

Supporting Information

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Table S1. Crystallographic data for **1²⁺** and **1⁴⁺**.

	1²⁺	1⁴⁺·C₄H₁₀O
Empirical formula	C ₉₇ H ₁₀₃ Cl ₂ F ₁₂ Fe ₂ N ₆ P ₆ Ru	C ₉₆ H ₁₀₁ F ₂₄ Fe ₂ N ₆ P ₈ Ru
Color and Habit	Light red block	Dark brown block
Crystal Size (mm)	0.25 × 0.18 × 0.11	0.240×0.150×0.130
Temperature(K)	99.98(11)	100.00(10)
Crystal system	Monoclinic	Triclinic
Space group	<i>P2₁</i>	<i>P$\bar{1}$</i>
a (Å)	15.0314(2)	14.1182(2)
b (Å)	17.2258(2)	14.2919(2)
c (Å)	19.1841(3)	29.4846(3)
alpha (deg.)	90	80.0220(10)
beta (deg.)	106.952(2)	80.4080(10)
gamma (deg.)	90	76.5650(10)
Volume (Å ³)	4751.46(12)	5649.14(13)
Z	2	2
Formula weight	2050.34	2255.35
Density(cal.) (Mg/m ³)	1.433	1.326
<i>M</i> (mm ⁻¹)	3.903	3.302
F (000)	2110.0	2302.0
Theta range (deg.)	4.186 to 120.668	5.338 to 120.16
Reflections collected / unique	37687 / 15869 [R(int) = 0.0354]	63857 / 24880 [R(int) = 0.0473]
Index range	-19 ≤ h ≤ 19, -22 ≤ k ≤ 14, -24 ≤ l ≤ 24	-17 ≤ h ≤ 18, -17 ≤ k ≤ 18, -38 ≤ l ≤ 35
Data/restraints/parameters (obs.)	15869/1/1143	24880/0/1242
Final R indices (obs.)	R ₁ = 0.0349, wR ₂ = 0.0837	R ₁ = 0.0569, wR ₂ = 0.1631

R indices (all)	R ₁ = 0.0388, wR ₂ = 0.0855	R ₁ = 0.0668, wR ₂ = 0.1700
Goodness-of-fit	1.036	1.062

Table S2. Crystallographic data for **2²⁺** and **2⁴⁺**.

	2²⁺	2⁴⁺·0.5C₄H₁₀O
Empirical formula	C ₉₉ H ₁₀₇ Cl ₂ F ₁₂ Fe ₂ N ₆ P ₆ Ru	C ₁₀₅ H ₁₂₂ Cl ₆ F ₂₄ Fe ₂ N ₆ OP ₈ Ru
Color and Habit	Light red block	Dark red block
Crystal Size (mm)	0.250×0.170×0.100	0.230×0.140×0.130
Temperature(K)	100.00(10)	99.97(10)
Crystal system	Monoclinic	Triclinic
Space group	<i>P</i> 2 ₁	<i>P</i> $\bar{1}$
a (Å)	15.2693(2)	15.78350(10)
b (Å)	16.9532(2)	16.41900(10)
c (Å)	19.1955(3)	24.0034(2)
alpha (deg.)	90	74.0600(10)
beta (deg.)	106.015(2)	77.9060(10)
gamma (deg.)	90	76.9500(10)
Volume (Å ³)	4776.16(12)	5754.12(8)
Z	2	2
Formula weight	2078.39	2613.31
Density(cal.) (Mg/m ³)	1.445	1.508
<i>M</i> (mm ⁻¹)	3.888	4.135
F (000)	2142.0	2672.0
Theta range (deg.)	4.164 to 120.348	3.37 to 120.17
Reflections collected / unique	39077 / 15784 [R(int) = 0.0480]	84120 / 25572 [R(int) = 0.0422]
Index range	-19≤h≤19, -12≤k≤21, -24≤l≤24	-20≤h≤20, -21≤k≤15, -30≤l≤30
Data/restraints/parameters (obs.)	15784/1/1163	25572/0/1390
Final R indices (obs.)	R ₁ = 0.0539, wR ₂ = 0.1368	R ₁ = 0.0429, wR ₂ = 0.1091
R indices (all)	R ₁ = 0.0608, wR ₂ = 0.1436	R ₁ = 0.0476, wR ₂ = 0.1118
Goodness-of-fit	1.029	1.028

Table S3. Crystallographic data for **3²⁺** and **3⁴⁺**.

	3²⁺	3⁴⁺·0.5C₄H₁₀O
Empirical formula	C ₁₀₃ H ₁₁₆ Cl ₂ F ₁₂ Fe ₂ N ₆ P ₆ Ru	C ₁₀₂ H ₁₁₄ F ₂₄ Fe ₂ N ₆ P ₈ Ru
Color and Habit	Dark red block	Dark brown block
Crystal Size (mm)	0.25 × 0.14 × 0.12	0.15 × 0.15 × 0.13
Temperature(K)	100.00(10)	99.99(10)
Crystal system	monoclinic	monoclinic
Space group	<i>P2₁</i>	<i>P2₁/n</i>
a (Å)	15.27300(10)	14.6751(3)
b (Å)	17.47840(10)	28.0911(7)
c (Å)	19.05300(10)	27.1789(5)
alpha (deg.)	90	90
beta (deg.)	105.5060(10)	101.114(2)
gamma (deg.)	90	90
Volume (Å ³)	4901.03(5)	10994.1(4)
Z	2	4
Formula weight	2135.50	2340.52
Density(cal.) (Mg/m ³)	1.447	1.414
<i>M</i> (mm ⁻¹)	3.798	3.407
F (000)	2208.0	4800.0
Theta range (deg.)	4.184 to 120.5	3.972 to 105.86
Reflections collected / unique	148502 / 22053 [R(int) = 0.0470]	71978 / 19186 [R(int) = 0.0625]
Index range	-19 ≤ h ≤ 19, -22 ≤ k ≤ 22, -24 ≤ l ≤ 24	-17 ≤ h ≤ 10, -33 ≤ k ≤ 33, -29 ≤ l ≤ 32
Data/restraints/parameters (obs.)	22053/1/1203	19186/24/1302
Final R indices (obs.)	R ₁ = 0.0524, wR ₂ = 0.1389	R ₁ = 0.0926, wR ₂ = 0.2432
R indices (all)	R ₁ = 0.0562, wR ₂ = 0.1420	R ₁ = 0.1184, wR ₂ = 0.2621
Goodness-of-fit	1.012	1.029

Table S4. Crystallographic data for 4²⁺ and 4⁴⁺.

