Dalton Transaction

Supporting Information

Different delocalized range in mixed valence cyanidometal-bridged Fe-Ru-Fe complexes controlled by terminal ligand substitution modification

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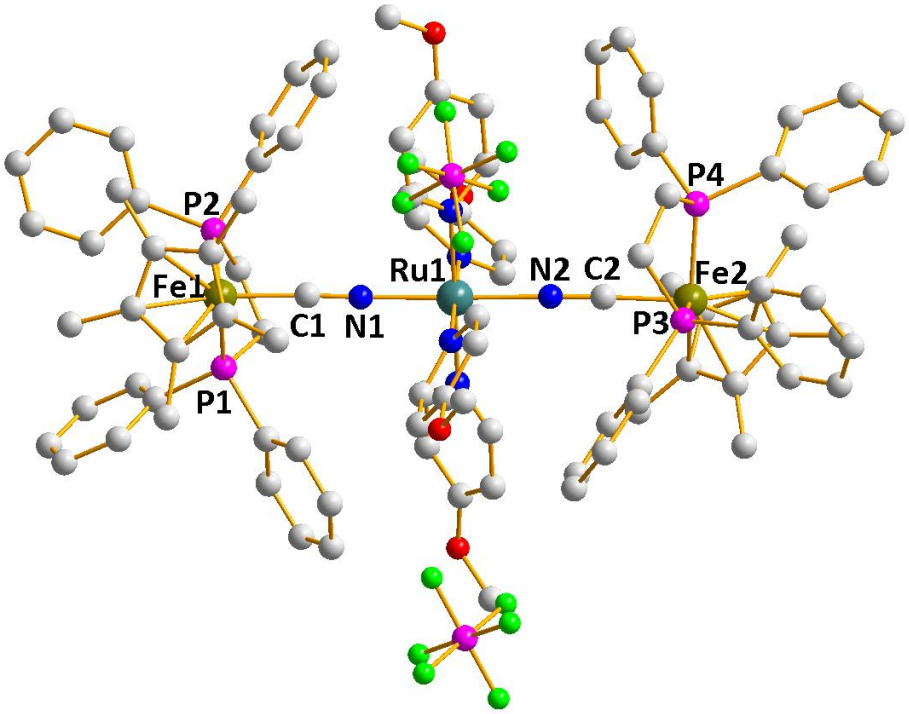

Fig. S1 Molecular structure of **2[PF_6]$_2$** (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink; F, bright green.

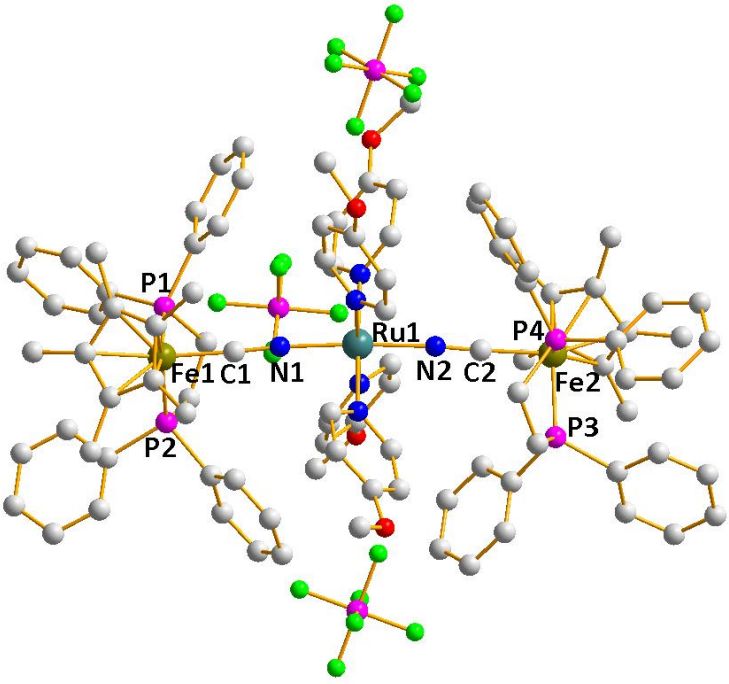

Fig. S2 Molecular structure of **2[PF_6]$_3$** (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink; F, bright green.

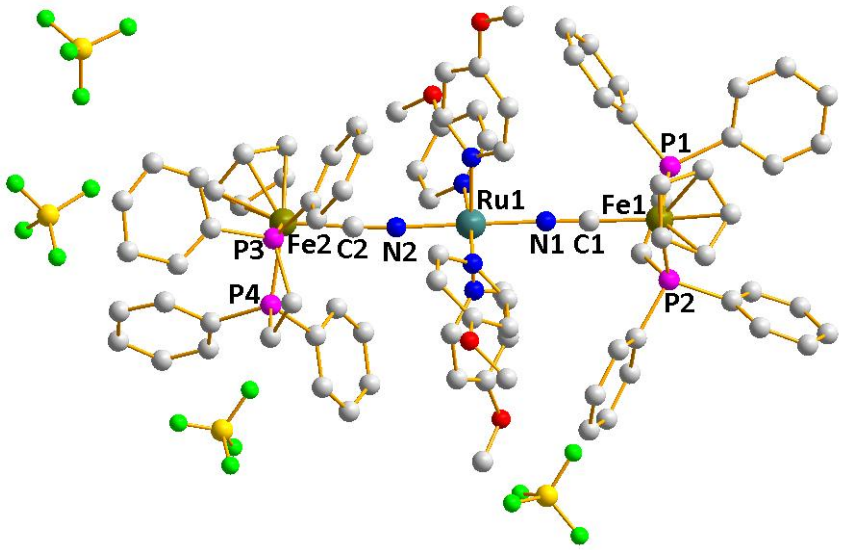

Fig. S3 Molecular structure of **2[BF$_4$]$_4$** (hydrogen atoms and solvent molecules have been removed for clarity). Ru, teal; Fe, dark yellow; C, gray; N, blue; P, pink; B, yellow; F, bright green.

Table S1. Selected bond lengths (Å), the distance between the metal centers (Å) and bond angle (°) of **1**$^{n+}$ (n = 2, 3, 4).

	1^{2+}	**1**$^{2+}_{average}$	**1**$^{3+}$	**1**$^{3+}_{average}$	**1**$^{4+}$	**1**$^{4+}_{average}$
Ru1-N1	2.055(5)	2.055(5)	1.991(3)	1.994(3)	2.002(4)	1.995(4)
Ru1-N2			1.996(3)		1.987(4)	
C1≡N1	1.166(7)	1.166(7)	1.162(4)	1.165(4)	1.157(6)	1.157(6)
C2≡N2			1.167(5)		1.157(6)	
Fe1-C1	1.893(6)	1.893(6)	1.841(3)	1.843(3)	1.900(5)	1.896(5)
Fe2-C2			1.844(3)		1.891(5)	
Fe1-P1	2.189(2)	2.187(2)	2.1926(10)	2.198(1)	2.2460(15)	2.244(1)
Fe1-P2	2.185(2)		2.2034(10)		2.2431(14)	
Fe2-P3	2.189(2)		2.2047(10)	2.197(1)	2.2265(16)	2.237(2)
Fe2-P4	2.185(2)		2.1899(10)		2.2471(18)	
Ru1···Fe1	5.077	5.077	4.982	4.990	5.048	5.033
Ru1···Fe2			4.998		5.018	
Ru1-N1-C1	171.9(5)	171.9(5)	172.9(3)	173.6	173.8(4)	173.4(4)
Ru1-N2-C2			174.3(3)		173.1(4)	
Fe1-C1-N1	172.5(5)	172.5(5)	175.7(3)	175.4	177.7(4)	176.8(5)
Fe2-C2-N2			175.2(3)		175.9(5)	
N1-Ru1-N2	180.0	--	177.69(12)	--	179.43(16)	--

Table S2. Selected bond lengths (Å), the distance between the metal centers (Å) and bond angle (°) of **2**$^{n+}$ (n = 2, 3, 4).

	2^{2+}	**2**$^{2+}_{average}$	**2**$^{3+}$	**2**$^{3+}_{average}$	**2**$^{4+}$	**2**$^{4+}_{average}$
Ru1-N1	2.062(3)	2.073(3)	2.024(5)		2.022(6)	2.020(6)
Ru1-N2	2.084(3)		2.008(5)		2.018(6)	
C1≡N1	1.163(4)	1.158(3)	1.190(8)	1.185	1.156(9)	

C2≡N2	1.152(4)		1.180(8)		1.143(9)	
Fe1-C1	1.904(3)	1.903(3)	1.873(6)		1.934(7)	1.930(7)
Fe2-C2	1.903(3)		1.875(6)		1.926(7)	
Fe1-P1	2.2202(10)		2.2270(19)	2.218(2)	2.298(2)	2.297(2)
Fe1-P2	2.2164(10)	2.214(1)	2.2090(19)		2.296(2)	
Fe2-P3	2.2120(11)		2.2352(19)	2.242(2)	2.312(2)	2.294(2)
Fe2-P4	2.2070(10)		2.2481(18)		2.276(2)	
Ru1---Fe1	5.126	5.132	5.085		5.108	5.096
Ru1---Fe2	5.137		5.058		5.085	
Ru1-N1-C1	177.2(3)	177.8(3)	175.3(5)		176.0(6)	
Ru1-N2-C2	178.4(3)		175.0(5)		176.8(6)	
Fe1-C1-N1	176.4(3)	177.2(3)	177.3(6)		176.9(7)	177.2(7)
Fe2-C2-N2	177.9(3)		177.8(6)		177.4(7)	
N1-Ru1-N2	178.81(11)		176.5(2)		176.8(2)	

Table S3. Crystallographic data for **1[X]$_n$ (X = PF_6 or BF_4, n = 2, 3, 4)**.

