Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information for

Tuning metal to metal charge transfer properties in cyanidometal-bridged complexes by changing the auxiliary ligand on the bridge

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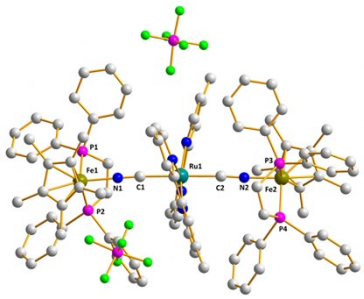

Fig. S1 Single crystal structure of **2**$(PF_6)_2$ (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink.

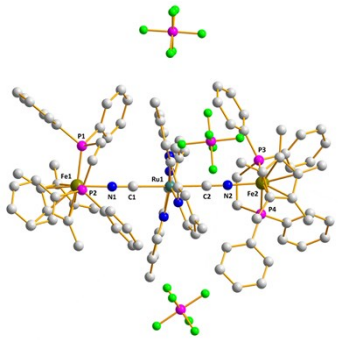

Fig. S2 Single crystal structure of **2**$(PF_6)_3$ (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink.

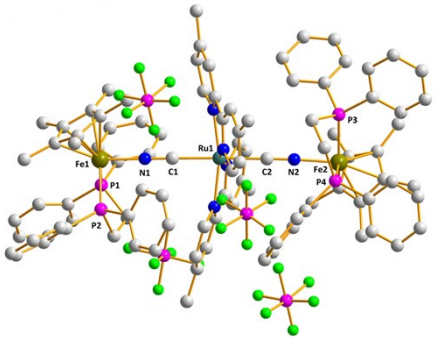

Fig. S3 Single crystal structure of **2**$(PF_6)_4$ (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink.

Table S1 Crystallographic data for **1**$(PF_6)_n$ (n = 2, 3, 4)

	1$(PF_6)_2$	**1**$(PF_6)_3$	**1**$(PF_6)_4$
Empirical formula	$C_{96}H_{98}Cl_4F_{12}Fe_2N_6P_6Ru$	$C_{188}H_{188}F_{42}Fe_4N_{12}O_{1.25}P_{15}Ru_2$	$C_{96}H_{97}F_{24}Fe_2N_7P_8Ru$
Formula weight	2104.19	4323.58	2265.33
Crystal size (mm)	0.420 × 0.305 × 0.280	0.252 × 0.210 × 0.125	0.408 × 0.310 × 0.306
Temperature/K	293(2)	293(2)	293(2)
Crystal system	triclinic	triclinic	monoclinic

Space group	Pī	Pī	$P2_1/n$
a/Å	11.9194(5)	23.186(2)	17.219(4)
b/Å	14.9993(5)	24.5526(19)	14.916(3)
c/Å	16.5490(5)	25.215(2)	20.604(5)
α/°	106.505(3)	113.495(8)	90
β/°	105.512(3)	113.588(9)	112.212(4)
γ/°	95.595(3)	90.261(7)	90
Volume/Å^3	2684.80(18)	11832(2)	4899(2)
Z	1	2	2
ρ_{calcd}/g cm^{-3}	1.301	1.214	1.536
μ/mm^{-1}	0.659	3.015	0.671
F(000)	1078.0	4410.0	2308.0
λ (Mo/Ga Kα, Å)	Mo, 0.71073	Ga, 1.3405	Mo, 0.71073
2θ range/°	4.542-54.966	4.548-104.096	5.466-55.016
Index range	-15 ≤ h ≤ 15 -19 ≤ k ≤ 19 -21 ≤ l ≤ 21	-27 ≤ h ≤ 27 -28 ≤ k ≤ 28 -29 ≤ l ≤ 29	-22 ≤ h ≤ 22 -19 ≤ k ≤ 19 -26 ≤ l ≤ 26
Reflections collected	43294	315602	72923
Independent reflections	12216 (R_{int} = 0.0493, R_{sigma} = 0.0440)	39934 (R_{int} = 0.3644, R_{sigma} = 0.1920)	11175 (R_{int} = 0.0631, R_{sigma} = 0.0476)
Data/restraints/parameters	12216/0/579	39934/4953/2322	11175/51/673
Goodness-of-fit on F^2	1.048	1.018	1.029
R_1, wR_2 (I ≥ 2σ (I))	R_1 = 0.0747, wR_2 = 0.1959	R_1 = 0.2318, wR_2 = 0.5523	R_1 = 0.0624, wR_2 = 0.1573
R_1, wR_2 (all data)	R_1 = 0.1001, wR_2 = 0.2121	R_1 = 0.3088, wR_2 = 0.6001	R_1 = 0.0689, wR_2 = 0.1632

Table S2 Crystallographic data for **2**$(PF_6)_n$ (n = 2, 3, 4)