	4²⁺	4⁴⁺
Empirical formula	C ₁₀₄ H ₁₁₈ F ₁₂ Fe ₂ N ₆ P ₆ Ru	C ₁₀₄ H ₁₁₆ F ₂₄ Fe ₂ N ₆ P ₈ Ru
Color and Habit	Dark red block	Dark brown block
Crystal Size (mm)	0.180×0.150×0.130	0.150×0.140×0.120

Temperature(K)	99.99(10)	100.00(10)
Crystal system	Monoclinic	Triclinic
Space group	$P2_1$	$P\bar{1}$
a (Å)	16.2245(3)	13.04330(10)
b (Å)	17.8873(3)	15.3889(2)
c (Å)	19.2837(4)	32.7979(4)
alpha (deg.)	90	94.4230(10)
beta (deg.)	109.935(2)	91.3690(10)
gamma (deg.)	90	113.6670(10)
Volume (Å ³)	5261.03(18)	6000.76(12)
Z	2	2
Formula weight	2078.63	2366.55
Density(cal.) (Mg/m ³)	1.312	1.310
M (mm ⁻¹)	3.224	3.124
F (000)	2156.0	2428.0
Theta range (deg.)	4.238 to 109.64	6.162 to 120.112
Reflections collected / unique	32694 / 14260 [R(int) = 0.0511]	83344 / 26508 [R(int) = 0.0575]
Index range	-19 ≤ h ≤ 19, -21 ≤ k ≤ 10, -23 ≤ l ≤ 23	-16 ≤ h ≤ 15, -19 ≤ k ≤ 19, -42 ≤ l ≤ 42
Data/restraints/parameters (obs.)	14260/703/1196	26508/0/1322
Final R indices (obs.)	R ₁ = 0.0563, wR ₂ = 0.1451	R ₁ = 0.0534, wR ₂ = 0.1426
R indices (all)	R ₁ = 0.0588, wR ₂ = 0.1467	R ₁ = 0.0631, wR ₂ = 0.1482
Goodness-of-fit	1.103	1.063

Table S5. Crystallographic data for **5⁴⁺**.

	5⁴⁺
Empirical formula	C ₁₀₆ H ₁₂₂ F ₂₄ Fe ₂ N ₆ P ₈ Ru
Color and Habit	Dark brown block
Crystal Size (mm)	0.2 × 0.13 × 0.12
Temperature(K)	100.01(10)
Crystal system	triclinic
Space group	$P\bar{1}$
a (Å)	12.48220(10)
b (Å)	14.6612(3)

c (Å)	17.9543(3)
alpha (deg.)	106.982(2)
beta (deg.)	101.5990(10)
gamma (deg.)	101.3990(10)
Volume (Å ³)	2960.78(9)
Z	1
Formula weight	2396.62
Density(cal.) (Mg/m ³)	1.344
M (mm ⁻¹)	3.170
F (000)	1232.0
Theta range (deg.)	4.654 to 120.228
Reflections collected / unique	35853 / 13050 [R(int) = 0.0336]
Index range	-16 ≤ h ≤ 13, -18 ≤ k ≤ 18, -23 ≤ l ≤ 23
Data/restraints/parameters (obs.)	13050/0/673
Final R indices (obs.)	R ₁ = 0.0409, wR ₂ = 0.1067
R indices (all)	R ₁ = 0.0468, wR ₂ = 0.1099
Goodness-of-fit	1.052

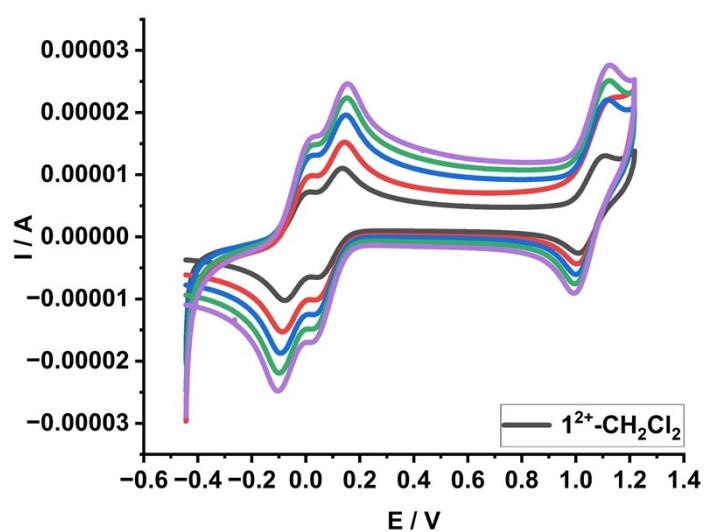


Figure S1. A cyclic voltammogram of 1^{2+} recorded in CH_2Cl_2 / 0.1 M [TBA] PF_6 at a n ($n=100, 200, 300, 400, 500$) $\text{mV}\cdot\text{s}^{-1}$ scan rate.

