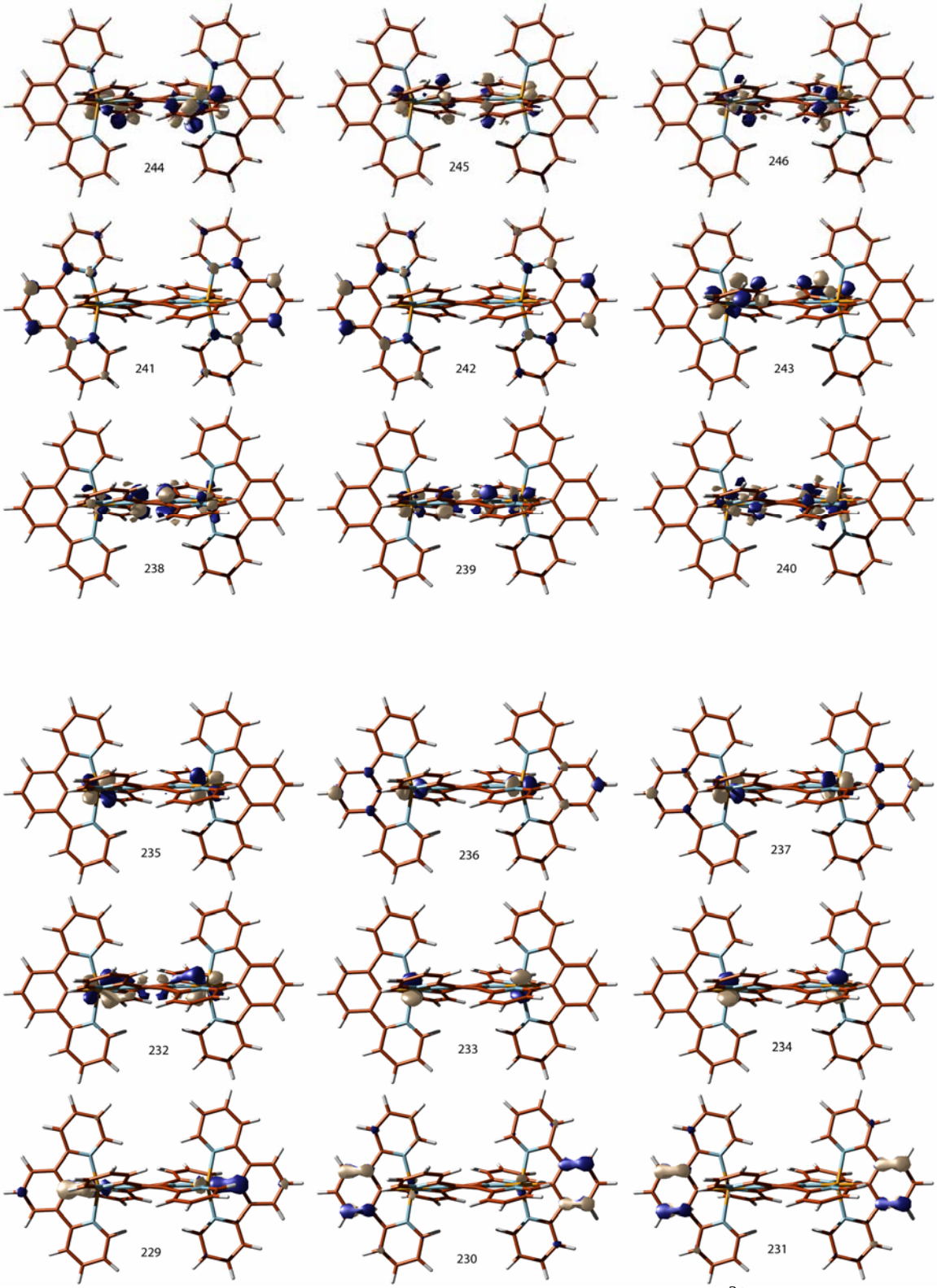

Figure S5. Isovalue (value = 0.05) plots of the frontier orbitals of $[\mathbf{5a}]^{2+}$.

Table S4.3 Complete listing of electronic transitions for [**5a**]$^{2+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	1.2414	998.71	H-2 →L (0.18063) H →L (0.65882)	0.0071	16	2.5071	494.53	H-7 →L (0.63163) H-5 →L+1 (0.13413) H-2 →L+2 (0.26523)	0.0000
2	1.2653	979.87	H-1 →L (0.69595)	0.0002	17	2.5908	478.56	H-4 →L+1 (-0.21975) H-3 →L+2 (0.65955)	0.0011
3	1.3354	928.43	H-2 →L (0.65367) H →L (-0.20448)	0.0070	18	2.7577	449.6	H-7 →L (-0.13943) H-5 →L+1 (0.58455) H-3 →L+8 (0.18148)	0.0000
4	1.4832	835.92	H-3 →L (0.51470) H-1 →L+2 (-0.10254) H →L+1 (0.46631)	0.0028	19	2.8121	440.9	H-6 →L+1 (-0.43107) H-4 →L+2 (0.47987) H-3 →L+1 (-0.16149)	0.0428
5	1.4954	829.13	H-1 →L+1 (0.66136) H →L+2 (-0.15251)	0.0000	20	2.841	436.41	H-6 →L+1 (0.53770) H-4 →L+2 (0.41399)	0.0328
6	1.537	806.66	H-3 →L (0.36121) H-2 →L+1 (0.42967) H-1 →L+2 (0.15248) H →L+1 (-0.37292)	0.0049	21	2.844	435.95	H-8 →L (0.33435) H-7 →L+1 (0.47459) H-1 →L+4 (-0.12464) H-1 →L+5 (0.19694) H-1 →L+6 (0.13487) H →L+8 (0.20595)	0.0069
7	1.6825	736.92	H-4 →L+2 (0.11882) H-3 →L+1 (0.66920)	0.0088	22	2.8519	434.75	H-8 →L (-0.31030) H-7 →L+1 (0.49181) H-1 →L+4 (0.16358) H-1 →L+5 (-0.18146) H-1 →L+6 (-0.12182) H →L+8 (-0.18772)	0.0118
8	1.7013	728.74	H-5 →L+1 (-0.16877) H-4 →L (0.66930)	0.0000	23	2.8527	434.63	H-9 →L (0.41397) H-4 →L+2 (-0.18606) H-1 →L+3 (0.10877) H-1 →L+8 (0.30285) H →L+4 (-0.17900) H →L+5 (0.24773) H →L+6 (0.16699)	0.0068
9	1.83	677.51	H-5 →L (-0.19294) H-4 →L+1 (0.61356) H-3 →L+2 (0.18971)	0.0005	24	2.9251	423.87	H-9 →L (-0.11134) H-1 →L+3 (0.44440) H-1 →L+8 (-0.11429) H →L+4 (-0.38290) H →L+5 (-0.19833) H →L+6 (-0.12816)	0.0005
10	2.0823	595.42	H-5 →L (0.65468) H-4 →L+1 (0.20304)	0.0015	25	2.9306	423.07	H-3 →L+9 (-0.12129) H-1 →L+4 (-0.37819) H-1 →L+5 (-0.18139) H-1 →L+6 (-0.12678) H →L+3 (0.46604)	0.1048
11	2.1525	576	H-6 →L (-0.12266) H-3 →L (-0.26209) H-2 →L+1 (0.45246) H →L+1 (0.24924)	0.4687	26	2.9435	421.21	H-8 →L (0.52267) H-1 →L+4 (0.11413) H-1 →L+5 (-0.30277) H-1 →L+6 (-0.19403) H →L+8 (-0.24990)	0.0039
12	2.3613	525.06	H-1 →L+1 (0.15664) H →L+2 (0.66568)	0.0000	27	2.9511	420.13	H-9 →L (0.50425) H-1 →L+7 (0.14815) H-1 →L+8 (-0.22585) H →L+5 (-0.38280)	0.0024
13	2.3651	524.22	H-2 →L+1 (-0.10558) H-1 →L+2 (0.66782) H →L+1 (0.16652)	0.0019	28	2.9539	419.72	H-9 →L (-0.19404) H-1 →L+7 (0.36068) H →L+5 (-0.18524) H →L+6 (0.49516)	0.0120
14	2.4438	507.34	H-7 →L (-0.25983) H-2 →L+2 (0.61236)	0.0000	29	2.9677	417.77	H-1 →L+5 (-0.28008) H-1 →L+6 (0.42264) H →L+7 (0.44774)	0.0000
15	2.5015	495.64	H-6 →L (0.68997)	0.0491	30	3.0209	410.43	H-10 →L (-0.11682) H-5 →L+2 (-0.20412) H-2 →L+5 (-0.31768) H-2 →L+6 (0.41098) H-1 →L+7 (-0.28910) H-1 →L+9 (-0.10484) H →L+10 (-0.19902)	0.0087

Table S5.1. Optimized geometry for [**5b**]$^{2+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	7.353558	-3.8672	-0.09785	C	-10.7552	-6.93179	0.176128	H	9.564653	0.468843	4.700833
C	9.926673	-4.40246	-0.14706	C	-8.99635	-8.90653	0.167615	H	-8.06404	-1.87085	9.695817
C	10.75329	-6.93164	-0.18365	C	-6.39668	-8.33486	0.112404	H	-3.47992	-2.88795	10.59951
C	8.993988	-8.90598	-0.17573	C	-5.66375	-5.80548	0.070195	H	-0.29306	-2.18591	7.235462
C	6.394502	-8.33374	-0.11825	C	-3.27868	0.60179	-4.29239	H	-15.3632	-3.75513	-0.07555
C	5.662227	-5.80423	-0.07328	C	-2.67775	1.513831	-6.72256	C	-18.2229	0.569689	-0.11765
C	11.54601	-2.15337	-0.18563	C	-4.59147	1.98312	-8.49089	H	-15.0862	4.337416	0.307741
C	10.12716	0.116052	-0.29755	C	-7.11921	1.52784	-7.81234	H	-3.33355	5.09459	0.364076
C	11.37508	2.483704	-0.35598	C	-7.64811	0.750301	-5.35124	H	-4.33099	9.704418	0.317528
C	14.02513	2.579007	-0.27455	N	-5.80453	0.358984	-3.59506	H	-8.91157	11.04535	0.400497
C	15.42569	0.308352	-0.09946	C	2.991795	-0.7639	-4.50632	H	-12.2583	7.735608	0.472822
C	14.2038	-2.06745	-0.07195	N	5.550749	-0.42734	-3.98944	H	-12.7642	-7.33312	0.225075
Ru	6.40499	-0.00646	-0.22373	C	7.281228	-0.77993	-5.86499	H	-9.63334	-10.8548	0.206422
N	7.08284	3.924589	-0.39479	C	6.608441	-1.59834	-8.27737	H	-4.97569	-9.80994	0.105095
C	9.615552	4.623765	-0.41344	C	4.05517	-2.13889	-8.77646	H	-3.68701	-5.27385	0.027105
C	10.28206	7.200752	-0.43287	C	2.253775	-1.71876	-6.88174	H	-9.22932	-0.44611	5.349361
C	8.402348	9.060803	-0.39048	C	-11.5466	-2.15332	0.182234	H	15.36245	-3.75663	0.065459
C	5.844726	8.324448	-0.34857	C	-10.1273	0.115576	0.298241	C	18.22359	0.56736	0.108487
C	5.273838	5.752946	-0.37199	C	-11.3745	2.483542	0.358184	H	15.08742	4.336488	-0.30757
N	2.553116	-0.10087	-0.08412	C	-14.0244	2.579663	0.273938	H	3.334644	5.096686	-0.354
C	1.412697	0.055781	2.269228	C	-15.4253	0.309648	0.094253	H	4.333315	9.706231	-0.3031
C	-1.25776	-0.26785	2.357839	C	-14.2042	-2.06652	0.065511	H	8.914151	11.04614	-0.38706
N	-2.55345	-0.10166	0.087001	C	-9.61453	4.623106	0.419405	H	12.2601	7.735609	-0.46485
C	-1.41302	0.057857	-2.26612	N	-7.082	3.92337	0.401522	H	12.76218	-7.33347	-0.23425
C	1.257369	-0.26502	-2.35506	C	-5.27257	5.751313	0.381721	H	9.630474	-10.8543	-0.21666
C	3.278716	0.597225	4.295925	C	-5.84279	8.32298	0.36073	H	4.973168	-9.8085	-0.11117
C	2.678362	1.505738	6.727594	C	-8.40025	9.059894	0.402041	H	3.685641	-5.27217	-0.02831
C	4.592495	1.9727	8.49612	C	-10.2804	7.200247	0.441326	O	-19.3581	2.617023	0.1112
C	7.120132	1.518684	7.816329	H	9.228279	-0.43534	-5.34885	O	-19.4029	-1.6853	-0.65055
C	7.648468	0.744597	5.354028	H	8.062459	-1.85424	-9.69704	C	-22.1863	-1.67752	-0.97464
N	5.804508	0.355536	3.597761	H	3.478772	-2.87392	-10.6004	H	-22.5731	-2.84318	-2.63131
C	-2.99232	-0.76973	4.5083	H	0.292534	-2.17846	-7.23427	H	-23.0282	-2.51249	0.716079
N	-5.55133	-0.43374	3.991199	H	-0.73287	1.904364	-7.21546	H	-22.8646	0.253729	-1.23839
C	-7.28223	-0.79021	5.865663	H	-4.12086	2.692572	-10.3545	O	19.35889	2.614888	-0.11843
C	-6.60971	-1.6117	8.277068	H	-8.66116	1.823198	-9.12755	O	19.40407	-1.6889	0.634971
C	-4.0562	-2.15095	8.776347	H	-9.56443	0.473498	-4.69891	C	22.18802	-1.68239	0.95386
C	-2.25447	-1.72706	6.882808	H	0.733582	1.895432	7.221583	H	22.57762	-2.84901	2.60921
Ru	-6.40519	-0.00776	0.226035	H	4.122256	2.679485	10.36089	H	23.02623	-2.5169	-0.73891
N	-7.35462	-3.86806	0.095438	H	8.66241	1.812403	9.131533	H	22.86756	0.248454	1.21725
C	-9.92787	-4.40279	0.142457								

Table S5.2. Orbital energies and Mulliken population on Ru for [**5b**]$^{2+}$.

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-11.2817	0.006561	0.000374	0.005862	0.000239	-1.5E-06	0.000224
H-11	-11.139	0.135266	0.002789	0.132428	0.139171	0.002885	0.136234
H-10	-11.1255	0.134587	0.003664	0.130892	0.130686	0.003569	0.127086
H-9	-10.8123	0.005413	0.000211	0.005153	0.00176	7.44E-05	0.001677
H-8	-10.8121	0.001082	1.38E-05	0.001053	0.004789	0.00015	0.004584
H-7	-10.6308	0.044338	4.15E-05	0.044276	0.04475	4.13E-05	0.044688
H-6	-10.6041	0.026862	2.9E-06	0.026884	0.026434	2.9E-06	0.026457
H-5	-10.4333	0.287312	0.007812	0.279499	0.287418	0.007812	0.279606
H-4	-9.9614	0.285246	-4.2E-05	0.285204	0.285873	-4.3E-05	0.285831
H-3	-9.8159	0.317935	0.000013	0.318033	0.317341	1.31E-05	0.317438
H-2	-9.6772	0.311995	0.003515	0.30848	0.312019	0.003513	0.308505
H-1	-9.5973	0.235072	0.001176	0.233895	0.234646	0.001173	0.233472
H	-9.5804	0.296401	0.003655	0.292749	0.29663	0.003657	0.292977
L	-7.6207	0.037498	0.001128	0.036557	0.037485	0.001124	0.036549
L+1	-7.2258	0.122176	-0.00061	0.122785	0.122189	-0.00061	0.122799
L+2	-6.602	0.031255	0.001831	0.029425	0.031254	0.001833	0.029423
L+3	-5.9348	0.004313	-3.3E-05	0.004352	0.004381	-3.3E-05	0.004421
L+4	-5.9222	0.014319	8.39E-05	0.014238	0.014254	8.51E-05	0.014171
L+5	-5.911	0.009545	0.003267	0.006121	0.009578	0.003271	0.006148
L+6	-5.8987	0.015315	0.002465	0.011641	0.015313	0.002464	0.011652
L+7	-5.8705	0.01363	0.003317	0.010311	0.013593	0.003306	0.010284
L+8	-5.8031	0.028251	-0.00062	0.028837	0.028234	-0.00061	0.028818
L+9	-5.7942	0.026211	0.00367	0.02255	0.026161	0.003665	0.022505
L+10	-5.7725	0.023789	0.002686	0.0211	0.023845	0.002695	0.021147
L+11	-5.3443	0.018363	-0.00156	0.020026	0.018372	-0.00157	0.02004
L+12	-5.2549	0.019297	0.000203	0.01864	0.019282	0.000201	0.018629

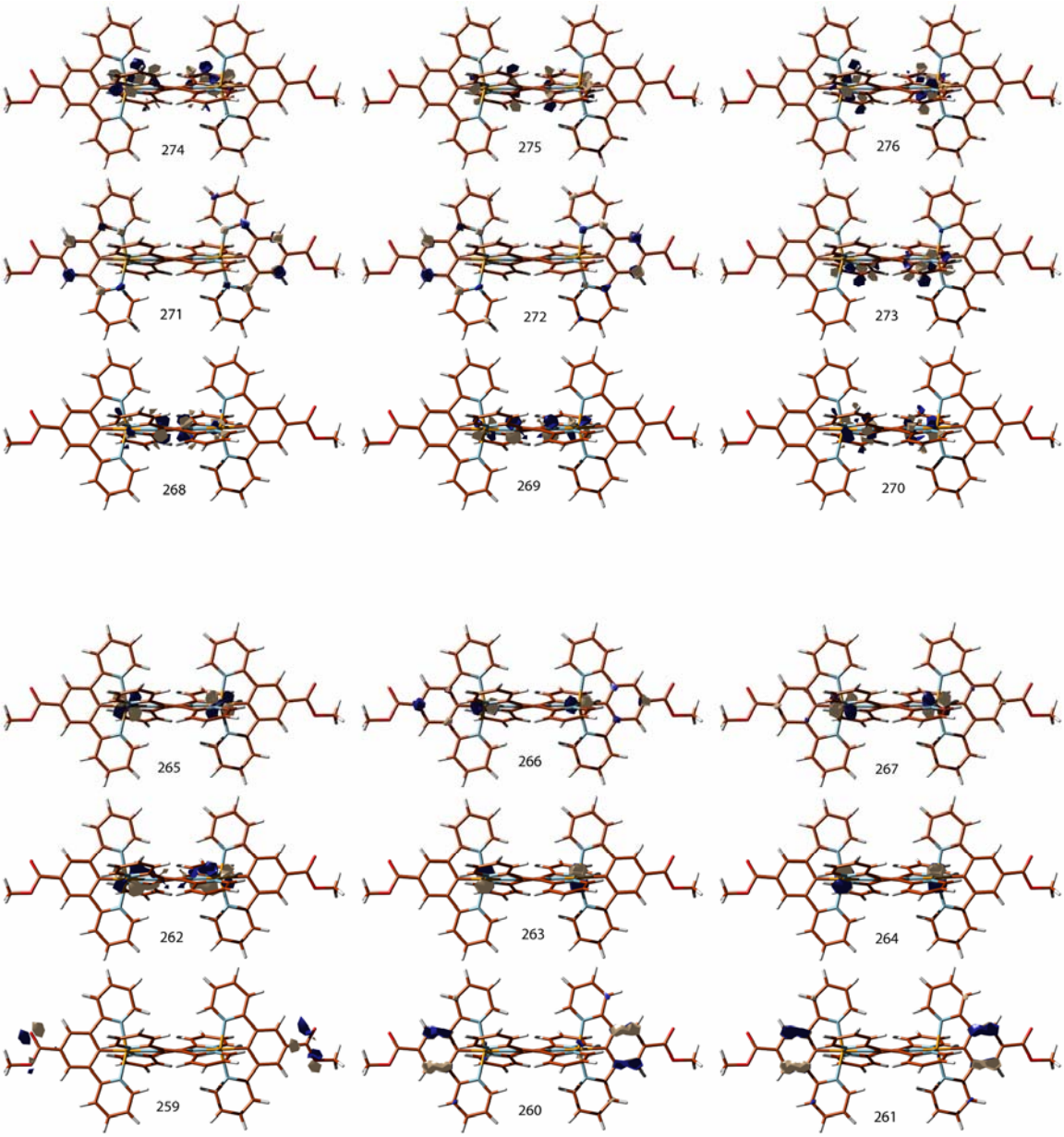

Figure S6. Isovalue (value = 0.05) plots of the frontier orbitals of [**5b**]$^{2+}$.