	2$(PF_6)_2$	**2**$(PF_6)_3$	**2**$(PF_6)_4$
Empirical formula	$C_{98}H_{102}F_{12}Fe_2N_6P_6Ru$	$C_{398}H_{420}Cl_{12}F_{72}Fe_8N_{24}O_3P_{28}Ru_4$	$C_{198}H_{208}Cl_4F_{48}Fe_4N_{12}O_5P_{16}Ru_2$
Formula weight	1990.44	9099.20	4810.61
Crystal size (mm)	0.412 × 0.360 × 0.341	0.286 × 0.110 × 0.102	0.408 × 0.360 × 0.355
Temperature/K	293(2)	110.6(3)	293(2)
Crystal system	orthorhombic	triclinic	monoclinic
Space group	$Pca2_1$	Pī	$P2_1/n$
a/Å	21.111(5)	15.54011(5)	13.159(3)
b/Å	15.961(3)	20.78264(9)	28.160(6)
c/Å	34.384(8)	33.67197(16)	36.422(7)
α/°	90	107.8851(4)	90
β/°	90	95.1931(3)	97.758(5)

γ/°	90	90.3443(3)	90
Volume/Å^3	11586(4)	10300.28(8)	13373(5)
Z	4	1	2
ρ_{calcd}/g cm^{-3}	1.141	1.467	1.195
μ/mm^{-1}	0.518	3.866	0.535
F(000)	4104.0	4656.0	4904.0
λ (Mo/Ga Kα, Å)	Mo, 0.71073	Ga, 1.3405	Mo, 0.71073
2θ range/°	2.368-54.97	4.818-104.096	4.258-55.018
Index range	-27 ≤ h ≤ 27 -20 ≤ k ≤ 20 -44 ≤ l ≤ 44	-18 ≤ h ≤ 18 -24 ≤ k ≤ 24 -39 ≤ l ≤ 39	-17 ≤ h ≤ 16 -36 ≤ k ≤ 36 -47 ≤ l ≤ 47
Reflections collected	164564	248527	186641
Independent reflections	26501 (R_{int} = 0.0899, R_{sigma} = 0.0467)	34905 (R_{int} = 0.0827, R_{sigma} = 0.0324)	30205 (R_{int} = 0.0650, R_{sigma} = 0.0503)
Data/restraints/parameters	26501/116/1081	34905/30/2531	30205/64/1365
Goodness-of-fit on F^2	1.054	1.047	0.999
R_1, wR_2 (I ≥ 2σ (I))	R_1 = 0.0832, wR_2 = 0.2227	R_1 = 0.0601, wR_2 = 0.1611	R_1 = 0.0904, wR_2 = 0.2450
R_1, wR_2 (all data)	R_1 = 0.0906, wR_2 = 0.2310	R_1 = 0.0630, wR_2 = 0.1634	R_1 = 0.1074, wR_2 = 0.2670

Table S3 Selected bond lengths (Å) of **1**$(PF_6)_3$

	$\mathbf{1}^{3+}$	$\mathbf{1}^{3+}_{av}$
Ru1-C1	1.967(9)	-
Ru1-C2	1.999(10)	-
C1≡N1	1.396(9)	-
C2≡N2	1.249(13)	-
Fe1-N1	1.938(8)	-
Fe2-N2	1.913(8)	-
Fe1-P1	2.302(6)	2.313
Fe1-P2	2.322(6)	
Fe2-P3	2.252(7)	2.245
Fe2-P4	2.237(6)	

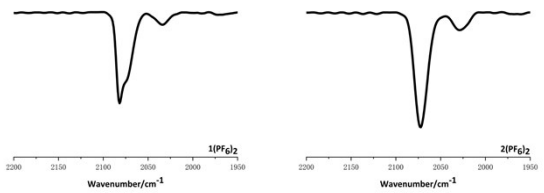

Fig. S4 IR spectra of **1**$(PF_6)_2$ and **2**$(PF_6)_2$ by the grinding and pressing tablet process.

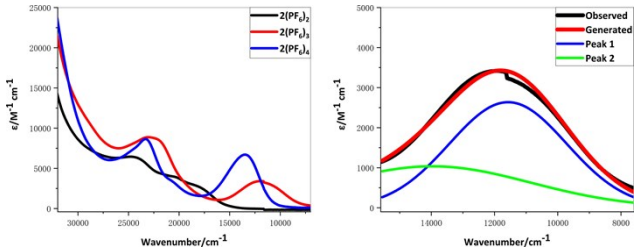

Fig. S5 The UV-vis-NIR spectroscopy of **2**$(PF_6)_n$ (n = 2, 3, 4; left) in CH_3CN and the Gaussian peak fitting of **2**$(PF_6)_3$ (right).