	1[PF_6]$_2$	**1[BF_4]$_3$**	**1[BF_4]$_4$**
Empirical formula	$C_{88}H_{86}F_{12}Fe_2N_6O_4P_6Ru$	$C_{96}H_{98}B_3F_{12}Fe_2N_{10}O_4P_4Ru$	$C_{92}H_{92}B_4F_{16}Fe_2N_8O_4P_4Ru$
Formula weight	1918.21	2052.92	2057.62
Crystal size (mm)	0.200 × 0.100 × 0.100	0.084 × 0.037 × 0.019	0.100 × 0.100 × 0.100
Temperature/K	293(2)	99.98(13)	100.15
Crystal system	triclinic	monoclinic	triclinic
Space group	Pī	$P2_1/n$	Pī
a/Å	11.366(4)	15.4029(2)	14.2053(3)
b/Å	13.418(6)	36.5766(4)	15.3072(3)
c/Å	15.982(6)	17.9000(2)	23.6959(6)
α/°	89.65(3)	90	82.436(2)
β/°	71.93(2)	108.3240(10)	78.481(2)
γ/°	67.437(16)	90	76.674(2)
Volume/Å^3	2122.1(15)	9573.3(2)	4893.0(2)
Z	1	4	2
ρcalcd/g cm-3	1.499	1.424	1.397
μ/mm^{-1}	0.707	3.293	3.320
F(000)	980.0	4220.0	2104.0
λ (Å)	$Mo_{Kα}$ (λ = 0.71073)	$Ga_{Kα}$ (λ = 1.3405)	$Ga_{Kα}$ (λ = 1.3405)
2θ range/°	4.378 - 49.994	4.2 - 120.32	5.18 - 105.862
Index range	-13 ≤ h ≤ 13 -15 ≤ k ≤ 15 -18 ≤ l ≤ 19	-19 ≤ h ≤ 18 -47 ≤ k ≤ 40 -21 ≤ l ≤ 23	-16 ≤ h ≤ 16 -18 ≤ k ≤ 18 -27 ≤ l ≤ 28
Reflections collected	18534	73200	45646
Independent reflections	7420 (R_{int} =0.0422, R_{sigma} = 0.0602)	21201 (R_{int} =0.0762, R_{sigma} = 0.0608)	16470 (R_{int} =0.0606, R_{sigma} = 0.0685)
Data/restraints/parameters	7420/0/547	21201/0/1197	16470/54/1174
Goodness-of-fit on F2	1.142	1.027	1.082

R1, wR2 (I ≥ 2σ (I))	0.0771, 0.1367	0.0642, 0.1662	0.0692, 0.1848
R1, wR2 (all data)	0.0960, 0.1544	0.0754, 0.1731	0.0909, 0.2045

Table S4. Crystallographic data for **2[X]$_n$ (X = PF_6 or BF_4, n = 2, 3, 4)**.

	2[PF_6]$_2$	**2[PF_6]$_3$**	**2[BF_4]$_4$**
Empirical formula	$C_{99}H_{108}Cl_2F_{12}Fe_2N_6O_4P_6Ru$	$C_{105}H_{122}Cl_6F_{18}Fe_2N_8O_5P_7Ru$	$C_{99}H_{108}B_4Cl_2F_{16}Fe_2N_6O_4P_4Ru$
Formula weight	2143.40	2532.34	2200.70
Crystal size (mm)	0.200 × 0.200 × 0.200	0.213 × 0.174 × 0.151	0.053 × 0.041 × 0.027
Temperature/K	293(2)	293(2)	99.9(3)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	C2/c	$P\bar{1}$
a/Å	13.7860(2)	29.9516(8)	12.8285(2)
b/Å	32.4422(4)	26.1705(4)	15.42782(19)
c/Å	25.3027(4)	31.3955(8)	28.5354(3)
α/°	90	90	96.4022(9)
β/°	100.979(2)	116.090(3)	101.3199(12)
γ/°	90	90	91.2395(12)
Volume/Å^3	11109.5(3)	22101.7(10)	5497.70(13)
Z	4	8	2
ρcalcd/g cm-3	1.282	1.522	1.329
μ/mm^{-1}	3.300	4.106	3.270
F(000)	4416.0	10392.0	2260.0
λ (Å)	$Ga_{K\alpha}$ (λ = 1.3405)	$Ga_{K\alpha}$ (λ = 1.3405)	$Ga_{K\alpha}$ (λ = 1.3405)
2θ range/°	3.896 - 105.862	4.166 - 105.862	5.016 - 105.862
Index range	-15 ≤ h ≤ 16 -25 ≤ k ≤ 38 -28 ≤ l ≤ 30	-35 ≤ h ≤ 35 -29 ≤ k ≤ 31 -37 ≤ l ≤ 37	-15 ≤ h ≤ 15 -17 ≤ k ≤ 18 -32 ≤ l ≤ 33
Reflections collected	79138	103307	62367
Independent reflections	19597 (R_{int} =0.0410, R_{sigma} = 0.0367)	10493 (R_{int} =0.0599, R_{sigma} = 0.0342)	19396 (R_{int} =0.0928, R_{sigma} = 0.0810)
Data/restraints/parameters	19597/0/1203	19493/0/1368	19396/12/1254
Goodness-of-fit on F2	1.047	1.073	1.031
R1, wR2 (I ≥ 2σ (I))	0.0538, 0.1558	0.0889, 0.2397	0.1104, 0.2919
R1, wR2 (all data)	0.0648, 0.1624	0.0940, 0.2430	0.1232, 0.3020

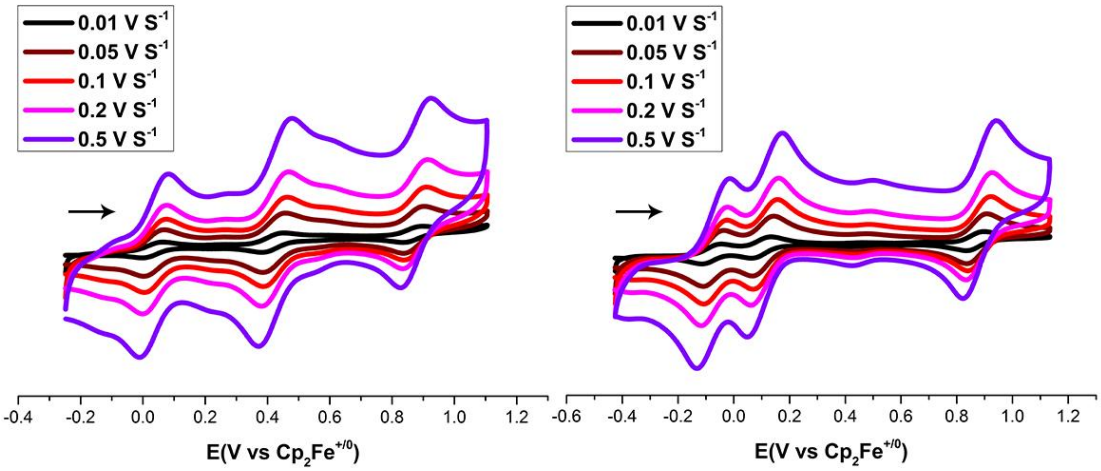

Fig S4. Cyclic voltammograms of **1[PF_6]$_2$** (left), and **2[PF_6]$_2$** (right) in a 0.1 M chloroform solution of Bu_4NPF_6 at a scan rate from 0.01 to 0.5 V s^{-1} at room temperature. Init E (**1[PF_6]$_2$**) =-0.248 V vs Ag/AgCl; Init E (**2[PF_6]$_2$**) = -0.425V.

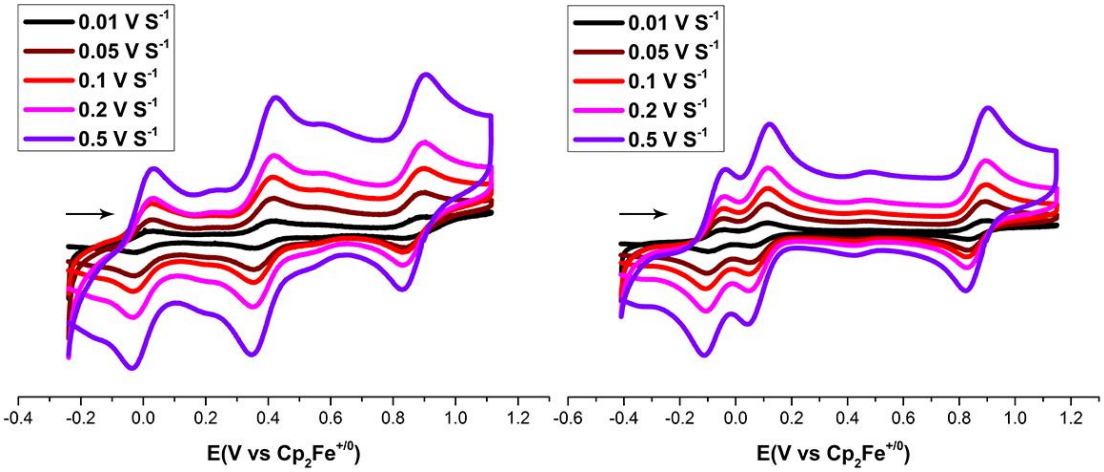

Fig S5. Cyclic voltammograms of **1[PF_6]$_2$** (left), and **2[PF_6]$_2$** (right) in a 0.1 M acetonitrile solution of Bu_4NPF_6 at a scan rate from 0.01 to 0.5 V s^{-1} at room temperature. Init E (**1[PF_6]$_2$**) =-0.239 V; Init E (**2[PF_6]$_2$**) = -0.409 V.

