Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

The redox series $[Ru(bpy)_2(L)]^n$, n = +3, +2, +1, 0, with L = bipyridine, "click" derived pyridyl-triazole or bis-triazole: A combined structural, electrochemical, spectroelectrochemical and DFT investigation‡

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Table S1 Crystallographic details for ligands.

	$L^3 \cdot 0.31\ Et_2O$
Chemical formula	$C_{14}H_9F_3N_4\,C_{1.31}O_{0.31}$
M_r	311.02
Crystal system, Space group	Tetragonal, I4(1)/a
a, b, c (Å)	15.3175(7), 15.3175(7), 23.0865(12)
α, β, γ (°)	90, 90, 90
V (Å^3)	5416.7(4)
Z	16
Densitiy (g cm^{-3})	1.526
F(000)	2534
Radiation Type	Mo K_α
μ (mm^{-1})	0.125
Crystal size	0.35 x 0.29 x 0.23
Meas. Refl.	19474
Indep. Refl.	2776
Obsvd. [$I > 2\sigma(I)$] refl.	2107
R_{int}	0.0340
R [$F^2 > 2\sigma(F^2)$], wR(F^2), S	0.0484, 0.1318, 1.055
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.572, -0.625

Table S2 Comparison between the bond lengths (in Å) of the experimental and calculated structures of $\mathbf{3}^{2+}$ and $\mathbf{6}^{2+}$.

	$\mathbf{3}^{2+}$ (expt)	$\mathbf{3}^{2+}$ (calc)	$\mathbf{6}^{2+}$ (expt)	$\mathbf{6}^{2+}$ (calc)
N1-Ru1	2.090(3)	2.088	2.054(4)	2.058
N2-Ru1	2.026(3)	2.029	2.060(4)	2.055
N7-Ru1	2.055(3)	2.050	2.057(4)	2.059
N8-Ru1	2.049(1)	2.049	2.048(4)	2.047
N9-Ru1	2.051(3)	2.050	2.049(4)	2.046
N10-Ru1	2.044(3)	2.062	2.062(4)	2.054

Table S3 Comparison between the bond angles (in °) of the experimental and calculated structures of $\mathbf{3}^{2+}$ and $\mathbf{6}^{2+}$.

	$\mathbf{3}^{2+}$ (expt)	$\mathbf{3}^{2+}$ (calc)	$\mathbf{6}^{2+}$ (expt)	$\mathbf{6}^{2+}$ (calc)
N1-Ru-N2	78.3(1)	78.5	77.4(2)	78.1
N2-Ru-N10	85.4(1)	85.3	89.9(2)	89.1

N10-Ru-N9	78.8(1)	79.0	78.9(2)	79.2
N9-Ru-N8	94.0(1)	91.4	90.3(2)	92.0
N8-Ru-N7	78.7(1)	79.1	79.2(2)	79.2
N2-Ru-N9	94.4(1)	94.3	95.9(1)	95.3
N2-Ru-N7	98.3(1)	98.5	95.8(2)	95.5
N9-Ru-N7	101.7(1)	96.5	94.9(2)	96.9
N8-Ru-N1	94.4(1)	96.0	96.5(2)	94.9
N10-Ru-N1	95.4(1)	96.2	99.5(2)	97.1
N7-Ru-N1	84.7(1)	88.6	87.2(2)	87.2
N8-Ru-N10	97.5(1)	97.4	95.8(2)	96.7
N1-Ru-N9	170.3(1)	171.7	173.1(2)	172.5
N2-Ru-N8	172.4(2)	174.1	172.3(2)	171.4
N10-Ru-N7	176.2(2)	174.3	172.1(2)	174.2

Table S4 Main contributions to the frontier orbitals of $\mathbf{3}^{2+}$.

Orbital	Energy (Eh)	pytz (%)	bpy1 (%)	bpy2 (%)	Ru (%)
HOMO-6	-0.31053	83.4	0	0.6	0.3
HOMO-5	-0.29573	49.7	24.4	7.5	2.1
HOMO-4	-0.29383	28	54.4	0.5	0.5
HOMO-3	-0.29135	3.4	4.5	75	0.4
HOMO-2	-0.25305	3.8	6.9	9.1	69.6
HOMO-1	-0.25223	8.7	7.3	4.6	69.1
HOMO	-0.2459	4.8	5.3	5.5	75.2
LUMO	-0.12082	2.1	55.9	12.7	2.4
LUMO+1	-0.11693	1.0	12.5	54.5	5.1
LUMO+2	-0.10653	66.5	0.7	1.7	5.0
LUMO+3	-0.09724	45.8	14.5	11.4	0.5
LUMO+4	-0.08898	34.8	25.6	10.2	2.5
LUMO+5	-0.08212	0.7	36.1	35.3	1.5
LUMO+6	-0.08033	47.5	9.6	15.8	0.6
LUMO+7	-0.07824	3.3	49	19.1	2.6
LUMO+8	-0.07559	17.7	7.1	48.6	1.3
LUMO+9	-0.07319	66.9	1.5	3.5	0.6
LUMO+10	-0.05921	72.4	0.1	0	0.5

Table S5 Main contributions to the frontier orbitals of $\mathbf{6}^{2+}$.