Table S5.3 Complete listing of electronic transitions for [**5b**]$^{2+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	1.2822	966.96	265 →268 (0.17700) 267 →268 (0.65604)	0.0096	16	2.545	487.16	260 →268 (0.62595) 262 →269 (-0.14533) 265 →270 (0.26981)	0
2	1.3391	925.9	266 →268 (0.69626)	0.0002	17	2.6166	473.84	263 →269 (-0.21594) 264 →270 (0.66112)	0.0018
3	1.4009	885.02	265 →268 (0.65930) 267 →268 (-0.20064)	0.005	18	2.769	447.76	260 →268 (0.15305) 262 →269 (0.58489) 263 →274 (-0.10390) 264 →276 (-0.18228)	0.0001
4	1.5168	817.39	264 →268 (0.57051) 267 →269 (0.40750)	0.0038	19	2.837	437.03	261 →269 (-0.36044) 263 →270 (0.54826) 264 →269 (-0.16302)	0.0546
5	1.5603	794.61	265 →270 (-0.10114) 266 →269 (0.66177) 267 →270 (0.13669)	0	20	2.8672	432.43	261 →269 (0.57922) 263 →270 (0.36877)	0.0257
6	1.5975	776.1	264 →268 (0.26290) 265 →269 (0.48152) 266 →270 (-0.16500) 267 →269 (-0.37835)	0.0041	21	2.8732	431.52	257 →268 (-0.31757) 258 →268 (-0.37451) 259 →268 (0.13833) 260 →269 (0.41671) 266 →274 (0.11094) 267 →276 (0.11786)	0.0024
7	1.7028	728.13	263 →270 (0.11913) 264 →269 (0.66918)	0.0086	22	2.8794	430.6	256 →268 (0.11040) 257 →268 (0.19689) 258 →268 (0.25160) 259 →268 (-0.27000) 260 →269 (0.51532)	0.002
8	1.7281	717.47	262 →269 (0.16847) 263 →268 (0.66894)	0	23	2.8795	430.58	256 →268 (-0.32585) 258 →268 (0.27616) 259 →268 (0.44307) 260 →269 (0.16832) 261 →269 (-0.10192) 266 →276 (0.14391) 267 →272 (0.10413) 267 →274 (0.10589)	0.0003
9	1.8476	671.06	262 →268 (0.18894) 263 →269 (0.61642) 264 →270 (0.18759)	0.0009	24	2.9263	423.68	256 →268 (0.29659) 258 →268 (0.19422) 259 →268 (0.39144) 265 →272 (0.10263) 266 →271 (0.15322) 266 →276 (-0.23350) 267 →272 (-0.21913) 267 →274 (-0.18392)	0.0012
10	2.1048	589.06	262 →268 (0.65593) 263 →269 (-0.19924)	0.0024	25	2.9267	423.63	257 →268 (-0.32113) 258 →268 (0.40956) 259 →268 (-0.19677) 266 →272 (0.21602) 266 →274 (0.18832) 267 →271 (-0.11004) 267 →276 (0.20373)	0.016
11	2.1647	572.75	261 →268 (-0.10938) 264 →268 (-0.26486) 265 →269 (0.41285) 267 →269 (0.31556)	0.5559	26	2.9811	415.89	256 →268 (0.27601) 266 →271 (-0.38971) 267 →272 (0.35810) 267 →274 (-0.22302)	0.0006
12	2.4029	515.97	266 →269 (-0.12948) 267 →270 (0.65847)	0	27	2.9836	415.56	257 →268 (-0.28292) 264 →277 (-0.12177) 266 →272 (-0.35276) 266 →274 (0.12613) 267 →271 (0.44260)	0.0758
13	2.4324	509.72	265 →269 (0.12715) 266 →270 (0.66851) 267 →269 (-0.14653)	0.005	28	2.9932	414.23	262 →270 (0.16241) 265 →273 (0.13659) 266 →271 (0.10974) 266 →275 (0.24688) 267 →273 (0.55728)	0.026
14	2.4958	496.77	260 →268 (-0.25849) 265 →270 (0.60956) 266 →269 (0.12613) 267 →270 (-0.10230)	0	29	3.0061	412.45	257 →268 (0.39199) 265 →276 (-0.13272) 266 →273 (0.12854) 266 →274 (0.41330)	0.001

15	2.5403	488.07	261 →268 (0.69227)	0.0522	30	3.0079	412.2	267 →271 (0.15820) 267 →276 (0.31124) 256 →268 (0.43045) 266 →276 (0.28660) 267 →274 (0.43801)	0.001

Table S6.1. Optimized geometry for [**3**]$^{5+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	-2.57445	-0.02819	0.00003	H	-9.35988	0.6917	-5.11083	N	7.23448	-3.87234	0.33409
C	-1.32912	0.13266	-2.32176	N	5.62856	-0.58069	-3.85424	H	12.65023	-7.34308	0.2526
C	1.3188	-0.24192	-2.31459	C	7.38266	-1.10349	-5.6513	H	9.5386	-10.8694	0.4598
N	2.56897	-0.02809	0.00062	C	6.73438	-2.05344	-8.0395	H	4.89679	-9.82903	0.64533
C	1.32069	0.1742	2.31641	C	4.18023	-2.54492	-8.56276	H	3.56723	-5.30518	0.55309
C	-1.32843	-0.20049	2.31988	C	2.34837	-1.93994	-6.73273	H	9.33692	-0.78936	-5.14034
C	-3.09137	0.72618	-4.43182	H	8.20273	-2.44282	-9.41599	N	-10.1724	0.02734	0.00701
C	3.07828	-0.87565	-4.41014	H	3.62152	-3.37776	-10.3517	C	-11.4452	-2.22363	-0.09069
C	3.0791	0.80406	4.41498	H	0.3784	-2.34461	-7.10839	C	-14.098	-2.24825	-0.09702
C	-3.09104	-0.79297	4.42744	Ru	6.30931	-0.00003	-0.00584	C	-15.4047	0.06406	-0.00005
N	-5.63916	-0.5129	3.85671	Ru	-6.30598	-0.00214	0.00699	C	-14.0653	2.35834	0.10393
C	-7.40371	-1.00206	5.65299	N	10.18269	0.03747	-0.00629	C	-11.4143	2.2958	0.10217
C	-6.76674	-1.89814	8.065	C	11.46588	-2.2058	0.12744	C	-9.76206	-4.43776	-0.19576
C	-4.21303	-2.37053	8.61229	C	14.11977	-2.22356	0.13087	H	-15.1423	-4.00686	-0.18024
C	-2.37199	-1.80351	6.77807	C	15.42402	0.0894	-0.00427	H	-17.4543	0.07943	0.00073
H	-9.35557	-0.7051	5.11987	C	14.07445	2.37601	-0.14052	H	-15.0846	4.13161	0.19178
H	-8.24481	-2.26401	9.43861	C	11.42185	2.3053	-0.13853	C	-9.70053	4.4868	0.20771
H	-3.66426	-3.1643	10.42334	C	9.79008	-4.4216	0.27119	N	-7.15593	3.89307	0.29789
H	-0.40371	-2.19857	7.17463	H	15.17071	-3.97736	0.24208	C	-5.43615	5.80299	0.42449
C	2.3484	1.81925	6.75938	H	17.47574	0.11013	-0.0045	C	-6.14525	8.34941	0.41368
C	4.18	2.41586	8.59195	H	15.08988	4.15051	-0.25347	C	-8.72477	8.97331	0.28766
C	6.73791	1.96536	8.05107	C	9.70469	4.48878	-0.27945	C	-10.5102	7.01152	0.19734
C	7.38707	1.0612	5.64617	N	7.16042	3.89157	-0.35339	H	-3.46548	5.26127	0.52772
N	5.63142	0.54818	3.84683	C	5.4401	5.79943	-0.50203	H	-4.71065	9.80991	0.49923
H	0.37623	2.19034	7.15331	C	6.14819	8.34579	-0.53718	H	-9.33115	10.93144	0.25217
H	3.61909	3.21127	10.39707	C	8.72776	8.97296	-0.43001	H	-12.5062	7.45649	0.10307
H	8.20738	2.35089	9.42719	C	10.5136	7.01321	-0.31423	C	-10.606	-6.95242	-0.19283
H	9.34269	0.77673	5.12219	H	3.4687	5.25736	-0.58397	C	-8.84647	-8.9385	-0.27781
C	-2.36866	1.69087	-6.79921	H	4.71464	9.80615	-0.64353	C	-6.25754	-8.34891	-0.39215
C	-4.20722	2.25173	-8.63708	H	9.33523	10.9315	-0.43658	C	-5.51431	-5.81228	-0.38418
C	-6.76434	1.82334	-8.07524	H	12.51002	7.46213	-0.23792	N	-7.20887	-3.87954	-0.27028
C	-7.40571	0.96608	-5.65077	C	10.64528	-6.93067	0.31881	H	-12.6093	-7.37047	-0.11322
N	-5.64179	0.48517	-3.85087	C	8.89501	-8.92243	0.43858	H	-9.48087	-10.8888	-0.26433
H	-0.39888	2.05255	-7.21131	C	6.30366	-8.34304	0.53432	H	-4.84277	-9.82931	-0.48209
H	-3.6565	3.01559	-10.4593	C	5.54871	-5.81054	0.48304	H	-3.53575	-5.29791	-0.45882
H	-8.2429	2.18838	-9.44721								

Table S6.2.1. Orbital energies and Mulliken population on Ru of alpha orbitals for [**3**]$^{5+}$.

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-19.37	0.04695	0.000244	0.046706	0.045484	0.00021	0.045274
H-11	-19.2989	0.016014	0.000247	0.015767	0.016925	0.000253	0.016672
H-10	-18.9593	0.031908	0.000166	0.031743	0.023739	0.000134	0.023605
H-9	-18.9526	0.018095	0.000155	0.01794	0.025401	0.000173	0.025228
H-8	-18.7758	0.185559	0.004586	0.180973	0.175339	0.004309	0.17103
H-7	-18.3992	0.037361	-0.00037	0.037895	0.034489	-0.00036	0.035016
H-6	-18.3286	0.298847	0.003827	0.295021	0.312496	0.003981	0.308515
H-5	-18.1173	0.179157	1.7E-06	0.179118	0.148227	7.2E-06	0.148183
H-4	-18.0944	0.38046	0.001639	0.37882	0.229029	0.000915	0.228114
H-3	-18.0512	0.080485	-9.5E-05	0.080632	0.095895	-8.1E-05	0.096024
H-2	-18.0474	0.231374	0.00117	0.230204	0.382532	0.001791	0.380742
H-1	-17.7898	0.176753	-9.7E-06	0.176772	0.129455	-4.8E-06	0.129461
H	-17.7367	0.163255	-3.6E-05	0.163351	0.230711	-4.2E-05	0.230819
L	-14.8533	0.054265	0.000414	0.053851	0.055607	0.000393	0.055213
L+1	-14.8086	0.01797	0.000832	0.017122	0.017735	0.000795	0.016912
L+2	-13.6876	0.012019	0.003962	0.008057	0.011607	0.003794	0.007813
L+3	-13.5956	0.015786	0.002507	0.01328	0.015438	0.002515	0.012923
L+4	-13.5213	0.01555	0.00268	0.01287	0.016534	0.002797	0.013737
L+5	-13.181	0.014409	0.000235	0.014167	3.09E-05	-3.3E-06	3.52E-05
L+6	-13.1781	4.67E-05	-3.3E-06	5.14E-05	0.014612	0.000245	0.014363
L+7	-12.8198	0.070107	0.002899	0.065013	0.031054	0.003174	0.025742
L+8	-12.7765	0.051949	-0.0018	0.054242	0.07342	-0.00211	0.076052
L+9	-12.728	0.001678	0.000773	0.000905	0.001485	0.000809	0.000676
L+10	-12.7114	0.008674	0.000901	0.00777	0.009182	0.000928	0.008252
L+11	-12.4773	0.426999	0.013293	0.405193	0.09773	0.005378	0.089011
L+12	-12.419	0.073622	-0.00144	0.075629	0.408826	0.007226	0.39651

Table S6.2.2. Orbital energies and Mulliken population on Ru of beta orbitals for [**3**]$^{5+}$.

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-11	-19.3279	0.008774	-0.00024	0.009015	0.008734	-0.00023	0.008968
H-10	-19.2944	0.002588	9.72E-05	0.002491	0.002922	9.76E-05	0.002824
H-9	-18.9407	0.023924	0.000185	0.023739	0.005304	0.000109	0.005194
H-8	-18.9394	0.004189	-4.6E-05	0.004235	0.022639	0.000028	0.022611
H-7	-18.4218	0.016583	-0.00051	0.017292	0.016006	-0.0005	0.016703
H-6	-18.04	0.080743	1.23E-05	0.08071	0.074704	1.62E-05	0.074668
H-5	-18.0123	0.046213	-4.4E-05	0.046283	0.042988	-4.3E-05	0.043054
H-4	-17.9038	0.622813	0.004207	0.618607	0.014949	0.00062	0.014329
H-3	-17.8953	0.017052	0.00058	0.016472	0.622233	0.004036	0.618197
H-2	-17.6571	0.270609	0.000942	0.269689	0.229646	0.000984	0.228673
H-1	-17.6045	0.283056	0.005089	0.277983	0.20794	0.005163	0.202775
H	-17.5744	0.2062	0.00019	0.206104	0.339552	9.02E-05	0.339582
L	-15.979	0.37883	0.005029	0.373801	0.372618	0.004801	0.367817
L+1	-14.8104	0.019266	0.000764	0.018487	0.019169	0.000731	0.018413
L+2	-14.4592	0.190546	-0.0003	0.190847	0.190912	-0.00031	0.191219
L+3	-13.6477	0.029737	0.003072	0.026665	0.028698	0.002879	0.025819
L+4	-13.5832	0.018244	0.002274	0.01597	0.018615	0.002355	0.01626
L+5	-13.5132	0.0237	0.00203	0.02167	0.024582	0.002134	0.022448
L+6	-13.1743	0.01457	0.000178	0.014404	0.000128	4.8E-06	0.000119
L+7	-13.1713	0.000268	-1.3E-06	0.000273	0.014967	0.000184	0.014804
L+8	-12.7988	0.031993	0.002345	0.027973	0.021065	0.002573	0.016746
L+9	-12.7618	0.002474	0.001065	0.001411	0.002366	0.001092	0.001276
L+10	-12.7445	0.030664	-0.00147	0.032536	0.036731	-0.00161	0.03883
L+11	-12.7235	0.00883	0.000901	0.007925	0.009139	0.000927	0.008211
L+12	-12.3584	0.015679	0.00019	0.015205	0.010497	-0.00036	0.010921
L+13	-12.3195	0.214432	0.007832	0.20285	0.068491	0.004343	0.061893

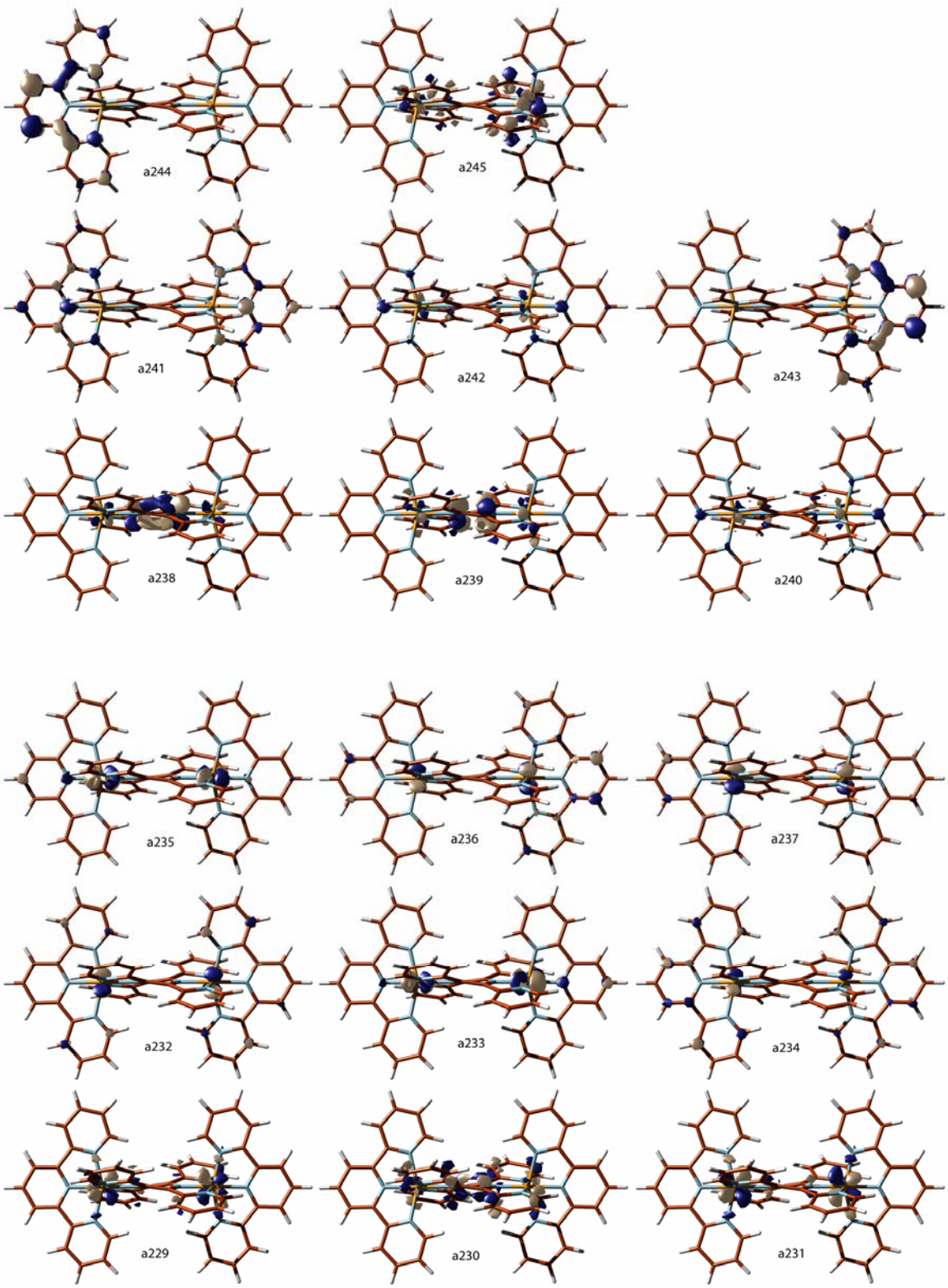

Figure S7.1. Isovalue (value = 0.05) plots of the alpha frontier orbitals of $[\mathbf{3}]^{5+}$.