Table S5. Half-wave potentials ($E_{1/2}$ vs Fc/Fc^+) and difference between the redox process (ΔE) of **1[PF_6]$_2$** and **2[PF_6]$_2$** from cyclic voltammetry at a scan rate of 0.1 V s^{-1} in acetronitrile.

	$E_{1/2}(1)$/V	$E_{1/2}(2)$/V	$E_{1/2}(3)$/V	$\Delta E_{1/2}(1)$/V	$\Delta E_{1/2}(2)$/V
1[PF_6]$_2$	-0.004	0.384	0.865	0.392	0.481
2[PF_6]$_2$	-0.076	0.080	0.861	0.156	0.781

Table S6. Half-wave potentials ($E_{1/2}$ vs Fc/Fc^+), and electron counts (n) of **1[PF_6]$_2$** and **2[PF_6]$_2$** from cyclic voltammetry at a scan rate of 0.01 V s^{-1} in dichloromethane.

	$E_{1/2}(1)$/V	n	$E_{1/2}(2)$/V	n	$E_{1/2}(3)$/V	n
1[PF_6]$_2$	0.031	1.07	0.416	1.28	0.866	0.95
2[PF_6]$_2$	-0.080	1.15	0.098	1.15	0.866	1.05

Table S7. Half-wave potentials ($E_{1/2}$ vs Fc/Fc^+), and electron counts (n) of **1[PF$_6$]$_2$** and **2[PF$_6$]$_2$** from cyclic voltammetry at a scan rate of 0.01 V s^{-1} in acetonitrile.

	$E_{1/2}(1)$/V	n	$E_{1/2}(2)$/V	n	$E_{1/2}(3)$/V	n
1[PF$_6$]$_2$	-0.002	1.00	0.384	0.95	0.866	0.83
2[PF$_6$]$_2$	-0.027	0.92	0.086	0.92	0.864	1.03

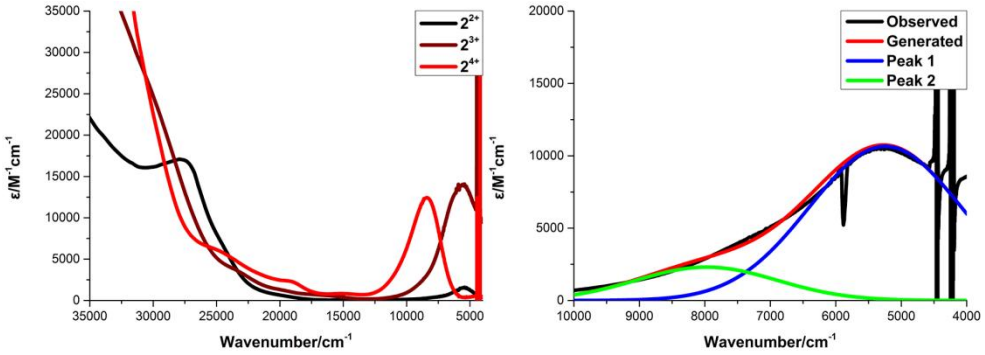

Fig. S6 The Gaussian peak fitting of the UV-Vis-NIR spectra of **2^{3+}** in dichlromethane at room temperature.

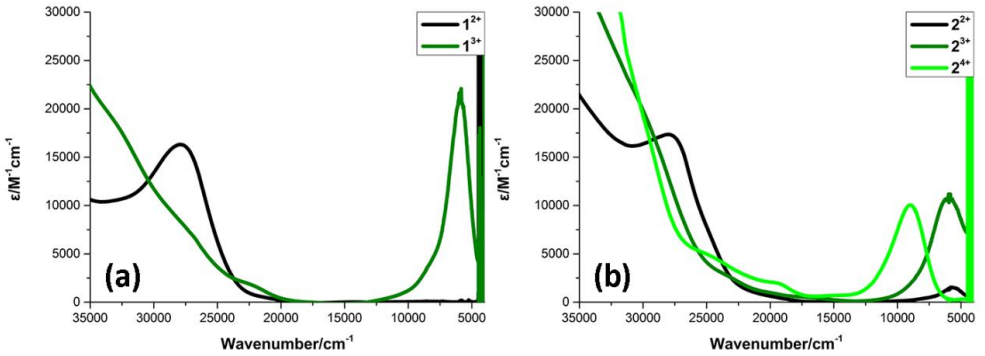

Fig. S7 The UV-vis-NIR spectroscopy of (a) **1^{n+}** and (b) **2^{n+}** (n = 2, black; n = 3, olive; n = 4, green) in acetonitrile at room temperature. The UV-vis-NIR spectroscopy of **1^{4+}** in acetonitrile could not be obtained since it gets reduced into **1^{3+}** immediately when dissolves.

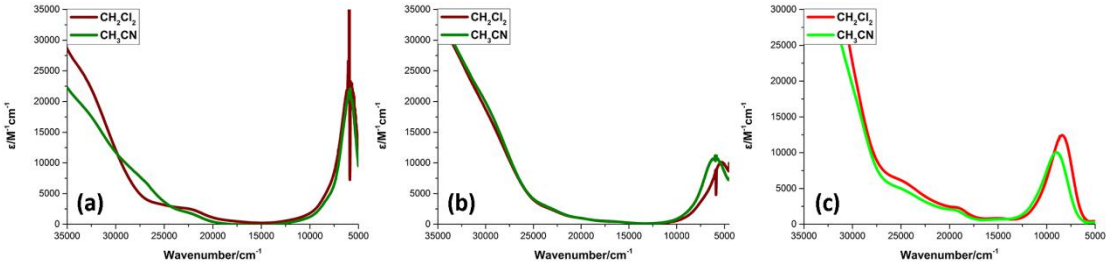

Fig. S8 UV-Vis-NIR spectra of (a) **1^{3+}**, (b) **2^{3+}** and (c) **2^{4+}** in different solvents

Table S8. The UV-vis-NIR absorption (cm^{-1}) of **N^{n+}** (N = 1, 2; n = 3, 4) in acetonitrile at room temperature.

N^{3+}	**λ_{max} (exp)/cm^{-1} (ε/$M^{-1}cm^{-1}$)**	**N^{4+}**	**λ_{max} (exp)/cm^{-1} (ε/$M^{-1}cm^{-1}$)**
1^{3+}	5872 (20939)	**1^{4+}**	_[a]
2^{3+}	5930 (10709)	**2^{4+}**	9004 (10012)

[a] The data could not be obtained because **1^{4+}** turns extremely fast into **1^{3+}** when dissolves in acetonitrile.

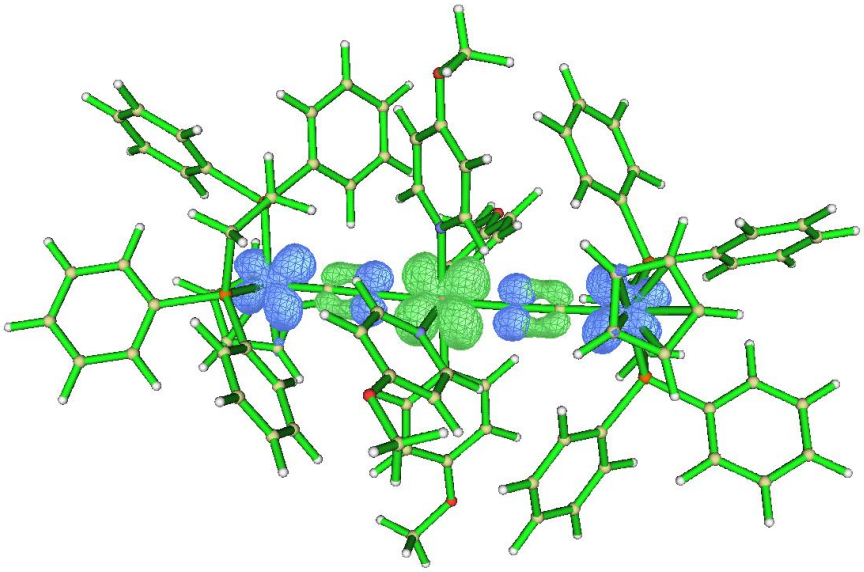

Fig. S9. Redistribution of the electron density for the electronic transition of $\mathbf{1}^{3+}$ in the calculated 1655 nm transition band. The green and blues areas represent gain and losses of density. The isosurface value is -0.0004 au.