Orbital	Energy (Eh)	bistz (%)	bpy (%)	Ru (%)
HOMO-5	-0.29756	73.3	7.7	2
HOMO-4	-0.29329	7.2	75.6	0.8
HOMO-3	-0.29187	0	82.6	0.5
HOMO-2	-0.25404	5.2	15.2	69.1
HOMO-1	-0.25363	6.7	13.4	68.9
HOMO	-0.24806	4.6	10.4	75.3
LUMO	-0.11983	0.7	70.3	2.2
LUMO+1	-0.11708	0.1	68.3	5.6

LUMO+2	-0.09549	41.1	31.2	1.0
LUMO+3	-0.0879	53.4	17.4	1.6
LUMO+4	-0.08698	49.3	20.3	2.6
LUMO+5	-0.08261	4.2	67.1	1.5
LUMO+6	-0.08059	63.3	7.1	2.2
LUMO+7	-0.07743	11.3	61.3	0.7
LUMO+8	-0.07663	2.9	68.6	2.3

Table S6 Main TD-DFT calculated transitions of $\mathbf{6}^{2+}$ compared with the experimental data.

	Main contributing excitation (%)	Transition wavelength (nm)	Oscillator strength	Exp. transition wavelength (nm)	Molar absorption coefficient, $M^{-1}cm^{-1}$
$\mathbf{6}^{2+}$	HOMO-2→LUMO (32)	422	0.137	433	30800 M→L
	HOMO-1→LUMO (24)				
	HOMO-1→LUMO+1 (25)				
	HOMO-2→LUMO+1 (37)	399	0.069	397	sh M→L
	HOMO-1→LUMO+1 (29)				
	HOMO-1→LUMO+3 (25)	324	0.043	296	67800 M→L
	HOMO-14→LUMO+5 (28)				
	HOMO→LUMO+8 (39)	323	0.042		
	mixed[a]	317	0.072		
	mixed[a]	317	0.045		
	HOMO-1→LUMO+6 (26)	312	0.063		
	HOMO-1→LUMO+7 (18)				
	HOMO-2→LUMO+6 (23)	312	0.030		
	HOMO-2→LUMO+8 (219)				
	HOMO-4→LUMO+1 (28)	271	0.254	279	63700 IL
	HOMO-3→LUMO (17)				
	HOMO-3→LUMO+1 (23)	266	0.498		
	HOMO-4→LUMO (18)				
	HOMO-5→LUMO+6 (43)	228	0.290	242	34200 IL

[a] Mixed refers to transitions where many different starting and target orbitals contribute to the transition.

Table S7 Main TD-DFT calculated transitions of $\mathbf{6}^{3+}$ compared with the experimental data.

Compound	Main contributing excitation (%)	Transition wavelength (nm)	Oscillator strength	Exp. transition wavelength (nm)	Molar absorption coefficient, $M^{-1}cm^{-1}$
$\mathbf{6}^{3+}$	HOMO-4(β)→LUMO(β) (65)	865	0.005	720	1500 L → M
	HOMO(β)→LUMO(β) (81)	771	0.005		
	HOMO-8(β)→LUMO(β) (39)	736	0.007		

HOMO-3(β)→LUMO(β) (29)				
HOMO-2(β)→LUMO(β) (20)				
HOMO-9(β)→LUMO(β) (94)	441	0.023	427	15200 L → M
HOMO-4(α)→LUMO+1(α) (31)	307	0.068	315	sh L → L
HOMO-4(α)→LUMO+1(α) (29)	301	0.065		
HOMO-24(β)→LUMO(β) (31)	291	0.065	301	37300 L → M
HOMO-14(β)→LUMO(β) (32)	290	0.076		
mixed[a]	284	0.141		

[a] Mixed refers to transitions where many different starting and target orbitals contribute to the transition.

Table S8 Main TD-DFT calculated transitions of $\mathbf{6}^{+}$ compared with the experimental data.

	Main contributing excitation (%)	Transition wavelength (nm)	Oscillator strength	Exp. transition wavelength (nm)	Molar absorption coefficient, $M^{-1}cm^{-1}$
$\mathbf{6}^{+}$	HOMO(α)→LUMO+8(α) (59)	866	0.016	998/869	4000 L→L
	HOMO(α)→LUMO+10(α) (20)				
	HOMO(α)→LUMO+12(α) (89)	462	0.072	525	sh L→L
	HOMO-1(β)→LUMO(β) (76)	437	0.069	486	28200 M→L
	HOMO-1(β)→LUMO+1 (β) (54)	399	0.098	430	31200 M→L
	HOMO-2(β)→LUMO+3(β) (31)	378	0.059		M→L
	HOMO-3(α)→LUMO+2(α) (33)				
	mixed[a]	377	0.054	357	58800
	mixed[a]	309	0.046	333	59700
	mixed[a]	304	0.023		
	mixed[a]	303	0.028		

[a] Mixed refers to transitions where many different starting and target orbitals contribute to the transition.

Table S9 Total energies from DFT calculations.

Compound	E/Eh BP86	E/Eh B3LYP
$\mathbf{3}^{+}$	-6630.09328325	-6628.21767318
$\mathbf{3}^{2+}$	-6629.95047609	-6628.08856704
$\mathbf{3}^{3+}$	-6629.70240195	-6627.85074640
$\mathbf{6}^{+}$	-7193.01686985	-7190.86418322
$\mathbf{6}^{2+}$	-7192.87105066	-7190.73500598
$\mathbf{6}^{3+}$	-7192.61880868	-7190.49260103

Fig. S1 Cyclic voltammogram of $\mathbf{1}^{2+}$ (top) and $\mathbf{5}^{2+}$ (bottom) in CH_2Cl_2 / 0.1 M Bu_4NPF_6 at 295 K. The ferrocene / ferrocenium couple was used as an internal standard.

