Supplementary Information for

The investigation on electron transfer properties between metal centers in binuclear and trinuclear cyanido-bridged mixed valence complexes with cis/trans-configuration

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Table S1 Crystallographic data for ***cis*-1[PF_6]$_n$** (n = 1, 2)

Complex	***cis*-1[PF_6]**	***cis*-1[PF_6]$_2$**
Empirical formula	$C_{58}H_{55}Cl_2F_6FeN_6OP_3Ru$	$C_{61}H_{63}F_{12}FeN_6OP_4Ru$
Formula weight	1286.81	1404.97
Crystal size (mm)	0.209 × 0.201 × 0.102	0.384 × 0.367 × 0.346
Temperature/K	100(2)	99.99(10)
Crystal system	triclinic	monoclinic
Space group	Pī	$P2_1/c$
a/Å	10.63212(19)	9.86160(10)
b/Å	12.3333(2)	41.2452(3)
c/Å	22.3815(3)	15.29680(10)
α/°	85.9555(13)	90
β/°	79.6473(13)	108.0130(10)
γ/°	73.0909(16)	90
Volume/Å^3	2761.75(9)	5916.92(9)
Z	2	4
ρ_{calcd}/g cm^{-3}	1.547	1.577
μ/mm^{-1}	4.463	3.917
F(000)	1312.0	2868.0
λ (Mo/Ga Kα, Å)	Ga, λ = 1.3405	Ga, λ = 1.3405
2θ range/°	6.514-120.894	5.6-120.81
Index range	-11 ≤ h ≤ 13 -15 ≤ k ≤ 15 -28 ≤ l ≤ 28	-12 ≤ h ≤ 12 -45 ≤ k ≤ 53 -19 ≤ l ≤ 19
Reflections collected	39034	75045
Independent reflections	12161 (R_{int} = 0.0416, R_{sigma} = 0.0406)	13076 (R_{int} = 0.0633, R_{sigma} = 0.0326)
Data/restraints/parameters	12161/32/745	13076/43/781
Goodness-of-fit on F^2	1.019	1.066
R_1, wR_2 (I ≥ 2σ (I))	R_1 = 0.0370, wR_2 = 0.0967	R_1 = 0.0437, wR_2 = 0.1097
R_1, wR_2 (all data)	R_1 = 0.0443, wR_2 = 0.1005	R_1 = 0.0450, wR_2 = 0.1107

Table S2 Crystallographic data for ***cis*-2[PF_6]$_n$** (n = 2, 4)

Complex	***cis*-2[PF_6]$_2$**	***cis*-2[PF_6]$_4$**
Empirical formula	$C_{88}H_{82}F_{12}Fe_2N_6O_{1.32}P_6Ru$	$C_{90}H_{85}F_{24}Fe_2N_7P_8Ru$
Formula weight	1871.46	2181.17
Crystal size (mm)	0.260 × 0.238 × 0.112	0.367 × 0.356 × 0.348
Temperature/K	293.15	100.01(10)
Crystal system	triclinic	orthorhombic
Space group	Pī	Pbca
a/Å	11.874(4)	28.1279(6)
b/Å	15.236(5)	19.5282(4)
c/Å	31.642(12)	36.8338(7)
α/°	95.91(3)	90
β/°	99.87(2)	90
γ/°	108.389(17)	90
Volume/Å^3	5276(3)	20232.3(7)
Z	2	8
ρ_{calcd}/g cm^{-3}	1.178	1.432
μ/mm^{-1}	0.566	3.604
F(000)	1913.0	8848.0
λ (Mo/Ga Kα, Å)	Mo, λ = 0.71073	Ga, λ = 1.3405
2θ range/°	3.652-49.426	4.172-96.268
Index range	-13 ≤ h ≤ 13 -17 ≤ k ≤ 17 -37 ≤ l ≤ 37	-31 ≤ h ≤ 19 -21 ≤ k ≤ 21 -40 ≤ l ≤ 40

Reflections collected	52540	67536
Independent reflections	17179 (R_{int} = 0.0692, R_{sigma} = 0.0535)	14530 (R_{int} = 0.0994, R_{sigma} = 0.0893)
Data/restraints/parameters	17179/171/1023	14530/24/1194
Goodness-of-fit on F^2	0.918	1.052
R_1, wR_2 (I ≥ 2σ (I))	R_1 = 0.1114, wR_2 = 0.2891	R_1 = 0.0622, wR_2 = 0.1531
R_1, wR_2 (all data)	R_1 = 0.1235, wR_2 = 0.3061	R_1 = 0.0964, wR_2 = 0.1715

Table S3 Crystallographic data for ***trans*-2[PF_6]$_n$** (n = 2, 4)

Complex	***trans*-2[PF_6]$_2$**	***trans*-2[PF_6]$_4$**
Empirical formula	$C_{88}H_{82}F_{12}Fe_2N_6P_6Ru$	$C_{92}H_{88}F_{24}Fe_2N_8P_8Ru$
Formula weight	1850.18	2222.23
Crystal size (mm)	0.296 × 0.287 × 0.281	0.397 × 0.112 × 0.107
Temperature/K	293(2)	293(2)
Crystal system	monoclinic	triclinic
Space group	C2/c	Pī
a/Å	36.990(6)	14.555(3)
b/Å	13.550(2)	16.261(3)
c/Å	18.366(3)	24.871(5)
α/°	90	73.893(6)
β/°	91.345(2)	85.450(7)
γ/°	90	87.854(8)
Volume/Å^3	9203(2)	5636.7(18)
Z	4	2
ρ_{calcd}/g cm^{-3}	1.335	1.309
μ/mm^{-1}	0.647	0.582
F(000)	3784.0	2256.0
λ (Mo/Ga Kα, Å)	Mo, λ = 0.71073	Mo, λ = 0.71073
2θ range/°	6.18-54.97	2.694-54.966
Index range	-48 ≤ h ≤ 48 -17 ≤ k ≤ 17 -23 ≤ l ≤ 23	-18 ≤ h ≤ 18 -21 ≤ k ≤ 21 -32 ≤ l ≤ 32
Reflections collected	67530	87619
Independent reflections	10364 (R_{int} = 0.0374, R_{sigma} = 0.0214)	25780 (R_{int} = 0.0483, R_{sigma} = 0.0449)
Data/restraints/parameters	10364/31/522	25780/8/1258
Goodness-of-fit on F^2	1.047	1.063
R_1, wR_2 (I ≥ 2σ (I))	R_1 = 0.0484, wR_2 = 0.1317	R_1 = 0.0625, wR_2 = 0.1674
R_1, wR_2 (all data)	R_1 = 0.0509, wR_2 = 0.1355	R_1 = 0.0737, wR_2 = 0.1794

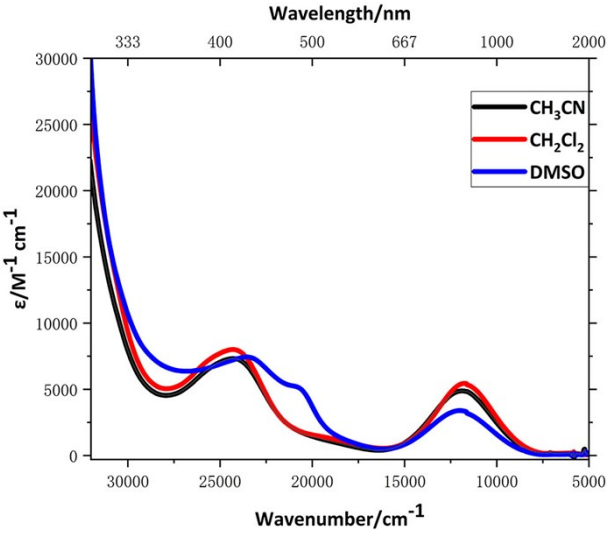

Fig. S1 The UV-vis-NIR spectra of ***cis*-1[PF_6]$_2$** in different solvents at room temperature.