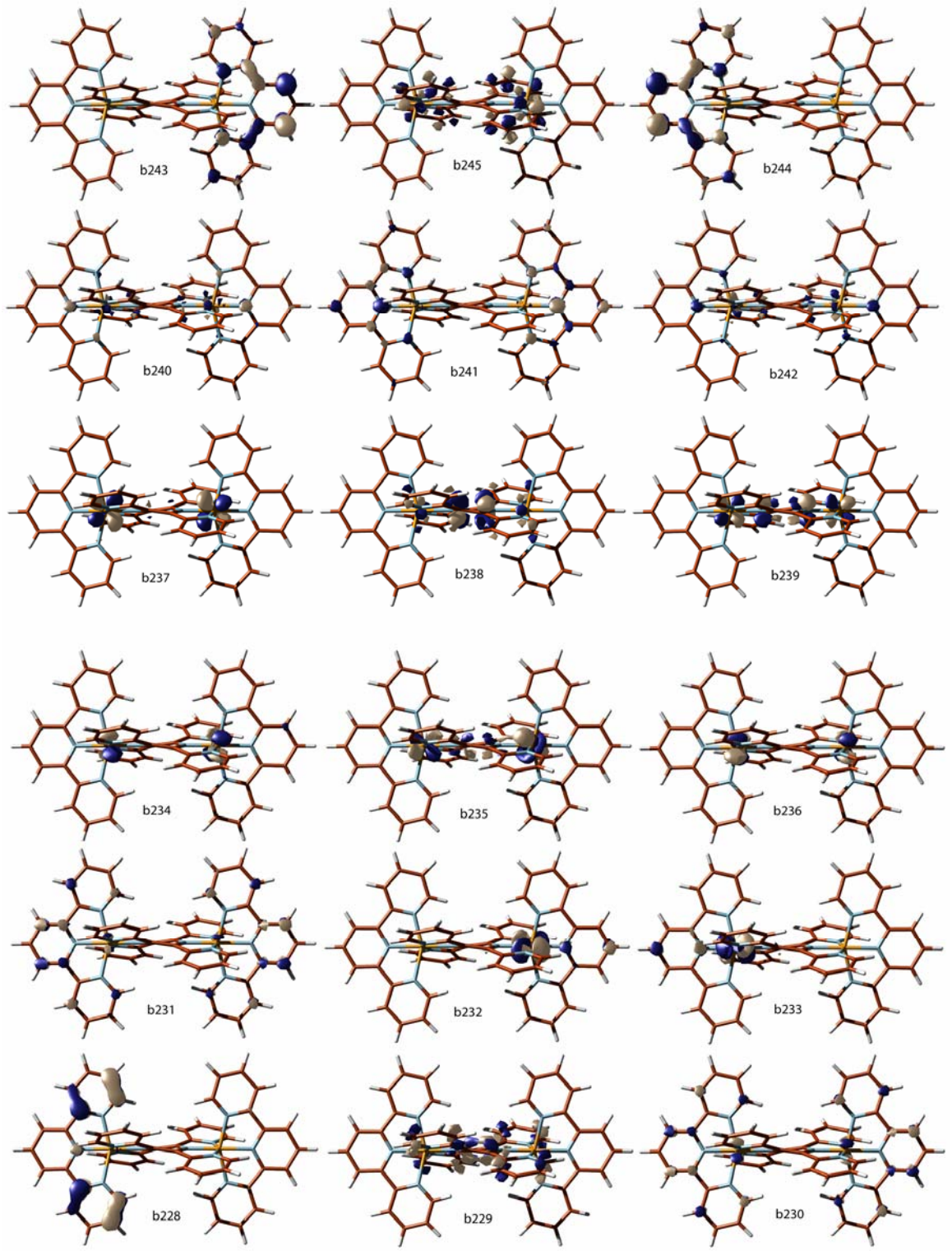

Figure S7.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**3**]$^{5+}$.

Table S6.3 Complete listing of electronic transitions for [**3**]$^{5+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	0.2024	6124.89	bH-23 →bL (0.11527) bH-6 →bL+2 (-0.12857) bH-5 →bL (0.27637) bH-2 →bL+2 (-0.26291) bH-1 →bL (0.20145) bH-1 →bL+2 (-0.10325) bH →bL (0.99604)	0.0000	16	2.2391	553.71	aH-6 →aL (0.13471) aH →aL (0.24258) aH →aL+1 (-0.22411) bH-7 →bL+1 (0.11502) bH-6 →bL (0.15837) bH-5 →bL+2 (0.15373) bH-2 →bL (0.22191) bH-2 →bL+3 (-0.10285) bH-1 →bL+2 (0.17382) bH →bL+1 (0.19407) bH →bL+2 (0.78593)	0.0030
2	0.2955	4195.35	bH-24 →bL (0.11399) bH-6 →bL (0.35172) bH-2 →bL (0.84899) bH-1 →bL (0.37318) bH →bL (-0.12106) bH →bL+2 (-0.29486)	0.0005	17	2.2922	540.89	aH-2 →aL (0.71561) bH-9 →bL (0.48868) bH-8 →bL (0.25365) bH-4 →bL+2 (-0.18823) bH-3 →bL (0.14657) bH-3 →bL+2 (-0.23280)	0.0000
3	0.4049	3062.45	bH-19 →bL (0.11256) bH-4 →bL (0.63774) bH-4 →bL+2 (-0.21060) bH-3 →bL (0.50632) bH-3 →bL+2 (0.21769) bH-2 →bL (0.25014) bH-1 →bL (-0.48021)	0.0046	18	2.3096	536.81	aH-4 →aL (-0.36215) bH-9 →bL (-0.41118) bH-8 →bL (0.73302) bH-4 →bL (0.14709) bH-4 →bL+2 (0.21472) bH-3 →bL+2 (-0.18397)	0.0001
4	0.4567	2715.07	bH-18 →bL (-0.12132) bH-4 →bL (-0.61547) bH-4 →bL+2 (0.20608) bH-3 →bL (0.74244) bH-3 →bL+2 (0.20054) bH-1 →bL+2 (-0.10771)	0.0000	19	2.3245	533.38	aH-2 →aL (0.10405) aH-1 →aL (0.31134) bH-7 →bL (0.15343) bH-6 →bL+2 (0.20261) bH-4 →bL+1 (0.20402) bH-3 →bL+1 (0.22007) bH-2 →bL+2 (0.72351) bH-1 →bL+2 (0.25414) bH →bL (0.20577) bH →bL+3 (-0.13005) bH →bL+5 (0.11027)	0.0013
5	0.9762	1270.05	aH-6 →aL (-0.33670) aH-3 →aL+1 (-0.11275) aH →aL+1 (-0.14928) bH-4 →bL (0.39243) bH-3 →bL (0.35916) bH-2 →bL (-0.31992) bH-1 →bL (0.76631) bH →bL (-0.14224) bH →bL+1 (0.12969)	0.1690	20	2.3265	532.91	aH-2 →aL+1 (0.13823) bH-4 →bL+1 (0.56538) bH-3 →bL+1 (0.71093) bH-2 →bL+2 (-0.25569) bH-1 →bL+1 (-0.13816)	0.0000
6	1.4329	865.29	bH-6 →bL (0.46961) bH-5 →bL (0.81707) bH-2 →bL (-0.19851) bH-1 →bL (-0.11511) bH →bL (-0.21252)	0.0003	21	2.3434	529.08	aH-2 →aL (-0.61230) bH-9 →bL (0.64144) bH-8 →bL (0.36767) bH-2 →bL+2 (0.13345)	0.0000
7	1.44	860.97	bH-6 →bL (0.78803) bH-5 →bL (-0.49314) bH-2 →bL (-0.29265) bH →bL (0.16785)	0.0002	22	2.3494	527.72	aH-4 →aL+1 (0.11778) bH-4 →bL+1 (0.75398) bH-3 →bL+1 (-0.61514)	0.0001
8	1.7162	722.45	bH-7 →bL (0.94088) bH-2 →bL+2 (-0.10552) bH-1 →bL+1 (0.25301) bH →bL (-0.13656)	0.0009	23	2.3695	523.24	aH-4 →aL (0.85014) aH →aL+1 (-0.10419) bH-9 →bL (-0.20210) bH-8 →bL (0.37398) bH-4 →bL+2 (-0.10405)	0.0035
9	1.9295	642.56	aH-8 →aL+1 (-0.10091) aH-1 →aL (-0.13304) bH-7 →bL (-0.24500) bH-4 →bL+1 (0.11105) bH-3 →bL+1 (0.10394) bH-2 →bL+1 (-0.27303) bH-1 →bL+1 (0.85114) bH →bL+1 (-0.26706)	0.0007	24	2.3964	517.37	aH-8 →aL (-0.15161) aH-5 →aL+1 (0.24390) aH-1 →aL+1 (0.80918) bH-9 →bL (0.13502) bH-2 →bL+1 (-0.25275) bH-2 →bL+2 (0.16069) bH-1 →bL+2 (-0.26815)	0.0001
10	1.9578	633.3	aH-7 →aL+1 (0.25954)	0.0072	25	2.4418	507.76	aH-7 →aL+1 (-0.52568)	0.0396

			aH-3 →aL+1 (0.27387) aH →aL+1 (0.45200) bH-7 →bL+1 (-0.24637) bH-5 →bL+1 (0.18956) bH-1 →bL+1 (0.25686) bH →bL+1 (0.73510)					aH-6 →aL (0.19248) aH-4 →aL (0.21096) aH-3 →aL+1 (-0.11117) aH-1 →aL+1 (0.11299) aH →aL+1 (0.60997) bH-11 →bL (0.19085) bH-7 →bL+1 (0.39319) bH-3 →bL+2 (-0.12245)	
11	2.0473	605.61	aH-3 →aL (0.34560) aH →aL (0.87514) bH →bL+2 (-0.26101)	0.0011	26	2.5137	493.24	aH-8 →aL (0.11516) aH-2 →aL (0.17048) aH-2 →aL+1 (0.65629) bH-9 →bL (0.13932) bH-8 →bL (0.15278) bH-4 →bL+2 (0.21885) bH-3 →bL (-0.17802) bH-3 →bL+2 (0.55847)	0.0001
12	2.1187	585.18	aH-8 →aL (-0.11705) aH-1 →aL (0.12872) bH-6 →bL+1 (0.16893) bH-2 →bL+1 (0.67419) bH-2 →bL+2 (0.14388) bH-1 →bL+1 (0.21602) bH-1 →bL+2 (-0.61427) bH →bL+2 (0.13793)	0.0000	27	2.5156	492.85	aH-2 →aL+1 (-0.71525) bH-9 →bL (0.11717) bH-8 →bL (0.14702) bH-4 →bL+2 (0.16903) bH-3 →bL (-0.16763) bH-3 →bL+2 (0.53095)	0.0001
13	2.1573	574.71	aH-12 →aL (0.13860) aH-8 →aL (0.19911) aH-5 →aL (0.18063) aH-5 →aL+1 (0.20300) aH-1 →aL (0.35919) aH-1 →aL+1 (0.34478) bH-6 →bL+1 (0.10469) bH-2 →bL+1 (0.43383) bH-2 →bL+2 (-0.27816) bH-1 →bL+1 (0.19822) bH-1 →bL+2 (0.52667) bH →bL+2 (-0.13077)	0.0000	28	2.5253	490.97	aH-7 →aL+1 (0.13677) aH-4 →aL (0.21112) bH-9 →bL (0.19918) bH-8 →bL (-0.17570) bH-7 →bL+1 (-0.13096) bH-4 →bL (0.24504) bH-4 →bL+2 (0.77430) bH-4 →bL+3 (-0.12429) bH-4 →bL+5 (0.10050) bH-3 →bL+2 (-0.26393)	0.0005
14	2.1628	573.25	aH-5 →aL (0.35723) aH-5 →aL+1 (-0.11067) aH-1 →aL (0.72442) aH-1 →aL+1 (-0.19311) bH-2 →bL+1 (-0.37568) bH-2 →bL+2 (-0.18522) bH-1 →bL+2 (-0.22508)	0.0001	29	2.5626	483.81	aH-4 →aL+1 (0.97270)	0.0001
15	2.2228	557.78	aH-7 →aL+1 (-0.20974) aH-6 →aL (0.39288) aH-3 →aL+1 (-0.21333) aH →aL (-0.14292) aH →aL+1 (-0.48969) bH-7 →bL+1 (0.31544) bH-1 →bL+1 (0.12239) bH →bL+1 (0.51276) bH →bL+2 (-0.29703)	0.0175	30	2.6249	472.34	aH-7 →aL (0.23241) aH-3 →aL (0.88237) aH →aL (-0.34690) bH-7 →bL+2 (0.12912)	0.0058

Table S7.1. Optimized geometry for [**4a**]$^{4+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	-2.5852	-0.02639	-0.00181	H	-9.35169	0.777095	-5.10713	N	7.3129	-3.94815	0.284819
C	-1.34539	0.174105	-2.30288	N	5.636635	-0.53443	-3.81243	H	12.67945	-7.48277	0.141309
C	1.320774	-0.20122	-2.28295	C	7.385023	-1.02641	-5.6391	H	9.517814	-10.976	0.275257
N	2.532369	-0.03251	0.001274	C	6.717995	-1.93892	-8.03131	H	4.87799	-9.8709	0.480096
C	1.320933	0.129228	2.286007	C	4.162877	-2.43082	-8.54895	H	3.63395	-5.31603	0.490805
C	-1.34588	-0.24055	2.298298	C	2.348181	-1.85039	-6.70289	H	9.342577	-0.72845	-5.13784
C	-3.09137	0.803269	-4.39768	H	8.180621	-2.30441	-9.41962	N	-10.1614	0.025175	0.004359
C	3.086971	-0.81484	-4.36984	H	3.592431	-3.24481	-10.3427	C	-11.4316	-2.22684	-0.11966
C	3.086441	0.73457	4.377805	H	0.374842	-2.24637	-7.06821	C	-14.0868	-2.24515	-0.12914
C	-3.09417	-0.87271	4.388192	Ru	6.52968	-0.00389	-0.00562	C	-15.3875	0.071377	-0.0014
N	-5.64377	-0.59089	3.82037	Ru	-6.34623	-0.0019	0.003245	C	-14.0466	2.363737	0.130166
C	-7.39644	-1.09903	5.629532	C	10.19298	0.031615	-0.0074	C	-11.3931	2.297474	0.126045
C	-6.74622	-2.01926	8.022116	C	11.53807	-2.29564	0.098529	C	-9.7342	-4.43618	-0.2442
C	-4.18863	-2.49491	8.557393	C	14.19277	-2.25852	0.100999	H	-15.14	-3.99826	-0.23969
C	-2.36131	-1.90717	6.726803	C	15.46538	0.096364	-0.00161	H	-17.4381	0.090982	-0.00473
H	-9.3504	-0.78636	5.11521	C	14.13559	2.418008	-0.10817	H	-15.0661	4.136698	0.239146
H	-8.21554	-2.39866	9.398496	C	11.48237	2.388689	-0.11018	C	-9.66476	4.480659	0.251846
H	-3.62473	-3.30188	10.35569	C	9.873089	-4.5246	0.207144	N	-7.11514	3.890871	0.334397
H	-0.38832	-2.29316	7.10579	H	15.30726	-3.97958	0.188339	C	-5.41046	5.809152	0.477596
C	2.346245	1.719694	6.732941	H	17.51803	0.123527	0.003319	C	-6.12288	8.35453	0.491691
C	4.161711	2.297144	8.579393	H	15.20258	4.168792	-0.19229	C	-8.704	8.970162	0.364977
C	6.72096	1.852235	8.041405	C	9.775507	4.583578	-0.21431	C	-10.4813	7.004017	0.260601
C	7.387534	0.978051	5.635013	N	7.22646	3.965193	-0.29876	H	-3.43911	5.269165	0.569401
N	5.637797	0.490489	3.80802	C	5.492268	5.855157	-0.41674	H	-4.69081	9.816886	0.593084
H	0.370044	2.077232	7.12025	C	6.161704	8.414509	-0.39855	H	-9.3214	10.92483	0.347611
H	3.588601	3.071985	10.38978	C	8.736401	9.063279	-0.27587	H	-12.48	7.439962	0.170969
H	8.18617	2.223435	9.425637	C	10.54414	7.122462	-0.2035	C	-10.5792	-6.95078	-0.26025
H	9.346193	0.705532	5.123878	H	3.528101	5.283114	-0.51846	C	-8.82302	-8.93671	-0.37054
C	-2.35527	1.789445	-6.75685	H	4.706853	9.855446	-0.4794	C	-6.23404	-8.35155	-0.48343
C	-4.1823	2.376791	-8.5882	H	9.328978	11.02742	-0.24017	C	-5.49295	-5.81506	-0.45701
C	-6.74397	1.946221	-8.03572	H	12.53778	7.580805	-0.12656	N	-7.17661	-3.87856	-0.32072
C	-7.39597	1.064878	-5.62924	C	10.67888	-7.0528	0.211283	H	-12.5829	-7.36532	-0.17309
N	-5.64328	0.560987	-3.81836	C	8.898353	-9.01989	0.292326	H	-9.46128	-10.8848	-0.36854
H	-0.37909	2.135457	-7.1564	C	6.313206	-8.41031	0.399327	H	-4.81735	-9.82891	-0.585
H	-3.61498	3.146478	-10.4018	C	5.606099	-5.86191	0.402065	H	-3.51555	-5.29566	-0.53397
H	-8.21396	2.327048	-9.41116								

Table S7.2.1. Orbital energies and Mulliken population on Ru of alpha orbitals for [**4a**]$^{4+}$. Ru^1 corresponds to RuN_5C (right in Figure S6.1), Ru^2 corresponds to RuN_6 (left in Figure S.2.5.1)

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-16.8503	0.143367	0.007711	0.10822	0.001189	0.00076	0.000123
H-11	-16.6566	0.000428	1.71E-05	0.000411	0.019378	3.68E-05	0.019341
H-10	-16.6386	0.100124	0.00183	0.098294	2.08E-05	5.9E-06	0.000015
H-9	-16.3031	0.211702	0.002016	0.209687	0.000226	0.000006	0.00022
H-8	-16.0194	0.018416	0.000182	0.018281	0.012027	-0.00026	0.012401
H-7	-15.752	0.002142	1.22E-05	0.002131	0.027239	3.6E-06	0.027222
H-6	-15.6611	0.460689	0.010233	0.450456	0.171822	0.004116	0.167706
H-5	-15.4305	0.430681	-5.4E-05	0.43072	0.005781	-1E-07	0.005776
H-4	-15.0822	0.085016	0.001046	0.083971	0.631763	0.005234	0.626529
H-3	-15.0328	0.190597	-2.7E-05	0.190641	0.024906	4E-07	0.024895
H-2	-14.998	0.162426	0.002055	0.160371	0.566939	0.006996	0.559943
H-1	-14.8819	0.023926	0.00008	0.023874	0.621007	-8.7E-05	0.621164
H	-14.8633	0.206239	0.000447	0.205792	0.002524	1.19E-05	0.002512
L	-12.4002	0.021611	0.001118	0.020684	0.027106	0.000928	0.026158
L+1	-12.1839	0.05304	-0.00103	0.054068	0.120029	-0.00028	0.120312
L+2	-11.3031	0.008351	0.001673	0.006678	0.033931	0.003583	0.030347
L+3	-11.1881	0.005359	0.001309	0.00405	0.043594	0.002867	0.040727
L+4	-10.9423	0.000149	9.3E-06	0.000139	0.016197	7.87E-05	0.016145
L+5	-10.5308	0.048	-0.0003	0.048123	0.004485	0.001974	0.001256
L+6	-10.4435	0.012399	0.00525	0.007146	0.001597	0.000871	0.000726
L+7	-10.4246	0.016865	0.000159	0.016652	0.000305	-1.6E-05	0.000352
L+8	-10.4071	0.005236	0.000861	0.004372	0.009783	0.000968	0.008815
L+9	-10.4037	0.012752	-3.1E-05	0.012067	0.029103	-0.00035	0.029629
L+10	-10.332	0.032755	0.007569	0.025187	0.000212	7.69E-05	0.000135
L+11	-10.0563	0.00062	0.00035	0.00027	0.014702	0.005468	0.009234
L+12	-10.0234	0.005363	-0.0003	0.004745	0.035954	-0.00064	0.036685

Table S7.2.2. Orbital energies and Mulliken population on Ru of beta orbitals for [**4a**]$^{4+}$. Ru^1 corresponds to RuN_5C (right in Figure S6.2), Ru^2 corresponds to RuN_6 (left in Figure S.2.5.2)