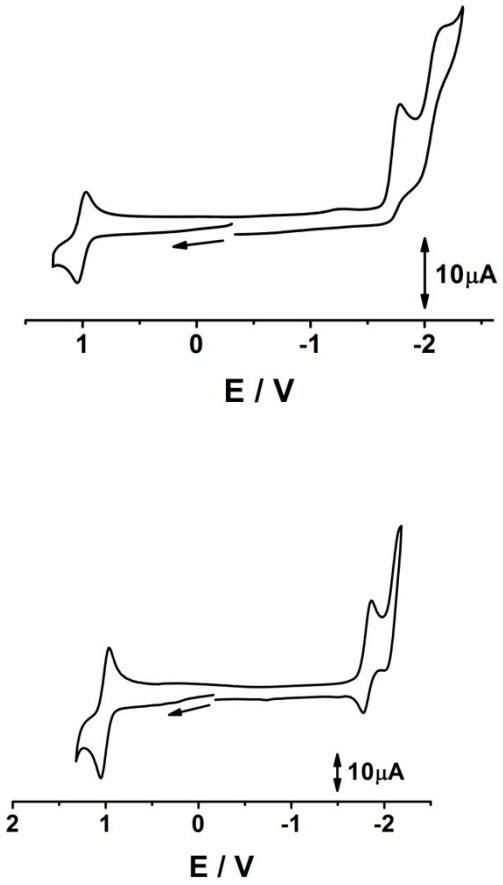
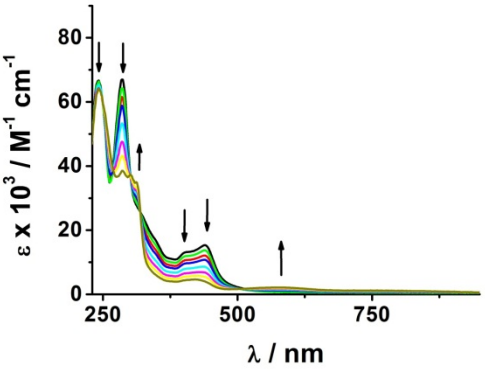
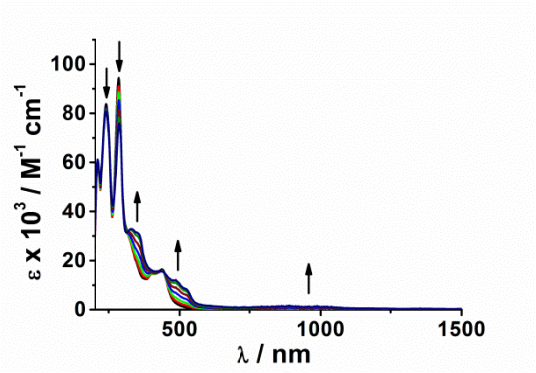


Fig. S2 Changes in the UV-vis-NIR spectra of $\mathbf{5}^{2+}$ during first oxidation (top), first reduction (middle) and second reduction (bottom) from OTTLE spectroelectrochemistry at 295 K.





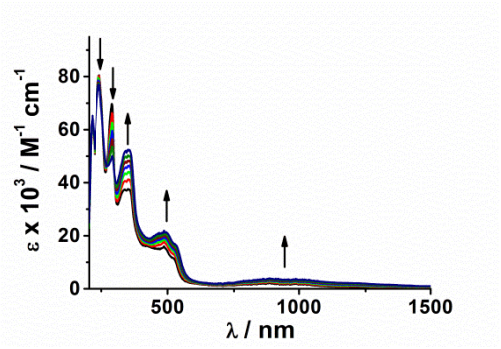


Fig. S3 Relevant calculated frontier orbitals (canonical orbitals) for the optical transitions observed in $\mathbf{6}^{2+}$. Orbitals are shown with an iso-value of 0.06.

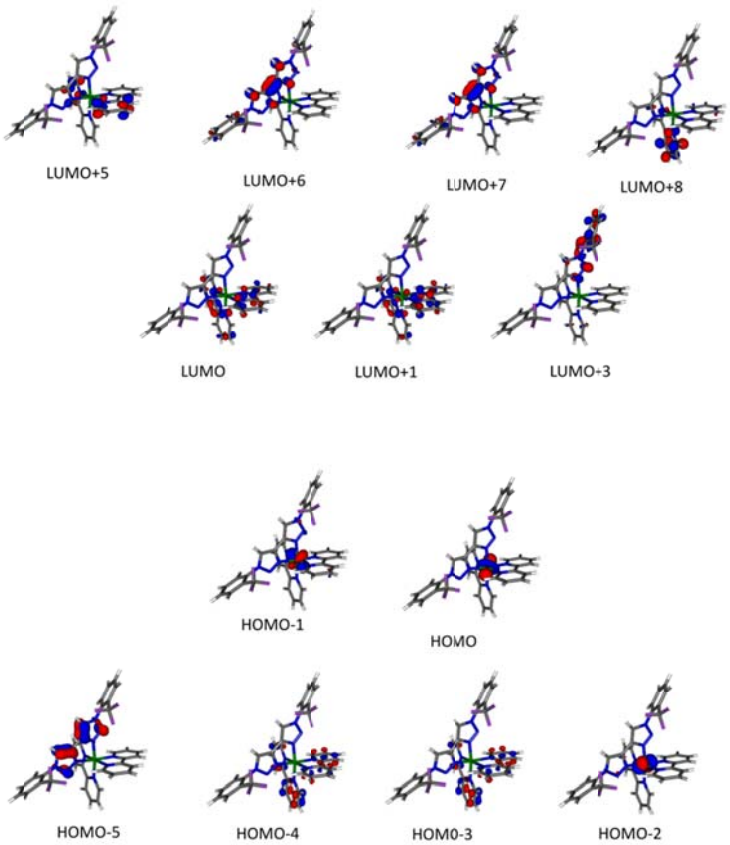


Fig. S4 Relevant calculated frontier orbitals (canonical orbitals) for the optical transitions observed in $\mathbf{6}^{3+}$. Orbitals are shown with an iso-value of 0.06.