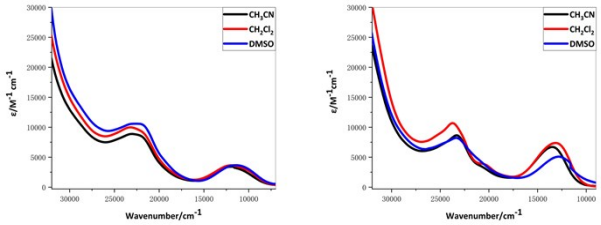

Fig. S6 The UV-vis-NIR spectroscopy of **2**$(PF_6)_n$ (n = 3 (left), 4 (right)) in different solvents.

Table S4 The maximum absorption (v_{max}/cm^{-1}(λ_{max}/nm)) of the broad MMCT absorption peak for **1**$(PF_6)_n$ and **2**$(PF_6)_n$ (n = 3 (before the Gaussian peak fitting), 4) in different solvents

	1$(PF_6)_3$	**1**$(PF_6)_4$	**2**$(PF_6)_3$	**2**$(PF_6)_4$
CH_3CN	13707(730)	14085(710)	11933(838)	13477(742)
CH_2Cl_2	13812(724)	13966(716)	11990(834)	13158(760)
DMSO	13369(748)	13123(762)	11468(872)	12853(778)

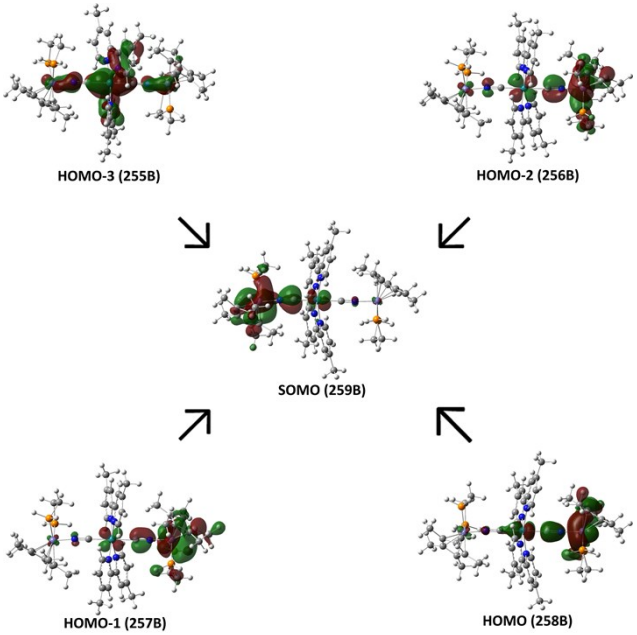

Fig. S7 Molecular orbital diagrams of HOMO-3 (255B), HOMO-2 (256B), HOMO-1 (257B), HOMO (258B) and SOMO (259B) of **2**$(PF_6)_3$ in dichloromethane (isocontour value: 0.02 $[e/b^3]^{1/2}$).

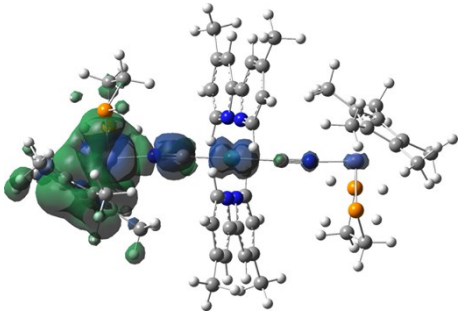

Fig. S8 The spin density distribution of **2**$(PF_6)_3$ (Ru, 0.103; Fe, 0.004 and 1.444; contour value: 0.0004 e/bohr^3).

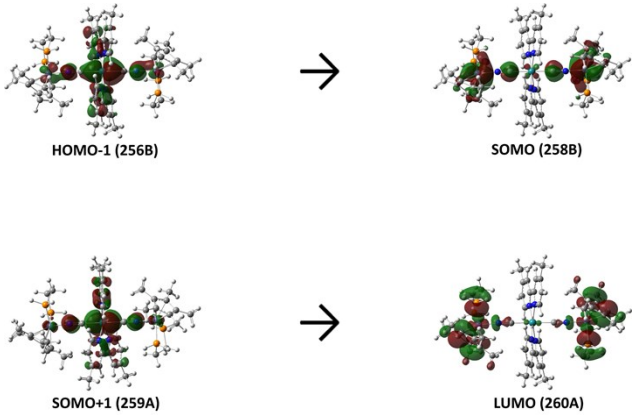

Fig. S9 Molecular orbital diagrams of HOMO-1 (256B), SOMO (258B), SOMO+1 (259A) and LUMO (260A) of **2**$(PF_6)_4$ in dichloromethane (isocontour value: 0.02 $[e/b^3]^{1/2}$).