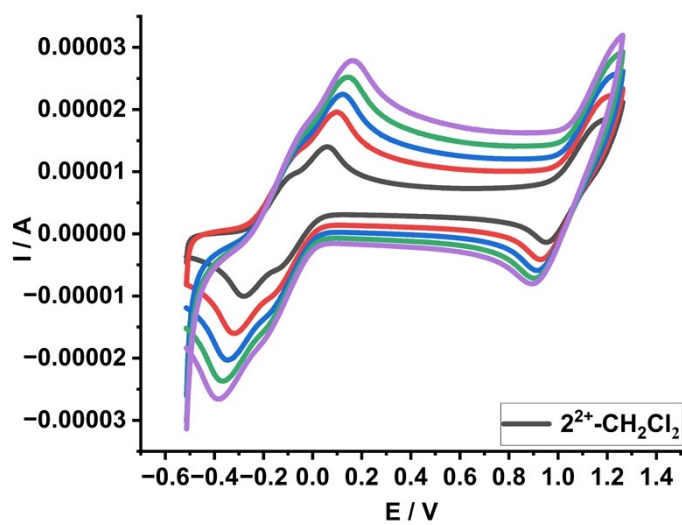


Figure S2. A cyclic voltammogram of 2^{2+} recorded in $\text{CH}_2\text{Cl}_2 / 0.1 \text{ M}$ $[\text{TBA}]\text{PF}_6$ at a $n(n=100, 200, 300, 400, 500) \text{ mV}\cdot\text{s}^{-1}$ scan rate.

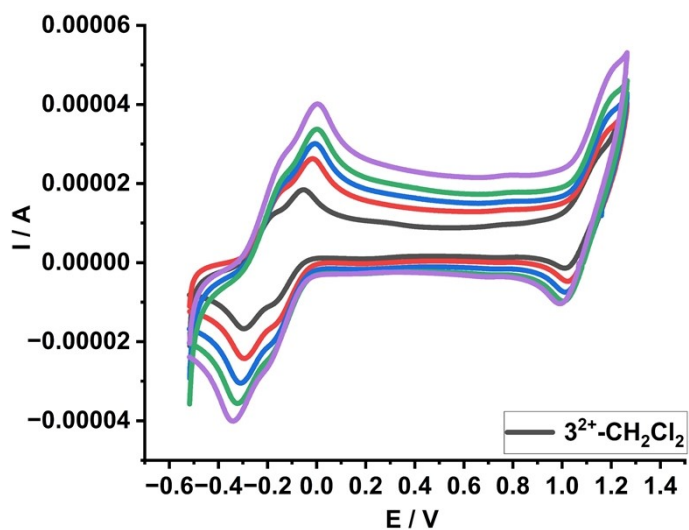


Figure S3. A cyclic voltammogram of 3^{2+} recorded in $\text{CH}_2\text{Cl}_2 / 0.1 \text{ M}$ $[\text{TBA}]\text{PF}_6$ at a $n(n=100, 200, 300, 400, 500) \text{ mV}\cdot\text{s}^{-1}$ scan rate.

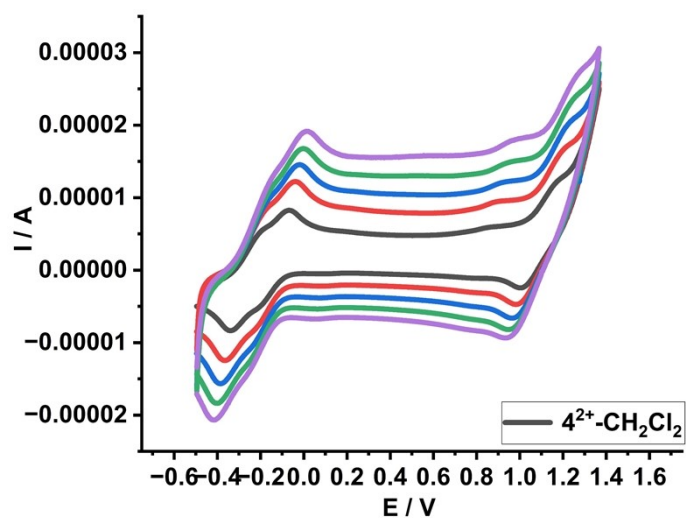


Figure S4. A cyclic voltammogram of 4^{2+} recorded in $\text{CH}_2\text{Cl}_2 / 0.1 \text{ M}$ $[\text{TBA}]\text{PF}_6$ at a n ($n=100, 200, 300, 400, 500$) $\text{mV}\cdot\text{s}^{-1}$ scan rate.

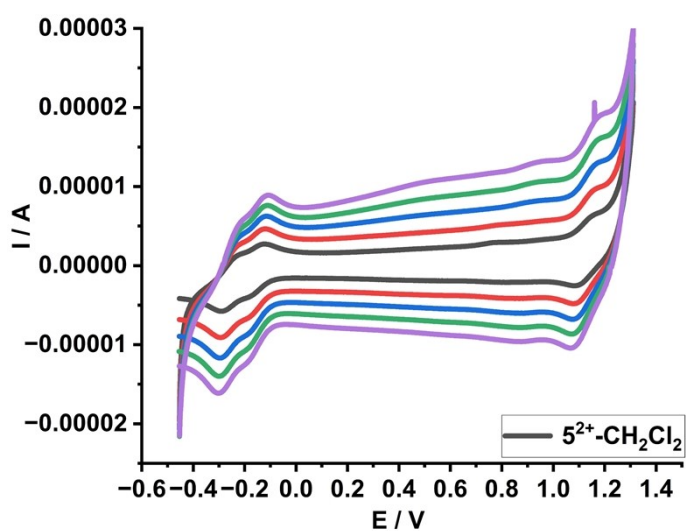


Figure S5. A cyclic voltammogram of 5^{2+} recorded in $\text{CH}_2\text{Cl}_2 / 0.1 \text{ M}$ $[\text{TBA}]\text{PF}_6$ at a n ($n=100, 200, 300, 400, 500$) $\text{mV}\cdot\text{s}^{-1}$ scan rate.