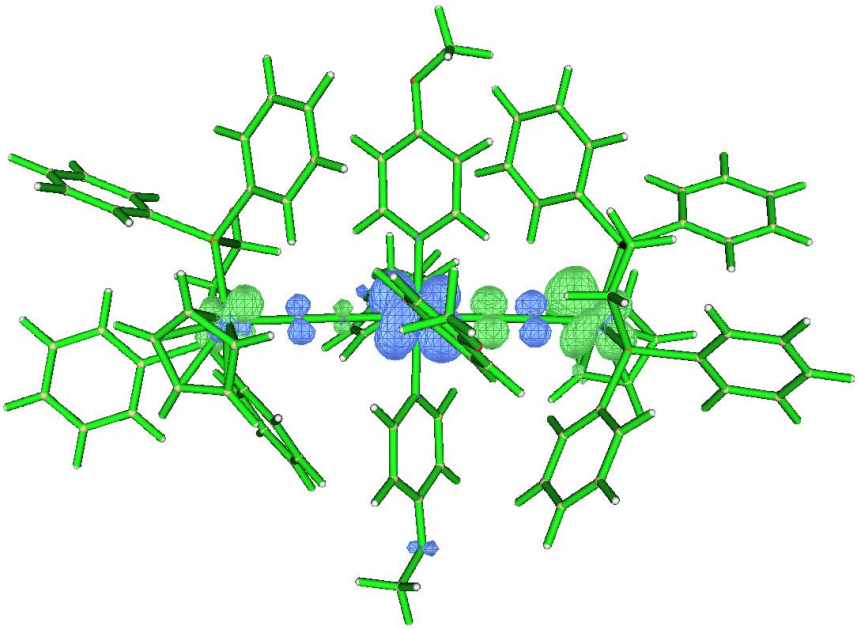

Fig. S10. Redistribution of the electron density for the electronic transition of $\mathbf{1}^{4+}$ in the calculated 950 nm transition band. The green and blues areas represent gain and losses of density. The isosurface value is -0.0004 au.

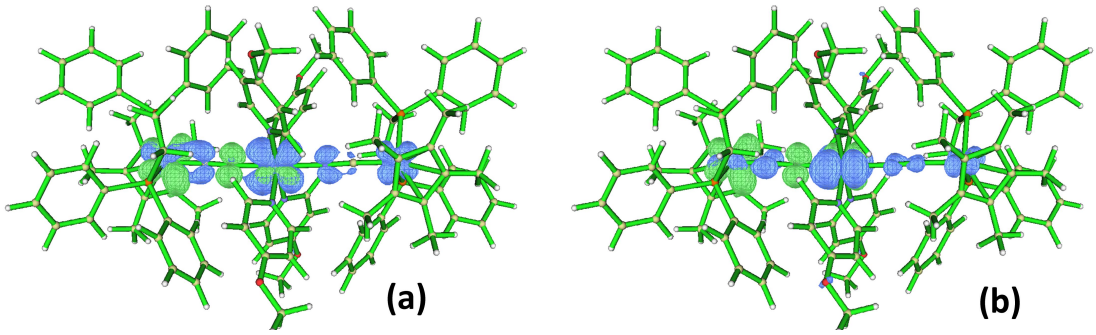

Fig. S11. Redistribution of the electron density for the electronic transition of $\mathbf{2}^{3+}$ in the calculated 1695 nm **(a)** and the calculated 1408 nm **(b)** transition band. The green and blues areas represent gain and losses of density. The isosurface value is -0.0004 au.

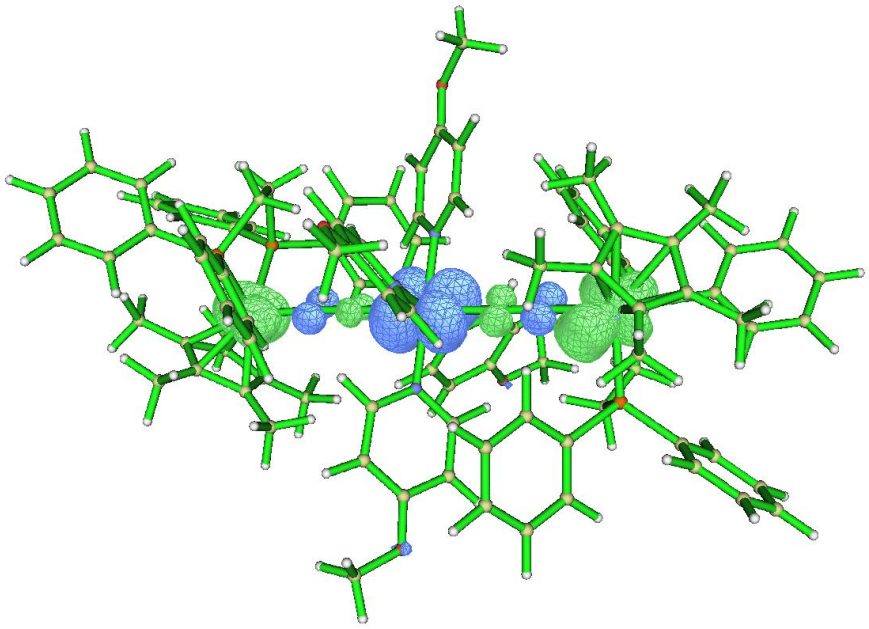

Fig. S12. Redistribution of the electron density for the electronic transition of $\mathbf{2}^{4+}$ in the calculated 733 nm transition band. The green and blues areas represent gain and losses of density. The isosurface value is -0.0004 au.

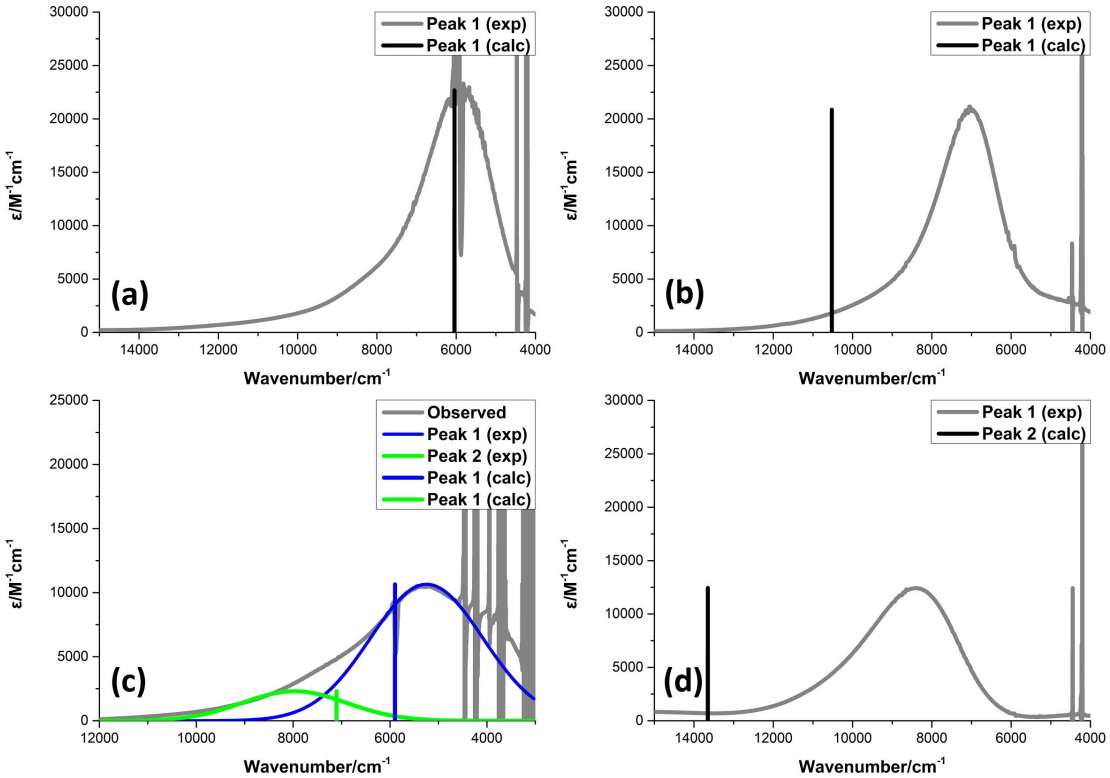

Fig. S13. The NIR spectra and calculated NIR absoprtion bands for $\mathbf{1}^{3+}$ (a), $\mathbf{1}^{4+}$ (b), $\mathbf{2}^{3+}$ (c), and $\mathbf{2}^{4+}$ (d).

Table S9. Calculated and experimental electronic absorption (in dichloromethane) of $\mathbf{1}^{3+}$, $\mathbf{1}^{4+}$, $\mathbf{2}^{3+}$, $\mathbf{2}^{4+}$.

Complex	Excitation (percentage)	f	λ_{max} (exp)/cm^{-1} (ε/M^{-1}cm^{-1})	ν_{max}(calc) /cm^{-1}	E(GS)/A.U.	E(ES)/A.U.
$\mathbf{1}^{3+}$	HOMO-1 (375β) → LUMO (377β) (23%) HOMO (376β) → LUMO (377β) (73%)	0.398	5860 (22957)	6044	-4397.427	-4397.399
$\mathbf{1}^{4+}$	HOMO-2 (373β) → LUMO (376β) (55%) HOMO-1 (374β) → LUMO+1 (377β) (19%)	0.1798	7038 (20869)	10524	-4396.727	-4396.679
$\mathbf{2}^{3+}$	HOMO (416β) → LUMO (417β) (66%)	0.1891	5244 (10650)	5898	-4789.934	-4789.907
	HOMO-1 (415β) → LUMO (417β) (59%) HOMO-9 (407β) → LUMO (417β) (21%)	0.0769	7973 (2304)	7104	-4789.934	-4789.902
$\mathbf{2}^{4+}$	HOMO-1 (414β) → LUMO (416β) (85%)	0.152	8409 (12448)	13652	-4790.052	-4789.990

Threshold of optimization: Maximum Force = 0.000450; RMS Force = 0.000300; Maximum Displacement = 0.001800; RMS Displacement = 0.001200.