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-11	-16.8287	0.137987	0.006552	0.105792	0.001059	0.000677	0.000104
H-10	-16.6566	6.42E-05	1.46E-05	4.97E-05	0.019446	3.82E-05	0.019408
H-9	-16.3854	0.017035	0.001502	0.015533	5.79E-05	6.7E-06	5.12E-05
H-8	-16.0187	0.010195	0.000167	0.010079	0.012424	-0.00027	0.012814
H-7	-15.7517	0.000797	1.18E-05	0.000788	0.027006	1.8E-06	0.026992
H-6	-15.7109	0.200596	0.008006	0.19259	0.000607	1.84E-05	0.000588
H-5	-15.516	0.27797	0.007403	0.270567	0.337412	0.006888	0.330524
H-4	-15.2366	0.273298	-1.7E-05	0.273314	0.009519	6.9E-06	0.009497
H-3	-15.0649	0.021118	0.00034	0.020778	0.690569	0.005155	0.685414
H-2	-14.9296	0.124169	-2.6E-05	0.124191	0.374691	-4.3E-05	0.374699
H-1	-14.8778	0.413772	0.006677	0.407095	0.350857	0.004176	0.346681
H	-14.8398	0.277986	6.12E-05	0.278034	0.268312	-2.5E-05	0.268436
L	-12.7968	0.514705	0.003393	0.511312	0.001488	1.7E-06	0.001486
L+1	-12.3943	0.026761	0.001098	0.025879	0.026898	0.000908	0.025972
L+2	-12.163	0.07784	-0.00115	0.078996	0.111632	-0.00024	0.111869
L+3	-11.3021	0.011238	0.001489	0.009748	0.032847	0.003569	0.029278
L+4	-11.1882	0.007232	0.001201	0.006031	0.0427	0.002844	0.039857
L+5	-10.9424	0.000122	8.3E-06	0.000113	0.016186	7.92E-05	0.016132
L+6	-10.5112	0.037908	0.000288	0.037516	0.006198	0.002264	0.00249
L+7	-10.4408	0.007085	0.001981	0.005102	0.001942	0.000956	0.000986
L+8	-10.4102	0.009959	-0.00018	0.010159	0.002255	-7.3E-05	0.00234
L+9	-10.4078	0.004893	0.000877	0.004015	0.009602	0.000989	0.008613
L+10	-10.3967	0.01439	-2E-05	0.013862	0.02553	-0.00051	0.026333
L+11	-10.203	0.085471	0.008359	0.077113	6.65E-05	1.54E-05	5.09E-05
L+12	-10.0561	0.000633	0.000343	0.00029	0.014663	0.005454	0.00921
L+13	-10.0226	0.002452	4.71E-05	0.001603	0.036502	-0.00069	0.037319

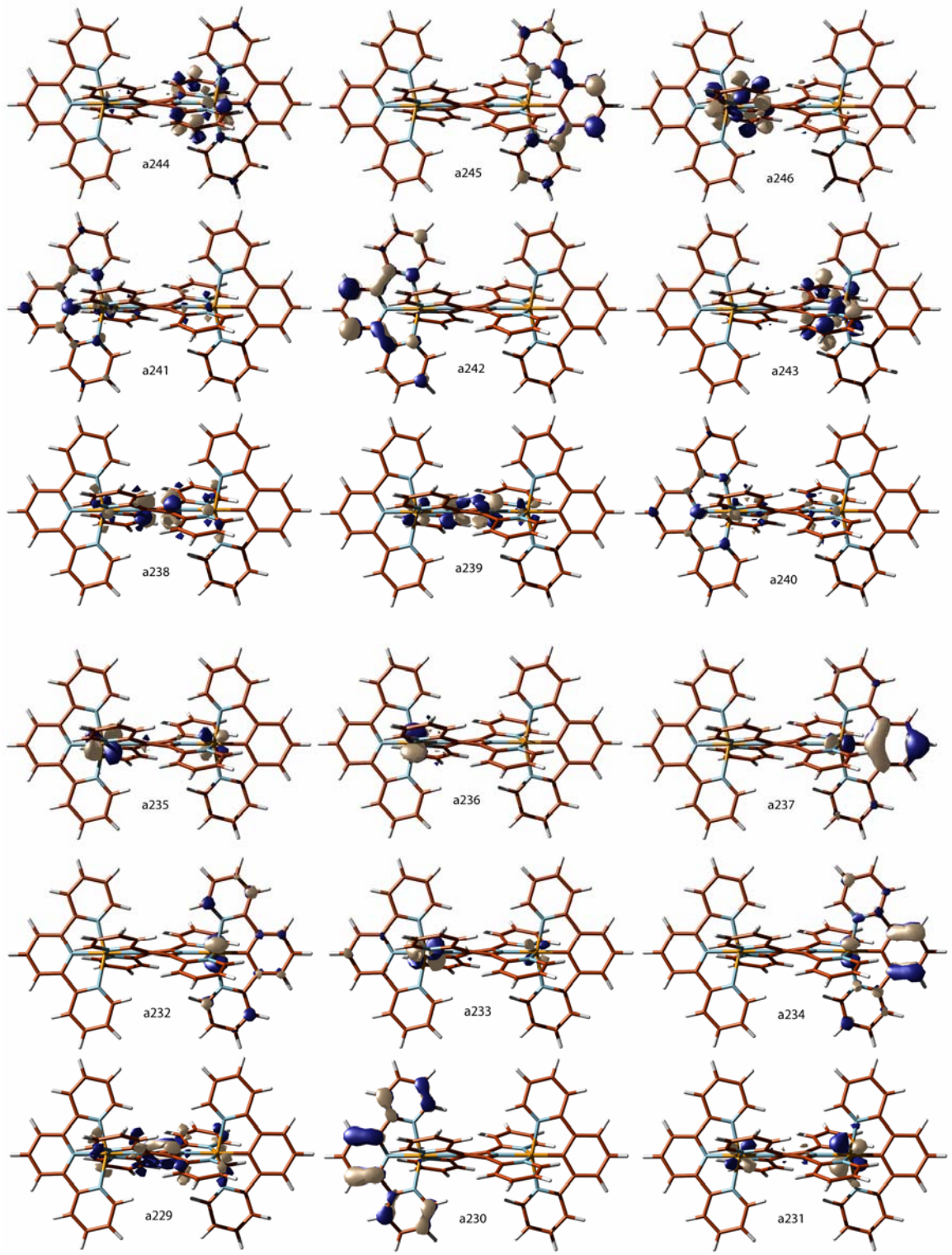

Figure S8.1. Isovalue (value = 0.05) plots of the alpha frontier orbitals of [**4a**]$^{4+}$.

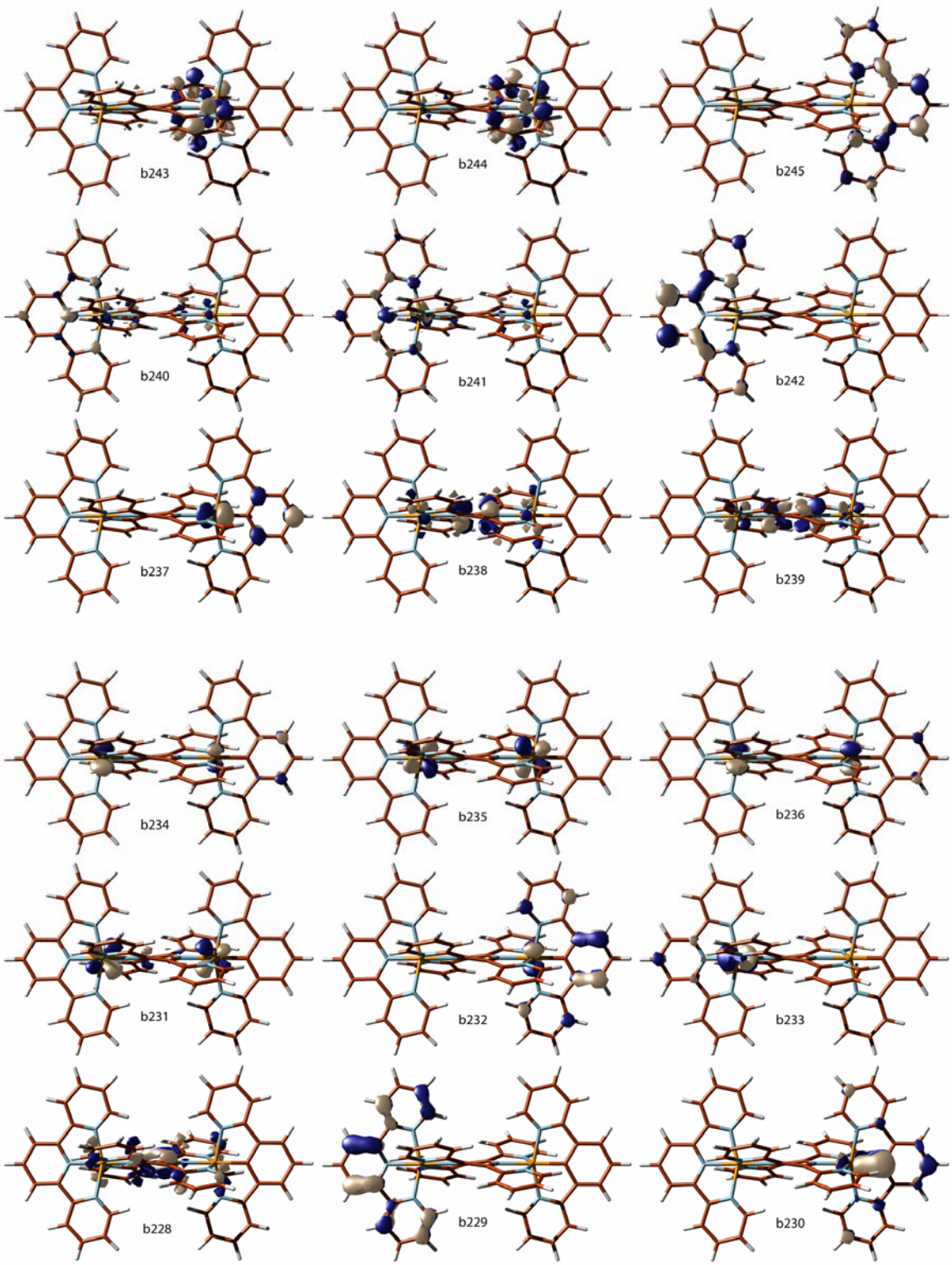

Figure S8.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**4a**]$^{4+}$.

Table S7.3 Complete listing of electronic transitions for [**4a**]$^{4+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	0.4622	2682.39	bH-4 →bL (0.47146) bH-2 →bL (-0.49549) bH →bL (0.76332)	0.0001	16	1.8943	654.51	aH-4 →aL (0.26889) aH-4 →aL+1 (0.37957) aH-2 →aL+1 (0.23123) aH-1 →aL (0.16328) aH →aL (0.25063) bH-3 →bL (0.65325) bH-3 →bL+1 (-0.20884) bH-3 →bL+2 (0.19551) bH-2 →bL+1 (0.15489) bH-1 →bL (-0.16599)	0.0032
2	0.5389	2300.51	bH-5 →bL (-0.47221) bH-3 →bL (0.17309) bH-1 →bL (0.88081)	0.0003	17	1.909	649.46	aH-5 →aL+1 (0.13635) aH-3 →aL+1 (0.14261) aH-2 →aL (0.15955) aH-1 →aL+1 (0.17170) aH →aL (-0.23765) bH-4 →bL+2 (-0.34458) bH-3 →bL+1 (0.10169) bH-2 →bL+2 (0.74259) bH →bL+2 (-0.31388) bH →bL+3 (0.14961) bH →bL+4 (-0.11349)	0.0009
3	1.3849	895.26	aH-8 →aL (-0.14654) aH-4 →aL+1 (-0.38372) aH-2 →aL+1 (0.67806) bH-8 →bL+1 (0.14749) bH-5 →bL+2 (0.24433) bH-5 →bL+3 (0.10954) bH-1 →bL+2 (0.78351)	0.0003	18	1.9128	648.18	aH-4 →aL (-0.14576) aH →aL (0.83677) bH-3 →bL+1 (0.47839) bH-2 →bL+2 (0.11679)	0.0001
4	1.4753	840.38	bH-4 →bL (0.84611) bH-2 →bL (0.44442) bH →bL (-0.25800)	0.0171	19	1.9592	632.83	aH-4 →aL (0.72123) aH →aL (-0.20045) bH-3 →bL+1 (0.58714) bH-3 →bL+2 (-0.13895) bH-1 →bL+1 (0.10291)	0.0034
5	1.5883	780.63	aH-4 →aL (-0.12644) aH-2 →aL (0.22475) aH-1 →aL+1 (0.63920) aH-1 →aL+2 (0.12356) bH-2 →bL (-0.19997) bH-2 →bL+2 (-0.37522) bH-2 →bL+3 (-0.10215) bH-1 →bL+1 (0.35077) bH →bL (-0.17670) bH →bL+2 (-0.47900)	0.0002	20	1.9745	627.92	aH-4 →aL (0.11848) aH-4 →aL+1 (0.31437) aH-2 →aL+1 (0.19922) bH-5 →bL (0.10472) bH-3 →bL (-0.49220) bH-3 →bL+1 (0.15173) bH-3 →bL+2 (0.67031) bH-3 →bL+3 (0.10429) bH-1 →bL (0.16059) bH-1 →bL+2 (-0.11203)	0.0002
6	1.6106	769.8	aH-8 →aL (-0.12390) aH-1 →aL (-0.67166) bH-8 →bL+1 (0.12037) bH-2 →bL+1 (0.32276) bH →bL+1 (0.67095)	0.0002	21	2.0283	611.28	aH-6 →aL+1 (-0.18391) aH-5 →aL (0.26061) aH-3 →aL (0.61148) aH →aL+1 (0.28813) bH-6 →bL (-0.12003) bH-5 →bL (-0.16582) bH-5 →bL+2 (-0.41530) bH-2 →bL+1 (-0.32523) bH-1 →bL+2 (0.26660) bH-1 →bL+3 (-0.14146)	0.0106
7	1.6661	744.17	aH-4 →aL (-0.17217) aH-2 →aL (0.36203) aH-1 →aL+1 (-0.22553) bH-2 →bL (0.14453) bH-2 →bL+2 (0.15511) bH-1 →bL+1 (0.81870) bH →bL (0.12369) bH →bL+2 (0.17288)	0.0014	22	2.0648	600.48	aH-5 →aL (-0.11131) aH-4 →aL+1 (-0.12505) aH-3 →aL (-0.27871) aH →aL+1 (0.88955) aH →aL+2 (-0.10260) bH-5 →bL (-0.16714) bH-1 →bL (-0.11089)	0.0010
8	1.7284	717.35	aH-1 →aL+1 (0.49674) bH-4 →bL (-0.16524) bH-2 →bL (0.63172) bH →bL (0.52275) bH →bL+2 (0.10115)	0.0005	23	2.1045	589.14	aH-6 →aL+1 (0.23949) aH-3 →aL (0.28199) aH →aL+1 (0.27280) bH-5 →bL (0.72979) bH-5 →bL+2 (0.19653) bH-3 →bL (0.18076)	0.0012

								bH-1 →bL (0.34678) bH-1 →bL+2 (-0.14567)	
9	1.7681	701.24	aH-4 →aL+1 (0.58198) aH-4 →aL+2 (0.10241) aH-4 →aL+3 (-0.10425) aH-2 →aL+1 (0.39919) aH-1 →aL (-0.13884) bH-3 →bL (-0.27587) bH-3 →bL+2 (-0.58248) bH-3 →bL+3 (-0.10912) bH →bL+1 (-0.17079)	0.0003	24	2.1548	575.39	aH-6 →aL+1 (0.49803) aH-3 →aL (0.41159) aH-2 →aL+2 (0.12184) bH-5 →bL (-0.39974) bH-5 →bL+2 (0.52663) bH-3 →bL (-0.10523) bH-1 →bL (-0.21506) bH-1 →bL+2 (-0.17796) bH-1 →bL+3 (0.15869) bH-1 →bL+4 (-0.10081) bH →bL+1 (0.13876)	0.0198
10	1.7912	692.18	aH-4 →aL+1 (0.19962) aH-3 →aL (-0.15817) aH-2 →aL+1 (-0.17265) aH-1 →aL (0.58135) bH-4 →bL+1 (0.17506) bH-3 →bL (-0.13699) bH-3 →bL+2 (-0.22641) bH-2 →bL+1 (-0.16392) bH-1 →bL+2 (0.15686) bH →bL+1 (0.59091) bH →bL+2 (-0.14430)	0.0134	25	2.161	573.74	aH-5 →aL+1 (0.41826) aH-3 →aL+1 (0.79344) aH-1 →aL+1 (0.10746) bH-5 →bL+1 (-0.28798) bH-2 →bL+2 (-0.17633) bH →bL+2 (0.13747)	0.0007
11	1.8039	687.3	aH-2 →aL (-0.24334) aH-1 →aL+1 (0.42882) bH-2 →bL (-0.30713) bH-2 →bL+1 (-0.10255) bH-2 →bL+2 (0.24155) bH-1 →bL+1 (0.13136) bH →bL (-0.23208) bH →bL+1 (0.14405) bH →bL+2 (0.61551)	0.0010	26	2.2495	551.16	aH-6 →aL (0.44576) aH-3 →aL+1 (0.27928) bH-5 →bL+1 (0.81832)	0.0013
12	1.8413	673.35	aH-6 →aL+1 (-0.10407) aH-5 →aL (0.12758) aH-3 →aL (0.16148) aH-2 →aL (0.56764) aH-2 →aL+1 (-0.12566) aH-1 →aL (0.20585) bH-4 →bL+1 (-0.17580) bH-2 →bL+1 (0.55748) bH-1 →bL+1 (-0.27135) bH-1 →bL+2 (0.17255) bH →bL+2 (0.25540)	0.0052	27	2.2968	539.81	aH-8 →aL (-0.19780) aH-5 →aL (-0.21521) aH-3 →aL (0.23361) bH-8 →bL+1 (0.19543) bH-4 →bL+1 (0.82832) bH-2 →bL+1 (0.22060) bH →bL+1 (-0.25340)	0.0015
13	1.8427	672.84	aH-6 →aL+1 (-0.10310) aH-5 →aL (0.12449) aH-3 →aL (0.15297) aH-2 →aL (-0.60905) aH-2 →aL+1 (-0.14489) aH-1 →aL (0.20662) bH-4 →bL+1 (-0.16771) bH-2 →bL+1 (0.55500) bH-1 →bL+1 (0.26588) bH-1 →bL+2 (0.15337) bH →bL+2 (-0.19058)	0.0053	28	2.3745	522.15	aH-8 →aL (0.35065) aH-6 →aL+1 (0.24915) aH-5 →aL (0.59238) aH-4 →aL+1 (0.12742) aH-3 →aL (-0.29883) aH-2 →aL+1 (-0.15988) aH-1 →aL (-0.16068) bH-8 →bL+1 (-0.34646) bH-5 →bL+2 (0.10044) bH-4 →bL+1 (0.30887) bH-1 →bL+2 (0.23332)	0.0247
14	1.8841	658.04	aH-5 →aL (0.11087) aH-4 →aL (0.20694) aH-4 →aL+1 (-0.15499) aH-3 →aL (0.16742) aH →aL (0.12941) bH-6 →bL (0.85420) bH-3 →bL (-0.25177) bH-3 →bL+1 (-0.22331) bH-1 →bL+2 (-0.10158)	0.0881	29	2.4814	499.66	aH-8 →aL (-0.46153) aH-6 →aL+1 (0.14542) aH-5 →aL (0.23963) aH-4 →aL+1 (0.24103) aH-4 →aL+3 (0.14203) aH-3 →aL (-0.10106) aH-2 →aL+1 (-0.31696) aH-2 →aL+2 (0.14353) bH-8 →bL+1 (0.53119) bH-7 →bL+1 (-0.10676) bH-5 →bL+2 (0.11944) bH-4 →bL+1 (-0.21899) bH-2 →bL+1 (-0.10839) bH-1 →bL+2 (0.17507)	0.1076
15	1.8859	657.42	aH-4 →aL (-0.51002) aH-4 →aL+1 (0.11650)	0.0229	30	2.4927	497.39	aH-6 →aL (0.50072) bH-5 →bL+1 (-0.26985)	0.0005

aH-2 →aL+1 (0.12491) aH →aL (-0.32752) bH-6 →bL (0.40278) bH-3 →bL (0.26515) bH-3 →bL+1 (0.52965)	bH-4 →bL+2 (0.70875) bH-2 →bL+2 (0.29942) bH →bL+2 (-0.21373)