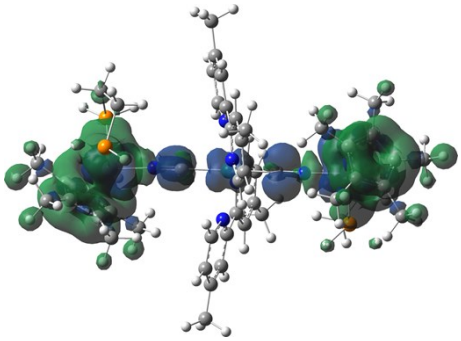

Fig. S10 The spin density distribution of **2**$(PF_6)_4$ (Ru, 0.108; Fe, 1.543 and 1.553; contour value: 0.0004 e/bohr^3).

Table S5 Calculated and experimental electronic transition absorption peak of **1**$(PF_6)_n$ and **2**$(PF_6)_n$ (n = 3, 4)

Complex	Electronic transition	f	ν_{max} (exp)/cm^{-1}	ν_{max} (calc)/cm^{-1}
1$(PF_6)_3$	HOMO (242B) → SOMO (243B) (52%)	0.0428	13337	13625
	HOMO-4 (238B) → SOMO (243B) (28%) HOMO-3 (239B) → SOMO (243B) (35%)	0.0514	16301	18879
1$(PF_6)_4$	HOMO-1 (220B) → SOMO (222B) (66%) HOMO (221B) → SOMO (222B) (20%)	0.1781	14085	17884
2$(PF_6)_3$	HOMO (258B) → SOMO (259B) (80%)	0.0697	11573	11457
	HOMO-3 (255B) → SOMO (259B) (9%) HOMO-2 (256B) → SOMO (259B) (22%) HOMO-1 (257B) → SOMO (259B) (54%)	0.0433	13976	14755
2$(PF_6)_4$	HOMO-1 (256B) → SOMO (258B) (39%) SOMO+1 (259A) → LUMO (260A) (14%)	0.1299	13477	17707

Optimized Cartesian Coordinates of 1^{3+}

Atomic Name	X	Y	Z
Ru	0.040958	0.061893	0.038158
Fe	-5.072719	0.007555	-0.069808
P	-5.201645	1.544789	1.582916
P	-5.439226	1.734245	-1.483452
N	-3.19711	0.263442	-0.112469
N	-0.113434	-1.70037	-1.101369
N	-0.272502	-1.431648	1.4837
C	-2.008282	0.269351	-0.077956
C	0.059231	-2.864149	-0.396675
C	-0.039222	-2.71388	1.061007
C	-4.996529	-1.942083	0.681224
C	-0.690942	-1.229583	2.755362
H	-0.990265	-0.21973	3.012044
C	-8.296043	-0.370931	-0.318571
H	-8.499116	0.316185	0.512897
H	-9.082963	-1.135178	-0.309978
H	-8.410314	0.199549	-1.248469

C	-0.354923	-1.773967	-2.431062
H	-0.620502	-0.846543	-2.924573
C	-6.933785	-0.98288	-0.208318
C	-4.892765	-1.972854	-0.764812
C	-6.27838	-1.376432	1.014061
C	-0.084118	-3.791193	1.955558
H	0.113461	-4.800216	1.610949
C	-6.08386	-1.396992	-1.311947
C	-3.75563	-2.535286	-1.552252
H	-3.608778	-1.982667	-2.489369
H	-3.938389	-3.58667	-1.810655
H	-2.816199	-2.486594	-0.983714
C	-3.982378	-2.470831	1.642058
H	-2.962644	-2.26785	1.281212
H	-4.081639	-3.555421	1.781864
H	-4.0832	-2.000283	2.628506
C	-0.775368	-2.265031	3.68824
H	-1.113136	-2.055933	4.696102
C	0.13217	-4.102283	-1.049383
H	0.275993	-5.013789	-0.479844
C	-0.316801	-2.979676	-3.13464
H	-0.52221	-2.989873	-4.198293
C	-0.430395	-3.56423	3.291527
H	-0.471553	-4.387103	3.995971
C	-6.419398	-1.3287	-2.76796
H	-7.220641	-0.613006	-2.979392
H	-6.771987	-2.306751	-3.11854
H	-5.549305	-1.057591	-3.37873
C	-0.032845	-4.162022	-2.436955
H	0.013722	-5.112959	-2.955522
C	-6.855749	-1.273824	2.389684
H	-6.092202	-1.056599	3.147927
H	-7.324566	-2.226006	2.666426
H	-7.634653	-0.506359	2.456678
C	-5.152796	3.286987	0.808237
H	-5.526006	4.034987	1.513321
H	-4.098593	3.509929	0.592906
C	-5.97728	3.26222	-0.481978
H	-5.850972	4.179447	-1.063835
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Fe	5.117664	-0.073716	0.053266
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P	5.492969	-2.020888	1.247645
N	3.239525	-0.253002	0.123206