Optimized Cartesian Coordinates of $\mathbf{1}^{3+}$

Atomic Name	X	Y	Z
Ru	0.000078	-0.248445	-0.000203
Fe	4.851510	-0.150713	1.308524
Fe	-4.851473	-0.151026	-1.308378
P	5.618481	-1.236870	-0.525219

P	5.248631	1.730588	0.107462
P	-5.618045	-1.237070	0.525504
P	-5.248641	1.730398	-0.107413
O	-0.864368	4.236942	4.289446
O	-0.995062	-4.461349	4.524560
O	0.995466	-4.461937	-4.524341
O	0.862963	4.235949	-4.291208
N	-1.959547	-0.230943	-0.419462
N	0.326913	-1.719329	-1.469951
N	-0.289458	1.227976	1.474497
N	1.959699	-0.230618	0.419132
N	-0.326458	-1.718968	1.469966
N	0.289262	1.227559	-1.475403
C	0.400166	-3.698554	2.652803
H	1.138536	-4.487580	2.749028
C	5.591001	0.679411	3.122093
H	5.791360	1.725480	3.312078
C	-0.195677	2.109363	-3.674107
H	-0.722359	1.982731	-4.613514
C	-0.714438	-3.609815	3.511355
C	0.551300	-2.737071	1.654583
H	1.396138	-2.765871	0.972612
C	6.518005	-0.296665	2.608614
H	7.553600	-0.131753	2.345675
C	7.392558	-1.825248	-0.463368
C	6.986965	2.400693	-0.064627
C	3.120098	-0.191556	0.728792
C	4.341402	0.029941	3.367833
H	3.452064	0.499916	3.763889
C	1.632673	-2.557390	-3.315400
H	2.496498	-2.480301	-3.965091
C	3.770128	-3.372757	-0.225059
H	3.572770	-2.917976	0.745705
C	-1.632311	-2.556949	3.315393
H	-2.496190	-2.479843	3.965004
C	4.788796	1.230143	-1.657598
H	3.703995	1.063578	-1.636835
H	4.982372	2.042345	-2.368430
C	5.831267	-1.560508	2.564530
H	6.261153	-2.497782	2.235692
C	1.105894	2.298520	-1.247572
H	1.602725	2.341187	-0.282660
C	0.714861	-3.610342	-3.511188
C	0.341330	1.150521	2.674068

H	0.981056	0.285985	2.823549
C	-4.341896	0.030999	-3.367725
H	-3.452869	0.501598	-3.763736
C	4.231245	3.251575	0.482550
C	-0.550792	-2.737514	-1.654396
H	-1.395567	-2.766336	-0.972348
C	4.488860	-1.361664	3.020610
H	3.722002	-2.120025	3.102476
C	7.687275	-3.190430	-0.299995
H	6.889871	-3.930541	-0.266939
C	-8.439116	-0.886565	0.504382
H	-8.236074	0.178613	0.608851
C	-4.231691	3.251541	-0.483083
C	7.737669	2.647034	1.099070
H	7.309384	2.462905	2.080649
C	0.644094	3.215928	-3.429769
C	1.413785	-1.649862	-2.295131
H	2.105371	-0.835626	-2.107895
C	-6.987060	2.400063	0.065561
C	8.439402	-0.886065	-0.502779
H	8.236163	0.179144	-0.606600
C	4.698250	-2.763053	-1.081146
C	-1.413404	-1.649501	2.295056
H	-2.105044	-0.835334	2.107710
C	-5.542724	-0.052857	2.025635
H	-6.575715	0.161144	2.325153
H	-5.055603	-0.576926	2.855835
C	-1.106126	2.298810	1.246167
H	-1.602644	2.341224	0.281090
C	3.129071	-4.559990	-0.610869
H	2.423424	-5.044089	0.060205
C	-5.591763	0.679714	-3.121391
H	-5.792628	1.725801	-3.310751
C	4.994640	-3.353549	-2.323817
H	5.749959	-2.915584	-2.974747
C	-4.488578	-1.360861	-3.021193
H	-3.721336	-2.118794	-3.103475
C	-0.341853	1.149725	-2.674788
H	-0.981507	0.285070	-2.823900
C	-3.120007	-0.191974	-0.728914
C	3.236943	3.207852	1.473649
H	3.058922	2.279026	2.016060
C	0.194741	2.110369	3.673126
H	0.721181	1.984020	4.612707

C	1.307910	3.295321	-2.187652
H	1.958428	4.137347	-1.977038
C	-0.212562	4.246642	5.591676
H	-0.523746	3.380612	6.186157
H	-0.545680	5.163286	6.073322
H	0.878080	4.263083	5.476759
C	4.351602	-4.536034	-2.711138
H	4.588654	-4.994294	-3.665762
C	-0.645086	3.216780	3.428287
C	-1.308517	3.295818	2.185940
H	-1.959031	4.137745	1.974916
C	10.062312	-2.676791	-0.247376
H	11.093001	-3.006403	-0.170262
C	-10.061763	-2.677434	0.248271
H	-11.092416	-3.007177	0.171237
C	-9.768881	-1.314524	0.403852
H	-10.572054	-0.585453	0.446209
C	-0.399680	-3.699074	-2.652550
H	-1.138007	-4.488158	-2.748642
C	5.543651	-0.052762	-2.025439
H	6.576753	0.161171	-2.324629
H	5.056776	-0.576862	-2.855762
C	-6.518173	-0.297095	-2.608186
H	-7.553797	-0.132831	-2.344947
C	3.418460	-5.140349	-1.853417
H	2.937465	-6.068332	-2.148472
C	-7.392103	-1.825525	0.464038
C	-4.697758	-2.763264	1.081247
C	9.020012	-3.612132	-0.193682
H	9.242651	-4.667374	-0.074113
C	-4.482751	4.452017	0.206325
H	-5.282152	4.505989	0.943362
C	9.769224	-1.313834	-0.402151
H	10.572259	-0.584568	-0.443781
C	3.726375	5.596579	0.079696
H	3.930795	6.524742	-0.443934
C	-3.237464	3.207830	-1.474257
H	-3.059289	2.278943	-2.016509
C	-3.769880	-3.373067	0.224977
H	-3.572713	-2.918324	-0.745854
C	-5.830783	-1.560607	-2.564869
H	-6.260179	-2.498261	-2.236482
C	2.725440	5.549118	1.063107
H	2.154356	6.441716	1.297255

C	4.482149	4.451958	-0.207064
H	5.281662	4.505943	-0.943982
C	-3.418054	-5.140655	1.853309
H	-2.937076	-6.068669	2.148289
C	-7.686625	-3.190658	0.299884
H	-6.889079	-3.930598	0.266190
C	-4.994006	-3.353728	2.323972
H	-5.749169	-2.915678	2.975026
C	-4.351017	-4.536268	2.711186
H	-4.587947	-4.994500	3.665852
C	7.555205	2.683637	-1.320008
H	6.999252	2.522053	-2.240757
C	-9.612389	3.404161	0.248207
H	-10.623953	3.789588	0.318819
C	-4.787959	1.230014	1.657474
H	-3.703177	1.063407	1.636191
H	-4.981176	2.042217	2.368401
C	-3.727227	5.596733	-0.080734
H	-3.931760	6.524937	0.442778
C	9.042790	3.146470	1.009950
H	9.611579	3.336485	1.914085
C	-7.738784	2.645490	-1.097673
H	-7.311312	2.460806	-2.079495
C	-3.128847	-4.560348	0.610694
H	-2.423388	-5.044555	-0.060499
C	-0.104204	-5.576503	4.807654
H	-0.052335	-6.256377	3.948958
H	-0.545598	-6.089998	5.659034
H	0.895781	-5.215072	5.072520
C	-2.485481	4.356564	-1.761654
H	-1.726060	4.328282	-2.540167
C	2.484696	4.356495	1.760741
H	1.725209	4.328215	2.539193
C	-2.726391	5.549283	-1.064238
H	-2.155491	6.441937	-1.298621
C	0.210784	4.245260	-5.593256
H	-0.879829	4.261544	-5.478033
H	0.521949	3.379157	-6.187638
H	0.543617	5.161854	-6.075196
C	-9.019310	-3.612551	0.193689
H	-9.241787	-4.667761	0.073538
C	-9.043958	3.144662	-1.007801
H	-9.613524	3.333973	-1.911594
C	0.104699	-5.577215	-4.807240

H	0.546096	-6.090777	-5.658578
H	-0.895336	-5.215917	-5.072094
H	0.052950	-6.256976	-3.948447
C	-8.863155	3.178702	1.411170
H	-9.292573	3.392137	2.384542
C	8.863946	3.178976	-1.409193
H	9.294103	3.391914	-2.382348
C	-7.554363	2.683648	1.321228
H	-6.997612	2.522801	2.241621
C	9.612179	3.405328	-0.245761
H	10.623707	3.790958	-0.315787