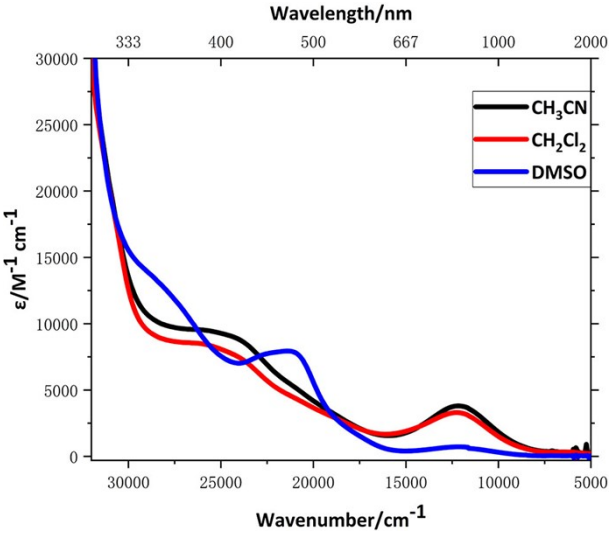

Fig. S2 The UV-vis-NIR spectra of ***cis*-2[PF_6]$_3$** in different solvents at room temperature.

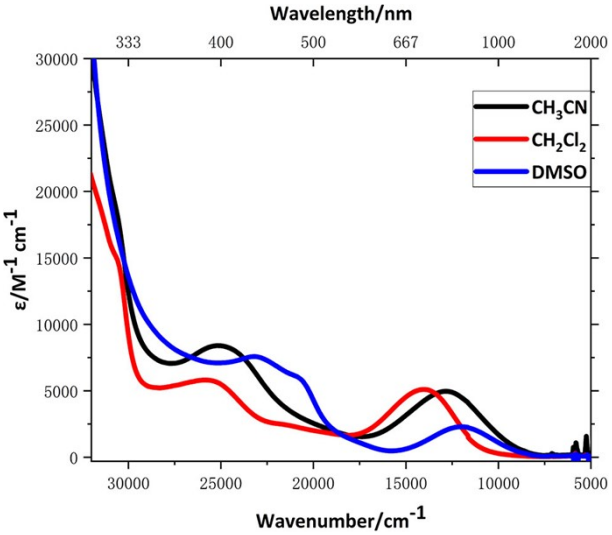

Fig. S3 The UV-vis-NIR spectra of ***cis*-2[PF_6]$_4$** in different solvents at room temperature.

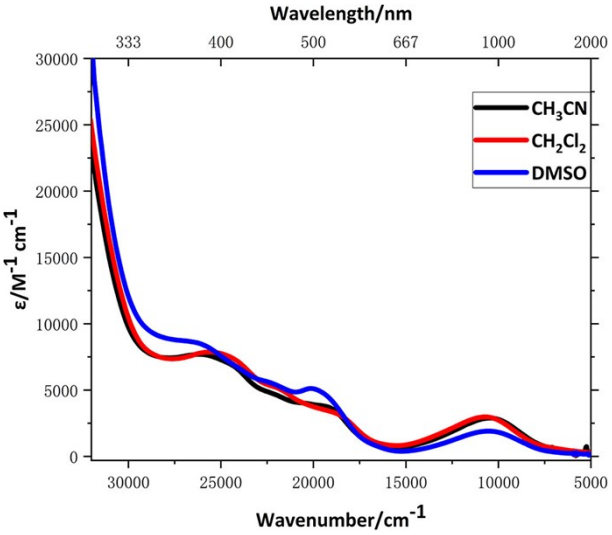

Fig. S4 The UV-vis-NIR spectra of ***trans*-2[PF_6]$_3$** in different solvents at room temperature.

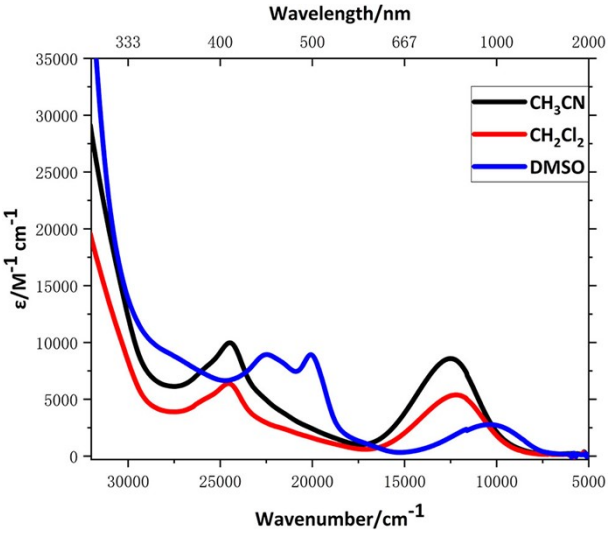

Fig. S5 The UV-vis-NIR spectra of ***trans*-2[PF_6]$_4$** in different solvents at room temperature.

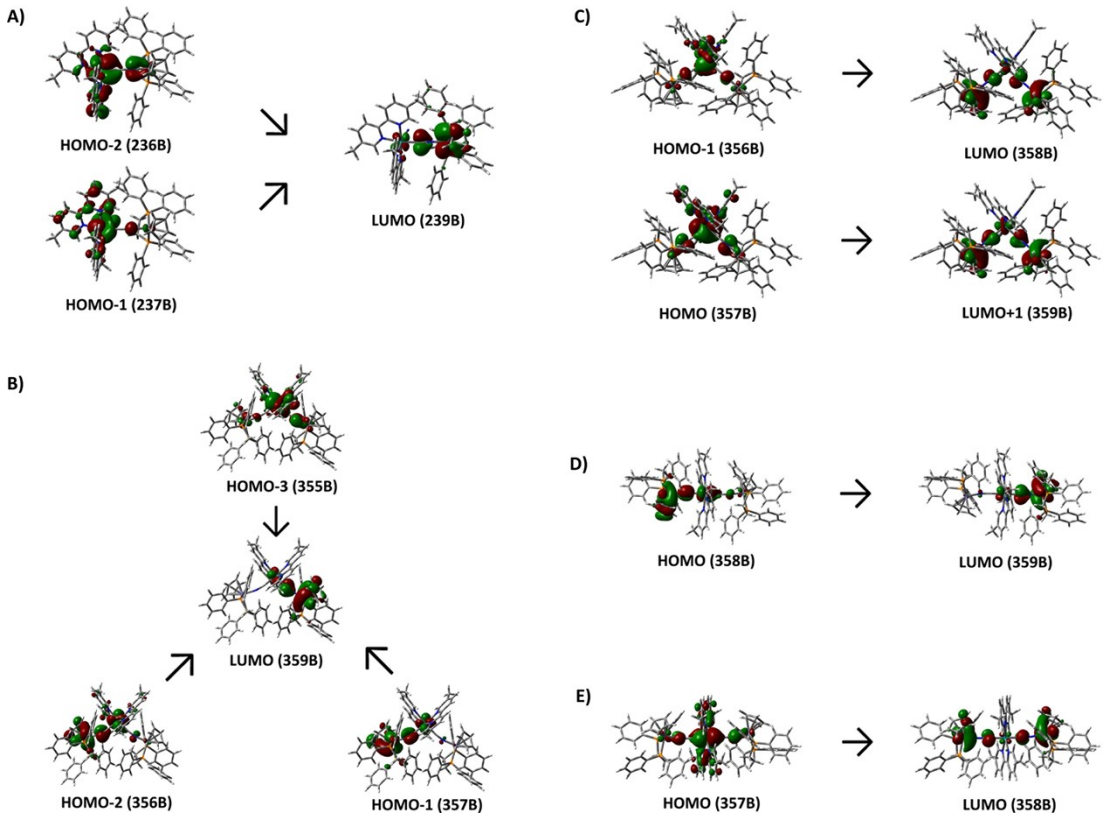

Fig. S6 Molecular orbital diagrams of ***cis*-1[PF_6]$_2$** (**A**), ***cis*-2[PF_6]$_3$** (**B**), ***cis*-2[PF_6]$_4$** (**C**), ***trans*-2[PF_6]$_3$** (**D**) and ***trans*-2[PF_6]$_4$** (**E**) in acetonitrile (isocontour value: 0.02 [e b^{-3}]$^{1/2}$).