Table S8.1. Optimized geometry for [**4b**]$^{4+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
Ru	-5.43343	0.018163	0.177737	N	-6.32094	-3.90546	0.036449	H	-8.36555	0.448005	-4.88012
Ru	7.426794	-0.04312	-0.08525	C	-8.90026	-4.40897	0.056219	H	1.649061	2.144756	7.190543
N	8.312454	-3.90378	0.217749	C	-9.7759	-6.91425	0.110728	H	4.960889	3.024873	10.39514
C	10.87824	-4.41909	0.162513	C	-8.04428	-8.92495	0.151255	H	9.51665	2.087254	9.32564
C	11.76282	-6.91932	0.213323	C	-5.44233	-8.39151	0.113417	H	10.54433	0.607773	4.966893
C	10.03721	-8.93253	0.318161	C	-4.66411	-5.86648	0.047494	H	-7.02372	-1.75854	9.691821
C	7.437585	-8.38978	0.388609	C	-2.09435	0.560407	-4.29554	H	-2.45482	-2.80756	10.60397
C	6.657394	-5.86532	0.342752	C	-1.42217	1.442493	-6.71064	H	0.747613	-2.11668	7.238015
C	12.53845	-2.18289	0.017488	C	-3.28604	1.906454	-8.5416	H	-14.3322	-3.69272	-0.19712
N	11.23496	0.047872	-0.13246	C	-5.82804	1.461053	-7.92686	C	-17.1783	0.634411	-0.26876
C	12.43033	2.339511	-0.27011	C	-6.42678	0.71461	-5.46222	H	-14.0126	4.419889	0.078147
C	15.08196	2.445863	-0.25548	N	-4.62892	0.336549	-3.65782	H	-2.27496	5.214098	0.522385
C	16.45811	0.175494	-0.10175	C	4.112098	-0.95142	-4.40741	H	-3.31411	9.816887	0.475559
C	15.1924	-2.15942	0.034074	N	6.665884	-0.60703	-3.89126	H	-7.88916	11.12859	0.295124
N	8.127339	3.855317	-0.44338	C	8.395503	-1.04465	-5.74073	H	-11.2149	7.807684	0.189937
C	10.66569	4.492875	-0.42365	C	7.725821	-1.95731	-8.13027	H	-11.7878	-7.30086	0.138231
C	11.42993	7.031058	-0.53053	C	5.175047	-2.51486	-8.61178	H	-8.71419	-10.8618	0.21282
C	9.61028	8.957636	-0.66505	C	3.368502	-2.00317	-6.73624	H	-4.05077	-9.89509	0.136346
C	7.039313	8.29043	-0.70881	C	-10.5034	-2.12936	0.053171	H	-2.67356	-5.3873	0.013097
C	6.381507	5.733625	-0.6007	C	-9.08851	0.15858	0.164029	H	-8.18328	-0.37364	5.332145
N	3.668202	-0.10847	-0.00338	C	-10.3112	2.555936	0.177167	H	16.26963	-3.8962	0.159336
C	2.475121	0.121506	2.322805	C	-12.9505	2.661866	0.072277	H	18.50871	0.226078	-0.08463
C	-0.19613	-0.225	2.361481	C	-14.3518	0.377986	-0.07412	H	16.07438	4.233831	-0.3604
N	-1.44457	-0.09651	0.091673	C	-13.1505	-2.02026	-0.07293	H	4.42165	5.147368	-0.6269
C	-0.28023	0.017104	-2.22305	C	-8.54746	4.706461	0.271651	H	5.576286	9.721624	-0.82142
C	2.387949	-0.34515	-2.28167	N	-6.01668	4.01056	0.354253	H	10.18668	10.92396	-0.735
C	4.273046	0.743023	4.380557	C	-4.22182	5.843738	0.440994	H	13.4203	7.511606	-0.50175
C	3.605617	1.737379	6.757183	C	-4.81127	8.419972	0.417394	H	13.7736	-7.30266	0.156825
C	5.476876	2.259392	8.564425	C	-7.36462	9.146483	0.320508	H	10.70688	-10.8702	0.340785
C	8.016625	1.768856	7.967026	C	-9.23884	7.26916	0.257744	H	6.044819	-9.89135	0.472286
C	8.605355	0.915986	5.534977	H	10.3492	-0.68263	-5.26086	H	4.671732	-5.37522	0.391588
N	6.810006	0.471067	3.750993	H	9.174612	-2.26915	-9.54498	O	-18.2492	2.7185	-0.15021
C	-1.94457	-0.7221	4.502214	H	4.601043	-3.32559	-10.4056	O	-18.3285	-1.63311	-0.61941
N	-4.49179	-0.38828	3.970175	H	1.404902	-2.46422	-7.07805	C	-21.1389	-1.71166	-0.90948
C	-6.23464	-0.723	5.835367	H	0.539322	1.807142	-7.1564	H	-21.4966	-3.05012	-2.43425
C	-5.56915	-1.52477	8.265846	H	-2.76135	2.594487	-10.4006	H	-21.9265	-2.38713	0.874214
C	-3.02373	-2.07665	8.774425	H	-7.32931	1.736863	-9.29583	H	-21.8538	0.170192	-1.36058
C	-1.21389	-1.66444	6.877363								

Table S8.2.1. Orbital energies and Mulliken population on Ru of alpha orbitals for [**4b**]$^{4+}$. Ru^1 corresponds to RuN_5C (right in Figure S6.1), Ru^2 corresponds to RuN_6 (left in Figure S.2.5.1)

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-12	-16.2907	0.004482	0.001277	0.145791	5.87E-05	5.9E-06	0.000137
H-11	-16.2403	0.147121	0.000178	0.016514	0.000144	-0.00023	0.012046
H-10	-15.9999	0.016633	1.44E-05	0.001958	0.011682	-3.1E-06	0.026149
H-9	-15.7329	0.001969	0.010379	0.437699	0.02615	0.004195	0.174365
H-8	-15.6284	0.448079	-5E-05	0.396684	0.17856	-2E-06	0.005711
H-7	-15.3904	0.39665	1.61E-05	0.105705	0.00571	4.42E-05	0.008213
H-6	-15.1027	0.105646	0.000871	0.067272	0.008262	0.005066	0.640293
H-5	-15.0522	0.068142	0.002335	0.178086	0.645359	0.006538	0.523178
H-4	-14.971	0.180421	9.31E-05	0.113513	0.529715	0.000119	0.050238
H-3	-14.9476	0.113662	9.62E-05	0.03314	0.050357	-8.6E-06	0.599849
H-2	-14.8473	0.03321	0.000378	0.17122	0.59978	0.000023	0.005269
H-1	-14.8099	0.171592	-5E-05	0.024821	0.00529	-2E-06	0.00101
H	-14.7277	0.024795	0.001111	0.020873	0.001004	0.000995	0.02591
L	-12.3643	0.021815	-0.00089	0.054924	0.026942	-0.00015	0.120981
L+1	-12.1621	0.054034	0.001525	0.006057	0.120837	0.003759	0.032556
L+2	-11.2689	0.007582	0.001407	0.004713	0.036315	0.002784	0.038112
L+3	-11.1668	0.006119	1.19E-05	0.000137	0.040896	2.17E-05	0.015869
L+4	-10.9175	0.000152	-0.00037	0.044323	0.015873	0.001938	0.001534
L+5	-10.487	0.044314	0.005382	0.005751	0.004819	0.000875	0.000532
L+6	-10.4124	0.011148	0.000986	0.006046	0.001404	0.000959	0.008683
L+7	-10.3819	0.007041	-0.00032	0.01372	0.009662	-0.00074	0.029818
L+8	-10.379	0.013948	0.000225	0.010591	0.029006	6.41E-05	0.000132
L+9	-10.3558	0.010883	0.00793	0.028658	0.000189	7.08E-05	0.000117
L+10	-10.3139	0.036564	0.000408	0.000344	0.000191	0.005335	0.010179
L+11	-10.0352	0.000807	-0.00038	0.004228	0.015504	-0.00062	0.0363
L+12	-9.9963	0.00467	0.001277	0.145791	0.035489	5.9E-06	0.000137

Table S8.2.2. Orbital energies and Mulliken population on Ru of beta orbitals for [**4b**]$^{4+}$. Ru^1 corresponds to RuN_5C (right in Figure S6.2), Ru^2 corresponds to RuN_6 (left in Figure S.2.5.2)

#	E (eV)	Ru^1	p	d	Ru^2	p	d
H-11	-16.2268	0.007437	0.000855	0.006571	0.000036	5.6E-06	0.00003
H-10	-15.9998	0.009455	0.000155	0.009365	0.012009	-0.00024	0.01239
H-9	-15.7326	0.000756	0.000011	0.000749	0.025971	-5.3E-06	0.025974
H-8	-15.6392	0.212491	0.008154	0.204293	0.002077	5.74E-05	0.002019
H-7	-15.4892	0.268785	0.007539	0.261242	0.339398	0.006827	0.332571
H-6	-15.2189	0.206212	-2.2E-05	0.206206	0.007199	5.3E-06	0.007185
H-5	-15.0403	0.016372	0.000268	0.016103	0.694522	0.005078	0.689444
H-4	-14.989	0.154298	4.42E-05	0.154354	0.036483	3.47E-05	0.036425
H-3	-14.8773	0.025886	0.000135	0.025734	0.457015	-3.7E-05	0.457079
H-2	-14.8473	0.398586	0.006562	0.392026	0.321246	0.003731	0.317515
H-1	-14.7863	0.293862	0.000293	0.293592	0.166531	0.000126	0.166457
H	-14.6979	0.014892	-9.8E-05	0.014987	0.007004	5.35E-05	0.006958
L	-12.8058	0.499376	0.003572	0.495761	0.001555	-1E-06	0.001556
L+1	-12.358	0.027867	0.001128	0.026936	0.026712	0.000975	0.025703
L+2	-12.141	0.079494	-0.00103	0.080525	0.112041	-9.4E-05	0.112134
L+3	-11.2681	0.010175	0.00134	0.008835	0.035351	0.003745	0.031606
L+4	-11.1668	0.008322	0.001282	0.007041	0.039908	0.002757	0.037152
L+5	-10.9176	0.000131	1.15E-05	0.000117	0.015855	0.000022	0.015851
L+6	-10.4698	0.035379	0.000268	0.034766	0.006881	0.00217	0.003185
L+7	-10.4109	0.005025	0.001955	0.003052	0.001414	0.000986	0.000429
L+8	-10.3833	0.006295	0.000861	0.005419	0.009655	0.000959	0.008684
L+9	-10.3728	0.013986	-0.00061	0.014292	0.026809	-0.00092	0.027899
L+10	-10.3494	0.009945	0.000122	0.009753	0.000473	0.000044	0.000449
L+11	-10.1729	0.092509	0.008933	0.083596	0.000113	4.48E-05	0.000053
L+12	-10.0351	0.00081	0.000406	0.000353	0.015463	0.005318	0.010155
L+13	-9.9956	0.002357	-0.00011	0.00173	0.035952	-0.00066	0.036829

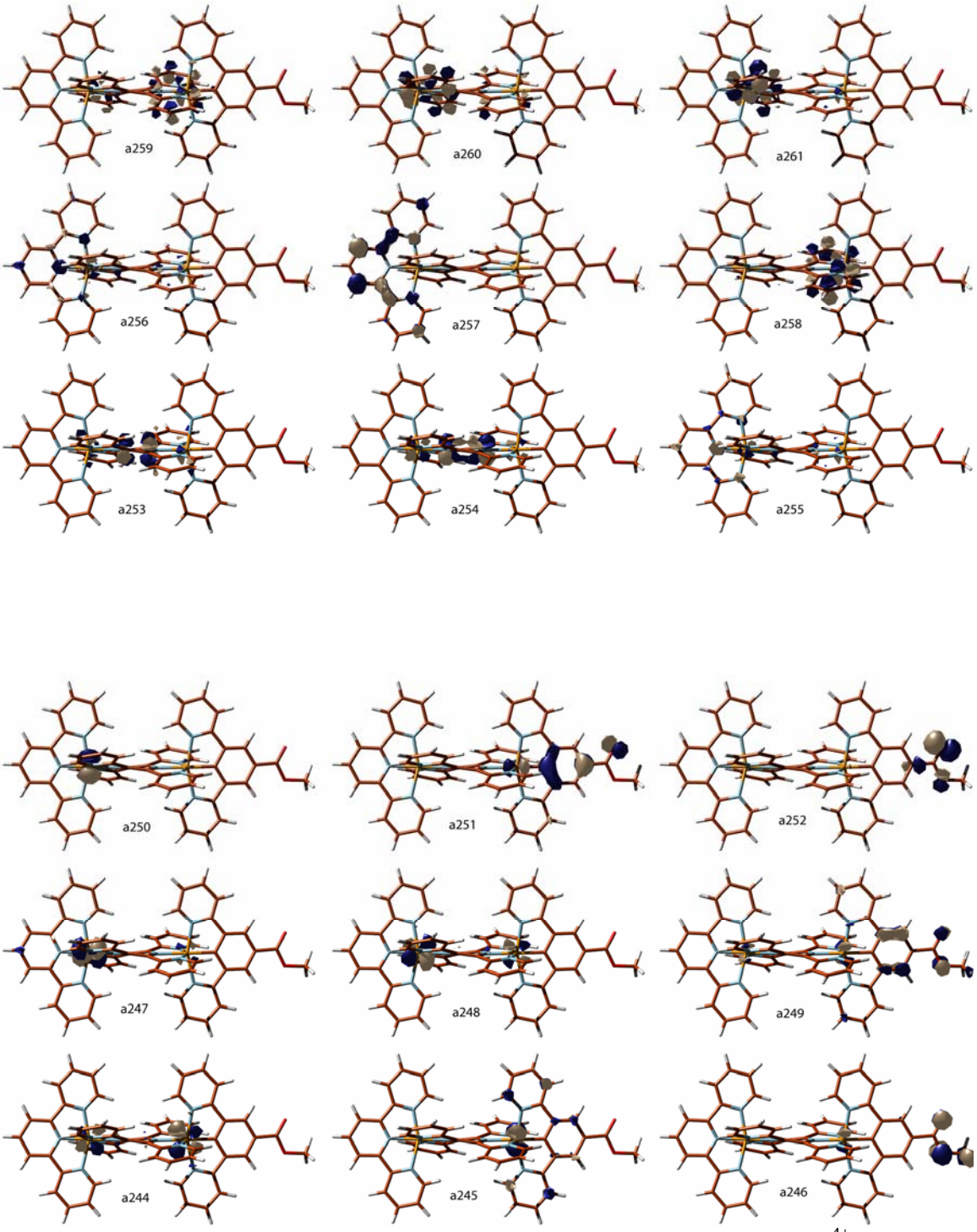

Figure S9.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**4b**]$^{4+}$.

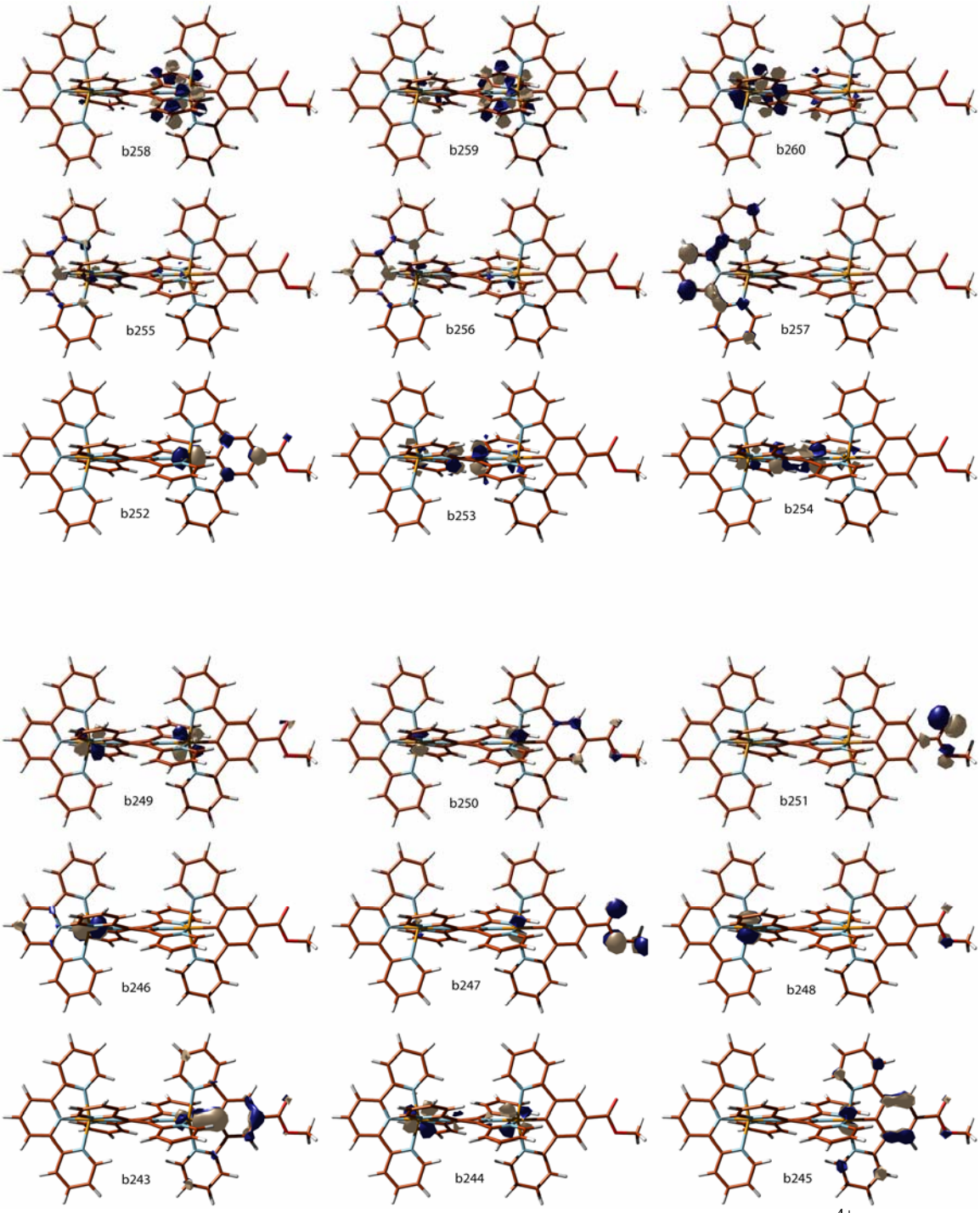

Figure S9.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**4b**]$^{4+}$.