Optimized Cartesian Coordinates of **1**$^{4+}$

Atomic Name	X	Y	Z
Ru	-0.011262	-0.284590	-0.020575
Fe	-4.972901	-0.398291	1.216885
Fe	4.935386	-0.395157	-1.292323
P	-5.766650	-0.984230	-0.903822
P	5.572496	-1.144352	0.813297
P	-5.388311	1.758766	0.517267
P	5.566687	1.668998	-0.473236
N	1.965918	-0.304678	-0.436959
O	0.138196	-6.524965	-0.567244
O	-1.512513	0.306025	-6.084278
O	1.410761	-0.981675	6.052111
N	-0.055192	-2.382408	-0.204447
N	0.431296	-0.492023	2.031235
N	-0.460575	-0.080694	-2.070710
C	3.123337	-0.334691	-0.714116
N	-1.997800	-0.299168	0.387343
C	4.665454	4.344796	-0.412547
H	5.516199	4.521559	0.243839
C	1.752384	-1.493227	3.790374
H	2.541791	-2.171958	4.094933
C	-0.019398	0.923304	-4.232864
H	0.595363	1.598457	-4.818624
C	3.872951	-3.424373	0.608111
H	3.601147	-3.041938	-0.375046
C	-5.059054	-2.495345	-3.177615
H	-5.785658	-1.878864	-3.704525
C	0.019468	-5.190151	-0.391134
C	8.642420	3.600217	-2.471274
H	8.733946	4.326480	-3.271836
C	-3.759285	5.391391	1.640829

H	-3.926826	6.437702	1.409265
C	0.005396	0.090359	4.345302
H	-0.577792	0.675503	5.048322
C	4.773257	-2.712738	1.417478
C	5.137558	-3.214426	2.681784
H	5.870105	-2.694021	3.296387
C	-4.411907	-3.529547	-3.865671
H	-4.621172	-3.690975	-4.917940
C	4.617657	-1.905042	-2.841470
H	3.800435	-2.612372	-2.869598
C	5.886623	-2.116050	-2.221925
H	6.194376	-3.031771	-1.735408
C	-1.860102	-0.626493	-3.962722
H	-2.692176	-1.184376	-4.379274
C	3.851835	5.419582	-0.793135
H	4.076203	6.417893	-0.430135
C	7.371730	3.195785	-2.041231
H	6.488709	3.622918	-2.513330
C	-4.328752	3.050238	1.334882
C	2.526858	3.932052	-2.184910
H	1.708091	3.781418	-2.883891
C	1.036054	-0.774181	4.772371
C	-3.921565	-3.146335	-1.124949
H	-3.731996	-2.998047	-0.063171
C	0.615663	-4.381000	-1.383037
H	1.102516	-4.856303	-2.227207
C	-7.726553	2.978881	-0.587716
H	-7.212975	3.001728	-1.546252
C	0.560634	-3.003609	-1.254455
H	1.009137	-2.351805	-1.997104
C	-6.725523	-0.838304	2.349756
H	-7.728952	-0.501435	2.128663
C	-1.109940	0.229133	-4.798795
C	-0.255382	0.197566	2.979655
H	-1.028984	0.865196	2.610702
C	3.345893	2.855536	-1.814863
H	3.168397	1.862215	-2.225624
C	-5.679343	0.574701	-1.996441
H	-5.191461	0.293650	-2.936043
H	-6.712833	0.860087	-2.224303
C	-4.806389	-2.296284	-1.805725
C	1.425904	-1.330851	2.454701
H	1.957292	-1.884179	1.685471
C	0.261006	0.738487	-2.879772

H	1.082330	1.267881	-2.405098
C	-0.646485	-3.165975	0.733946
H	-1.128447	-2.645876	1.556482
C	-4.914908	1.704835	-1.304382
H	-5.095778	2.674576	-1.783312
H	-3.835029	1.513168	-1.325238
C	-5.748683	-0.159176	3.165180
H	-5.881987	0.781140	3.682300
C	4.585641	-4.418197	3.138639
H	4.876273	-4.812039	4.106777
C	-2.577575	3.675996	2.895610
H	-1.834935	3.400502	3.640244
C	-0.633855	-4.559555	0.686965
H	-1.107446	-5.124820	1.481867
C	-8.577992	-0.641337	-0.765805
H	-8.371835	0.406542	-0.549575
C	10.086925	-1.722489	1.894681
H	11.131435	-1.870520	2.146508
C	9.672205	2.139841	-0.826805
H	10.560513	1.734042	-0.353699
C	-3.350212	2.685924	2.273431
H	-3.207571	1.635855	2.528216
C	7.376553	-1.340068	1.242242
C	-3.521477	-4.375949	-3.185093
H	-3.037720	-5.189786	-3.715055
C	-3.282087	-4.185500	-1.816973
H	-2.614619	-4.858243	-1.284675
C	-6.159103	-2.100533	1.951274
H	-6.654039	-2.846346	1.342545
C	5.886419	0.018589	-3.150357
H	6.212685	0.997075	-3.476552
C	3.689851	-5.132544	2.327318
H	3.294036	-6.082930	2.670503
C	3.337692	-4.637878	1.063202
H	2.677338	-5.212575	0.419184
C	-9.713447	3.505404	0.709653
H	-10.716018	3.915243	0.766674
C	-3.160467	-0.342582	0.638733
C	9.793004	3.074989	-1.865340
H	10.774949	3.394094	-2.197527
C	-0.793410	1.141867	-7.038422
H	-0.834023	2.194037	-6.735617
H	-1.314058	1.010474	-7.984208
H	0.244375	0.804963	-7.137624

C	-4.832833	-2.184450	2.474050
H	-4.147446	-3.008836	2.336917
C	9.530274	-2.381303	0.787915
H	10.142229	-3.045743	0.187415
C	-7.801808	2.468465	1.790009
H	-7.326074	2.105180	2.698492
C	-0.463661	-7.451181	0.384591
H	-0.026405	-7.318922	1.380904
H	-0.229623	-8.443893	0.006821
H	-1.550908	-7.314450	0.418865
C	-4.540987	4.406175	1.023855
H	-5.326347	4.699403	0.329070
C	7.251463	2.263947	-0.992638
C	-4.577879	-0.988965	3.228812
H	-3.657178	-0.754604	3.746177
C	-2.780307	5.026640	2.577826
H	-2.194910	5.797806	3.069062
C	7.932430	-0.701108	2.367007
H	7.335073	-0.059810	3.010860
C	-1.511267	-0.756278	-2.629154
H	-2.068625	-1.418192	-1.972564
C	-9.167073	-3.333244	-1.303029
H	-9.395437	-4.372397	-1.514441
C	4.614923	-0.588282	-3.414577
H	3.792513	-0.135210	-3.951612
C	0.722091	-0.305871	7.145067
H	0.833859	0.780547	7.057298
H	1.211223	-0.654530	8.051721
H	-0.336572	-0.587442	7.164134
C	-7.115764	2.444431	0.561537
C	9.283675	-0.891053	2.687921
H	9.704093	-0.399446	3.558824
C	4.974210	0.264536	1.916974
H	3.880923	0.259003	1.832048
H	5.224595	0.063792	2.965677
C	-9.023981	3.504923	-0.511219
H	-9.490222	3.919638	-1.398585
C	8.181001	-2.193410	0.464782
H	7.764666	-2.738522	-0.378348
C	4.411685	3.057793	-0.925093
C	2.780662	5.214124	-1.678111
H	2.164171	6.053082	-1.986727
C	6.674501	-0.916864	-2.388412
H	7.696046	-0.765160	-2.067534

C	-9.909143	-1.073363	-0.810665
H	-10.711055	-0.362367	-0.639749
C	-7.831642	-2.909063	-1.263850
H	-7.037551	-3.629079	-1.452241
C	-9.096666	2.995212	1.862805
H	-9.619430	3.017978	2.812953
C	5.569038	1.589363	1.428267
H	6.605019	1.718914	1.761578
H	4.990532	2.443513	1.797448
C	-10.205713	-2.418545	-1.078603
H	-11.237712	-2.750258	-1.115002
C	8.406061	1.727589	-0.392494
H	8.341422	0.992958	0.409062
C	-7.536455	-1.558018	-1.003974
N	0.045708	1.815698	0.178159
C	-0.920176	2.596113	-0.392040
H	-1.676042	2.072821	-0.967545
C	-0.949681	3.973459	-0.261547
H	-1.729524	4.569436	-0.721888
C	0.043269	4.611882	0.509602
C	1.053899	3.820560	1.090289
H	1.857645	4.252138	1.676785
C	1.017761	2.441764	0.891182
H	1.787466	1.804439	1.315626
O	-0.064587	5.956779	0.624144
C	0.853818	6.688815	1.482562
H	0.768809	6.342736	2.519934
H	0.549060	7.730979	1.412995
H	1.886412	6.579707	1.130783

Optimized Cartesian Coordinates of **2**$^{3+}$

Atomic Name	X	Y	Z
Ru	-0.050930	-0.351386	-0.014895
Fe	4.961331	-0.171770	1.110796
Fe	-5.016028	-0.189296	-1.131957
P	-5.259502	1.906727	-0.152915
P	-5.453744	-1.017282	0.995320
P	5.220118	1.870363	0.129158
P	5.420834	-1.039828	-0.950318
O	0.983157	3.825816	-4.560848
O	-1.031052	3.960231	4.428238
O	0.896805	-4.554458	-4.574717
O	-0.724247	-4.783480	4.381479
N	-2.013734	-0.314884	-0.426809