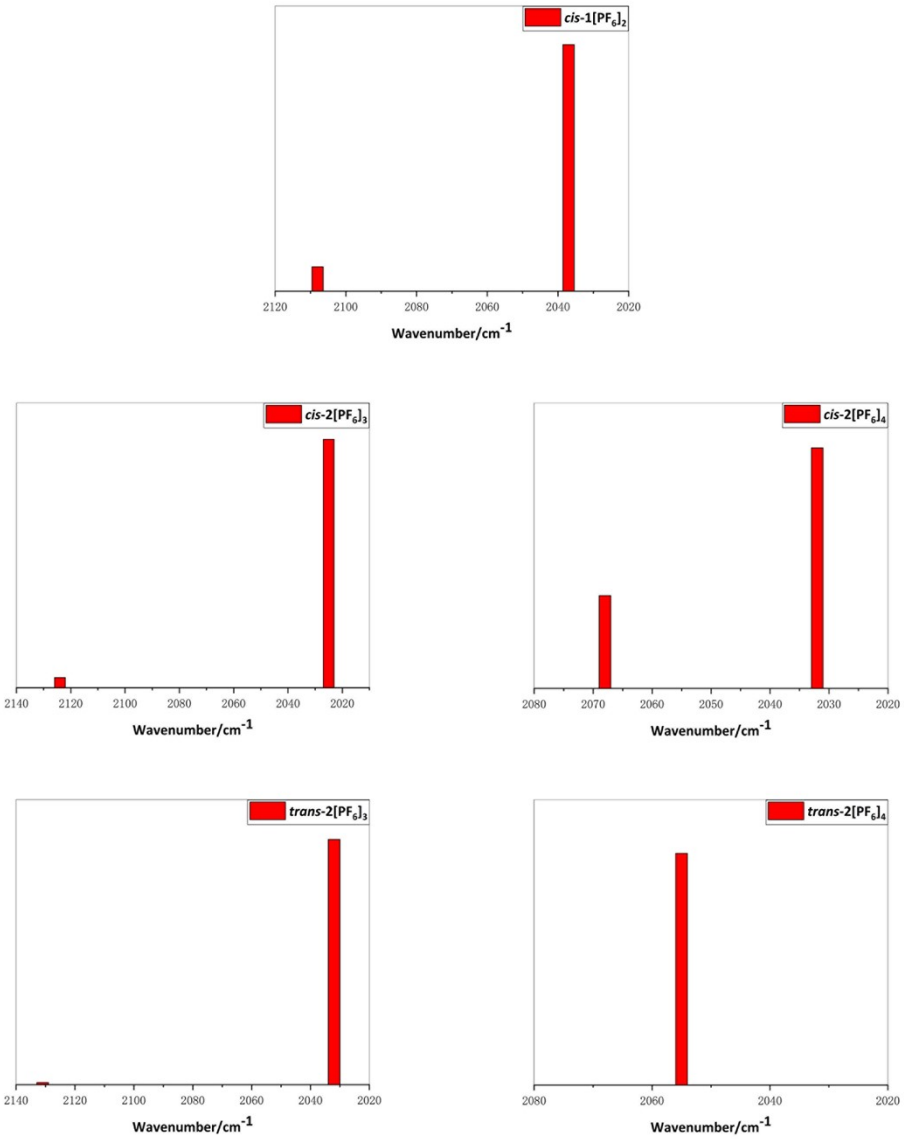

Fig. S7 The calculated C≡N stretching frequencies of ***cis*-1[PF_6]$_2$**, ***cis*-2[PF_6]$_3$**, ***cis*-2[PF_6]$_4$**, ***trans*-2[PF_6]$_3$** and ***trans*-2[PF_6]$_4$** in acetonitrile.

Table S4 The experimental and calculated C≡N stretching frequencies of ***cis*-1[PF_6]$_2$**, ***cis*-2[PF_6]$_3$**, ***cis*-2[PF_6]$_4$**, ***trans*-2[PF_6]$_3$** and ***trans*-2[PF_6]$_4$**

Complex	$\nu_{C\equiv N}$/cm^{-1} (exp)	$\nu_{C\equiv N}$/cm^{-1} (calc)
***cis*-1[PF_6]$_2$**	2077, 2010	2108, 2037
***cis*-2[PF_6]$_3$**	2087, 2015	2124, 2025
***cis*-2[PF_6]$_4$**	2056, 2018	2068, 2032
***trans*-2[PF_6]$_3$**	2098, 2037	2131, 2032
***trans*-2[PF_6]$_4$**	2040	2055

Optimized Cartesian Coordinates of *cis*-1^{2+}

Atomic Name	X	Y	Z
Ru	-2.48727	0.093405	-0.282929
Fe	2.293211	0.220273	1.364518

P	2.8756	1.512523	-0.550583
P	2.779684	-1.59144	-0.070476
N	-2.452509	-1.974928	-0.669901
N	-4.352537	0.384124	-1.293701
N	-2.912419	2.104011	0.155971
N	-3.508576	-0.700679	1.433306
N	0.466617	0.139183	0.859894
N	-0.799364	0.788198	-2.912774
C	-0.681737	0.083695	0.515786
C	-4.85937	1.653901	-1.203557
C	-1.909971	-2.54815	-1.780954
H	-1.430935	-1.867098	-2.474918
C	-3.102514	-2.764293	0.249697
C	2.44038	0.453553	-2.086713
H	1.584986	0.897876	-2.605187
H	3.311889	0.511996	-2.745415
C	-4.085021	2.592346	-0.371814
C	4.561751	-2.087124	-0.360127
C	-4.00743	0.019307	2.471628
H	-3.847562	1.090749	2.430284
C	1.85444	5.477018	0.104355
H	2.244976	6.288405	0.712816
C	-4.999098	-0.539716	-2.04999
H	-4.54852	-1.523341	-2.09807
C	1.94173	-3.211925	0.364519
C	2.448412	4.206354	0.174195
H	3.30736	4.061165	0.825145
C	2.080492	-1.009919	-1.736224
H	2.408857	-1.693244	-2.527395
H	0.996375	-1.102926	-1.641948
C	4.670593	2.014917	-0.824177
C	5.21174	-1.848764	-1.588827
H	4.700429	-1.353816	-2.408847
C	1.969297	3.148793	-0.636457
C	0.876348	3.368507	-1.498688
H	0.468251	2.579095	-2.121677
C	-2.153062	2.915711	0.944882
H	-1.231516	2.486219	1.317139
C	2.360625	-4.406262	-0.2647
H	3.163268	-4.393782	-0.99724
C	0.91681	-3.253724	1.333061
H	0.582589	-2.340657	1.814939
C	3.697378	1.378996	2.666616
H	4.372454	2.150166	2.323804