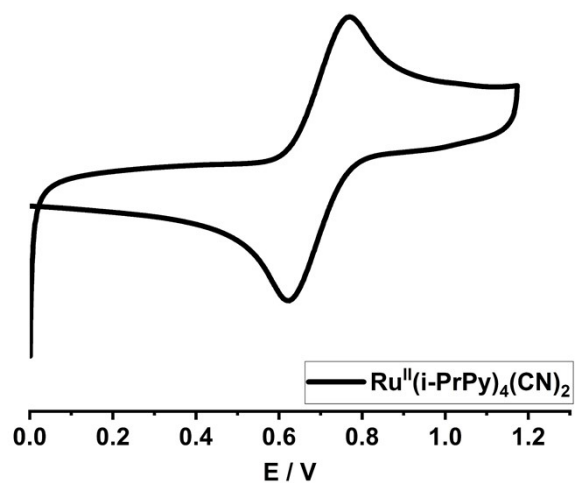


Figure S6. Cyclic voltammograms of $\text{Ru}^{\text{II}}(\text{i-PrPy})_4(\text{CN})_2$ recorded in $\text{CH}_2\text{Cl}_2 / 0.1 \text{ M } [\text{TBA}]\text{PF}_6$ at a 100 mV s^{-1} scan rate.

Table S6. Electrochemical data vs. Ag/AgCl .

	$E_{1/2} / \text{V}$
$\text{CpFe}(\text{dppe})\text{CN}^{\text{I}}$	0.48
$\text{CpMeFe}(\text{dppe})\text{CN}^{\text{I}}$	0.44
$\text{CpMe}^3\text{Fe}(\text{dppe})\text{CN}^{\text{I}}$	0.34
$\text{CpMe}^4\text{Fe}(\text{dppe})\text{CN}^{\text{I}}$	0.30
$\text{CpMe}^5\text{Fe}(\text{dppe})\text{CN}^{\text{I}}$	0.25
$\text{Ru}^{\text{II}}(\text{i-PrPy})_4(\text{CN})_2$	0.69

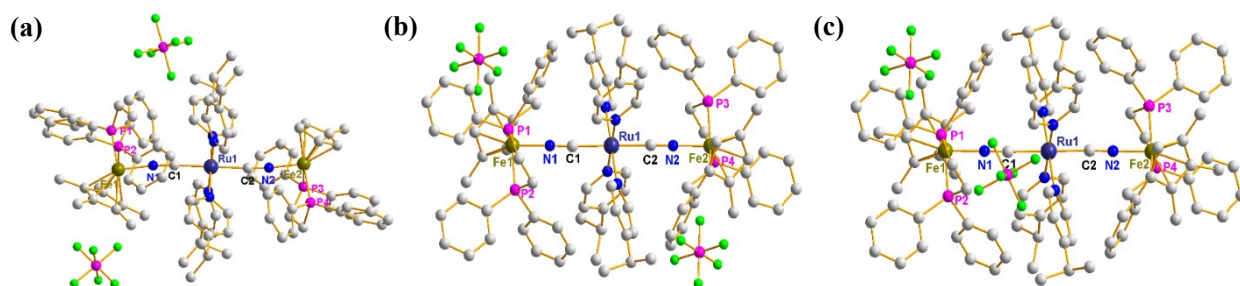


Figure S7. (a), (b), (c) Molecular structure of 2^{2+} , 3^{2+} , 4^{2+} , respectively. Hydrogen atoms and solvent molecules have been omitted for clarity. Dark blue, Ru; yellow, Fe; pink, P; gray, C; blue, N; green, F.

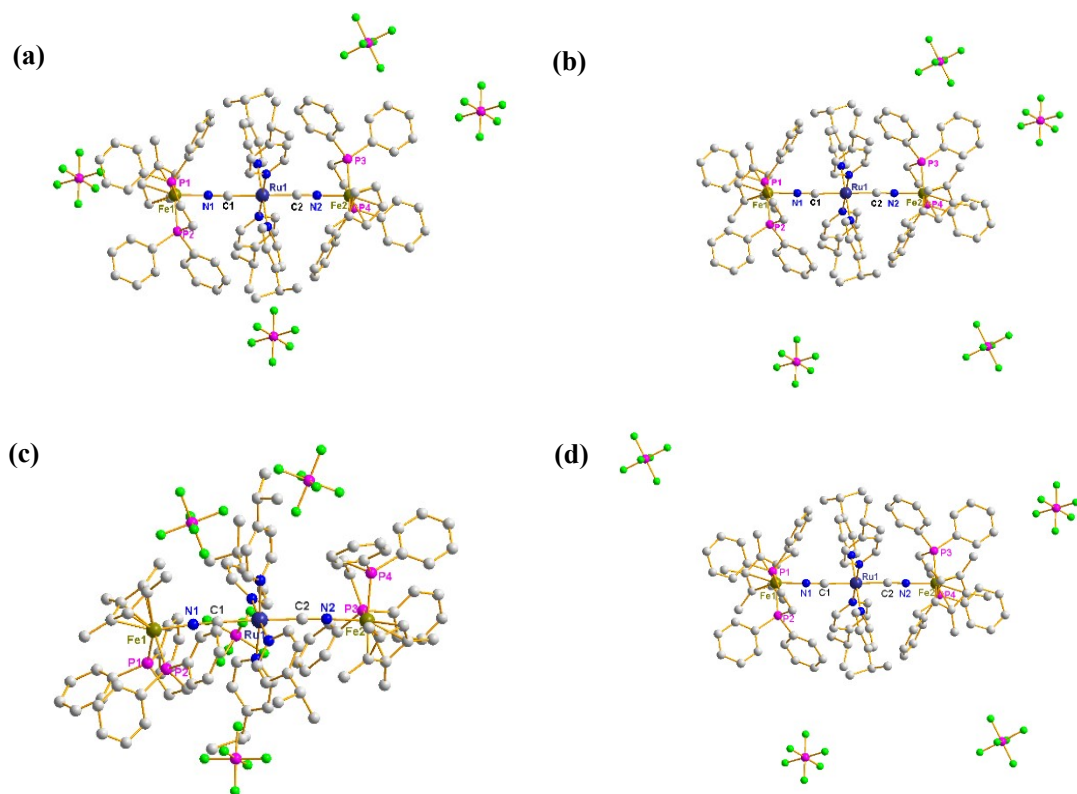


Figure S8. (a), (b), (c), (d) Molecular structure of 2^{2+} , 3^{4+} , 4^{4+} , 5^{4+} , respectively. Hydrogen atoms and solvent molecules have been omitted for clarity. Dark blue, Ru; yellow, Fe; pink, P; gray, C; blue, N; green, F.