Table S8.3 Complete listing of electronic transitions for [**4b**]$^{4+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	0.4408	2812.6	245B →252B (0.38691) 247B →252B (-0.45799) 248B →252B (-0.22354) 250B →252B (0.79687)	0.0001	16	1.8459	671.67	247A →254A (-0.11201) 248A →253A (0.75493) 248A →254A (0.13435) 250A →253A (0.10613) 243B →252B (0.11414) 244B →253B (-0.10022) 245B →254B (-0.10844) 246B →252B (-0.17085) 247B →254B (0.13383) 248B →253B (0.25760) 248B →254B (0.10217) 249B →253B (0.30273) 250B →254B (-0.23735) 251B →253B (-0.10472)	0.0114
2	0.5255	2359.49	244B →252B (-0.45446) 246B →252B (0.15057) 249B →252B (0.86009) 251B →252B (-0.18900)	0.0004	17	1.87	663.03	247A →253A (-0.19466) 247A →254A (0.37950) 248A →253A (0.15573) 248A →254A (-0.16019) 250A →253A (0.17730) 251A →253A (-0.12486) 246B →252B (0.71670) 246B →253B (0.27278) 248B →253B (0.21660) 249B →252B (-0.14460)	0.002
3	1.2053	1028.68	249B →252B (0.18102) 251B →252B (0.97498) 251B →273B (-0.10213)	0.0013	18	1.8873	656.92	245A →254A (0.11884) 247A →253A (0.20798) 248A →253A (-0.25737) 249A →254A (0.10178) 250A →254A (0.18581) 251A →253A (0.28533) 252A →253A (0.18480) 245B →254B (-0.24581) 246B →252B (0.12188) 246B →253B (-0.11384) 247B →254B (0.38112) 248B →254B (0.52293) 250B →254B (-0.32456) 250B →255B (0.11299) 250B →256B (-0.10662)	0.0007
4	1.3711	904.29	242A →253A (-0.14211) 244A →254A (0.10100) 247A →254A (-0.33468) 248A →254A (-0.68873) 241B →253B (0.14297) 244B →254B (0.24181) 244B →255B (0.10319) 249B →254B (0.75727) 250B →254B (-0.15928) 251B →254B (-0.13864)	0.0003	19	1.8914	655.52	247A →253A (0.25407) 251A →253A (0.73319) 252A →253A (0.35004) 245B →254B (0.12041) 246B →252B (0.13580) 246B →253B (-0.14885) 247B →254B (-0.19120) 248B →254B (-0.27765) 250B →254B (0.14377)	0.001
5	1.4045	882.76	245B →252B (0.64460) 247B →252B (-0.37297) 248B →252B (0.49074) 249B →252B (-0.16204) 250B →252B (-0.40071)	0.0127	20	1.9111	648.76	247A →253A (-0.53512) 247A →254A (-0.16695) 251A →253A (0.34432) 252A →253A (0.23468) 246B →252B (-0.15145) 246B →253B (0.64898) 246B →254B (-0.10958) 249B →253B (-0.11038)	0.0007
6	1.5759	786.76	248A →253A (-0.19596) 249A →254A (-0.10718) 250A →253A (0.11482) 250A →254A (0.61005) 250A →255A (0.11045) 247B →252B (-0.11117) 248B →252B (-0.27406) 248B →254B (-0.45541) 249B →253B (0.28708) 250B →252B (-0.17678)	0.0001	21	1.9587	632.99	247A →253A (0.56439) 247A →254A (-0.26326) 248A →254A (0.14060) 246B →252B (0.24640) 246B →253B (0.42266) 246B →254B (-0.49970)	0.0014

			250B →253B (-0.15176) 250B →254B (-0.39037)						
7	1.611	769.59	242A →253A (0.11859) 250A →253A (0.64361) 250A →254A (-0.15531) 241B →253B (-0.11415) 248B →253B (-0.44037) 248B →254B (0.10318) 250B →253B (-0.58543)	0.0002	22	1.9744	627.95	247A →253A (0.42085) 247A →254A (0.25762) 248A →254A (-0.12970) 246B →252B (-0.33343) 246B →253B (0.51258) 246B →254B (0.51773) 249B →252B (0.10738)	0.0011
8	1.6318	759.8	245B →252B (0.59515) 247B →252B (0.77318) 250B →252B (0.10724)	0.0088	23	2.0131	615.88	244A →254A (-0.17611) 245A →253A (0.22454) 246A →253A (-0.27974) 249A →253A (0.51173) 251A →254A (0.34579) 252A →254A (0.17526) 244B →252B (-0.21091) 244B →254B (-0.39057) 247B →253B (-0.10984) 248B →253B (-0.28311) 249B →254B (0.23642) 249B →255B (-0.12201) 250B →253B (0.13601)	0.0085
9	1.6638	745.17	247A →253A (-0.15435) 248A →253A (-0.36324) 250A →254A (-0.10526) 245B →252B (-0.11293) 248B →252B (0.27489) 248B →253B (0.14638) 248B →254B (0.14355) 249B →253B (0.77787) 250B →252B (0.13924) 250B →253B (-0.11356) 250B →254B (0.10049) 251B →253B (-0.17733)	0.0015	24	2.0384	608.23	245A →253A (-0.12757) 246A →253A (0.16151) 247A →254A (-0.12385) 249A →253A (-0.30344) 251A →254A (0.75897) 252A →254A (0.38509) 244B →252B (-0.13026) 244B →254B (0.13595) 248B →253B (0.12022)	0.0024
10	1.7009	728.95	250A →253A (0.10175) 250A →254A (0.49386) 245B →252B (-0.17797) 247B →252B (0.16505) 248B →252B (0.67304) 249B →253B (-0.18937) 250B →252B (0.37885)	0.0009	25	2.0567	602.83	249B →253B (0.21379) 251B →253B (0.96098)	0.0002
11	1.7634	703.11	247A →254A (0.58931) 247A →256A (-0.10501) 248A →254A (-0.34175) 250A →253A (-0.13675) 246B →252B (-0.33575) 246B →254B (-0.57932) 246B →255B (-0.10316) 250B →253B (-0.16079)	0.0002	26	2.0787	596.44	244A →254A (0.19027) 246A →253A (-0.11358) 249A →253A (0.23992) 251A →254A (0.24173) 243B →252B (-0.10778) 244B →252B (0.75638) 244B →254B (0.13930) 246B →252B (0.16833) 249B →252B (0.34741) 249B →254B (-0.12061)	0.0003
12	1.7794	696.78	247A →254A (0.15368) 248A →253A (-0.15806) 248A →254A (0.11312) 250A →253A (0.46990) 250A →254A (-0.31770) 246B →252B (-0.13122) 246B →254B (-0.19172) 247B →253B (-0.13423) 248B →252B (0.17432) 248B →254B (-0.23398) 250B →253B (0.43187) 250B →254B (-0.40880)	0.0094	27	2.0912	592.9	251A →253A (-0.46302) 252A →253A (0.86797)	0.0001
13	1.7922	691.78	248A →254A (0.12326) 249A →253A (-0.14876) 249A →254A (-0.11119) 250A →253A (0.30641) 250A →254A (0.33982) 243B →252B (0.13207) 245B →253B (0.13902) 247B →253B (-0.21432)	0.0148	28	2.1325	581.39	244A →254A (-0.32895) 245A →254A (0.28662) 246A →254A (-0.32483) 249A →253A (-0.24613) 249A →254A (0.52114) 250A →254A (0.10051) 244B →252B (0.26689) 244B →253B (-0.10127)	0.0092

			248B →252B (-0.19742) 248B →253B (-0.13006) 248B →254B (0.28085) 249B →253B (0.13162) 249B →254B (0.10040) 250B →253B (0.42266) 250B →254B (0.46124)					244B →254B (-0.36802) 249B →252B (0.14276) 249B →254B (0.13464) 249B →255B (-0.10142) 250B →254B (0.10376)	
14	1.8338	676.12	248A →254A (-0.14044) 249A →253A (0.14304) 243B →252B (0.92860) 244B →252B (0.10127) 249B →254B (-0.14997)	0.1336	29	2.1373	580.09	244A →254A (0.38382) 245A →254A (0.26935) 246A →253A (-0.11280) 246A →254A (-0.27151) 249A →253A (0.31903) 249A →254A (0.46341) 250A →254A (0.10181) 244B →252B (-0.20477) 244B →253B (-0.19715) 244B →254B (0.38976) 248B →254B (-0.10289) 249B →252B (-0.10530) 249B →254B (-0.10220) 249B →255B (0.10850) 250B →253B (0.11664) 250B →254B (0.12759) 251B →254B (0.12449)	0.0137
15	1.8385	674.37	244A →254A (-0.14198) 245A →253A (0.16339) 246A →253A (-0.12669) 247A →254A (-0.13665) 248A →253A (-0.23861) 248A →254A (0.17077) 249A →253A (0.21000) 250A →253A (0.29182) 245B →253B (-0.16950) 246B →252B (-0.16107) 247B →253B (0.32186) 248B →253B (0.60179) 249B →253B (-0.22086) 249B →254B (0.21939) 250B →254B (0.17614)	0.0023	30	2.2373	554.18	242A →253A (0.10354) 245A →253A (0.11698) 249A →253A (-0.20437) 245B →253B (-0.52042) 247B →253B (0.59975) 248B →253B (-0.33499) 249B →253B (0.13599) 250B →253B (0.35408)	0.0011

Table S9.1. Optimized geometry for [**5a**]$^{3+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	2.545703	-0.05139	0.002373	H	9.389893	0.033615	5.094954	N	-7.3043	-3.89696	-0.04327
C	1.325147	0.095219	2.331147	N	-5.68099	-0.23392	3.846908	H	-12.6424	-7.46758	0.134141
C	-1.32832	-0.19859	2.328989	C	-7.46766	-0.4283	5.680754	H	-9.44531	-10.9236	0.152472
N	-2.54584	-0.05222	-0.00109	C	-6.87806	-1.14474	8.157982	H	-4.8172	-9.80173	0.024205
C	-1.32544	0.097731	-2.32981	C	-4.36993	-1.79984	8.727093	H	-3.59997	-5.25252	-0.10588
C	1.328316	-0.19495	-2.32808	C	-2.50836	-1.55055	6.849513	H	-9.39015	-0.04683	5.097806
C	3.143809	0.541269	4.442495	H	-8.36095	-1.24114	9.569514	C	10.15561	0.043125	-0.00115
C	-3.15146	-0.63066	4.439332	H	-3.86061	-2.48055	10.5927	C	11.5123	-2.25215	-0.01557
C	-3.14499	0.545245	-4.44024	H	-0.57853	-2.09775	7.251233	C	14.18261	-2.21704	-0.02305
C	3.152138	-0.62427	-4.43861	Ru	-6.37676	-0.01304	0.001135	C	15.46106	0.120252	-0.00954
N	5.681739	-0.23057	-3.84439	Ru	6.376724	-0.01308	0.001443	C	14.11531	2.419346	0.008215
C	7.469414	-0.42447	-5.67732	C	-10.1554	0.044733	0.001611	C	11.44512	2.376753	0.009198
C	6.880835	-1.13668	-8.15595	C	-11.513	-2.25003	0.012463	C	9.860083	-4.477	-0.01877
C	4.372251	-1.7875	-8.72775	C	-14.1833	-2.2138	0.01553	H	15.28124	-3.95353	-0.03519
C	2.509783	-1.53922	-6.8509	C	-15.4607	0.124047	0.000263	H	17.51275	0.15008	-0.01353
H	9.391892	-0.04606	-5.09243	C	-14.1141	2.422646	-0.01483	H	15.16347	4.186914	0.015831
H	8.364725	-1.23305	-9.56645	C	-11.4439	2.378932	-0.01088	C	9.729982	4.553057	0.014384
H	3.863293	-2.46428	-10.5949	C	-9.86172	-4.47555	0.014834	N	7.190643	3.899842	-0.0397
H	0.57973	-2.0838	-7.25487	H	-15.2827	-3.94978	0.024749	C	5.402553	5.755441	-0.03782
C	-2.49391	1.447994	-6.85488	H	-17.5123	0.154702	0.000103	C	6.015953	8.316328	0.03619
C	-4.35409	1.71109	-8.73178	H	-15.1616	4.190606	-0.02489	C	8.585829	9.0099	0.098909
C	-6.86883	1.085519	-8.15889	C	-9.72792	4.554595	-0.01375	C	10.43663	7.11896	0.083018
C	-7.46483	0.38855	-5.67778	N	-7.18893	3.900384	0.044527	H	3.44951	5.146604	-0.09565
N	-5.6791	0.183349	-3.84427	C	-5.40012	5.755296	0.045885	H	4.532747	9.730598	0.035543
H	-0.55895	1.972873	-7.26013	C	-6.0124	8.316405	-0.02979	H	9.126534	10.98689	0.155065
H	-3.83852	2.379905	-10.5999	C	-8.58189	9.010949	-0.09785	H	12.42187	7.626613	0.130537
H	-8.35116	1.190716	-9.57039	C	-10.4335	7.12074	-0.08467	C	10.64036	-7.02117	-0.09255
H	-9.39111	0.033458	-5.09056	H	-3.44744	5.145643	0.107599	C	8.844208	-8.96418	-0.10713
C	2.490865	1.441242	6.857646	H	-4.52868	9.730119	-0.02647	C	6.255513	-8.34499	-0.03695
C	4.350001	1.704607	8.735467	H	-9.12178	10.98809	-0.15602	C	5.568104	-5.80319	0.042528
C	6.865536	1.082009	8.162821	H	-12.4184	7.629105	-0.13625	N	7.30291	-3.89754	0.042267
C	7.463107	0.387006	5.68149	C	-10.643	-7.01955	0.083641	H	12.63959	-7.46987	-0.14543
N	5.678306	0.181326	3.847088	C	-8.84753	-8.96323	0.095642	H	9.441183	-10.9246	-0.16835
H	0.555221	1.96371	7.262625	C	-6.25855	-8.34488	0.028356	H	4.813582	-9.80128	-0.03483
H	3.833004	2.371369	10.60397	C	-5.57013	-5.80319	-0.04566	H	3.598171	-5.25195	0.105262
H	8.347163	1.187847	9.574976								

Table S9.2.1. Orbital energies and Mulliken population on Ru of alpha orbitals for [**5a**]$^{3+}$.

#	E (eV)	Ru1	p	d	Ru2	p	d
H-12	-14.2276	0.07504	-0.00631	0.065985	0.075653	-0.00632	0.066514
H-11	-14.1669	0.084412	0.01309	0.060651	0.08371	0.013001	0.06014
H-10	-13.8466	0.01547	0.000497	0.014775	0.015471	0.000497	0.014775
H-9	-13.7952	0.236421	0.006035	0.230385	0.237642	0.00605	0.231591
H-8	-13.7719	0.212265	0.002607	0.209658	0.211084	0.002586	0.208498
H-7	-13.697	0.242844	0.004762	0.238082	0.242937	0.004765	0.238172
H-6	-13.1955	0.332901	0.005234	0.327667	0.332721	0.005231	0.327491
H-5	-13.1372	0.246944	1.27E-05	0.246885	0.24779	1.27E-05	0.24773
H-4	-13.0435	0.210722	1.95E-05	0.210753	0.210027	1.98E-05	0.210058
H-3	-12.6244	0.085022	-1.6E-05	0.085031	0.085535	-1.6E-05	0.085544
H-2	-12.6005	0.116102	1.45E-05	0.116087	0.115445	1.44E-05	0.11543
H-1	-12.3091	0.139475	-1.4E-05	0.139489	0.144456	-1.5E-05	0.144471
H	-12.2911	0.149504	4.24E-05	0.149461	0.144489	0.000042	0.144447
L	-10.0926	0.020236	0.001314	0.01904	0.020217	0.001311	0.019024
L+1	-9.9238	0.05704	-0.0001	0.05714	0.057038	-0.0001	0.057141
L+2	-9.017	0.012844	0.002842	0.010002	0.012839	0.00284	0.009999
L+3	-8.3114	0.022478	0.001601	0.019305	0.022144	0.001601	0.018984
L+4	-8.2646	0.006136	0.00353	0.002606	0.006036	0.003501	0.002535
L+5	-8.2531	0.025862	-0.00178	0.027811	0.026089	-0.00179	0.028048
L+6	-8.2431	0.009582	0.002766	0.006816	0.00964	0.002794	0.006846
L+7	-8.1979	0.008594	2.03E-05	0.008557	0.008786	2.54E-05	0.008742
L+8	-8.1911	0.005518	3.78E-05	0.005442	0.00531	3.53E-05	0.005242
L+9	-8.1643	0.020142	0.005637	0.014504	0.020361	0.00569	0.014671
L+10	-8.1434	0.016606	0.003635	0.01297	0.0164	0.003586	0.012812
L+11	-7.7196	0.009392	-0.00227	0.011333	0.009366	-0.00227	0.011317
L+12	-7.5861	0.00847	4.64E-05	0.008295	0.008464	4.73E-05	0.008285

Table S9.2.2. Orbital energies and Mulliken population on Ru of beta orbitals for [**5a**]$^{3+}$.

#	E (eV)	Ru1	p	d	Ru2	p	d
H-11	-14.2076	0.07459	-0.00734	0.066668	0.075277	-0.00737	0.067261
H-10	-14.1534	0.085281	0.011709	0.062612	0.084515	0.011628	0.062039
H-9	-13.8902	0.010289	0.000591	0.00942	0.010294	0.000592	0.009423
H-8	-13.6328	0.19461	0.003028	0.191582	0.194229	0.003021	0.191208
H-7	-13.6115	0.188698	0.003611	0.185087	0.189076	0.003617	0.185459
H-6	-12.9731	0.164712	7.9E-06	0.164679	0.165162	0.000008	0.165129
H-5	-12.9126	0.120589	0.000014	0.120632	0.12029	1.41E-05	0.120333
H-4	-12.5793	0.18648	0.006761	0.179719	0.18645	0.006753	0.179697
H-3	-12.5222	0.172871	-3E-05	0.172895	0.173561	-0.00003	0.173584
H-2	-12.4637	0.222114	3.35E-05	0.222134	0.221257	3.36E-05	0.221278
H-1	-12.1981	0.181477	0.000271	0.181205	0.182603	0.000269	0.182334
H	-12.1308	0.182069	0.000526	0.181544	0.180882	0.000525	0.180357
L	-10.6962	0.355994	0.006702	0.349293	0.356032	0.006703	0.34933
L+1	-10.0959	0.024959	0.00119	0.02389	0.024941	0.001187	0.023875
L+2	-9.4675	0.23161	0.000688	0.230923	0.231693	0.000689	0.231004
L+3	-8.9537	0.059154	0.000858	0.058296	0.059172	0.000856	0.058316
L+4	-8.3199	0.004607	0.003249	0.001334	0.004588	0.003238	0.001328
L+5	-8.3022	0.021005	0.001619	0.017861	0.020717	0.001621	0.017584
L+6	-8.2639	0.009076	0.002317	0.006757	0.009094	0.002318	0.006774
L+7	-8.2474	0.017429	-0.00152	0.019121	0.017568	-0.00152	0.01926
L+8	-8.1878	0.006766	0.000002	0.006778	0.008391	0.000012	0.008386
L+9	-8.1865	0.017742	-0.00015	0.017869	0.016134	-0.00016	0.016278
L+10	-8.1561	0.023453	0.005794	0.017659	0.023841	0.005879	0.017962
L+11	-8.1399	0.022198	0.004301	0.017896	0.021804	0.004218	0.017585
L+12	-7.7167	0.007971	-0.00228	0.009774	0.007951	-0.00228	0.009764
L+13	-7.5751	0.01075	5.57E-05	0.010531	0.010746	5.71E-05	0.010522

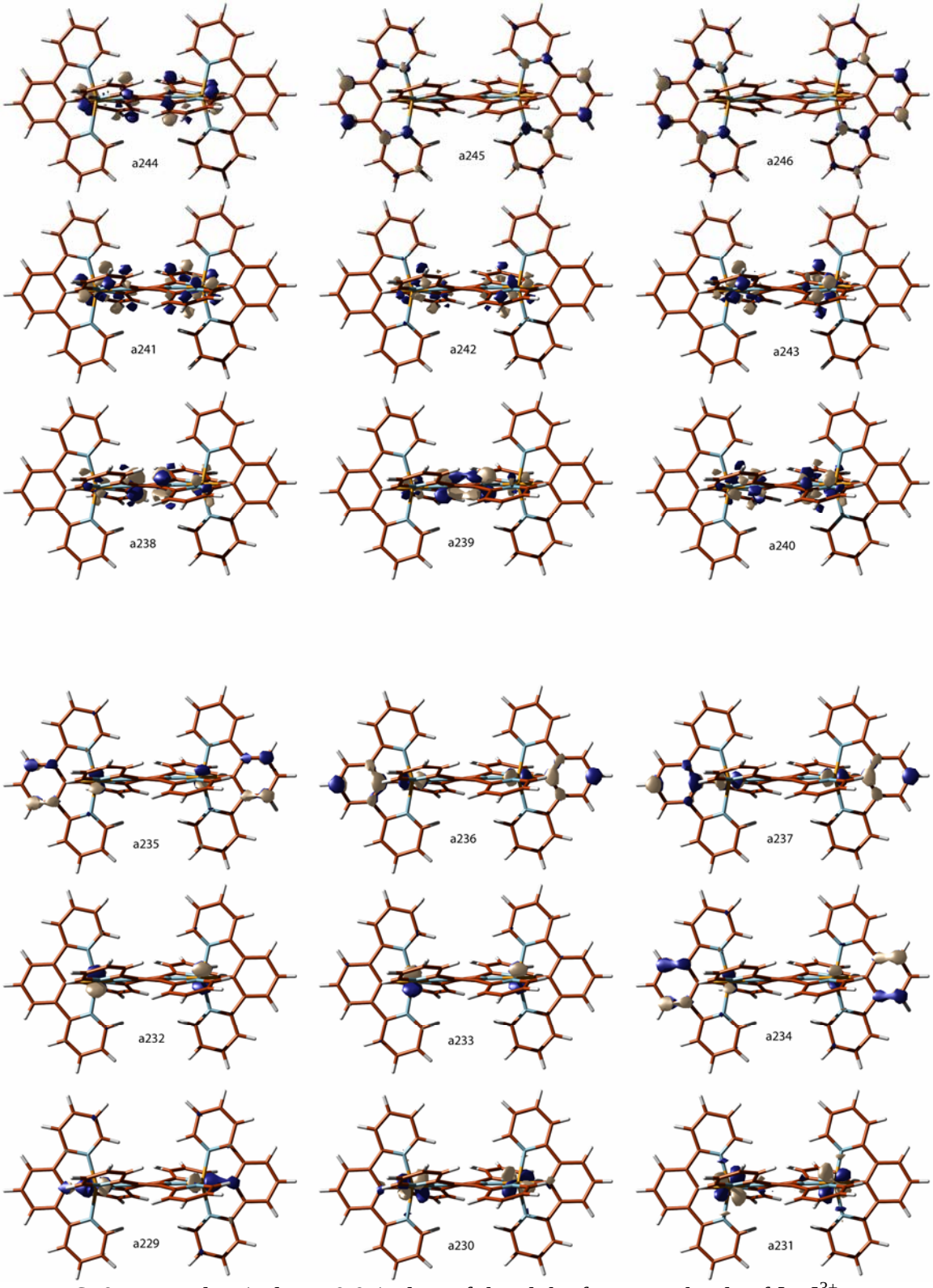

Figure S10.1. Isovalue (value = 0.05) plots of the alpha frontier orbitals of [**5a**]$^{3+}$.