C	-3.673154	-2.062505	1.417007
C	5.731892	1.350801	-0.176389
H	5.535637	0.538151	0.51355
C	-6.182181	-0.269112	-2.761423
C	-4.494651	3.9123	-0.098906
H	-5.41912	4.293598	-0.516064
C	-4.699882	-0.555021	3.553609
C	-1.501028	0.578531	-1.970437
C	-3.20932	-4.153394	0.04179
H	-3.733284	-4.775116	0.758451
C	3.996415	-0.024995	2.731779
H	4.94273	-0.484134	2.486953
C	-2.509536	4.235695	1.269897
C	5.261707	-2.742432	0.679984
H	4.766461	-2.970098	1.621641
C	-1.977518	-3.927574	-2.047511
C	2.350393	1.570139	3.124877
H	1.829457	2.515604	3.184459
C	1.828625	0.285957	3.512582
H	0.833604	0.097089	3.890501
C	0.324462	-4.482866	1.676951
H	-0.451772	-4.511818	2.437469
C	-4.354108	-2.709523	2.468024
H	-4.488935	-3.784921	2.456853
C	-3.714129	4.732585	0.722168
H	-4.034943	5.748082	0.938679
C	-6.852627	-1.333392	-3.599881
H	-6.869085	-1.045146	-4.658809
H	-7.894246	-1.48458	-3.289854
H	-6.33494	-2.295289	-3.523545
C	2.840493	-0.703527	3.270549
H	2.765035	-1.759271	3.489482
C	-2.649744	-4.734853	-1.101793
H	-2.738517	-5.805693	-1.265031
C	0.775585	5.703464	-0.775187
H	0.334496	6.694047	-0.852123
C	-6.702327	1.041361	-2.663563
H	-7.611287	1.307341	-3.196471
C	0.74471	-5.67279	1.053303
H	0.298188	-6.623665	1.332069
C	0.289126	4.648343	-1.56738
H	-0.536681	4.813371	-2.254021
C	-4.866796	-1.959095	3.532895
H	-5.39589	-2.455928	4.341846

C	6.545737	-2.259252	-1.775472
H	7.035348	-2.075649	-2.727702
C	1.759189	-5.631105	0.076992
H	2.093746	-6.546921	-0.402711
C	-1.63741	5.082374	2.168911
H	-2.185801	5.403457	3.063851
H	-1.302642	5.98886	1.650119
H	-0.744707	4.537769	2.493771
C	7.064697	1.72041	-0.437424
H	7.875351	1.203429	0.068831
C	-6.041607	1.99983	-1.886907
H	-6.439444	3.005823	-1.824285
C	6.593629	-3.149103	0.491964
H	7.119775	-3.661537	1.292723
C	7.347007	2.75121	-1.352395
H	8.375756	3.038252	-1.55177
C	-1.356721	-4.507923	-3.298169
H	-0.977354	-3.723981	-3.961447
H	-2.084435	-5.10362	-3.863045
H	-0.520346	-5.173763	-3.047263
C	-5.244684	0.29729	4.677513
H	-4.851231	-0.0279	5.648883
H	-6.338411	0.223268	4.732439
H	-4.987741	1.353626	4.546145
C	4.956706	3.048175	-1.747401
H	4.153997	3.577482	-2.253543
C	7.240266	-2.906263	-0.737271
H	8.268044	-3.22604	-0.88474
C	6.289821	3.410753	-2.009593
H	6.499925	4.206169	-2.719215

Optimized Cartesian Coordinates of cis-2^{3+}

Atomic Name	X	Y	Z
Ru	-0.047917	2.372604	0.002202
Fe	-4.058878	-0.40476	-1.216558
Fe	4.144172	-0.171149	1.126181
P	-3.270923	-2.623234	-1.136158
P	-5.070959	-0.929766	0.845545
P	4.902738	-0.814769	-1.008281
P	3.539543	-2.440947	1.339189
N	2.45049	0.426308	0.427594
N	-2.451935	0.312978	-0.430982
C	-1.506465	1.004832	-0.196071
C	1.464389	1.065564	0.210878

N	-0.036675	2.512583	-2.103791
N	-1.500885	3.907807	-0.353543
N	1.349314	3.964217	0.333179
C	-1.299028	-4.380265	-2.251846
H	-1.912421	-5.192024	-1.870912
N	-0.061732	2.540294	2.105503
C	-0.208921	2.811081	-4.88632
H	-0.281481	2.935027	-5.963472
C	4.925179	-0.182024	3.185861
H	4.78213	-0.989912	3.88941
C	-1.681507	-3.035381	-2.050261
C	0.699828	1.876574	-4.339296
C	-4.48293	-0.465954	-3.367217
H	-4.079273	-1.190301	-4.060644
C	0.741722	1.767135	-2.936308
H	1.418155	1.073295	-2.453745
C	-1.706128	4.210632	-1.674577
C	-3.892766	0.798291	-3.056545
H	-2.959993	1.175138	-3.450945
C	1.986681	4.671578	-0.636007
H	1.792611	4.364892	-1.657149
C	-3.067102	5.646927	0.319932
C	-1.011797	3.582866	-4.038198
H	-1.702402	4.302074	-4.462706
C	4.941141	0.480035	-2.370713
C	-2.163726	4.605493	0.605287
H	-1.958677	4.321054	1.630682
C	-0.914363	3.426125	-2.641873
C	1.426113	-4.184594	2.141429
H	1.99938	-4.972409	1.658112
C	0.242328	-4.51851	2.822187
H	-0.091065	-5.552502	2.84758
C	-0.485627	-3.520636	3.501073
H	-1.381406	-3.786076	4.057345
C	-0.033957	-2.188342	3.478558
H	-0.586347	-1.419357	4.011075
C	1.148764	-1.850185	2.792098
H	1.496072	-0.82171	2.777999
C	1.888629	-2.848648	2.129505
C	-5.710469	-0.588673	-2.613238
H	-6.412077	-1.408525	-2.652909
C	-3.285781	5.947742	-1.044759
H	-3.973473	6.741849	-1.323277
C	1.54292	4.293604	1.649611

C	4.07327	0.958257	3.021069
H	3.176607	1.169665	3.586586
C	-5.888448	0.633134	-1.875007
H	-6.727821	0.859214	-1.232482
C	0.784576	3.491145	2.628976
C	4.649512	1.793977	1.99463
H	4.249343	2.733284	1.640444
C	2.403781	5.354278	1.997697
H	2.557442	5.622495	3.036404
C	0.642847	-3.646316	-3.53158
H	1.521012	-3.884611	-4.12674
C	-2.607709	5.23128	-2.03832
H	-2.772513	5.476778	-3.080948
C	-4.190055	-2.487814	1.540165
H	-3.921414	-2.292739	2.583323
H	-4.916651	-3.305736	1.531861
C	-5.00115	0.343148	2.221956
C	-0.760189	1.901015	4.351255
C	-0.893705	-1.997613	-2.590174
H	-1.186588	-0.962988	-2.441841
C	-4.760296	1.480508	-2.125147
H	-4.601633	2.466675	-1.711753
C	-5.392319	-0.012233	3.534003
H	-5.688608	-1.032854	3.765599
C	5.152383	2.472962	-4.361829
H	5.257927	3.244161	-5.120348
C	3.519321	6.520874	-1.481772
H	4.612468	6.4434	-1.419195
H	3.272449	7.588239	-1.423786
H	3.2084	6.162067	-2.468687
C	6.005281	-0.083276	2.240091
H	6.826912	-0.777824	2.146301
C	4.511823	1.79683	-2.103481
H	4.113819	2.046844	-1.124456
C	-0.807985	1.775085	2.94976
H	-1.46035	1.050924	2.478047
C	5.475149	0.164677	-3.641017
H	5.849511	-0.833903	-3.850897
C	0.263844	-2.305794	-3.329347
H	0.854496	-1.504633	-3.765936
C	5.574414	1.156312	-4.633746
H	6.001393	0.909393	-5.601885
C	4.620712	2.788628	-3.097575
H	4.316353	3.809079	-2.879308