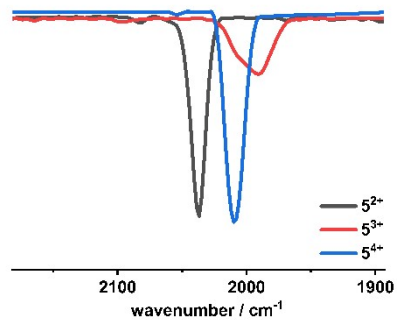
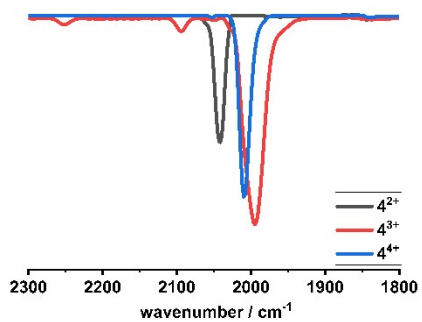
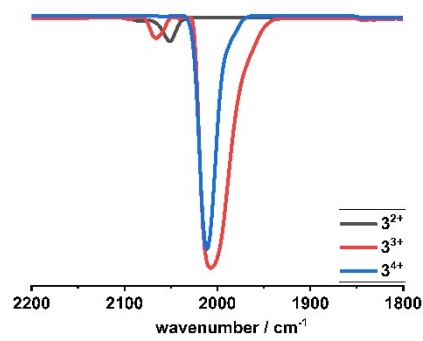
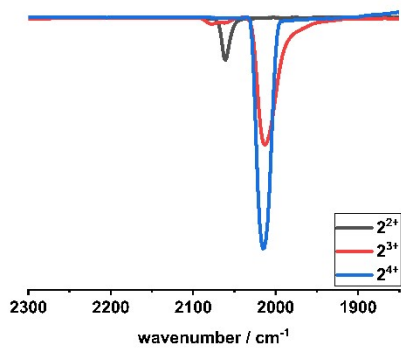


Figure S9. The $\nu(\text{CN})$ bands in solid state.

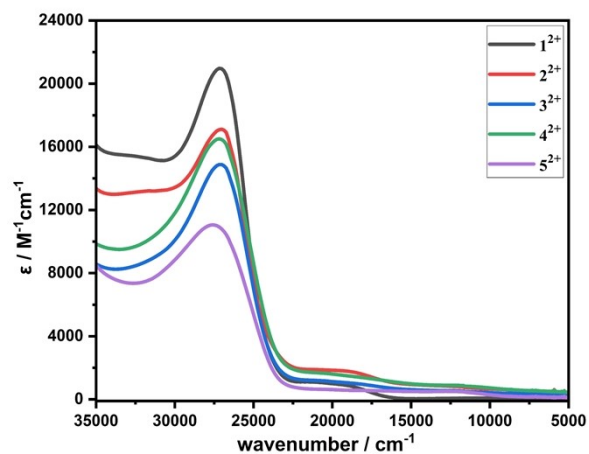


Figure S10. UV-vis-NIR spectra of the 1^{2+} - 5^{2+} in CH_2Cl_2 .

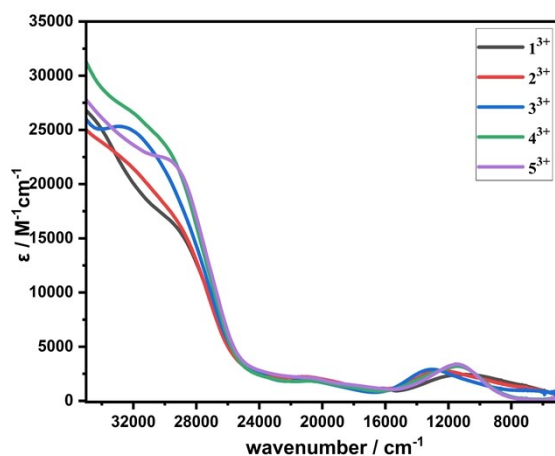


Figure S11. UV-vis-NIR spectra of the 1^{3+} - 5^{3+} in CH_2Cl_2 .

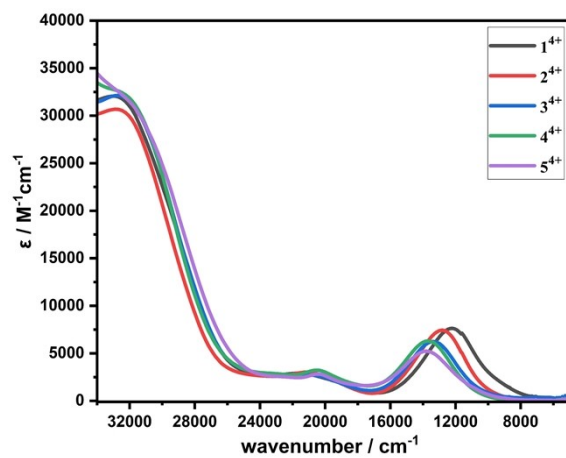


Figure S12. UV-vis-NIR spectra of the 1^{4+} - 5^{4+} in CH_2Cl_2 .