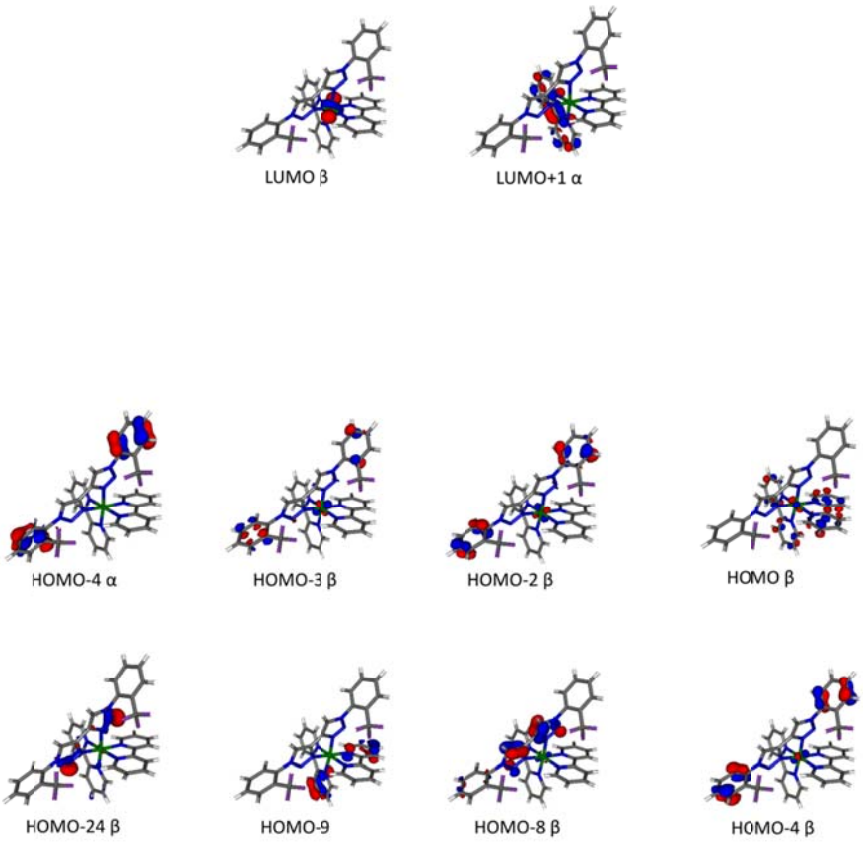


Fig. S5 Relevant calculated frontier orbitals (canonical orbitals) for the optical transitions observed in $\mathbf{6}^{+}$. Orbitals are shown with an iso-value of 0.06.

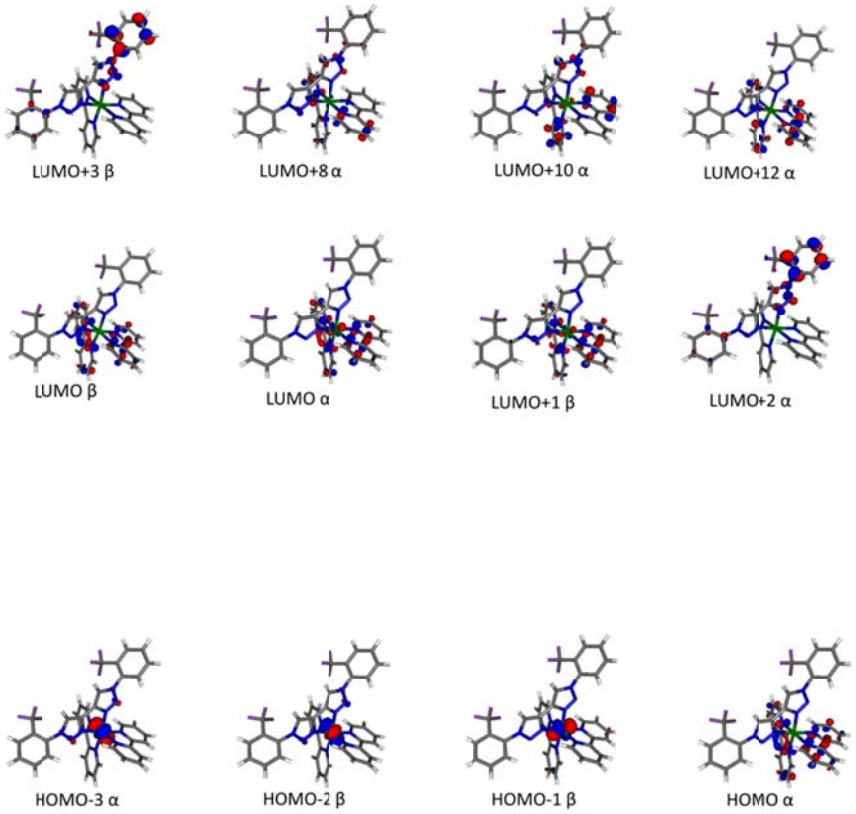
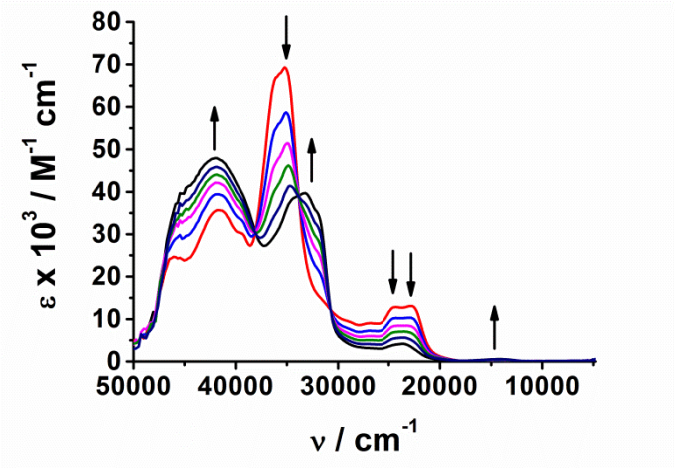


Fig. S6 Changes in the UV-vis-NIR spectra of $\mathbf{3}^{2+}$ in cm^{-1} during first oxidation (top) and first reduction (bottom) from OTTLE spectroelectrochemistry at 295 K.