C	-0.138033	-4.683669	-2.985992
H	0.139214	-5.721289	-3.150949
C	2.85071	5.749925	-0.366514
C	-5.456975	0.963721	4.544401
H	-5.779921	0.6851	5.543782
C	1.588033	1.026727	-5.218702
H	0.99864	0.281918	-5.770415
H	2.352096	0.501661	-4.637023
H	2.104899	1.641238	-5.964893
C	-7.874948	-0.459158	1.241946
H	-7.584001	0.492817	1.676754
C	-6.900332	-1.377094	0.790687
C	-7.313955	-2.608875	0.236452
H	-6.591455	-3.328586	-0.136845
C	-8.682577	-2.924916	0.155077
H	-8.988889	-3.879647	-0.26358
C	-9.651456	-2.011247	0.612095
H	-10.707619	-2.257614	0.549671
C	-9.243259	-0.777532	1.152563
H	-9.984242	-0.067445	1.509388
C	5.841793	1.160621	1.522883
H	6.509566	1.562385	0.773862
C	5.370115	-4.679874	4.364844
H	5.131479	-4.975799	5.382757
C	4.447825	-3.912419	3.628952
H	3.504544	-3.637005	4.092321
C	4.74074	-3.528078	2.30106
C	5.973798	-3.909283	1.727382
H	6.239712	-3.613837	0.716843
C	6.890169	-4.681452	2.465019
H	7.831442	-4.976885	2.009707
C	6.592317	-5.069087	3.785235
H	7.300647	-5.666014	4.352707
C	-6.004356	-6.247363	-2.407275
H	-6.621357	-7.086018	-2.717183
C	-5.417876	-6.234537	-1.128115
H	-5.578725	-7.065571	-0.446797
C	-4.612788	-5.150351	-0.728085
H	-4.163562	-5.179743	0.260539
C	-4.391813	-4.061559	-1.600546
C	-4.978439	-4.086028	-2.886025
H	-4.801419	-3.278847	-3.590325
C	-5.77765	-5.171006	-3.287451
H	-6.216999	-5.178844	-4.281101

C	3.601905	-2.104089	-1.506678
H	2.663049	-1.551081	-1.600861
H	3.831583	-2.543242	-2.483735
C	-2.930797	-2.841594	0.717612
H	-2.582974	-3.855717	0.940842
H	-2.108511	-2.156609	0.944558
C	6.558733	-1.680286	-1.229892
C	7.731585	-1.037747	-0.773518
H	7.67771	-0.070348	-0.28307
C	8.992971	-1.625549	-0.974118
H	9.887059	-1.116838	-0.624515
C	9.099249	-2.866715	-1.631958
H	10.073837	-3.320154	-1.788829
C	7.93647	-3.51034	-2.09456
H	8.010484	-4.462785	-2.612316
C	6.673221	-2.919429	-1.898305
H	5.797613	-3.437354	-2.279574
C	-3.760735	6.412319	1.423837
H	-3.445777	6.072091	2.416043
H	-4.85134	6.3078	1.356705
H	-3.539857	7.484835	1.355685
C	-4.670095	1.682513	1.93533
H	-4.371546	1.960877	0.929063
C	-5.139208	2.30535	4.25065
H	-5.219403	3.064219	5.024637
C	3.055192	6.080686	0.993533
H	3.7117	6.904698	1.260103
C	0.117544	2.872969	4.883361
H	0.192771	3.009455	5.958871
C	3.471883	-3.196768	-0.422609
H	4.275968	-3.934844	-0.497093
H	2.519214	-3.724459	-0.532714
C	-4.742983	2.65986	2.947817
H	-4.516709	3.696941	2.714866
C	0.885659	3.665531	4.022829
H	1.552762	4.413203	4.435607
C	-1.612689	1.03262	5.247732
H	-2.206024	1.645561	5.936606
H	-0.99006	0.371627	5.865414
H	-2.309986	0.416455	4.672016

Optimized Cartesian Coordinates of cis-2^{4+}

Atomic Name	X	Y	Z
Ru	-0.000004	1.760687	0.00056

Fe	-3.810495	-1.661985	-0.461793
Fe	3.810417	-1.662381	0.460795
P	4.481773	-1.540209	-1.823599
P	5.573403	-0.076708	0.769916
P	-5.573756	-0.076086	-0.769611
P	-4.481498	-1.541713	1.822604
N	2.40086	-0.350745	0.222598
N	-0.406294	1.941814	2.06889
N	-1.439562	3.355615	0.038383
C	6.024966	-2.410748	-2.439218
C	5.871542	0.76082	-0.92741
H	5.818163	1.843406	-0.774842
H	6.891844	0.518226	-1.237178
C	4.836176	0.316701	-1.985331
H	5.179053	0.559321	-2.997017
H	3.875496	0.814153	-1.826373
C	-6.107397	2.379534	-2.095005
H	-6.955829	2.467526	-1.420159
C	3.611234	-3.855832	0.414703
H	3.502821	-4.456834	-0.476919
C	3.170918	-2.052248	-3.06383
C	9.323801	-1.927357	0.888276
H	9.994263	-2.411066	0.183717
C	3.100998	-2.649544	2.337481
H	2.546289	-2.160922	3.126576
C	3.094162	5.985562	2.173122
H	4.18312	6.102822	2.22539
H	2.761663	5.499312	3.095218
H	2.665104	6.995754	2.150889
C	-0.136113	1.170595	-3.049429
H	-0.806054	0.388344	-2.716095
C	3.53056	-2.262248	-4.414687
H	4.550058	-2.096045	-4.751155
C	-5.216905	1.284761	-2.002501
C	-1.46926	0.398064	-0.145225
C	7.028054	-1.714223	-3.151329
H	6.962154	-0.644191	-3.326435
N	0.406227	1.942709	-2.06773
C	-4.883887	3.213937	-4.033825
H	-4.777554	3.938885	-4.836355
C	-2.686542	5.204355	-0.943985
C	5.216052	1.283324	2.003578
C	-7.590138	-0.653989	-2.704243
H	-6.946975	-0.1455	-3.417184