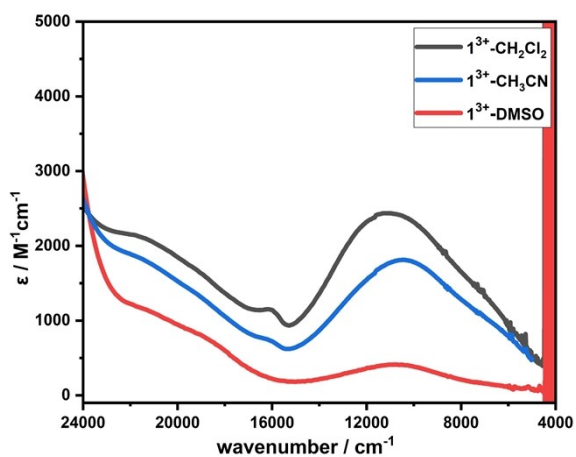


Figure S13. UV-vis-NIR spectra of 1^{3+} in different solvents.

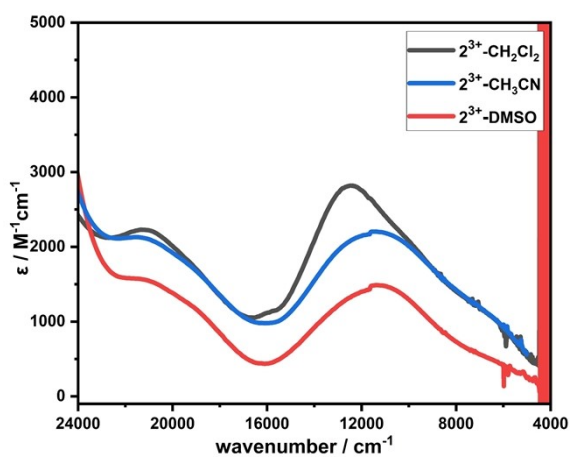


Figure S14. UV-vis-NIR spectra of 2^{3+} in different solvents.

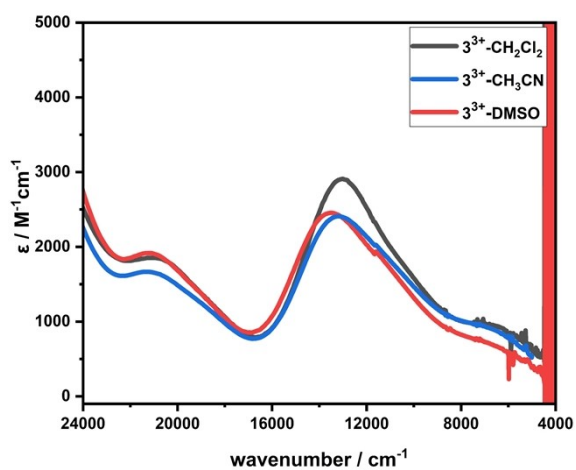


Figure S15. UV-vis-NIR spectra of 3^{3+} in different solvents.

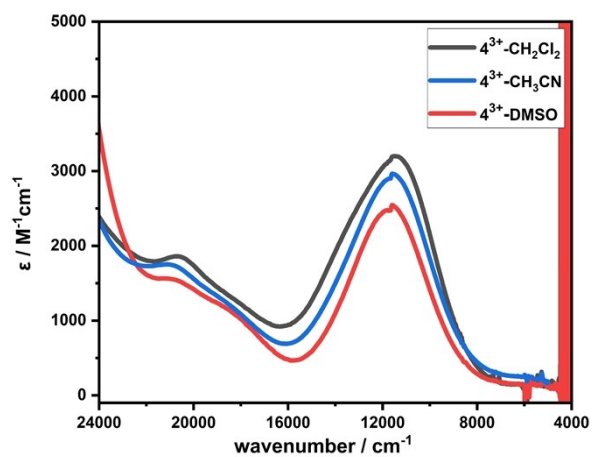


Figure S16. UV-vis-NIR spectra of 4^{3+} in different solvents.

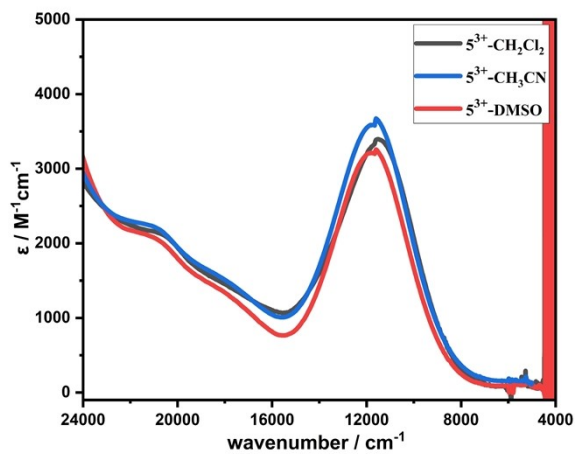


Figure S17. UV-vis-NIR spectra of 5^{3+} in different solvents.

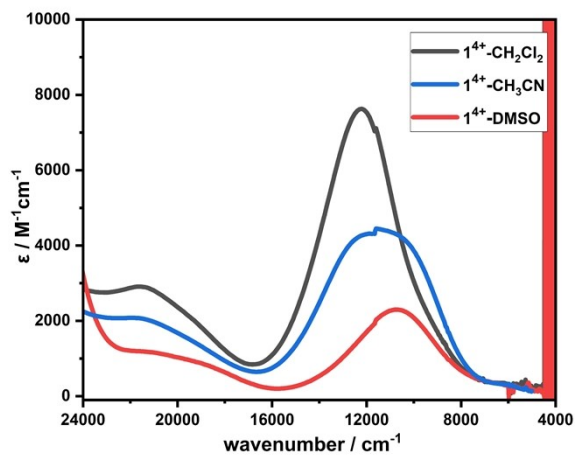


Figure S18. UV-vis-NIR spectra of 1^{4+} in different solvents.