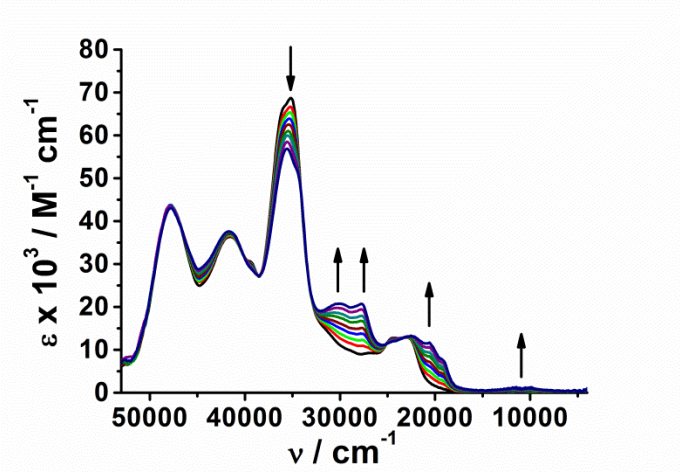


Fig. S7 EPR spectrum of in-situ electrochemically generated $\mathbf{1}^{+}$ at 295 K.

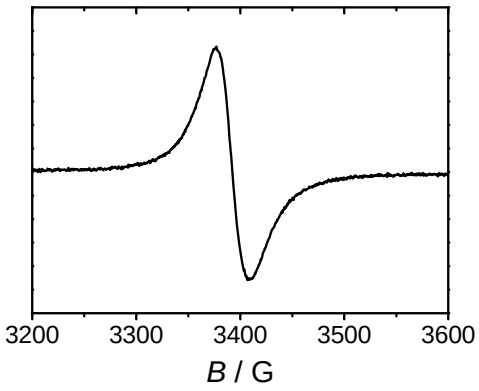
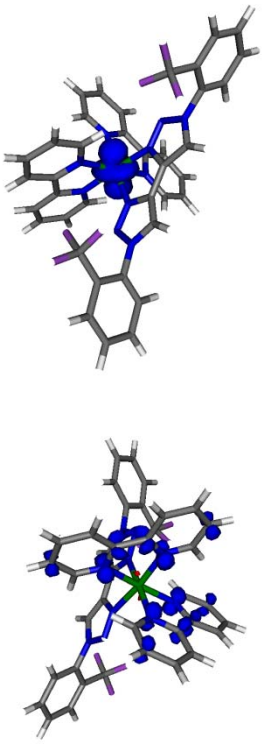


Fig. S8 Spin density plots for $\mathbf{6}^{3+}$ (top) and $\mathbf{6}^{+}$ (bottom). Spin densities are shown with an iso-value of 0.01.



Coordinates from geometry optimizations

3^{2+}

C	11.429694	2.818657	0.138611
N	10.714543	3.161267	1.232584
C	11.183059	3.362204	-1.117455
C	10.160493	4.303025	-1.266866
C	9.419862	4.673343	-0.146635
C	9.715411	4.093197	1.087417
C	9.023831	4.384594	2.326249
N	9.512311	3.771562	3.460391
C	7.911444	5.106611	2.714806
N	7.803087	4.878937	4.051488
C	6.768234	5.322576	4.933906
C	5.940657	4.398907	5.599295
C	6.598768	6.696105	5.103303
C	5.602353	7.168450	5.958669
C	4.790850	6.264867	6.646229
C	4.958458	4.890345	6.465292
C	6.061237	2.900810	5.407894
F	7.038733	2.354942	6.187730
F	4.907393	2.261219	5.731582
F	6.345296	2.558201	4.116551
C	12.406305	-0.148143	2.358632
N	12.537025	1.156712	2.687599
C	13.496063	-0.951329	2.046538
C	14.778228	-0.396928	2.074517
C	14.922367	0.944283	2.417880
C	13.791791	1.708498	2.723607

C	13.826935	3.125780	3.095713
N	12.600850	3.676768	3.362946
C	14.994575	3.889559	3.191730
C	14.915497	5.229348	3.561064
C	13.660316	5.782340	3.827954
C	12.531809	4.979370	3.718155
C	8.760126	0.703467	1.987965
N	9.477345	1.024167	3.087094
C	7.687551	-0.179052	2.028458
C	7.332353	-0.755912	3.249819
C	8.069185	-0.433081	4.385366
C	9.141039	0.459175	4.287642
C	9.988266	0.860146	5.414183
N	10.981390	1.749551	5.101652
C	9.829283	0.390594	6.721192
C	10.695448	0.822372	7.721414
C	11.714400	1.717588	7.388888
C	11.824520	2.156280	6.074876
Ru	10.994511	2.418168	3.163754
N	8.788027	4.066719	4.513264
H	12.214840	2.079265	0.288340
H	11.790555	3.045282	-1.963961
H	9.945477	4.743304	-2.240074
H	8.618296	5.407891	-0.217986
H	7.194914	5.708426	2.169093
H	7.258531	7.384583	4.574982
H	5.471273	8.242078	6.093146
H	4.017010	6.626881	7.322956