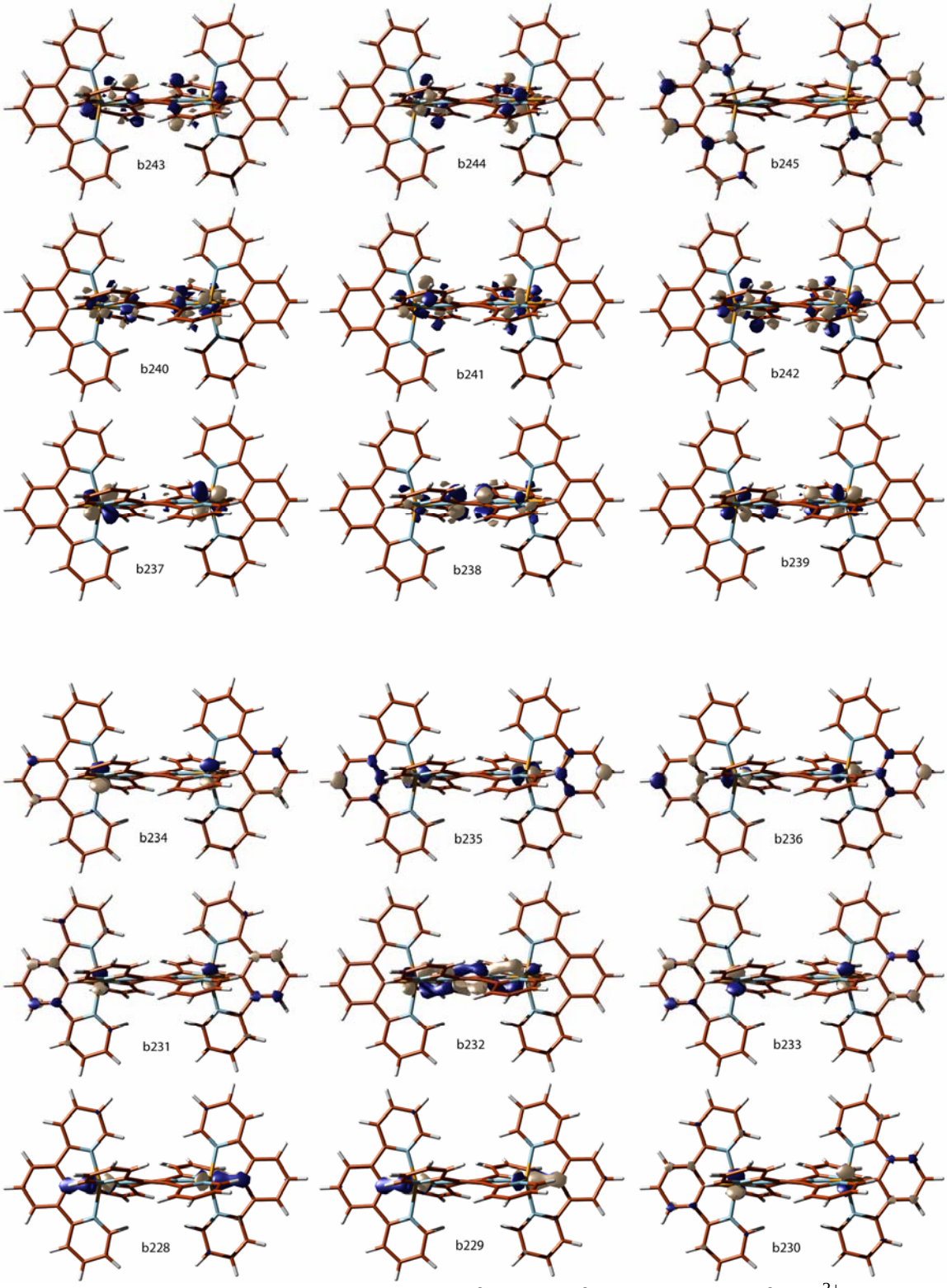

Figure S10.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**5a**]$^{3+}$.

Table S9.3 Complete listing of electronic transitions for [**5a**]$^{3+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	0.2638	4700.08	bH-8 →bL+2 (-0.14887) bH-7 →bL (0.27661) bH-4 →bL (-0.18239) bH-1 →bL+2 (0.31918) bH →bL (0.92232) bH →bL+3 (0.11688)	0.0033	16	1.7409	712.18	aH →aL+1 (0.48370) bH-8 →bL (-0.36122) bH-7 →bL+2 (0.15971) bH-6 →bL+1 (-0.10104) bH-4 →bL+2 (0.13280) bH-3 →bL+1 (-0.28616) bH-1 →bL (-0.33759) bH-1 →bL+3 (0.15865) bH →bL+2 (0.58192)	0.0000
2	0.2939	4218.72	bH-8 →bL (-0.27912) bH-7 →bL+2 (0.14660) bH-4 →bL+2 (-0.11579) bH-1 →bL (0.92852) bH-1 →bL+3 (0.12095) bH →bL+2 (0.30514)	0.0000	17	1.7864	694.03	aH-5 →aL (0.17391) aH-3 →aL (0.25462) bH-8 →bL (-0.13663) bH-6 →bL+1 (0.27003) bH-3 →bL+1 (0.86719) bH-1 →bL (-0.11560) bH →bL+2 (0.17740)	0.0000
3	0.393	3154.89	bH-6 →bL+2 (0.22000) bH-5 →bL (0.43050) bH-4 →bL+1 (0.12475) bH-3 →bL+2 (0.29159) bH-2 →bL (0.89063) bH-2 →bL+3 (0.12410)	0.0000	18	1.7877	693.55	aH-1 →aL+1 (0.43440) bH-8 →bL+2 (-0.20103) bH-7 →bL (0.48638) bH-4 →bL (0.15923) bH-1 →bL+2 (0.54761) bH →bL (-0.35175) bH →bL+3 (0.20606)	0.0031
4	0.5069	2445.79	bH-6 →bL (0.49333) bH-5 →bL+2 (0.18995) bH-3 →bL (0.80198) bH-3 →bL+3 (0.12189) bH-2 →bL+2 (0.34415)	0.0010	19	1.9471	636.77	aH-6 →aL+1 (0.11928) aH-5 →aL+2 (-0.10390) aH-4 →aL (-0.10425) aH-4 →aL+1 (0.40504) aH-3 →aL+2 (-0.11781) aH-2 →aL (-0.32856) aH-2 →aL+1 (0.77624) bH-6 →bL (0.12621) bH-2 →bL+1 (0.14836) bH-2 →bL+2 (-0.15320)	0.0058
5	1.0684	1160.47	aH-10 →aL (-0.10008) aH-6 →aL+1 (0.34236) aH-4 →aL (0.16431) aH-2 →aL (0.14371) bH-4 →bL (0.96205) bH-2 →bL+1 (-0.17834) bH →bL (0.22737)	0.1451	20	1.9492	636.08	aH-6 →aL+1 (-0.27935) aH-4 →aL (0.23469) aH-4 →aL+1 (0.17531) aH-2 →aL (0.74569) aH-2 →aL+1 (0.34183) bH-9 →bL+1 (-0.11403) bH-2 →bL+1 (-0.33864)	0.0307
6	1.3684	906.07	bH-4 →bL+1 (0.36048) bH →bL+1 (0.93014)	0.0000	21	1.9564	633.74	aH-9 →aL+1 (0.10524) aH-7 →aL+1 (-0.11215) aH-5 →aL (0.27525) aH-3 →aL (0.74189) bH-8 →bL (0.21945) bH-4 →bL+2 (0.51291) bH-3 →bL+1 (-0.19590) bH-1 →bL (0.10673)	0.0000
7	1.4862	834.22	bH-1 →bL+1 (0.98491)	0.0003	22	2.0265	611.82	aH-5 →aL+1 (0.40088) aH-4 →aL+2 (-0.10971) aH-3 →aL+1 (0.82835) aH-2 →aL+2 (-0.15783) bH-6 →bL+2 (-0.11418) bH-5 →bL (0.12379) bH-3 →bL+2 (-0.23154) bH-2 →bL+3 (-0.13305)	0.0001
8	1.5431	803.47	bH-6 →bL+2 (0.15574) bH-5 →bL (0.85711) bH-4 →bL+1 (0.14990) bH-2 →bL (-0.45835)	0.0006	23	2.0775	596.81	aH-9 →aL+1 (0.17736) aH-7 →aL+1 (-0.19374) aH-3 →aL (-0.48766) bH-8 →bL (0.52857) bH-7 →bL+2 (-0.10362) bH-4 →bL+2 (0.43893) bH-3 →bL+1 (0.16160) bH →bL+2 (0.42679)	0.0000
9	1.5475	801.19	bH-6 →bL (0.78615) bH-5 →bL+2 (0.17255) bH-3 →bL (-0.57502)	0.0000	24	2.1231	583.98	aH-6 →aL+1 (0.10960) bH-7 →bL (0.73649) bH-1 →bL+2 (-0.62615)	0.0051

								bH →bL+3 (-0.16824)	
10	1.5995	775.16	aH-7 →aL (0.10858) aH →aL (-0.58922) bH-4 →bL+1 (0.74614) bH →bL+1 (-0.25288)	0.0002	25	2.1592	574.23	aH-6 →aL (-0.14370) aH-2 →aL+1 (0.23646) bH-6 →bL (-0.32247) bH-6 →bL+3 (0.11830) bH-5 →bL+2 (0.23246) bH-3 →bL (-0.23315) bH-3 →bL+3 (0.23027) bH-2 →bL+2 (0.79307)	0.0041
11	1.6256	762.7	aH →aL (0.79560) bH-4 →bL+1 (0.53571) bH →bL+1 (-0.22817)	0.0004	26	2.1654	572.57	aH-9 →aL+1 (0.18133) aH-7 →aL+1 (-0.18156) aH-3 →aL (-0.25859) bH-8 →bL (-0.54842) bH-4 →bL+2 (0.60860) bH-1 →bL+3 (-0.19454) bH →bL+2 (-0.37880)	0.0000
12	1.6392	756.37	aH-1 →aL (0.98389)	0.0001	27	2.1848	567.5	aH-3 →aL+1 (0.33415) bH-9 →bL (0.26479) bH-6 →bL+2 (0.28824) bH-5 →bL (-0.22233) bH-5 →bL+3 (0.11746) bH-3 →bL+2 (0.69610) bH-2 →bL (-0.24575) bH-2 →bL+3 (0.29858)	0.0007
13	1.6501	751.37	aH-9 →aL+1 (-0.10054) aH-1 →aL+2 (-0.13897) aH →aL+1 (0.83853) bH-8 →bL (0.25937) bH-7 →bL+2 (-0.12656) bH-1 →bL (0.24607) bH-1 →bL+3 (-0.11336) bH →bL+2 (-0.33256)	0.0000	28	2.2486	551.39	aH-10 →aL (-0.27554) aH-6 →aL+1 (-0.18936) aH-4 →aL (0.54572) aH-2 →aL (-0.40179) bH-9 →bL+1 (-0.23893) bH-5 →bL+1 (0.56744) bH-2 →bL+1 (-0.20701)	0.0060
14	1.6678	743.41	aH-10 →aL (-0.12308) aH-4 →aL (0.26348) aH-2 →aL (0.33721) bH-5 →bL+1 (0.26253) bH-2 →bL+1 (0.86109)	0.0156	29	2.3103	536.66	aH-10 →aL (0.15019) aH-6 →aL+1 (0.45652) aH-4 →aL (-0.38216) aH-2 →aL (0.17551) bH-9 →bL+1 (0.14332) bH-5 →bL+1 (0.72424) bH-4 →bL+3 (0.10919) bH-2 →bL+1 (-0.18111)	0.0042
15	1.6757	739.89	aH-8 →aL+1 (-0.13238) aH-1 →aL+1 (0.86799) aH →aL+2 (-0.14993) bH-8 →bL+2 (0.11804) bH-7 →bL (-0.24952) bH-1 →bL+2 (-0.26080) bH →bL (0.19342) bH →bL+3 (-0.10770)	0.0000	30	2.3202	534.37	aH-5 →aL (0.26318) aH-3 →aL (-0.16759) bH-6 →bL+1 (0.89650) bH-3 →bL+1 (-0.29170)	0.0000

Table S10.1. Optimized geometry for [**5b**]$^{3+}$.

atom	X	Y	Z	atom	X	Y	Z	atom	X	Y	Z
N	7.367806	-3.86609	-0.08946	C	-10.7635	-6.92532	0.16804	H	9.560639	0.472023	4.717619
C	9.933456	-4.39822	-0.13415	C	-9.00485	-8.901	0.164319	H	-8.05833	-1.88546	9.727322
C	10.76162	-6.9252	-0.17557	C	-6.4052	-8.33065	0.109486	H	-3.48167	-2.90804	10.61893
C	9.002523	-8.90046	-0.17243	C	-5.66987	-5.80283	0.066748	H	-0.28769	-2.21145	7.242044
C	6.403048	-8.32954	-0.11531	C	-3.27636	0.597954	-4.32083	H	-15.3667	-3.7382	-0.08651
C	5.66839	-5.80159	-0.06973	C	-2.67237	1.525677	-6.73981	C	-18.2357	0.569756	-0.11166
C	11.54267	-2.14537	-0.17387	C	-4.59288	1.994927	-8.51361	H	-15.0862	4.33443	0.308175
C	10.13428	0.115036	-0.28833	C	-7.11853	1.535347	-7.84108	H	-3.33976	5.094498	0.384771
C	11.37434	2.47347	-0.35173	C	-7.64476	0.745722	-5.37387	H	-4.34898	9.698656	0.336668
C	14.0263	2.575537	-0.27348	N	-5.7988	0.342319	-3.63497	H	-8.91858	11.03293	0.404787
C	15.42501	0.311398	-0.10043	C	2.988685	-0.76262	-4.53183	H	-12.2691	7.722278	0.46622
C	14.20313	-2.05624	-0.06634	N	5.542549	-0.41467	-4.02434	H	-12.7705	-7.33294	0.218946
Ru	6.36162	-0.0106	-0.21876	C	7.276967	-0.77813	-5.88289	H	-9.63587	-10.8512	0.2034
N	7.099794	3.915314	-0.40794	C	6.607351	-1.60929	-8.30179	H	-4.9904	-9.81275	0.095917
C	9.623845	4.613349	-0.41891	C	4.057387	-2.15519	-8.79544	H	-3.69134	-5.28458	0.021143
C	10.29358	7.186866	-0.43327	C	2.249226	-1.73388	-6.89545	H	-9.2249	-0.45001	5.362439
C	8.414351	9.047167	-0.39517	C	-11.5434	-2.14534	0.170368	H	15.36578	-3.73968	0.076487
C	5.856497	8.310752	-0.3601	C	-10.1345	0.114585	0.288948	C	18.23639	0.567343	0.102555
C	5.282481	5.740935	-0.38665	C	-11.3738	2.473329	0.353886	H	15.08741	4.333517	-0.30795
N	2.541904	-0.10478	-0.08297	C	-14.0256	2.576191	0.272872	H	3.340887	5.096538	-0.37459
C	1.402138	0.053562	2.285801	C	-15.4247	0.312671	0.095256	H	4.351277	9.700413	-0.32218
C	-1.24657	-0.26813	2.37222	C	-14.2037	-2.05535	0.059889	H	8.921075	11.03364	-0.39131
N	-2.5422	-0.10554	0.08582	C	-9.62278	4.612688	0.424843	H	12.27086	7.722406	-0.45829
C	-1.40238	0.055842	-2.28272	N	-7.09893	3.914022	0.41469	H	12.76847	-7.33328	-0.22818
C	1.246271	-0.26514	-2.36951	C	-5.28121	5.739286	0.396415	H	9.633031	-10.8508	-0.21366
C	3.276408	0.59327	4.324384	C	-5.85457	8.309285	0.372274	H	4.987885	-9.81129	-0.10212
C	2.672912	1.517526	6.744813	C	-8.41227	9.046321	0.406741	H	3.690002	-5.28292	-0.02236
C	4.593796	1.984452	8.518857	C	-10.2919	7.186335	0.44172	O	-19.34	2.630041	0.111749
C	7.119367	1.526139	7.84514	H	9.223982	-0.43938	-5.36189	O	-19.3984	-1.67967	-0.62903
C	7.645092	0.740019	5.376717	H	8.056817	-1.8691	-9.7285	C	-22.1897	-1.68887	-0.96797
N	5.798787	0.338836	3.637674	H	3.480599	-2.894	-10.6198	H	-22.5606	-2.86039	-2.62301
C	-2.98912	-0.76857	4.533773	H	0.287225	-2.20385	-7.24092	H	-23.0228	-2.52002	0.726966
N	-5.54307	-0.42116	4.026079	H	-0.72573	1.926641	-7.2254	H	-22.8648	0.240831	-1.24129
C	-7.27784	-0.7883	5.883552	H	-4.12044	2.704202	-10.3788	O	19.3407	2.627856	-0.11889
C	-6.60853	-1.62248	8.301512	H	-8.65603	1.832812	-9.16449	O	19.39946	-1.68332	0.61352
C	-4.05835	-2.16719	8.795328	H	-9.56042	0.476664	-4.71555	C	22.19145	-1.69384	0.947241
C	-2.24984	-1.74223	6.896452	H	0.726353	1.917671	7.231436	H	22.56504	-2.86628	2.601013
Ru	-6.36185	-0.01196	0.22102	H	4.12173	2.69104	10.38519	H	23.02087	-2.52458	-0.74969
N	-7.36886	-3.86697	0.087146	H	8.657162	1.821944	9.168585	H	22.86791	0.235451	1.220197
C	-9.93466	-4.39852	0.129559								

Table S10.2.1. Orbital energies and Mulliken population on Ru of alpha orbitals for [**5b**]$^{3+}$.

#	E (eV)	Ru1	p	d	Ru2	p	d
H-12	-13.8112	0.219162	0.002705	0.21636	0.217023	0.002673	0.214251
H-11	-13.7246	0.242375	0.004928	0.237429	0.242466	0.004928	0.237519
H-10	-13.2269	0.327684	0.005344	0.322343	0.327802	0.005345	0.322461
H-9	-13.1911	0.209439	-9.1E-06	0.209366	0.209633	-9.6E-06	0.20956
H-8	-13.1239	0.099601	5.16E-05	0.099472	0.099043	5.23E-05	0.098913
H-7	-13.0635	0.041348	5.19E-05	0.041319	0.042349	5.27E-05	0.042321
H-6	-13.0363	0.117798	2.76E-05	0.117883	0.116999	2.75E-05	0.117083
H-5	-12.6716	0.003705	-9E-07	0.003704	0.007018	-1.5E-05	0.007019
H-4	-12.6715	0.00553	-4.1E-05	0.005544	0.002303	-2.7E-05	0.002315
H-3	-12.6657	0.078493	-1.7E-05	0.078487	0.08015	-1.7E-05	0.080143
H-2	-12.6438	0.111847	1.56E-05	0.111811	0.110261	1.56E-05	0.110225
H-1	-12.3575	0.13265	-2E-07	0.132657	0.130845	-2E-07	0.130852
H	-12.34	0.136222	4.14E-05	0.136182	0.137951	4.19E-05	0.137911
L	-10.1184	0.019761	0.001248	0.018664	0.019754	0.001244	0.018661
L+1	-9.9514	0.057339	-0.00038	0.057721	0.057349	-0.00038	0.057734
L+2	-9.0454	0.013054	0.002866	0.010189	0.013057	0.002868	0.010191
L+3	-8.3277	0.021816	0.002127	0.018165	0.021781	0.002126	0.018137
L+4	-8.2927	0.006828	0.003743	0.003082	0.006857	0.003753	0.003102
L+5	-8.2643	0.014257	0.001772	0.012571	0.014185	0.001769	0.012499
L+6	-8.264	0.02074	-0.00029	0.0211	0.020808	-0.00029	0.021171
L+7	-8.2103	0.008477	0.00032	0.008147	0.008501	0.00032	0.00817
L+8	-8.2036	0.005994	0.000141	0.00583	0.005966	0.000137	0.005809
L+9	-8.1915	0.020349	0.005159	0.015209	0.020311	0.005151	0.01518
L+10	-8.1703	0.017251	0.003542	0.013707	0.01729	0.003552	0.013736
L+11	-7.7313	0.008046	-0.00222	0.010412	0.008031	-0.00222	0.0104
L+12	-7.5964	0.008476	5.02E-05	0.00823	0.008485	0.00005	0.00824

Table S10.2.2. Orbital energies and Mulliken population on Ru of beta orbitals for [**5b**]$^{3+}$.