N	0.246754	1.120684	-1.481408
N	-0.333840	1.106942	1.471730
N	1.979698	-0.295959	0.402302
N	0.248242	-1.818189	-1.499580
N	-0.280683	-1.869172	1.435347
C	4.539761	-2.619850	-1.463252
C	-3.995213	3.209043	-0.590386
C	3.977766	3.234872	0.469720
C	-4.584143	-2.612734	1.451057
C	-7.160235	-1.313055	1.711030
C	-6.870751	-0.597915	-2.167521
C	1.080059	2.168793	-1.266031
H	1.527473	2.243730	-0.279151
C	-7.821618	-2.525520	1.434019
H	-7.327398	-3.299588	0.852403
C	-3.720231	-3.240690	0.540711
H	-3.531042	-2.770054	-0.422787
C	-5.078839	1.705045	1.740132
H	-4.316222	2.417223	2.076680
H	-6.034134	2.013844	2.178720
C	-0.076111	1.890189	-3.749133
H	-0.529117	1.767023	-4.726682
C	8.012014	2.145513	-0.126077
H	7.959747	1.137492	-0.533183
C	0.100161	1.897865	3.720267
H	0.626208	1.740101	4.655614
C	-7.788393	-0.366110	2.539322
H	-7.289624	0.559030	2.817137
C	7.142894	-1.407117	-1.611986
C	-3.161148	3.049987	-1.706150
H	-3.195705	2.124222	-2.275775
C	1.379221	3.111268	-2.249224
H	2.045571	3.927617	-1.995255
C	-0.564267	-2.897617	-1.618139
H	-1.361335	-2.975891	-0.883726
C	-0.325371	1.002997	-2.715838
H	-0.982142	0.149792	-2.852745
C	-0.411162	-3.864377	-2.612547
H	-1.093881	-4.707474	-2.643896
C	-6.875087	2.842014	-0.301527
C	3.651798	-3.242959	-0.573810
H	3.459015	-2.768426	0.387732
C	-9.101671	-2.768037	1.945404
H	-9.598226	-3.708482	1.730360

C	7.846614	-0.481417	-2.402089
H	7.396046	0.464598	-2.693587
C	3.088649	3.110687	1.546938
H	3.086818	2.188614	2.125358
C	0.286810	0.996413	2.673841
H	0.951184	0.145789	2.784744
C	3.977525	4.419076	-0.293279
H	4.692270	4.546158	-1.105905
C	-1.407504	3.114399	2.270237
H	-2.058974	3.961780	2.086555
C	6.844359	2.802411	0.300273
C	3.148655	-0.212209	0.665665
C	1.261410	-1.685967	-2.406844
H	1.905440	-0.825108	-2.273656
C	6.757702	-0.625127	2.216876
C	-0.768099	2.988036	3.519700
C	9.359195	4.042826	0.565342
H	10.327009	4.522558	0.667506
C	9.262338	2.763425	-0.002281
H	10.155138	2.244193	-0.338241
C	1.903293	4.941573	-4.414097
H	2.913533	4.580825	-4.182480
H	1.557749	5.628984	-3.631869
H	1.903201	5.446638	-5.377678
C	6.060437	0.436171	2.889834
C	-4.688476	0.281879	2.142353
H	-4.967707	0.060693	3.180161
H	-3.604526	0.146630	2.039499
C	6.946384	4.080268	0.874346
H	6.062687	4.599490	1.236899
C	-6.965362	4.097931	-0.925031
H	-6.082119	4.580581	-1.335905
C	4.741501	-0.028020	3.223749
C	-1.166996	2.171844	1.282372
H	-1.637055	2.252182	0.306299
C	-4.830450	-3.208786	2.701800
H	-5.517407	-2.744484	3.407030
C	-8.038155	2.231914	0.201145
H	-7.993443	1.245271	0.659227
C	4.642387	-1.410052	2.809829
C	3.046390	-4.461326	-0.915106
H	2.383667	-4.960065	-0.209627
C	-4.218514	-4.425274	3.032250
H	-4.412888	-4.884412	3.995996

C	-6.023324	-1.776368	-2.168661
C	0.527555	-2.958793	1.427271
H	1.274330	-2.992909	0.639534
C	-3.118292	-4.463716	0.867746
H	-2.469547	-4.962053	0.149883
C	-3.177632	-0.233916	-0.705668
C	-9.276474	2.876984	0.098077
H	-10.167679	2.399646	0.494079
C	4.750171	0.240459	-2.188397
H	5.106131	0.000934	-3.198398
H	3.661364	0.107143	-2.167615
C	-0.518492	-3.875246	3.395661
C	-3.932528	4.397669	0.162721
H	-4.600657	4.551829	1.009004
C	-1.350996	-2.737473	3.418854
H	-2.088769	-2.635041	4.205729
C	-3.368420	-5.057594	2.112510
H	-2.917527	-6.013168	2.363999
C	4.191940	-4.428327	-3.055600
H	4.405489	-4.888815	-4.014825
C	-0.382784	3.926487	5.730592
H	0.707414	3.978055	5.620434
H	-0.668723	3.024321	6.282844
H	-0.741799	4.809263	6.255311
C	0.624855	-3.705184	-3.553584
C	1.465400	-2.579869	-3.441969
H	2.270505	-2.443335	-4.154122
C	5.107771	1.672080	-1.780101
H	4.351384	2.377164	-2.147713
H	6.077197	1.984638	-2.185364
C	0.438561	-3.983440	2.369811
H	1.120895	-4.824255	2.303605
C	-9.070463	-0.610808	3.052099
H	-9.540984	0.124767	3.696428
C	-6.183402	0.432798	-2.905725
C	8.199526	4.696091	1.005227
H	8.269471	5.682138	1.453167
C	4.805924	-3.217298	-2.708460
H	5.516115	-2.758647	-3.394374
C	2.210385	4.158569	1.863626
H	1.547186	4.069304	2.720717
C	0.795733	2.975478	-3.520556
C	5.881736	-1.780232	2.200161
C	-1.214148	-1.781665	2.428622

H	-1.848895	-0.902901	2.411766
C	2.206341	5.332412	1.097818
H	1.538627	6.148818	1.354951
C	-3.035045	5.411505	-0.195629
H	-2.999944	6.329523	0.382268
C	-4.805878	-1.445910	-2.856214
C	-8.207365	4.739631	-1.031659
H	-8.270797	5.709911	-1.513055
C	-9.363677	4.133471	-0.520656
H	-10.322440	4.634275	-0.603560
C	0.084431	-5.744144	-4.759639
H	0.502008	-6.249154	-5.628170
H	0.149963	-6.398915	-3.881908
H	-0.959933	-5.474735	-4.956628
C	-4.898828	-0.078724	-3.301013
C	3.092551	5.461183	0.015301
H	3.116591	6.380701	-0.562415
C	3.762133	0.671093	4.110490
H	3.900292	1.758878	4.103632
H	3.887071	0.336519	5.149734
H	2.727335	0.449568	3.818769
C	-8.292445	-0.562983	-1.708764
H	-8.422190	-1.018043	-0.718161
H	-8.927595	-1.120422	-2.409717
H	-8.678715	0.459659	-1.659763
C	-9.735349	-1.805487	2.745863
H	-10.727086	-1.994323	3.142707
C	3.317343	-5.055706	-2.155277
H	2.868663	-6.010424	-2.415698
C	-6.447026	-3.152289	-1.765948
H	-5.733719	-3.651246	-1.098342
H	-6.544131	-3.778813	-2.661887
H	-7.426806	-3.135687	-1.280242
C	7.749744	-2.641175	-1.309321
H	7.204431	-3.397298	-0.749903
C	-2.276134	4.073931	-2.075222
H	-1.659294	3.958743	-2.962378
C	-3.699950	-2.387686	-3.197516
H	-2.714056	-1.920018	-3.078797
H	-3.788907	-2.708707	-4.244101
H	-3.729175	-3.291174	-2.576085
C	6.632140	1.745819	3.327231
H	7.534461	2.017261	2.770514
H	6.906202	1.682588	4.388646

H	5.915908	2.571116	3.223415
C	9.144801	-0.767259	-2.850416
H	9.673428	-0.043902	-3.463171
C	-2.208053	5.251868	-1.319219
H	-1.531938	6.049163	-1.612086
C	-6.748117	1.741898	-3.345169
H	-7.603292	2.055727	-2.739546
H	-7.095976	1.648460	-4.382463
H	-6.005052	2.548502	-3.324339
C	8.201641	-0.636493	1.823833
H	8.363742	-1.097012	0.839824
H	8.790855	-1.208560	2.552888
H	8.618807	0.375023	1.789337
C	3.508368	-2.327540	3.131486
H	2.533400	-1.857759	2.939602
H	3.535329	-2.612174	4.192536
H	3.560650	-3.253955	2.544348
C	0.118251	-5.965830	4.458241
H	1.169000	-5.684085	4.592744
H	0.001177	-6.584149	3.559808
H	-0.229194	-6.514001	5.331460
C	9.752366	-1.985001	-2.518187
H	10.756862	-2.205763	-2.863472
C	-3.921284	0.590862	-4.209238
H	-4.063561	1.675797	-4.248860
H	-4.047974	0.212771	-5.232604
H	-2.884996	0.383660	-3.914264
C	6.290509	-3.172273	1.831665
H	5.601005	-3.658720	1.129886
H	6.327569	-3.795042	2.734985
H	7.293801	-3.183471	1.395082
C	9.045322	-2.926883	-1.755897
H	9.498472	-3.883648	-1.517137

Optimized Cartesian Coordinates of **2**$^{4+}$

Atomic Name	X	Y	Z
Ru	-0.008068	-0.241994	0.009179
Fe	5.062706	-0.302694	1.077841
Fe	-5.070747	-0.255883	-1.114724
P	-5.365397	1.884069	-0.135301
P	-5.580165	-1.081563	1.029995
P	5.366208	1.842059	0.115912
P	5.536538	-1.111276	-1.082855
O	0.827902	3.994686	-4.536154