C	1.603871	3.179022	-3.762465
H	2.288135	3.973914	-4.034598
C	2.536523	-3.331579	1.200934
H	1.48335	-3.436018	0.980623
C	-4.527315	-2.752525	-2.26003
H	-5.24292	-2.369745	-2.973881
C	2.687009	5.20362	0.946506
C	3.080732	5.601145	-0.351653
H	3.70683	6.479325	-0.485292
C	-4.154638	1.168054	-2.919954
H	-3.470107	0.327554	-2.853621
C	-2.536332	-3.329244	-1.205569
H	-1.482884	-3.433126	-0.9863
C	7.589235	-0.655647	2.704772
H	6.945839	-0.147638	3.417843
C	2.575827	-2.735089	-5.333474
H	2.863572	-2.909489	-6.366339
C	4.154075	1.165411	2.921198
H	3.469951	0.324601	2.854443
C	-3.102305	-2.646117	-2.340697
H	-2.548659	-2.156227	-3.129748
C	1.279264	2.949231	-2.410711
C	1.469198	0.397888	0.145647
N	-2.4009	-0.350539	-0.222737
C	-1.87309	4.057919	-1.040562
H	-1.555493	3.695179	-2.010417
C	0.138063	1.348667	-4.417934
C	8.814675	-1.183443	3.150499
H	9.091492	-1.089367	4.196676
C	-4.852631	-3.464989	-1.048157
H	-5.848248	-3.734554	-0.727095
C	-3.991202	2.130334	-3.935252
H	-3.190025	2.021918	-4.661532
C	0.135513	1.168863	3.050244
H	0.805089	0.386447	2.716569
C	8.138739	-2.405859	-3.671829
H	8.900479	-1.861971	-4.223208
C	4.853075	-3.465528	1.045494
H	5.849141	-3.733997	0.724907
C	7.252893	-4.497421	-2.792546
H	7.330295	-5.573205	-2.663774
C	-8.815679	-1.181553	-3.149963
H	-9.092791	-1.086829	-4.196004
C	1.033855	2.385847	-4.764658

H	1.278743	2.569951	-5.807281
C	6.143657	-3.809193	-2.270428
H	5.369307	-4.379041	-1.765273
C	-8.097546	-1.406648	-0.435531
H	-7.84553	-1.513653	0.61462
C	-1.27898	2.948488	2.412318
C	-1.034253	2.383613	4.765975
H	-1.279281	2.567164	5.808665
C	-9.686659	-1.817548	-2.244296
H	-10.635933	-2.216688	-2.589513
N	1.43982	3.35541	-0.036592
C	1.873324	4.057314	1.042623
H	1.555493	3.694358	2.012322
C	-9.324128	-1.926913	-0.888071
H	-9.994356	-2.411109	-0.183625
C	-5.937195	3.342016	-3.105859
H	-6.641462	4.165098	-3.188804
C	-2.574545	-2.736402	5.331959
H	-2.861906	-2.910297	6.365017
C	-3.09403	5.986544	-2.170332
H	-2.667399	6.997715	-2.146651
H	-4.183215	6.101255	-2.223773
H	-2.759344	5.501929	-3.092503
C	-7.027455	-1.717775	3.150668
H	-6.961966	-0.647851	3.326614
C	-1.262641	-3.01958	4.904583
H	-0.53968	-3.423166	5.608561
C	-3.529427	-2.263257	4.413476
H	-4.548673	-2.096339	4.750369
C	-8.137743	-2.410314	3.670809
H	-8.899613	-1.867214	4.222788
C	1.851579	-2.318558	-2.640368
H	1.570029	-2.161254	-1.603384
C	-3.170311	-2.053947	3.062384
C	-6.02423	-2.413302	2.437777
C	1.263507	-3.017217	-4.90667
H	0.540634	-3.420567	-5.610871
C	-5.871714	0.76004	0.928404
H	-5.818359	1.842768	0.776774
H	-6.892004	0.517202	1.238012
C	8.25659	-3.796981	-3.490847
H	9.111198	-4.329598	-3.897791
C	-1.603712	3.177643	3.764156
H	-2.287735	3.972632	4.036613

C	0.905152	-2.804241	-3.561784
H	-0.100416	-3.047923	-3.227295
C	-3.079857	5.601667	0.354362
H	-3.705677	6.479992	0.488364
C	1.819562	3.749519	-1.294609
C	-0.90483	-2.807359	3.559432
H	0.100334	-3.052048	3.224469
C	5.935632	3.340078	3.108304
H	6.639535	4.16342	3.191732
C	-1.851375	-2.321323	2.638334
H	-1.570265	-2.164589	1.601143
C	-4.836317	0.315024	1.985877
H	-5.179174	0.556708	2.9978
H	-3.875679	0.812709	1.827371
C	9.685939	-1.818826	2.244677
H	10.635137	-2.218133	2.58991
C	-7.251176	-4.500784	2.789632
H	-7.328145	-5.576496	2.659997
C	4.882593	3.210808	4.036423
H	4.776147	3.935088	4.839542
C	8.097321	-1.406871	0.435723
H	7.845593	-1.51318	-0.614573
C	-8.255032	-3.80134	3.488701
H	-9.109333	-4.334654	3.895377
C	3.990401	2.126865	3.937254
H	3.189455	2.017478	4.66364
C	-3.609973	-3.855229	-0.418971
H	-3.500378	-4.457383	0.471737
C	4.526169	-2.754849	2.257989
H	5.240833	-2.372501	2.973019
C	-0.138857	1.346229	4.418786
C	2.652596	4.872415	-1.468039
H	2.949081	5.192757	-2.459968
C	-0.492608	0.464678	-5.469281
H	-1.282471	-0.168322	-5.050033
H	0.25595	-0.197839	-5.92178
H	-0.926772	1.05915	-6.282202
C	-6.142335	-3.811653	2.267863
H	-5.367796	-4.380727	1.7621
C	-1.819034	3.749432	1.296575
C	6.106065	2.37844	2.096695
H	6.954343	2.467305	1.421774
C	-7.228054	-0.757491	-1.340446
C	0.491358	0.4615	5.469784

H	-0.258546	-0.19684	5.926082
H	0.930754	1.055692	6.280144
H	1.277084	-0.175705	5.049181
C	7.227544	-0.75833	1.340815
C	-2.651709	4.87252	1.47047
H	-2.947922	5.192678	2.462541

Optimized Cartesian Coordinates of trans-2^{3+}

Atomic Name	X	Y	Z
Ru	-0.045133	-0.074363	0.032017
Fe	4.990657	-0.188634	-1.224227
P	5.759498	1.696389	-0.068268
P	5.705943	-1.388213	0.652063
N	3.176773	-0.068108	-0.520245
C	2.013294	-0.04659	-0.282513
N	-0.14716	-1.330074	-1.670894
C	-0.627619	-0.747777	-2.814532
C	7.516808	-1.874355	0.852374
C	4.695852	3.245479	-0.00402
C	4.840006	-2.98558	1.153077
C	-0.77277	-1.498511	-3.997905
H	-1.158031	-1.034911	-4.898363
C	0.295305	-2.615466	-1.726946
H	0.764077	-2.999101	-0.831088
C	4.48907	0.266988	-3.312967
H	3.73925	0.96997	-3.648158
C	7.440123	2.379508	-0.587248
C	0.204959	-3.420258	-2.876562
C	6.017731	1.20179	1.77231
H	7.096496	1.184257	1.955064
H	5.585271	1.977097	2.413062
C	5.377075	-0.171056	2.077345
H	4.286398	-0.084514	2.13094
H	5.731283	-0.568205	3.035652
C	4.964962	4.283134	0.917097
H	5.771993	4.18412	1.639485
C	8.281105	-1.518566	1.984965
H	7.85611	-0.91818	2.784681
C	8.596188	1.590678	-0.390849
H	8.5328	0.612515	0.078471
C	8.114252	-2.667695	-0.153194
H	7.543262	-2.971234	-1.02604
C	3.679295	3.421359	-0.963946
H	3.472981	2.626283	-1.674667