N	0.128856	1.814241	1.18832
N	0.240098	1.58346	-1.403515
C	2.043206	-0.165147	0.119531
C	-0.151946	2.96771	0.50242
C	-0.100843	2.83486	-0.958633
C	5.229745	1.968268	-0.584548
C	0.574856	1.42294	-2.705489
H	0.935419	0.441457	-2.99346
C	8.382919	0.077576	0.308453
H	8.501043	-0.641076	-0.512686
H	9.211998	0.79177	0.231161
H	8.514216	-0.462886	1.251465
C	0.374708	1.888539	2.51806
H	0.696913	0.97222	2.999905
C	7.068602	0.785956	0.245235
C	5.096267	1.894489	0.852201
C	6.472763	1.333181	-0.949635
C	-0.234469	3.908845	-1.84895
H	-0.531489	4.887166	-1.487678
C	6.225648	1.163089	1.37172
C	3.997731	2.480254	1.670515
H	3.763079	1.849388	2.535687
H	4.291608	3.467067	2.049741
H	3.080328	2.604254	1.084012
C	4.263925	2.607004	-1.524824
H	3.232666	2.505357	-1.163543
H	4.47749	3.677104	-1.638707
H	4.314171	2.155762	-2.522845
C	0.484774	2.459557	-3.636176
H	0.751443	2.28146	-4.671093
C	-0.310804	4.188654	1.171717
H	-0.551221	5.089359	0.617784
C	0.252243	3.078997	3.236831
H	0.452032	3.089695	4.30165
C	0.037581	3.717362	-3.206826
H	-0.070152	4.535402	-3.909895
C	6.522588	0.956536	2.82086
H	7.289478	0.193441	2.986552
H	6.903731	1.886566	3.260717
H	5.627413	0.675358	3.387953
C	-0.130257	4.24477	2.556963
H	-0.2549	5.180656	3.089625
C	7.080481	1.31768	-2.312291
H	6.333822	1.241425	-3.111523

H	7.619285	2.259894	-2.475386
H	7.81345	0.513981	-2.434529
C	4.80783	-3.213838	-1.188948
H	5.012389	-3.940955	-1.979666
H	3.738909	-3.259245	-0.944885
C	5.676577	-3.47884	0.045943
H	5.399901	-4.4146	0.538763
H	6.737363	-3.548258	-0.223679
H	6.575723	-2.177135	2.168936
H	4.37524	-2.383528	2.064263
H	4.174206	-1.204799	-2.801129
H	6.347088	-1.594388	-2.585975
H	-6.337741	1.636194	2.457643
H	-4.144068	1.628768	2.559453
H	-4.298655	2.259254	-2.193232
H	-6.392099	1.703686	-2.555267

Optimized Cartesian Coordinates of 1^{4+}

Atomic Name	X	Y	Z
Ru	-0.000012	-0.000143	0.000315
Fe	-5.144491	0.048684	-0.049038
P	-5.383187	1.714577	1.551758
P	-5.61676	1.76841	-1.554292
N	-3.229496	0.29343	-0.056427
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N	-0.238715	-1.638289	1.31115
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H	-0.805652	-2.589154	4.506945
C	0.098751	-4.042723	-1.490161
H	0.288785	-5.00234	-1.022663
C	-0.437091	-2.732037	-3.441297
H	-0.661877	-2.641519	-4.497359
C	-0.212751	-3.939197	2.912878
H	-0.179477	-4.825901	3.535758
C	-6.486249	-1.444227	-2.665037
H	-7.259951	-0.724549	-2.949565
H	-6.864394	-2.435413	-2.94527
H	-5.59653	-1.255451	-3.276405
C	-0.111881	-3.97129	-2.871415
H	-0.058249	-4.86491	-3.482912
C	-7.110265	-1.111405	2.459917
H	-6.38027	-0.934382	3.258146
H	-7.641542	-2.036632	2.719056
H	-7.857077	-0.311399	2.477918
C	-5.245974	3.391738	0.682806
H	-5.589973	4.191117	1.344844
H	-4.183757	3.557832	0.465168
C	-6.078055	3.339564	-0.60185
H	-5.913268	4.223501	-1.223764
H	-7.151109	3.287353	-0.381397
Fe	5.144507	-0.048466	0.048934
P	5.382906	-1.714015	-1.552371
P	5.617672	-1.768546	1.553496
N	3.229521	-0.293455	0.056665
N	0.191878	1.652344	1.298224
N	0.238479	1.638065	-1.310481
C	2.036382	-0.239571	0.037135
C	-0.026655	2.875436	0.717787
C	0.002133	2.867698	-0.751067
C	5.203502	1.90025	-0.862785
C	0.557435	1.571462	-2.625691
H	0.844585	0.597504	-3.004975