O	-1.090326	3.999422	4.501027
O	0.897676	-4.540063	-4.479371
O	-0.968072	-4.571295	4.454939
N	-2.026270	-0.205086	-0.401526
N	0.269857	1.233861	-1.464273
N	-0.283113	1.217041	1.501897
N	2.009106	-0.222881	0.410795
N	0.257091	-1.728046	-1.467567
N	-0.290023	-1.737852	1.471696
C	4.603224	-2.672433	-1.510811
C	-4.089632	3.193985	-0.506086
C	4.113623	3.168118	0.512641
C	-4.657335	-2.647973	1.462978
C	-7.301825	-1.435732	1.655396
C	-6.921880	-0.631967	-2.222826
C	1.085101	2.300911	-1.266367
H	1.549408	2.379958	-0.287051
C	-7.897228	-2.677709	1.357627
H	-7.341768	-3.441677	0.818718
C	-3.752427	-3.218637	0.553585
H	-3.558010	-2.723560	-0.397146
C	-5.280609	1.653764	1.761298
H	-4.555629	2.381534	2.143312
H	-6.265284	1.939411	2.147228
C	-0.135493	2.020197	-3.715209
H	-0.614190	1.897964	-4.680644
C	8.154682	2.105995	-0.189288
H	8.097357	1.126924	-0.663455
C	0.096286	1.973170	3.776009
H	0.594104	1.799054	4.724031
C	-8.012204	-0.498518	2.427397
H	-7.565361	0.449150	2.718879
C	7.245144	-1.461557	-1.745384
C	-3.233018	3.066051	-1.608987
H	-3.241311	2.150290	-2.195150
C	1.333227	3.263445	-2.246492
H	1.985851	4.096217	-2.006777
C	-0.536768	-2.826669	-1.540467
H	-1.315935	-2.902654	-0.786174
C	-0.332192	1.115954	-2.686176
H	-0.973592	0.250065	-2.815079
C	-0.387237	-3.817333	-2.512628
H	-1.056294	-4.671845	-2.508944
C	-6.977871	2.806344	-0.347888

C	3.703915	-3.240325	-0.594084
H	3.520385	-2.745889	0.359159
C	-9.194981	-2.961742	1.798415
H	-9.642599	-3.923747	1.572264
C	7.930935	-0.531430	-2.547613
H	7.473858	0.411922	-2.837539
C	3.230965	3.025313	1.592731
H	3.214985	2.096311	2.157633
C	0.314070	1.094315	2.716056
H	0.973394	0.239268	2.833092
C	4.117149	4.365389	-0.230679
H	4.826261	4.507705	-1.045080
C	-1.394995	3.199310	2.316751
H	-2.062059	4.035693	2.138943
C	6.997453	2.736250	0.304066
C	3.173224	-0.193114	0.663886
C	1.239174	-1.599356	-2.409808
H	1.852265	-0.708608	-2.333048
C	6.922838	-0.710807	2.162913
C	-0.783315	3.057466	3.579545
C	9.507361	3.972847	0.573290
H	10.474609	4.453356	0.673863
C	9.403999	2.724622	-0.060619
H	10.291503	2.235991	-0.450571
C	1.686250	5.163096	-4.416087
H	2.725821	4.861116	-4.241163
H	1.336064	5.818977	-3.609751
H	1.608481	5.678240	-5.371006
C	6.270065	0.351561	2.887514
C	-4.884406	0.240003	2.188900
H	-5.205546	0.025944	3.216168
H	-3.795612	0.117597	2.137229
C	7.103253	3.982904	0.944570
H	6.224562	4.480195	1.347938
C	-7.046466	4.061165	-0.977160
H	-6.150160	4.545817	-1.356343
C	4.953428	-0.097140	3.254388
C	-1.126497	2.276569	1.317479
H	-1.588821	2.364052	0.338059
C	-4.904421	-3.282447	2.694781
H	-5.623475	-2.863230	3.396090
C	-8.156873	2.193358	0.114526
H	-8.127759	1.208667	0.579397
C	4.812703	-1.467903	2.824298

C	3.051723	-4.442052	-0.901714
H	2.378312	-4.899045	-0.179302
C	-4.249162	-4.480346	3.009257
H	-4.442606	-4.969691	3.957915
C	-6.048038	-1.788383	-2.221399
C	0.500930	-2.838477	1.544653
H	1.286468	-2.910569	0.796596
C	-3.108664	-4.424084	0.864979
H	-2.431377	-4.883286	0.147600
C	-3.185678	-0.164736	-0.673092
C	-9.391268	2.836990	-0.033919
H	-10.295984	2.361676	0.332225
C	4.824067	0.224674	-2.214351
H	5.119608	0.017579	-3.250722
H	3.736125	0.109766	-2.138882
C	-0.685167	-3.693363	3.464418
C	-4.064590	4.373406	0.263953
H	-4.754062	4.507441	1.096146
C	-1.501345	-2.544632	3.402956
H	-2.287020	-2.412925	4.137706
C	-3.358657	-5.056277	2.090791
H	-2.878083	-6.000942	2.327863
C	4.172106	-4.499561	-3.056672
H	4.353511	-4.987286	-4.008493
C	-0.500723	3.942589	5.832195
H	0.591734	4.018418	5.772821
H	-0.795993	3.021461	6.346593
H	-0.900499	4.804527	6.361692
C	0.627263	-3.669190	-3.479370
C	1.445293	-2.521731	-3.418733
H	2.219909	-2.382749	-4.163803
C	5.240401	1.631139	-1.781870
H	4.511641	2.368332	-2.138819
H	6.219463	1.913033	-2.184810
C	0.339709	-3.836090	2.507887
H	1.006584	-4.692355	2.504495
C	-9.311306	-0.787448	2.869117
H	-9.847315	-0.063611	3.474094
C	-6.249218	0.426719	-2.935429
C	8.356655	4.597812	1.074750
H	8.433916	5.561989	1.565961
C	4.836255	-3.305588	-2.745958
H	5.550010	-2.888098	-3.453648
C	2.360593	4.071519	1.933100

H	1.696739	3.963813	2.787143
C	0.710205	3.129862	-3.501499
C	6.034900	-1.856303	2.162536
C	-1.283176	-1.614669	2.403326
H	-1.896954	-0.724315	2.323874
C	2.362092	5.261084	1.192180
H	1.701720	6.076345	1.469241
C	-3.183696	5.411095	-0.067900
H	-3.182855	6.324617	0.518019
C	-4.814668	-1.410223	-2.868008
C	-8.284926	4.701299	-1.127037
H	-8.333291	5.671871	-1.609205
C	-9.457537	4.093421	-0.656577
H	-10.413181	4.593394	-0.772161
C	0.086201	-5.737019	-4.644095
H	0.497796	-6.249547	-5.510864
H	0.162013	-6.381277	-3.759573
H	-0.959554	-5.471037	-4.835748
C	-4.935252	-0.036278	-3.293493
C	3.241687	5.405957	0.106644
H	3.268981	6.336449	-0.452013
C	3.992373	0.623338	4.139571
H	4.158240	1.705623	4.140724
H	4.113810	0.277174	5.174801
H	2.952240	0.426392	3.850913
C	-8.347442	-0.634511	-1.780312
H	-8.478413	-1.110893	-0.799727
H	-8.959617	-1.196623	-2.497881
H	-8.759375	0.376995	-1.722001
C	-9.910042	-2.012472	2.544681
H	-10.914834	-2.234533	2.887381
C	3.287495	-5.073014	-2.131058
H	2.799625	-6.014492	-2.365787
C	-6.448108	-3.177036	-1.843434
H	-5.716670	-3.680390	-1.199075
H	-6.552006	-3.784658	-2.751576
H	-7.419398	-3.185603	-1.341043
C	7.851902	-2.698726	-1.450639
H	7.312821	-3.457735	-0.888578
C	-2.364520	4.113279	-1.950368
H	-1.734501	4.024318	-2.831189
C	-3.677736	-2.318276	-3.200358
H	-2.706014	-1.831553	-3.045154
H	-3.732690	-2.618144	-4.255291

H	-3.703756	-3.236347	-2.600650
C	6.890678	1.630869	3.329748
H	7.746647	1.921414	2.714189
H	7.256554	1.504477	4.357987
H	6.179687	2.465254	3.341526
C	9.217815	-0.822559	-3.022501
H	9.734772	-0.104579	-3.650580
C	-2.335802	5.283894	-1.180118
H	-1.677377	6.102061	-1.454984
C	-6.849374	1.716121	-3.376315
H	-7.708856	2.013203	-2.768826
H	-7.204312	1.600651	-4.409692
H	-6.128403	2.541913	-3.374911
C	8.343181	-0.727020	1.704814
H	8.457828	-1.202363	0.721822
H	8.957565	-1.297119	2.414132
H	8.765094	0.280227	1.643771
C	3.670089	-2.366371	3.163248
H	2.701645	-1.868303	3.025557
H	3.736490	-2.677748	4.214145
H	3.677782	-3.278621	2.554230
C	-0.166813	-5.775981	4.613091
H	0.879105	-5.520214	4.817293
H	-0.239193	-6.409291	3.720431
H	-0.590171	-6.295659	5.469885
C	9.828375	-2.042710	-2.701768
H	10.823380	-2.266650	-3.070792
C	-3.958743	0.672809	-4.170709
H	-4.116900	1.755993	-4.183830
H	-4.069113	0.320176	-5.204995
H	-2.923333	0.471321	-3.869188
C	6.413763	-3.247268	1.771262
H	5.673287	-3.734785	1.125110
H	6.512059	-3.864215	2.673718
H	7.383322	-3.265376	1.265771
C	9.137272	-2.985079	-1.924771
H	9.593402	-3.943619	-1.700984