C	5.880161	0.546679	-3.108996
H	6.358081	1.510918	-3.21545
C	4.291022	-1.147088	-3.079311
H	3.351579	-1.676587	-3.161593
C	5.546008	-1.717555	-2.710632
H	5.724948	-2.762845	-2.498019
C	9.448093	-3.094742	-0.029809
H	9.892024	-3.709793	-0.807906
C	5.216882	-3.682346	2.32251
H	5.991392	-3.28597	2.974682
C	7.560241	3.631097	-1.228968
H	6.687764	4.255953	-1.396026
C	-0.376494	-2.839304	-4.025673
H	-0.480317	-3.419442	-4.938645
C	9.619749	-1.940058	2.105376
H	10.196457	-1.657494	2.982082
C	6.537085	-0.662184	-2.701226
H	7.594217	-0.772865	-2.509931
C	4.229449	5.481843	0.875837
H	4.465148	6.283907	1.570702
C	3.871803	-3.545421	0.294445
H	3.592574	-3.012512	-0.610831
C	0.726551	-4.839438	-2.884045
H	1.572219	-4.945498	-3.575726
H	-0.046417	-5.54361	-3.216026
H	1.066468	-5.15331	-1.891774
C	3.226316	5.660463	-0.098562
H	2.688515	6.603837	-0.15709
C	2.953381	4.627622	-1.01543
H	2.206789	4.77267	-1.792049
C	9.854604	2.05836	-0.810272
H	10.737159	1.445744	-0.64664
C	3.301645	-4.798161	0.594082
H	2.590634	-5.250595	-0.094266
C	-0.813397	0.710295	-2.747422
C	-1.280317	1.48388	-3.828234
H	-1.628312	1.002324	-4.734648
C	-0.324166	2.664277	-1.544243
H	0.112705	3.098303	-0.6581
C	-1.274438	2.880387	-3.743136
H	-1.634813	3.47992	-4.574877
C	-0.762652	3.50512	-2.584817
C	-0.687358	5.010457	-2.461921
H	-0.276121	5.319553	-1.495713

H	-1.682251	5.462483	-2.561747
H	-0.059599	5.441673	-3.252195
C	3.682242	-5.491877	1.758205
H	3.271064	-6.476126	1.97064
C	9.971705	3.310948	-1.44338
H	10.944136	3.670669	-1.76803
C	4.635032	-4.92608	2.628538
H	4.949264	-5.465401	3.518271
C	10.207164	-2.72877	1.099191
H	11.238221	-3.057626	1.194688
C	8.821126	4.092712	-1.654116
H	8.901869	5.059475	-2.14389
N	-0.382928	1.30748	-1.586104
Fe	-5.020662	-0.246812	1.215018
P	-5.87252	-1.378595	-0.701064
P	-5.667004	1.707593	0.027733
N	-3.232345	-0.140409	0.551876
C	-2.052266	-0.114187	0.338065
N	0.350272	1.136158	1.770446
C	0.924248	0.430093	2.801573
C	-7.459587	2.263297	-0.019674
C	-4.857828	-2.829091	-1.305492
C	-4.739432	3.274441	0.469332
C	1.500378	1.095508	3.900822
H	1.968523	0.529721	4.697772
C	0.267307	2.487274	1.884471
H	-0.265828	3.003266	1.099781
C	-4.686158	-1.563122	2.989688
H	-3.940262	-2.343504	3.051266
C	-7.611154	-2.077138	-0.560319
C	0.815667	3.223818	2.951257
C	-5.921254	-0.107993	-2.133459
H	-6.971618	0.045808	-2.39651
H	-5.423326	-0.559117	-2.997358
C	-5.229965	1.218662	-1.75071
H	-4.141723	1.110987	-1.763417
H	-5.497444	2.01857	-2.449934
C	-5.120306	-3.373478	-2.583626
H	-5.868046	-2.929103	-3.236645
C	-8.140825	2.472529	-1.239683
H	-7.662449	2.280971	-2.195924
C	-8.730484	-1.214711	-0.568206
H	-8.615235	-0.14057	-0.678805
C	-8.117103	2.55964	1.195911

H	-7.604928	2.448118	2.147329
C	-3.918075	-3.451392	-0.46015
H	-3.707641	-3.035505	0.520567
C	-6.034812	-1.717316	2.53046
H	-6.497164	-2.633688	2.191267
C	-4.499313	-0.18939	3.376653
H	-3.586477	0.238564	3.767173
C	-5.728743	0.51008	3.150165
H	-5.912705	1.548066	3.387983
C	-9.436408	3.04502	1.192325
H	-9.928381	3.277385	2.132565
C	-5.140715	4.506542	-0.095377
H	-5.966918	4.552688	-0.800059
C	-7.803414	-3.467923	-0.396966
H	-6.959619	-4.151965	-0.397448
C	1.465293	2.492185	3.969342
H	1.920279	3.009393	4.809754
C	-9.463073	2.95703	-1.241032
H	-9.97476	3.11994	-2.185455
C	-6.677945	-0.428012	2.591025
H	-7.710892	-0.228461	2.34618
C	-4.448234	-4.533109	-3.008647
H	-4.667797	-4.955417	-3.985213
C	-3.697236	3.243412	1.418342
H	-3.383996	2.300862	1.856584
C	0.734828	4.732934	2.985782
H	0.364921	5.092985	3.953587
H	1.728449	5.172963	2.832604
H	0.080865	5.124021	2.199178
C	-3.521441	-5.163931	-2.155222
H	-3.028906	-6.079655	-2.471471
C	-3.257609	-4.620175	-0.884445
H	-2.558224	-5.118775	-0.21826
C	-10.027698	-1.742346	-0.434268
H	-10.883881	-1.073897	-0.45377
C	-3.06936	4.441003	1.809231
H	-2.295593	4.417757	2.571621
C	0.790831	-1.03245	2.716915
C	1.122613	-1.912749	3.765793
H	1.616184	-1.543176	4.656773
C	-0.185016	-2.805588	1.520694
H	-0.73472	-3.105049	0.637532
C	0.795624	-3.268211	3.667136
H	1.059988	-3.952302	4.468715

C	0.094313	-3.738763	2.533906
C	-0.323734	-5.186063	2.408733
H	-0.883232	-5.37106	1.485239
H	0.555273	-5.84259	2.404159
H	-0.95134	-5.496801	3.253315
C	-3.466466	5.668228	1.245553
H	-2.996226	6.594983	1.563444
C	-10.218542	-3.12886	-0.277984
H	-11.22134	-3.533858	-0.176947
C	-4.497366	5.697711	0.285466
H	-4.817561	6.643459	-0.142667
C	-10.115479	3.240727	-0.026672
H	-11.133444	3.619589	-0.029557
C	-9.103687	-3.988176	-0.257921
H	-9.243782	-5.059296	-0.142824
N	0.190563	-1.498928	1.576796

Optimized Cartesian Coordinates of trans-2^{4+}

Atomic Name	X	Y	Z
Ru	0.005754	-0.054618	-0.428331
Fe	5.123864	-0.584625	-0.885885
Fe	-5.10057	0.606856	-0.881255
P	5.757661	1.585724	-0.125596
P	5.735554	-1.252344	1.329583
P	-5.593496	1.361008	1.331331
P	-5.916167	-1.491403	-0.063336
N	-0.331927	-1.080552	1.414327
C	2.057806	-0.218882	-0.431591
N	3.247821	-0.306102	-0.479961
N	-3.23369	0.248092	-0.490227
C	-2.046265	0.125369	-0.455073
C	-4.99592	0.709027	-3.11644
H	-4.325917	0.131891	-3.738927
N	0.112661	-1.62384	-1.882622
C	4.855598	-1.039553	-3.048575
H	4.014616	-0.707743	-3.641521
N	-0.111254	1.0052	-2.292304
C	7.43075	-2.02918	1.540825
C	-6.857224	1.368539	-1.888671
H	-7.853163	1.386387	-1.470723
C	-6.319394	0.326554	-2.728275
H	-6.831697	-0.58502	-3.002472
N	0.34415	1.470538	1.032587
C	4.943912	-2.284467	-2.329434