#	E (eV)	Ru1	p	d	Ru2	p	d
H-11	-13.6442	0.194424	0.003702	0.190685	0.193814	0.003691	0.190084
H-10	-13.1046	0.032524	8.2E-06	0.032454	0.03323	8.9E-06	0.033157
H-9	-13.0953	0.012262	3.87E-05	0.012166	0.01148	3.84E-05	0.011386
H-8	-12.984	0.136375	5.55E-05	0.136345	0.13702	5.56E-05	0.13699
H-7	-12.9324	0.112165	1.22E-05	0.112253	0.111501	1.23E-05	0.111589
H-6	-12.6805	0.038679	0.001568	0.037093	0.038879	0.00157	0.037291
H-5	-12.6702	0.003055	3.19E-05	0.003	0.003024	2.94E-05	0.002972
H-4	-12.6183	0.144929	0.004306	0.14062	0.145543	0.004309	0.141231
H-3	-12.562	0.17246	0.00053	0.171922	0.172431	0.000528	0.171895
H-2	-12.512	0.219268	3.01E-05	0.219278	0.218789	2.93E-05	0.218799
H-1	-12.2542	0.172002	0.000246	0.171759	0.171238	0.000245	0.170996
H	-12.1792	0.176288	0.00069	0.175596	0.176903	0.000689	0.176212
L	-10.7441	0.356266	0.006748	0.349522	0.356267	0.006748	0.349523
L+1	-10.1216	0.024444	0.001123	0.023478	0.024437	0.00112	0.023475
L+2	-9.4996	0.229135	0.000655	0.228484	0.229118	0.000655	0.228468
L+3	-8.9827	0.0585	0.000893	0.057609	0.058481	0.000894	0.057588
L+4	-8.3447	0.004896	0.003421	0.001451	0.004902	0.003424	0.001453
L+5	-8.319	0.020613	0.002142	0.017002	0.020589	0.00214	0.01699
L+6	-8.2838	0.009812	0.002139	0.007662	0.009809	0.002137	0.007659
L+7	-8.2587	0.01749	-0.00099	0.018633	0.0175	-0.00099	0.01864
L+8	-8.2004	0.015868	0.000201	0.015667	0.015763	0.000198	0.015565
L+9	-8.1999	0.008105	0.000125	0.008007	0.008216	0.000126	0.008118
L+10	-8.183	0.024127	0.005412	0.018743	0.024093	0.005405	0.018716
L+11	-8.1674	0.022684	0.004147	0.018534	0.022719	0.004155	0.018561
L+12	-7.7287	0.007294	-0.00218	0.009532	0.00729	-0.00218	0.009531
L+13	-7.5858	0.010613	5.42E-05	0.010325	0.01062	5.33E-05	0.010333

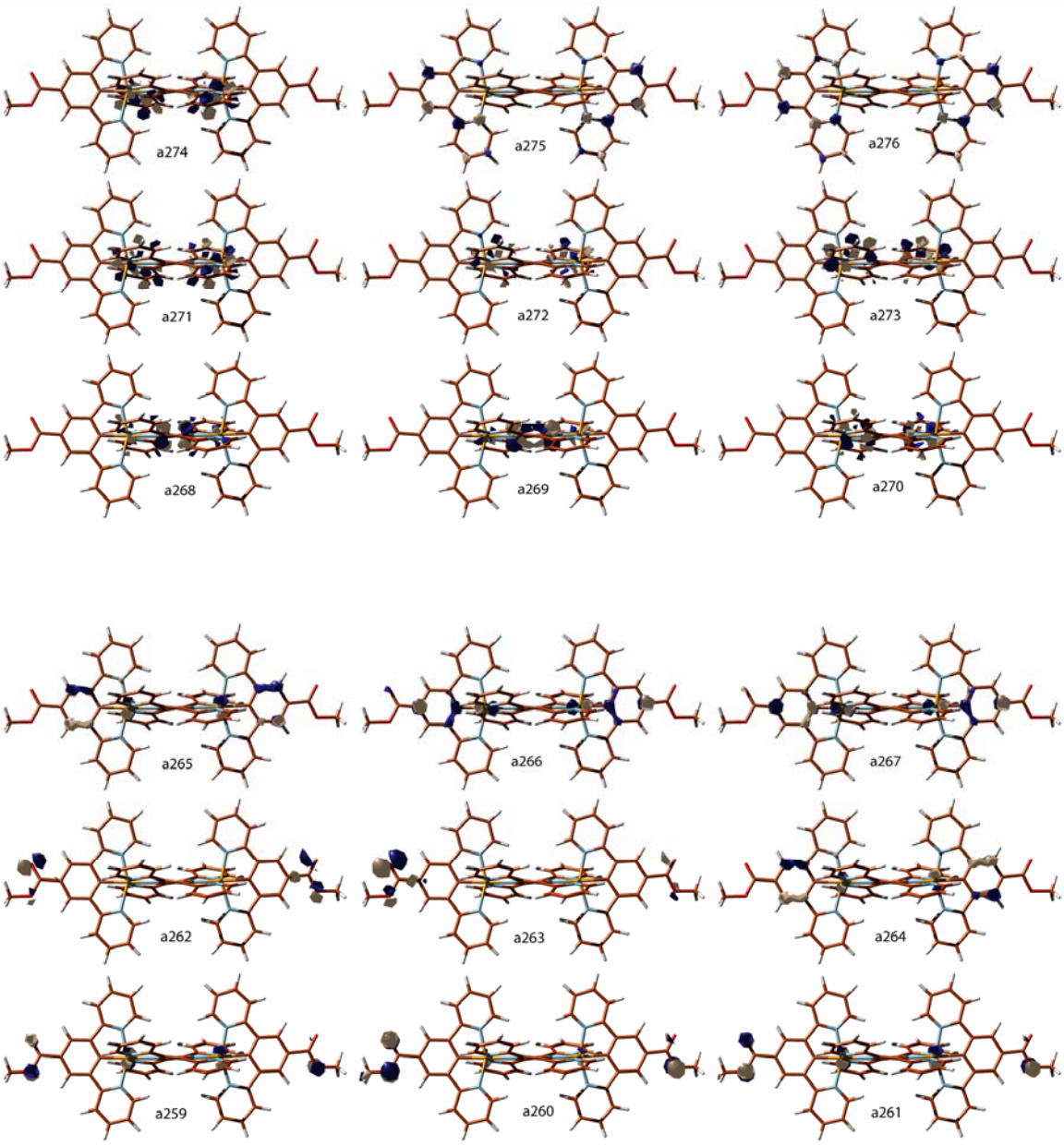

Figure S11.1. Isovalue (value = 0.05) plots of the alpha frontier orbitals of [**5b**]$^{3+}$.

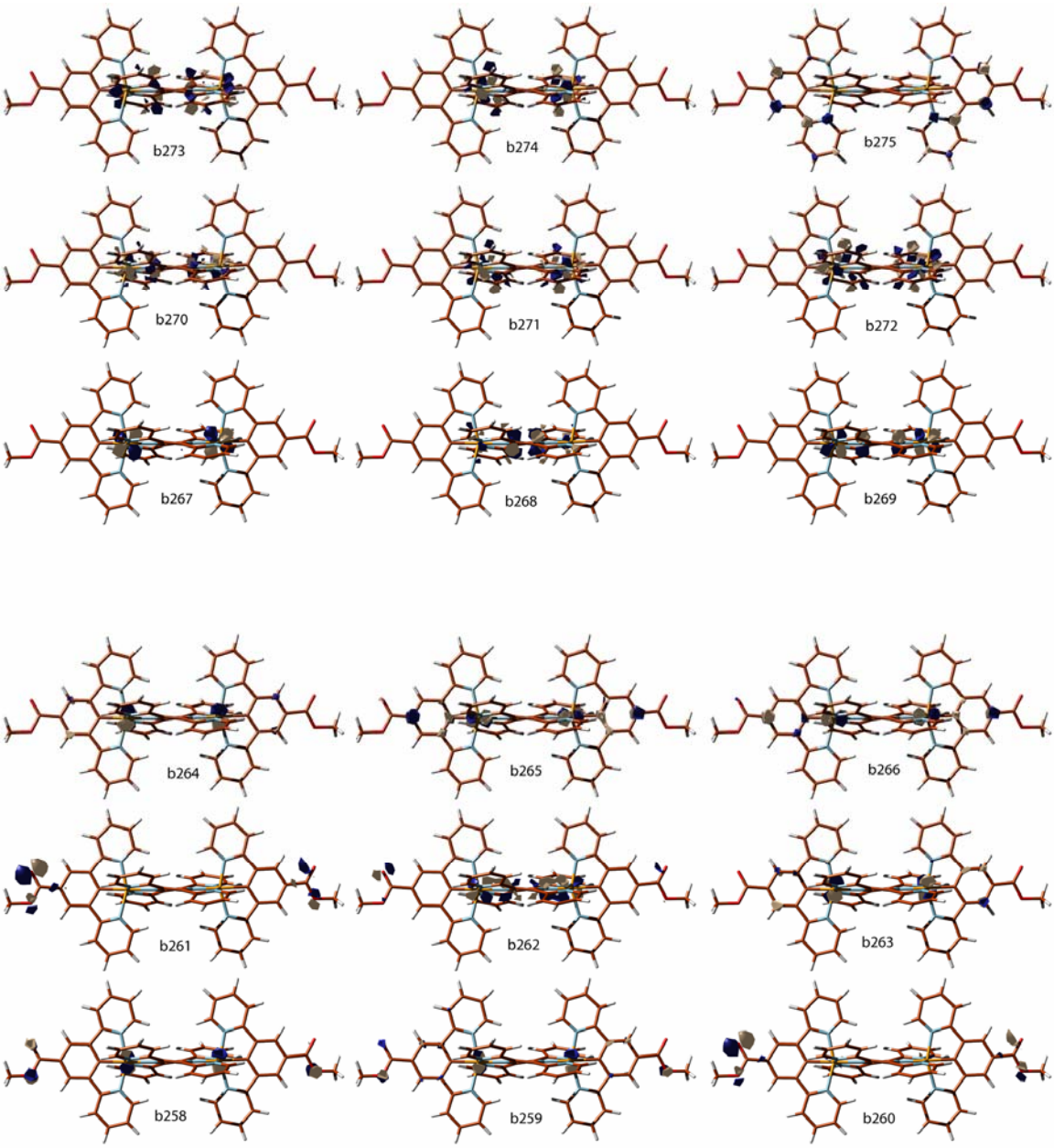

Figure S11.2. Isovalue (value = 0.05) plots of the beta frontier orbitals of [**5b**]$^{3+}$.

Table S10.3 Complete listing of electronic transitions for [**5b**]$^{3+}$ calculated by TDDFT.

#	E(eV)	E(nm)	character	*f*	#	E(eV)	E(nm)	character	*f*
1	0.2975	4168.07	254B →269B (-0.15123) 255B →267B (0.28550) 260B →267B (-0.12101) 262B →267B (-0.12277) 265B →269B (0.30471) 266B →267B (0.91565) 266B →270B (0.11106)	0.0055	16	1.6922	732.69	253A →268A (-0.12162) 259A →268A (-0.16992) 261A →268A (-0.18850) 265A →268A (-0.32014) 266A →268A (0.29081) 259B →268B (0.25177) 264B →268B (0.81965)	0.0163
2	0.3325	3728.65	254B →267B (-0.28727) 255B →269B (0.14775) 265B →267B (0.91569) 265B →270B (0.11475) 266B →269B (0.28867)	0.0000	17	1.7111	724.59	255A →269A (0.13310) 266A →269A (0.82137) 267A →270A (-0.14061) 254B →269B (0.13158) 255B →267B (-0.29191) 260B →267B (-0.19367) 264B →268B (-0.10364) 265B →269B (-0.27595) 266B →267B (0.20000) 266B →270B (-0.11079)	0.0000
3	0.3986	3110.55	257B →267B (0.11949) 258B →269B (-0.19834) 259B →267B (0.41992) 262B →268B (0.10237) 263B →269B (0.27320) 264B →267B (0.88452) 264B →270B (0.12097)	0.0000	18	1.7596	704.6	256A →269A (-0.10182) 267A →269A (0.58110) 254B →267B (-0.34153) 255B →269B (0.14471) 261B →267B (-0.13578) 262B →268B (0.10358) 262B →269B (0.14765) 263B →268B (-0.20038) 265B →267B (-0.29214) 265B →270B (0.12999) 266B →269B (0.53252)	0.0000
4	0.5108	2427.41	256B →267B (-0.20449) 258B →267B (-0.46137) 259B →269B (0.18284) 262B →267B (-0.21338) 263B →267B (0.76593) 263B →270B (0.11323) 264B →269B (0.33665)	0.0011	19	1.8097	685.12	266A →269A (0.50233) 254B →269B (-0.19380) 255B →267B (0.49931) 260B →267B (0.18749) 265B →269B (0.47656) 266B →267B (-0.31925) 266B →270B (0.17906)	0.0060
5	1.0607	1168.91	253A →268A (-0.10061) 257A →269A (0.34019) 259A →268A (-0.11193) 261A →268A (-0.12096) 265A →268A (-0.13698) 260B →267B (0.38206) 262B →267B (0.83488) 263B →267B (0.28690) 264B →268B (-0.16929) 266B →267B (0.23366)	0.1613	20	1.8104	684.85	258A →268A (-0.15697) 264A →268A (0.24687) 254B →267B (-0.12370) 258B →268B (-0.27183) 262B →268B (-0.33596) 263B →268B (0.80395) 266B →269B (0.13502)	0.0000
6	1.3878	893.38	260B →268B (0.13170) 262B →268B (0.35676) 263B →268B (0.13577) 266B →268B (0.91339)	0.0001	21	1.964	631.28	258A →270A (-0.10161) 259A →269A (0.28459) 261A →269A (0.35511) 264A →270A (0.12239) 265A →268A (0.16529) 265A →269A (0.81388) 258B →267B (-0.14950) 264B →269B (-0.17439)	0.0013
7	1.5301	810.32	254B →268B (-0.10220) 258B →267B (0.14570) 263B →267B (0.12314) 265B →268B (0.96130)	0.0006	22	1.9675	630.15	257A →269A (0.30410) 259A →268A (0.15697) 261A →268A (0.22209) 265A →268A (0.78883) 265A →269A (-0.17668) 253B →268B (-0.12666) 264B →268B (0.36440)	0.0355

8	1.5378	806.27	257B →267B (0.25796) 258B →269B (-0.13153) 259B →267B (0.81581) 264B →267B (-0.46922)	0.0005	23	1.9712	628.96	254A →269A (0.11295) 256A →269A (-0.12645) 258A →268A (-0.23500) 260A →268A (-0.14634) 264A →268A (0.67058) 254B →267B (0.27952) 257B →267B (0.15988) 260B →269B (0.20747) 262B →269B (0.43597) 263B →268B (-0.16119) 263B →269B (0.20571) 265B →267B (0.11187) 266B →269B (0.13485)	0.0000
9	1.5423	803.9	256B →267B (0.34551) 258B →267B (0.67941) 259B →269B (-0.15318) 262B →267B (-0.23984) 263B →267B (0.51892) 265B →268B (-0.20903)	0.0002	24	2.0217	613.27	264A →268A (-0.20014) 257B →267B (0.90379) 259B →267B (-0.30230) 266B →269B (0.12141)	0.0001
10	1.5939	777.88	254B →267B (-0.12731) 261B →267B (0.95294) 265B →267B (-0.17916) 266B →269B (0.12196)	0.0000	25	2.0224	613.04	256B →267B (0.87543) 258B →267B (-0.44285) 265B →269B (-0.12278)	0.0000
11	1.5949	777.4	255B →267B (-0.11323) 260B →267B (0.87070) 262B →267B (-0.41327) 263B →267B (-0.11313) 266B →267B (0.12876)	0.0000	26	2.0425	607.02	258A →269A (-0.35458) 260A →269A (-0.20957) 262A →269A (0.11724) 264A →269A (0.79027) 265A →270A (0.15322) 257B →267B (-0.16492) 258B →269B (-0.11347) 263B →269B (0.23492) 264B →270B (0.13470)	0.0001
12	1.632	759.7	256A →268A (-0.10908) 267A →268A (0.52021) 260B →268B (0.30984) 262B →268B (0.64383) 263B →268B (0.30969) 266B →268B (-0.31482)	0.0003	27	2.0834	595.11	254A →269A (0.15548) 256A →269A (-0.17915) 264A →268A (-0.51362) 264A →269A (-0.13153) 254B →267B (0.51051) 257B →267B (-0.15269) 260B →269B (0.13925) 262B →269B (0.31492) 263B →268B (0.16250) 263B →269B (0.14626) 266B →269B (0.42329)	0.0000
13	1.6627	745.66	267A →268A (0.84011) 260B →268B (-0.18285) 262B →268B (-0.38097) 263B →268B (-0.20487) 266B →268B (0.21921)	0.0004	28	2.1368	580.24	257A →269A (0.13329) 255B →267B (0.69424) 265B →269B (-0.65179) 266B →270B (-0.17484)	0.0067
14	1.6762	739.66	266A →268A (0.93906) 264B →268B (-0.25856)	0.0007	29	2.1728	570.63	257A →268A (0.14856) 265A →269A (0.24062) 256B →267B (0.16934) 258B →267B (0.26580) 258B →270B (-0.11170) 259B →269B (0.23616) 263B →267B (-0.21559) 263B →270B (0.21962) 264B →269B (0.78433)	0.0037
15	1.6843	736.12	254A →269A (-0.10612) 266A →270A (-0.12544) 267A →269A (0.76379) 254B →267B (0.30122) 255B →269B (-0.14161) 261B →267B (0.23086)	0.0000	30	2.1863	567.09	254A →269A (0.16939) 256A →269A (-0.18711) 264A →268A (-0.25264) 254B →267B (-0.51248)	0.0000

265B →267B (0.25474) 265B →270B (-0.11905) 266B →269B (-0.36917)	260B →269B (0.23525) 262B →269B (0.47497) 263B →269B (0.33515) 265B →270B (-0.19608) 266B →269B (-0.38736)

Table S11. Complete listing of applied basis set.

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S       1       1.00
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P       4       1.00
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        0.359400000     0.640089000
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N       0
S       6       1.00
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        59.8376000      0.253364000
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S       1       1.00
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        0.700000000     1.00000000
S       1       1.00
        0.213300000     1.00000000
P       4       1.00
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P       1       1.00
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P       4       1.00
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        0.7171000     0.6273750
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S       1       1.00
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S       1       1.00
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P       2       1.00
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P       1       1.00
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D       4       1.00
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        2.10428000    0.265739200
        0.921500000   0.481239800
        0.388598000   0.409977800
D       1       1.00
        0.152836000   1.00000000
D       1       1.00
        0.510000000E-01       1.00000000
        ****

RU      0
RU-ECP      4       28
G       POTENTIAL
        1
2       1.00000000    0.00000000
S-G     POTENTIAL
        2
2       11.10526900   209.82297100
2       5.41474500    30.65472600
P-G     POTENTIAL
        2
2       9.77127100    146.33618200
2       5.07399100    24.12787700
D-G     POTENTIAL
        2
2       7.67142300    67.51589700
2       4.13656500    9.87010400
F-G     POTENTIAL
        2
2       11.36000000   -28.34061600
2       5.68000000    -4.94462900
```