H	4.308957	4.190521	6.988879
H	11.391549	-0.541697	2.347030
H	13.332764	-1.996231	1.786448
H	15.653018	-1.000212	1.833796
H	15.911738	1.397164	2.448338
H	15.961736	3.437436	2.979300
H	15.819578	5.832315	3.639737
H	13.548091	6.825536	4.119940
H	11.536182	5.368262	3.924488
H	9.069740	1.175482	1.057012
H	7.142614	-0.402109	1.112330
H	6.492656	-1.446921	3.317680
H	7.808952	-0.870916	5.347080
H	9.030860	-0.310760	6.955672
H	10.578307	0.463380	8.743478
H	12.420844	2.080075	8.134311
H	12.601217	2.859098	5.779555

3^{3+}

C	11.494951	2.906318	0.166032
N	10.742867	3.224913	1.241031
C	11.273411	3.476539	-1.081909
C	10.251077	4.417870	-1.231870
C	9.479730	4.766563	-0.125349
C	9.745169	4.160792	1.101414
C	9.036346	4.430293	2.333268
N	9.501154	3.790934	3.460738
C	7.905633	5.124945	2.722184

N	7.772081	4.846388	4.047460
C	6.722845	5.271693	4.926594
C	5.905482	4.331225	5.581394
C	6.535047	6.642790	5.093185
C	5.525932	7.097647	5.942720
C	4.721081	6.180012	6.619159
C	4.907853	4.807311	6.436244
C	6.047829	2.836305	5.384442
F	7.036553	2.303339	6.161553
F	4.908821	2.176439	5.697397
F	6.347391	2.508061	4.088790
C	12.359708	-0.183269	2.479348
N	12.520485	1.133632	2.734225
C	13.438211	-1.011768	2.198542
C	14.725821	-0.470109	2.194487
C	14.896165	0.883817	2.472820
C	13.779877	1.677544	2.743571
C	13.833109	3.104868	3.063110
N	12.616317	3.687214	3.304234
C	15.005823	3.860861	3.124539
C	14.932764	5.217458	3.430426
C	13.684298	5.798753	3.664202
C	12.546530	5.005441	3.586899
C	8.672736	0.811179	2.024439
N	9.431986	1.074754	3.108683
C	7.596608	-0.065582	2.078474
C	7.285848	-0.680263	3.293457
C	8.061429	-0.401226	4.414950

C	9.136057	0.484423	4.307821
C	10.012640	0.862373	5.416584
N	11.017613	1.736502	5.092909
C	9.886199	0.381403	6.720677
C	10.793749	0.789040	7.695062
C	11.822272	1.666876	7.345787
C	11.906316	2.117241	6.034767
Ru	10.990808	2.431112	3.162572
N	8.746986	4.031862	4.504042
H	12.279586	2.167199	0.318383
H	11.899395	3.179354	-1.921523
H	10.060348	4.879381	-2.200128
H	8.681763	5.503808	-0.201979
H	7.194710	5.738429	2.181891
H	7.189077	7.342505	4.572777
H	5.378856	8.168600	6.079640
H	3.935393	6.529179	7.288637
H	4.260305	4.098171	6.949403
H	11.340561	-0.564523	2.494999
H	13.261743	-2.065369	1.989083
H	15.590733	-1.097147	1.980890
H	15.892949	1.320077	2.481169
H	15.969794	3.393331	2.934169
H	15.841834	5.815505	3.483039
H	13.583255	6.855626	3.904829
H	11.554339	5.415405	3.766543
H	8.951081	1.310704	1.098099
H	7.016500	-0.255781	1.177215

H	6.444388	-1.368107	3.368225
H	7.830454	-0.868599	5.369744
H	9.085401	-0.310073	6.974130
H	10.701416	0.420767	8.716214
H	12.555580	2.006353	8.075186
H	12.689548	2.805078	5.722769

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C	11.463746	2.759567	0.203571
N	10.748776	3.119626	1.293187
C	11.266719	3.334209	-1.047706
C	10.293524	4.327814	-1.200606
C	9.548125	4.711080	-0.088424
C	9.791633	4.096001	1.141627
C	9.074120	4.382833	2.365580
N	9.495616	3.715572	3.499392
C	7.967459	5.125539	2.727542
N	7.787691	4.857052	4.049289
C	6.745499	5.329711	4.901765
C	5.870463	4.437663	5.550423
C	6.615904	6.709355	5.068879
C	5.618137	7.216897	5.901525
C	4.762805	6.342688	6.574635
C	4.888635	4.963450	6.397210
C	5.936506	2.936432	5.358132
F	6.859824	2.348287	6.170228
F	4.742046	2.345726	5.646288
F	6.240315	2.583432	4.078015

C	12.484115	-0.189811	2.521699
N	12.555498	1.140442	2.739002
C	13.578305	-0.953851	2.139957
C	14.825365	-0.310373	1.980098
C	14.922275	1.047758	2.226550
C	13.782767	1.785089	2.624168
C	13.779022	3.180011	2.970926
N	12.560031	3.674067	3.428383
C	14.907446	4.031835	2.928438
C	14.815210	5.337854	3.373710
C	13.579023	5.809452	3.873607
C	12.492176	4.948332	3.873161
C	8.780974	0.630491	2.017341
N	9.483686	0.969086	3.120077
C	7.669304	-0.199949	2.058750
C	7.246383	-0.702010	3.301382
C	7.967650	-0.372553	4.439557
C	9.099608	0.454359	4.341228
C	9.964671	0.807125	5.452774
N	10.994407	1.668880	5.142285
C	9.831437	0.303079	6.757821
C	10.745466	0.663536	7.739057
C	11.802898	1.522151	7.401507
C	11.891229	1.993163	6.096711
Ru	10.987714	2.375818	3.219003
N	8.729685	3.997577	4.529033
H	12.210294	1.982454	0.358966
H	11.875538	3.002818	-1.887887