H	4.182688	-3.051708	-2.296276
C	7.562364	2.087862	-0.03803
C	-5.87522	2.430152	-1.81874
H	-5.992267	3.385223	-1.326921
C	5.138608	1.53845	1.66631
H	5.382124	2.474166	2.181597
H	4.049012	1.465415	1.598207
C	6.223813	-2.340452	-1.689752
H	6.610628	-3.154708	-1.093025
C	9.66869	2.52755	-1.203238
H	10.249019	2.532791	-2.121426
C	6.917126	-1.107033	-1.972282
H	7.922809	-0.865874	-1.660369
C	8.3332	2.089048	-1.223397
H	7.899547	1.785277	-2.171843
C	7.550519	-3.420893	1.758391
H	6.670485	-4.051399	1.847367
C	0.07832	-1.221869	-3.194605
C	6.076709	-0.319851	-2.849149
H	6.328675	0.627036	-3.304732
C	5.728607	0.324556	2.414543
H	5.141627	0.110955	3.313211
H	6.760611	0.506243	2.726883
C	8.824378	-4.004359	1.892176
H	8.909893	-5.072357	2.071118
C	-4.723643	2.009273	-2.558322
H	-3.807445	2.570215	-2.678594
C	-0.12564	0.218244	-3.417478
C	9.863942	-1.823238	1.582407
H	10.754599	-1.204496	1.519853
C	9.98288	-3.208919	1.806534
H	10.964129	-3.661217	1.917035
C	-0.827199	-2.342819	1.527405
H	-1.004352	-2.876276	0.603564
C	4.566742	-2.469152	2.137518
C	-7.680602	-1.942597	-0.516437
C	3.89403	2.802589	-1.92914
H	3.540012	1.794803	-2.12299
C	4.933025	3.025146	-1.000878
C	0.613317	-3.907903	-2.593719
C	0.405559	-2.924813	-1.608897
H	0.50424	-3.184314	-0.563869
C	8.594815	-1.233015	1.442622
H	8.535443	-0.162948	1.265046

C	-5.107903	-0.161879	2.35117
H	-4.027137	-0.271015	2.219232
H	-5.300097	0.013139	3.415514
C	-1.153969	-2.950089	2.753667
C	0.215381	1.074788	2.340327
C	-10.08542	-1.600838	-0.262458
H	-10.915208	-1.094856	0.222773
C	-0.976544	-2.174103	3.921144
H	-1.209948	-2.59157	4.896876
C	3.688701	-3.249196	1.358784
H	3.620956	-3.088147	0.286919
C	-5.857101	-1.413363	1.848584
H	-6.890125	-1.435632	2.206126
H	-5.362626	-2.322434	2.204649
C	-0.213904	-0.316539	2.548451
C	4.649221	-2.687467	3.532108
H	5.348592	-2.124696	4.146098
C	-8.765054	-1.275484	0.097655
H	-8.605111	-0.511524	0.853225
C	-0.602627	2.971124	-3.661925
C	10.250508	2.970431	0.001463
H	11.281125	3.312838	0.015929
C	-7.352719	1.778125	1.829512
C	-0.348812	0.782902	-4.690525
H	-0.358427	0.156151	-5.574536
C	8.146567	2.544452	1.165382
H	7.58155	2.585327	2.092176
C	3.328245	3.889491	-2.622775
H	2.552335	3.710685	-3.363092
C	0.84445	2.709837	0.773438
H	1.032058	2.948088	-0.264548
C	2.907629	-4.249485	1.968466
H	2.257818	-4.875049	1.360854
C	-0.371808	2.335055	-2.427956
H	-0.421345	2.910196	-1.513862
C	-7.930001	-2.919618	-1.507418
H	-7.113393	-3.45148	-1.987384
C	-10.333944	-2.580042	-1.244115
H	-11.354547	-2.831111	-1.517896
C	-7.977993	1.155059	2.933413
H	-7.475627	0.384631	3.511281
C	-8.036987	2.804072	1.137762
H	-7.565017	3.333294	0.314828
C	0.273222	-2.14991	-4.238492

H	0.243895	-1.827189	-5.272603
C	-4.594744	2.825938	1.938306
C	-1.664573	-4.372316	2.807631
H	-2.009312	-4.719419	1.82773
H	-2.495629	-4.472292	3.51529
H	-0.876536	-5.057412	3.148525
C	0.916145	-5.341506	-2.219419
H	1.845641	-5.689765	-2.686766
H	0.12181	-6.015312	-2.565292
H	1.011879	-5.47033	-1.135918
C	-3.494508	3.305245	1.196657
H	-3.196266	2.809154	0.278119
C	0.525797	-3.493902	-3.942952
H	0.674559	-4.209773	-4.747035
C	-3.349446	-4.102303	-2.067853
H	-2.675032	-4.057454	-2.919124
C	-0.573936	2.157481	-4.818409
H	-0.742221	2.593417	-5.799551
C	-4.981958	3.484199	3.128007
H	-5.846917	3.149007	3.693621
C	-0.525118	-0.854408	3.813122
H	-0.427854	-0.24762	4.705494
C	-3.173193	5.093178	2.829181
H	-2.64268	5.980917	3.162766
C	-9.329156	3.190547	1.534162
H	-9.841876	3.986291	1.001425
C	-9.253911	-3.23569	-1.865544
H	-9.4397	-3.995475	-2.619321
C	-5.159148	-4.227822	0.084081
H	-5.889118	-4.30393	0.886784
C	1.167361	3.649856	1.768973
C	-2.789282	4.438192	1.643541
H	-1.958226	4.823541	1.057631
C	-3.593201	-5.331368	-1.426
H	-3.110454	-6.239486	-1.777278
C	-0.870073	4.457724	-3.741386
H	-0.892854	4.924416	-2.750895
H	-1.827246	4.665427	-4.236197
H	-0.098353	4.966378	-4.333304
C	0.517812	1.961653	3.393102
H	0.407784	1.64605	4.42375
C	-4.916228	-2.992983	-0.561792
C	5.40043	4.339525	-0.771119
H	6.225983	4.524884	-0.089314

C	-4.266812	4.610232	3.573769
H	-4.575414	5.118141	4.482962
C	2.991956	-4.468246	3.35646
H	2.4106	-5.258718	3.823569
C	9.485141	2.981444	1.182792
H	9.922419	3.33688	2.111515
C	1.692845	5.020603	1.406688
H	2.014733	5.07149	0.361423
H	2.545511	5.299546	2.036493
H	0.923654	5.789728	1.560213
C	3.858746	-3.679623	4.139038
H	3.942332	-3.855227	5.207774
C	3.791395	5.199347	-2.391568
H	3.373588	6.03547	-2.945778
C	-9.953719	2.55704	2.627103
H	-10.950384	2.858666	2.935812
C	4.82479	5.422545	-1.460313
H	5.198617	6.428276	-1.290696
C	0.975323	3.252929	3.111712
H	1.202514	3.939042	3.923165
C	-4.006073	-2.933569	-1.635705
H	-3.815944	-1.991056	-2.139847
C	-4.494689	-5.391103	-0.343824
H	-4.704651	-6.340466	0.140832
C	-9.273208	1.543004	3.327097
H	-9.741444	1.062946	4.181712