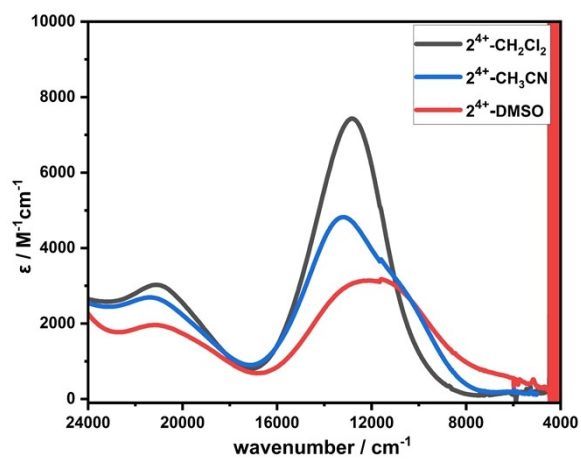


Figure S19. UV-vis-NIR spectra of 2^{4+} in different solvents.

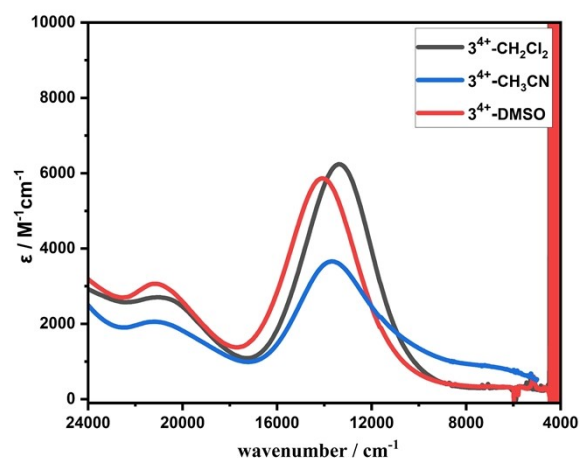


Figure S20. UV-vis-NIR spectra of 3^{4+} in different solvents.

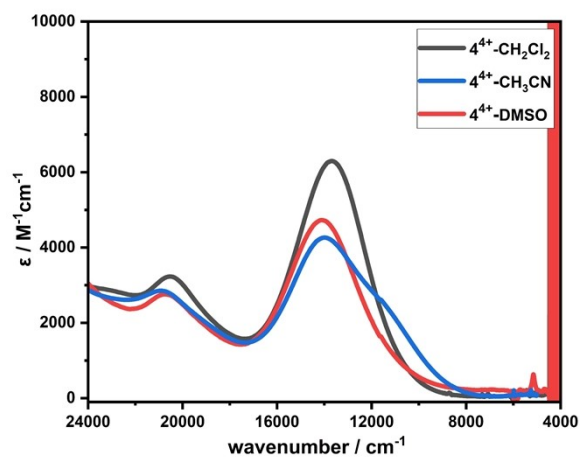


Figure S21. UV-vis-NIR spectra of 4^{4+} in different solvents.

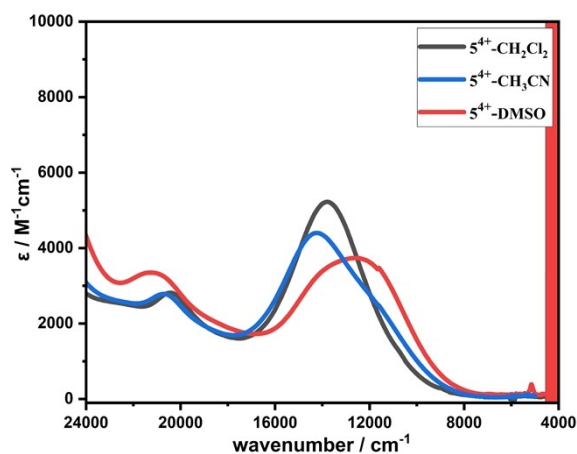


Figure S22. UV-vis-NIR spectra of 5^{4+} in different solvents.

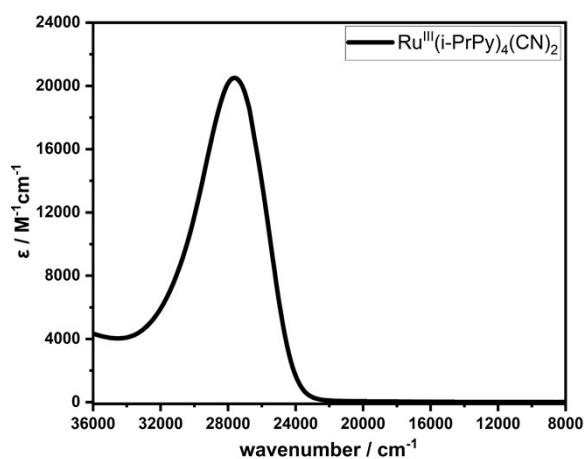


Figure S23. UV-vis-NIR spectra of $\text{Ru}^{\text{III}}(\text{i-PrPy})_4(\text{CN})_2$ in CH_2Cl_2 .

Table S7. Mulliken spin densities of the MV compounds.