H	10.120353	4.795841	-2.169261
H	8.781546	5.482166	-0.161255
H	7.296229	5.767433	2.170123
H	7.310677	7.374562	4.555965
H	5.521282	8.294717	6.031771
H	3.988639	6.731278	7.236077
H	4.205467	4.286466	6.907769
H	11.497254	-0.636003	2.644816
H	13.457019	-2.021172	1.962020
H	15.705608	-0.876098	1.673382
H	15.881204	1.554580	2.123678
H	15.853003	3.651330	2.543032
H	15.686211	5.992817	3.340207
H	13.461419	6.827248	4.242339
H	11.514954	5.271664	4.232189
H	9.133997	1.057731	1.079224
H	7.140815	-0.437681	1.136682
H	6.364296	-1.338039	3.374053
H	7.653660	-0.746970	5.412597
H	9.015433	-0.377853	6.994697
H	10.644353	0.276228	8.752959
H	12.546992	1.828572	8.135324
H	12.690491	2.665809	5.788265

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C	9.615981	6.633686	12.886669
N	9.005968	5.855676	11.950016
C	9.161108	7.908775	12.629065

H	10.295772	6.230487	13.625845
C	9.994538	9.862849	14.183190
N	9.611244	11.166528	14.098670
C	9.309123	9.232886	13.167127
H	10.695463	9.509440	14.928335
N	8.305697	7.819985	11.544483
N	8.551539	10.201911	12.531160
C	9.114944	4.437697	11.760377
C	9.767614	3.979673	10.618054
C	8.555660	3.541183	12.687837
C	9.883636	2.606041	10.396233
H	10.183460	4.701615	9.915781
C	9.351287	1.704290	11.318969
H	10.395349	2.245120	9.504160
C	8.689508	2.169101	12.457941
H	9.444178	0.631130	11.153117
H	8.263022	1.462480	13.167958
C	7.814167	4.031812	13.910064
F	8.664949	4.580522	14.833618
F	7.141582	3.040804	14.538347
F	6.902418	5.001406	13.601732
C	10.005165	12.263122	14.936712
C	10.887090	13.205913	14.415137
C	9.493201	12.386225	16.240081
C	11.282155	14.287294	15.205951
H	11.259475	13.083365	13.398404
C	10.794732	14.413477	16.507698
H	11.974426	15.026063	14.802361

C	9.903236	13.468904	17.022477
H	11.103986	15.253397	17.129566
H	9.516779	13.577066	18.034552
C	8.519279	11.374717	16.797756
F	7.478821	11.136275	15.939044
F	7.977476	11.769635	17.971028
F	9.116562	10.163578	17.021358
C	5.680820	9.194224	13.501382
N	5.787712	8.973358	12.172090
C	4.611506	8.722861	14.252547
H	6.481941	9.771780	13.958754
C	3.607050	7.990940	13.614679
H	4.573920	8.928753	15.321277
C	3.707941	7.762616	12.245219
H	2.756462	7.604711	14.175296
C	4.805586	8.261455	11.536492
H	2.934939	7.197304	11.728020
C	5.004771	8.094076	10.093648
N	6.149166	8.661924	9.599779
C	4.115991	7.419054	9.251434
C	4.389326	7.325682	7.889763
H	3.212646	6.969181	9.659124
C	5.553862	7.916710	7.395157
H	3.702859	6.801514	7.225599
C	6.404427	8.572932	8.276687
H	5.809765	7.874570	6.337453
H	7.322845	9.041989	7.929232
C	5.501916	11.955442	11.002597

N	6.640940	11.417082	10.516533
C	5.078812	13.235308	10.665006
H	4.925270	11.332324	11.683368
C	5.855405	13.997426	9.789501
H	4.152001	13.620431	11.087695
C	7.027991	13.447073	9.280035
H	5.552251	15.004906	9.506300
C	7.406216	12.153229	9.651520
H	7.647847	14.021233	8.593861
C	8.614704	11.476986	9.171626
N	8.792843	10.209293	9.659154
C	9.533263	12.038555	8.279005
C	10.646101	11.304301	7.878792
H	9.378509	13.046566	7.898586
C	10.818368	10.012296	8.381967
H	11.366904	11.733469	7.183548
C	9.875780	9.502644	9.266431
H	11.671546	9.398534	8.096730
H	9.968741	8.498919	9.677164
N	8.205643	6.578833	11.126996
Ru	7.362243	9.560245	10.982713
N	8.732460	11.377932	13.087084

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C	9.670245	6.628623	12.883157
N	9.016940	5.852228	11.976159
C	9.283103	7.917102	12.577770
H	10.319609	6.216265	13.645311

C	10.154456	9.900551	14.080267
N	9.763085	11.201135	13.976772
C	9.443120	9.245731	13.097266
H	10.878162	9.564811	14.812100
N	8.425266	7.821800	11.496503
N	8.668826	10.206290	12.469514
C	9.029126	4.414160	11.878245
C	9.958234	3.817160	11.033515
C	8.109286	3.655491	12.622145
C	9.978142	2.424038	10.923184
H	10.654745	4.438781	10.471496
C	9.073341	1.654225	11.654716
H	10.702592	1.946466	10.264062
C	8.143410	2.264946	12.501359
H	9.087279	0.567788	11.571117
H	7.441399	1.658471	13.071019
C	7.114994	4.321468	13.545122
F	7.742457	5.030451	14.534472
F	6.291847	3.439213	14.146928
F	6.323005	5.221096	12.879807
C	10.143080	12.306250	14.816570
C	11.009129	13.262040	14.294981
C	9.624993	12.409811	16.119160
C	11.386356	14.344322	15.093496
H	11.386490	13.150548	13.278925
C	10.893661	14.456125	16.394388
H	12.068148	15.095268	14.695313
C	10.015028	13.496047	16.904836