C	8.408227	0.292786	0.326616
H	8.59264	-0.504277	-0.404286
H	9.200186	1.039615	0.187033
H	8.543677	-0.126933	1.32845
C	0.470513	1.600766	2.622997
H	0.747487	0.631657	3.021495
C	7.064031	0.918522	0.148166
C	5.036839	2.011445	0.569918
C	6.473857	1.274672	-1.121507
C	-0.041009	4.02613	-1.538882
H	-0.244224	4.991103	-1.088296
C	6.18675	1.416487	1.202049
C	3.896357	2.660993	1.276042
H	3.760472	2.245786	2.280674
H	4.080363	3.737148	1.385671
H	2.955723	2.532094	0.72509
C	4.245684	2.379504	-1.899015
H	3.222311	2.417779	-1.506838
H	4.514186	3.388139	-2.237936
H	4.247229	1.728678	-2.78208
C	0.550254	2.692692	-3.458218
H	0.804873	2.589269	-4.506265
C	-0.099027	4.04226	1.491034
H	-0.289203	5.001892	1.023622
C	0.437306	2.731488	3.441977
H	0.662306	2.640933	4.49799
C	0.211706	3.939055	-2.91208
H	0.178131	4.825789	-3.534903
C	6.48524	1.444886	2.664802
H	7.259203	0.725582	2.949564
H	6.862721	2.436261	2.945251
H	5.595398	1.25556	3.275826
C	0.111834	3.970745	2.872245
H	0.058221	4.86431	3.483824
C	7.111086	1.111502	-2.459871
H	6.381376	0.934737	-3.258414
H	7.642681	2.036638	-2.718697
H	7.85774	0.311337	-2.477642
C	5.247204	-3.391534	-0.68384
H	5.59156	-4.190446	-1.346256
H	4.185187	-3.558502	-0.465902
C	6.079666	-3.339183	0.600561
H	5.915566	-4.223353	1.222324
H	7.152624	-3.2863	0.379814

H	6.602368	-1.653478	2.582586
H	4.460956	-2.143696	2.307499
H	4.40895	-1.752826	-2.599051
H	6.60284	-1.813343	-2.29458
H	-6.603595	1.814809	2.293061
H	-4.409931	1.753174	2.599096
H	-4.460049	2.142787	-2.308678
H	-6.601754	1.653379	-2.583098

Optimized Cartesian Coordinates of 2^{3+}

Atomic Name	X	Y	Z
Ru	-0.087127	0.043562	0.077826
Fe	5.064563	-0.077242	-0.084296
Fe	-5.164436	0.021152	-0.033041
P	5.069569	-2.111989	0.899345
P	5.029641	-1.192059	-2.047383
P	-5.190615	1.364098	-1.913733
P	-5.335208	2.012361	1.125937
N	-3.293949	0.141413	0.064054
N	3.166314	-0.090271	-0.051286
N	-0.247137	1.741457	-1.16968
N	0.095359	-1.606439	-1.238065
N	0.300504	1.646945	1.395018
C	-2.093901	0.114545	0.099796
N	-0.281748	-1.613879	1.360253
C	0.138514	-2.840508	-0.645257
C	1.978983	-0.047126	0.000351
C	1.196358	2.570541	3.435776
H	1.557367	2.390901	4.443565
C	0.78456	-3.912363	-2.737307
C	0.33381	2.897673	0.842024
C	0.469926	-3.990571	-1.372147
H	0.504662	-4.955281	-0.875
C	0.754057	4.012857	1.577404
H	0.780816	4.993413	1.112069
C	-5.171329	3.195405	-1.402934
H	-4.60292	3.778978	-2.133225
H	-6.207267	3.552213	-1.42605
C	1.187888	3.875475	2.90411
C	-0.055241	2.957815	-0.569884
C	0.764535	1.498488	2.660814
H	0.827121	0.485712	3.040229
C	-4.572409	3.330921	0.001348
H	-4.744052	4.33097	0.409002

H	-3.492595	3.1373	-0.0063
C	-0.25229	4.155613	-1.269016
H	-0.082583	5.107347	-0.774714
C	-0.716369	1.726683	-2.441716
H	-0.940316	0.752472	-2.86281
C	-0.365665	-4.020931	1.533109
H	-0.264612	-4.992013	1.057893
C	-0.712061	-3.957713	2.891553
C	-0.895987	-2.672459	3.439872
H	-1.201772	-2.556049	4.474829
C	-5.85684	-1.764077	-0.912836
C	-7.030708	-0.998593	-0.522898
C	0.783747	-2.62707	-3.314723
H	1.055306	-2.492649	-4.356954
C	-0.6824	-1.543055	2.654349
H	-0.858442	-0.550244	3.052979
C	0.45085	-1.516853	-2.54331
H	0.507665	-0.520194	-2.964198
C	-5.105304	-2.058159	0.285446
C	-0.163748	-2.85097	0.789583
C	-3.870142	-2.88958	0.348842
H	-3.25242	-2.754045	-0.54645
H	-4.135854	-3.952007	0.418167
H	-3.258599	-2.638946	1.223213
C	5.526771	1.310154	1.410803
C	6.988624	0.778765	-0.333257
C	4.695509	-3.038769	-1.700357
H	3.608965	-3.140362	-1.560281
H	4.994977	-3.655763	-2.552756
C	-6.981854	-0.802215	0.897195
C	8.17995	0.252313	-1.070724
H	8.396188	-0.790809	-0.804317
H	9.075529	0.838983	-0.830597
H	8.050896	0.301198	-2.157713
C	-0.934477	2.886228	-3.181736
H	-1.289464	2.811775	-4.205003
C	-5.311483	-1.455336	2.8192
H	-4.219772	-1.36834	2.885812
H	-5.59942	-2.398578	3.299661
H	-5.749401	-0.644995	3.411736
C	3.896876	2.906991	0.143121
H	3.444253	2.890726	-0.856444
H	4.178485	3.943357	0.371984
H	3.1284	2.597188	0.863322