H	11.188305	15.298066	17.020259
H	9.623810	13.595322	17.915951
C	8.667179	11.377974	16.668153
F	7.643171	11.114577	15.789956
F	8.102196	11.759108	17.829409
F	9.288526	10.179362	16.892978
C	5.892701	8.914398	13.514499
N	5.936024	8.796919	12.170249
C	4.897605	8.311054	14.272330
H	6.669997	9.519293	13.978297
C	3.920380	7.552830	13.623306
H	4.895336	8.437485	15.353550
C	3.965159	7.426833	12.237904
H	3.130877	7.062732	14.191605
C	4.985427	8.056116	11.520520
H	3.211978	6.838978	11.717500
C	5.137793	7.993516	10.066232
N	6.208295	8.687431	9.562758
C	4.269279	7.315207	9.210013
C	4.490222	7.352886	7.835315
H	3.422948	6.763167	9.613473
C	5.575145	8.077771	7.337293
H	3.818181	6.825524	7.159292
C	6.410682	8.737477	8.228891
H	5.780426	8.137019	6.269941
H	7.268541	9.310442	7.883250
C	5.383993	11.775557	11.033666
N	6.574497	11.364766	10.547878

C	4.874528	13.036026	10.750466
H	4.843609	11.075202	11.667140
C	5.609572	13.895689	9.930915
H	3.914418	13.330122	11.170684
C	6.830527	13.467672	9.415639
H	5.233500	14.889597	9.691183
C	7.301948	12.192502	9.731597
H	7.411847	14.121333	8.768606
C	8.553104	11.622910	9.232112
N	8.819418	10.349786	9.663615
C	9.444102	12.282469	8.382404
C	10.609973	11.638317	7.976448
H	9.229413	13.293215	8.041512
C	10.869360	10.342298	8.429801
H	11.310850	12.143995	7.313270
C	9.955430	9.730723	9.278446
H	11.768206	9.803779	8.134868
H	10.113678	8.721527	9.654578
N	8.253642	6.575772	11.130485
Ru	7.428789	9.554304	10.954066
N	8.865739	11.395042	12.988740

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C	9.666440	6.607338	12.950740
N	9.072581	5.829901	12.002970
C	9.163020	7.870282	12.730170
H	10.377875	6.216321	13.665884
C	9.956746	9.806162	14.320513

N	9.569112	11.109046	14.247258
C	9.291022	9.187036	13.285545
H	10.651552	9.444847	15.067302
N	8.296496	7.782587	11.650836
N	8.536987	10.159300	12.644768
C	9.259278	4.435893	11.739679
C	9.795914	4.078768	10.502720
C	8.891213	3.453605	12.677225
C	9.990429	2.731608	10.195081
H	10.064199	4.862700	9.795160
C	9.653944	1.748671	11.127711
H	10.412427	2.454949	9.229009
C	9.106319	2.108385	12.360698
H	9.810303	0.695203	10.896387
H	8.828403	1.338205	13.078162
C	8.259750	3.814773	14.001380
F	9.171225	4.347491	14.875870
F	7.713239	2.739971	14.621035
F	7.267097	4.740720	13.864938
C	9.953995	12.200372	15.090917
C	10.776407	13.187800	14.552200
C	9.493471	12.285078	16.417032
C	11.164562	14.269809	15.344933
H	11.109895	13.096011	13.518928
C	10.732090	14.354160	16.669646
H	11.809960	15.041321	14.925274
C	9.899309	13.367640	17.202818
H	11.037257	15.193650	17.294079

H	9.552665	13.444049	18.231989
C	8.571545	11.238365	16.996736
F	7.520818	10.959660	16.167806
F	8.043398	11.616587	18.185620
F	9.217936	10.050555	17.213732
C	5.605778	9.212564	13.551550
N	5.725729	9.075314	12.211311
C	4.411899	9.016132	14.227429
H	6.507752	9.515903	14.081814
C	3.266443	8.658620	13.486472
H	4.374296	9.150456	15.307360
C	3.379398	8.484563	12.117259
H	2.306054	8.516423	13.981933
C	4.621185	8.673866	11.475989
H	2.507990	8.198415	11.529669
C	4.870617	8.443332	10.073462
N	6.169853	8.686348	9.657080
C	3.919268	7.941392	9.160027
C	4.282988	7.670965	7.852017
H	2.898266	7.758560	9.492511
C	5.616140	7.897128	7.452534
H	3.549069	7.281899	7.146104
C	6.513938	8.400843	8.381486
H	5.951004	7.694826	6.436334
H	7.550910	8.597765	8.113505
C	5.620892	12.011333	11.101623
N	6.666008	11.363204	10.540943
C	5.143520	13.224296	10.628602

H	5.158841	11.519152	11.956152
C	5.772901	13.811379	9.511761
H	4.292132	13.694443	11.118301
C	6.855903	13.168703	8.937062
H	5.419243	14.760669	9.109143
C	7.313578	11.940550	9.460255
H	7.365590	13.612912	8.083041
C	8.482795	11.233948	8.996618
N	8.803156	10.092807	9.716288
C	9.303918	11.644891	7.925941
C	10.454335	10.938605	7.617154
H	9.030115	12.523991	7.343918
C	10.795729	9.812669	8.395180
H	11.087369	11.253582	6.787591
C	9.946095	9.432091	9.422178
H	11.697628	9.234564	8.199928
H	10.157345	8.553103	10.030216
N	8.236059	6.548233	11.204209
Ru	7.375578	9.524399	11.075537
N	8.703689	11.329135	13.220480