C	-5.769136	-1.419153	1.399166
C	6.735384	0.592412	1.064897
C	5.084477	2.007128	0.222911
C	5.443322	-3.433695	-0.423375
H	6.528302	-3.430526	-0.587328
H	5.157859	-4.430463	-0.07486
C	5.961908	1.668659	-0.858567
C	-8.152272	-0.564382	-1.407644
H	-8.504075	0.444637	-1.160745
H	-9.008875	-1.239094	-1.285749
H	-7.879857	-0.584765	-2.467445
C	5.893472	2.213393	-2.250725
H	6.342599	1.531297	-2.982826
H	6.438492	3.162662	-2.324624
H	4.858881	2.402192	-2.561882
C	-0.67414	4.146739	-2.607
C	-8.042168	-0.135202	1.707475
H	-7.671369	0.225101	2.672823
H	-8.84398	-0.852913	1.923263
H	-8.505417	0.703339	1.175194
C	-0.833594	5.415674	-3.390345
H	-1.082586	6.265164	-2.747778
H	-1.604402	5.324375	-4.161289
H	0.103289	5.664206	-3.903687
C	4.907169	1.407922	2.767846
H	3.811769	1.460371	2.69837
H	5.252856	2.300288	3.307053
H	5.156578	0.536562	3.385275
C	1.679586	5.043443	3.704592
H	1.257418	5.040661	4.714564
H	1.432735	5.99766	3.232365
H	2.770211	4.998892	3.815237
C	1.127443	-5.129297	-3.543384
H	1.403402	-5.976011	-2.909162
H	1.954036	-4.931095	-4.233269
H	0.271648	-5.441195	-4.154049
C	-5.519617	-2.260255	-2.280237
H	-6.07203	-1.729326	-3.062582
H	-5.770135	-3.323795	-2.377897
H	-4.447213	-2.156681	-2.48717
C	-0.88117	-5.195124	3.721127
H	-1.135789	-6.065862	3.110513
H	-1.655522	-5.068697	4.483479
H	0.051343	-5.42933	4.248944

C	7.626792	-0.1572	2.001948
H	7.098078	-0.517311	2.892116
H	8.432812	0.49937	2.352749
H	8.106789	-1.015624	1.515523
H	3.802436	-2.587956	1.400481
H	5.924692	-2.501014	1.984103
H	4.029099	-0.896405	-3.040838
H	6.187106	-1.251886	-2.897985
H	-6.602208	2.565032	1.502244
H	-4.605485	2.11469	2.351435
H	-6.208131	1.296879	-2.918568
H	-4.009672	1.204099	-2.707453

Optimized Cartesian Coordinates of 2^{4+}

Atomic Name	X	Y	Z
Ru	-0.014652	0.028268	-0.034189
Fe	5.136644	0.00963	-0.01635
Fe	-5.169827	-0.034596	-0.028545
P	5.355026	-0.913748	-2.139676
P	5.18741	-2.206576	0.700278
P	-5.285983	2.051967	1.001409
P	-5.406208	1.182644	-1.995366
N	0.208917	1.699655	1.246592
N	-0.206201	1.681373	-1.349032
N	3.22172	-0.050492	-0.048136
N	0.216612	-1.661501	-1.300542
N	-3.255568	0.0824	-0.050481
N	-0.238507	-1.60847	1.288797
C	2.027185	-0.009586	-0.033268
C	-2.060259	0.059446	-0.043902
C	0.211072	-2.885341	-0.683342
C	-0.348355	-4.012484	1.508846
H	-0.251271	-4.994311	1.055565
C	0.518778	-4.059141	-1.382442
H	0.504587	-5.016125	-0.869453
C	-0.590267	1.599794	-2.647227
H	-0.736405	0.604256	-3.049271
C	5.202647	2.027441	0.602602
C	0.908148	-2.747194	-3.346222
H	1.1877	-2.64339	-4.389884
C	0.850996	-4.021275	-2.747039
C	0.583736	1.631355	2.549037
H	0.706612	0.639426	2.968197
C	0.412475	4.103625	1.387976

H	0.371438	5.071682	0.898155
C	-0.364314	4.086362	-1.529732
H	-0.294564	5.061741	-1.057838
C	-0.135361	2.925378	-0.779987
C	-0.726859	-3.920945	2.858751
C	-0.830119	2.720084	-3.439223
H	-1.117474	2.591043	-4.477948
C	0.600767	-1.611342	-2.600272
H	0.691991	-0.627098	-3.043671
C	4.745707	-3.284619	-0.792393
H	4.9562	-4.335956	-0.576978
H	3.666277	-3.173716	-0.961492
C	-0.69282	4.012035	-2.893547
C	0.163484	2.934914	0.656959
C	-7.131885	-0.97899	-0.181113
C	5.548339	1.187296	1.727633
C	5.554065	-2.794111	-1.997422
H	5.233787	-3.281176	-2.922716
H	6.623268	-3.00202	-1.869495
C	7.141981	0.832519	0.055039
C	-0.12003	-2.859765	0.746206
C	6.176652	1.80282	-0.441967
C	-6.068634	-1.820411	-0.708293
C	-5.152292	-2.100384	0.376049
C	-0.670532	-1.51084	2.571252
H	-0.852271	-0.510606	2.947586
C	-5.576671	3.028859	-1.591827
H	-5.218859	3.633826	-2.429472
H	-6.646072	3.238397	-1.4695
C	-0.911867	-2.622358	3.374936
H	-1.243987	-2.481622	4.398762
C	0.73503	4.045769	2.753772
C	-4.80098	3.332458	-0.306376
H	-5.01526	4.342623	0.053635
H	-3.71808	3.24087	-0.460043
C	6.775832	0.497481	1.407088
C	0.839825	2.760386	3.323177
H	1.122417	2.643547	4.364736
C	-6.870468	-0.754863	1.215719
C	4.058668	2.979008	0.530202
H	4.380996	3.981395	0.839009
H	3.238032	2.670933	1.188927
H	3.663262	3.055453	-0.48944
C	-3.950611	-2.977804	0.304296

H	-3.514085	-2.984654	-0.700666
H	-4.222745	-4.009957	0.55814
H	-3.178055	-2.648683	1.009838
C	-5.620397	-1.399772	1.550916
C	-8.355472	-0.518586	-0.902498
H	-8.606284	0.523268	-0.665911
H	-9.2193	-1.126172	-0.603922
H	-8.265107	-0.612287	-1.988909
C	8.374075	0.353716	-0.639767
H	8.542975	-0.719647	-0.482963
H	9.258204	0.8734	-0.24948
H	8.345859	0.542811	-1.71727
C	-5.997091	-2.410205	-2.077935
H	-6.552297	-1.82295	-2.816301
H	-6.436408	-3.415622	-2.080398
H	-4.9628	-2.507504	-2.426479
C	-0.887375	5.241809	-3.727699
H	-1.174189	6.107712	-3.124728
H	-1.644387	5.092109	-4.503085
H	0.04493	5.50295	-4.243404
C	4.815656	1.097945	3.022422
H	3.744049	1.286775	2.890715
H	5.198675	1.838205	3.736292
H	4.931712	0.112737	3.4883
C	6.243845	2.544577	-1.735828
H	6.81474	2.008356	-2.500687
H	6.744056	3.510303	-1.590173
H	5.246629	2.755058	-2.138625
C	1.130708	-5.271673	-3.52469
H	1.548906	-6.061982	-2.89454
H	1.816188	-5.089948	-4.357361
H	0.203277	-5.665942	-3.958029
C	7.58066	-0.345015	2.336651
H	6.968666	-0.873834	3.07609
H	8.263287	0.302489	2.90309
H	8.208784	-1.070409	1.809222
C	-4.977158	-1.414834	2.895956
H	-3.884451	-1.459829	2.816727
H	-5.303975	-2.290041	3.471755
H	-5.23853	-0.528508	3.484451
C	-0.934286	-5.139764	3.70535
H	-1.723617	-4.988817	4.447357
H	-0.01936	-5.379463	4.261084
H	-1.187352	-6.018285	3.105642

C	-7.784291	-0.052532	2.160665
H	-7.259575	0.398522	3.010093
H	-8.491894	-0.779677	2.581108
H	-8.387683	0.71683	1.667431
C	0.965372	5.284016	3.56557
H	1.752461	5.138347	4.311305
H	0.056116	5.555657	4.11579
H	1.234707	6.140619	2.942
H	6.390065	-2.800125	1.202428
H	4.244472	-2.568706	1.712753
H	6.370544	-0.512415	-3.062481
H	4.172983	-0.750404	-2.930531
H	-4.245046	1.105821	-2.827841
H	-6.446299	0.928545	-2.94258
H	-4.391662	2.277133	2.094081
H	-6.518389	2.557727	1.526447