	Ru	Fe1	Fe2
1^{3+}	0.080415	0.006824	1.179786
2^{3+}	0.059975	0.004731	1.260200
3^{3+}	0.038135	0.004455	1.354057
4^{3+}	0.030960	0.002665	1.368360
5^{3+}	0.038744	0.007840	1.369491
1^{4+}	0.048250	1.293172	1.296249
2^{4+}	0.037271	1.297464	1.301171
3^{4+}	0.027491	1.448378	1.448494
4^{4+}	0.021001	1.441631	1.487646
5^{4+}	0.013958	1.536410	1.511494

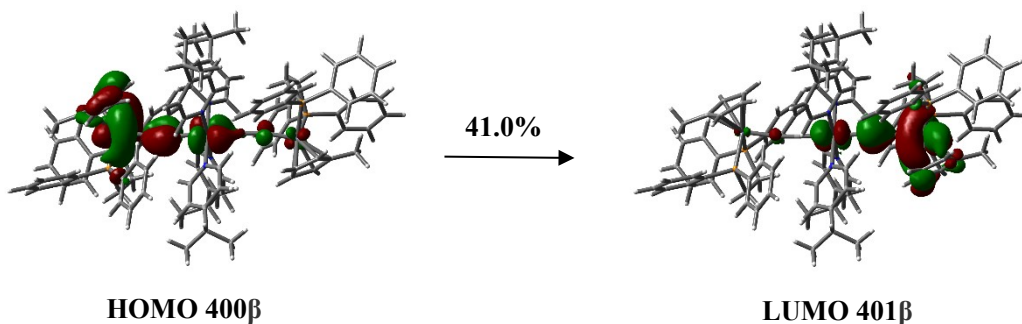


Figure S24. The major electronic transitions corresponding to the NIR band ($\lambda = 921$ nm, $f = 0.0528$) of 2^{3+} .

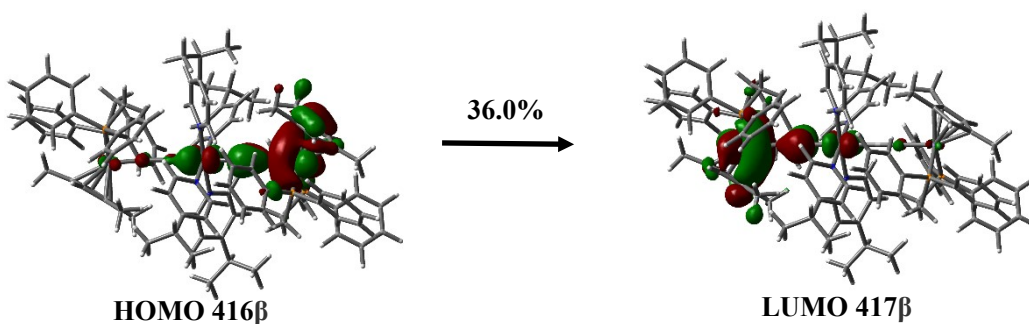
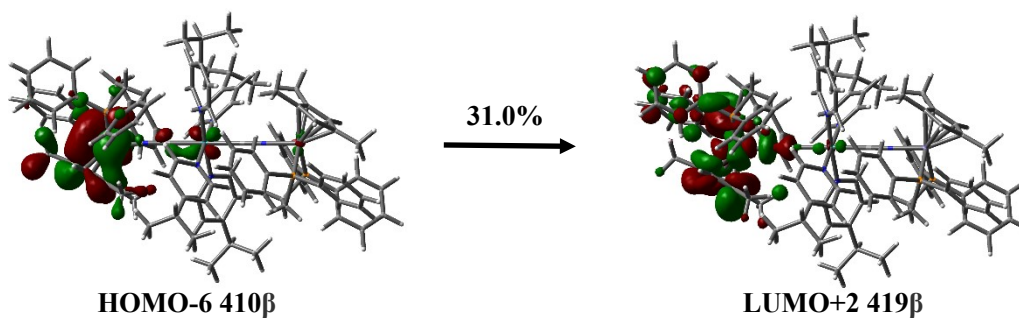


Figure S25. The major electronic transitions corresponding to the NIR band ($\lambda = 878$ nm, $f = 0.0422$) of 3^{3+} .

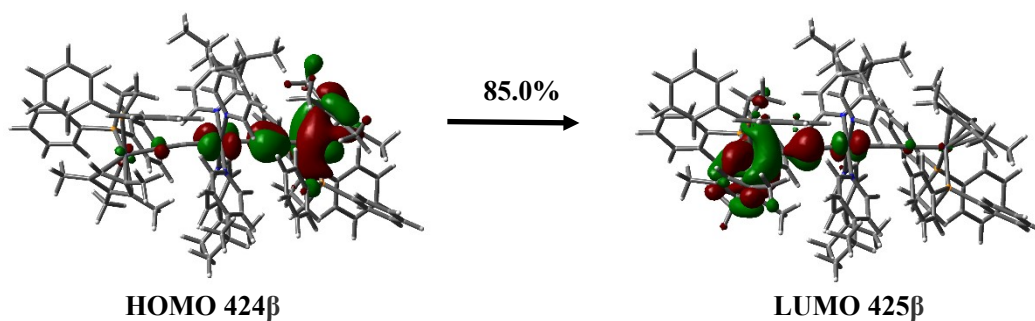


Figure S26. The major electronic transitions corresponding to the NIR band ($\lambda = 801$ nm, $f = 0.0415$) of 4^{3+} .

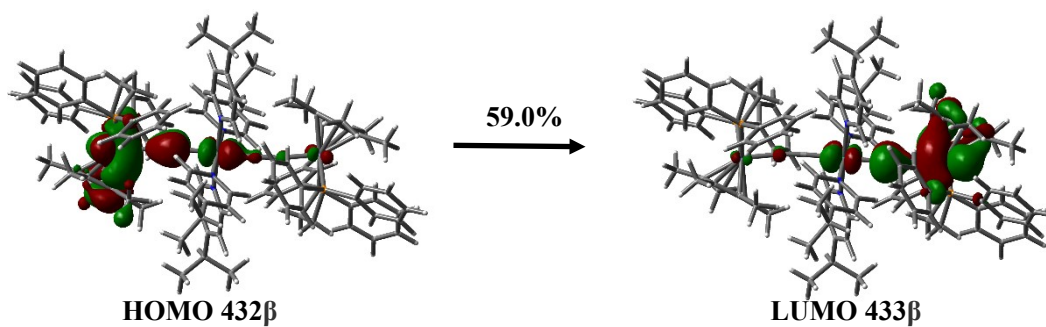


Figure S27. The major electronic transitions corresponding to the NIR band ($\lambda = 1052$ nm, $f = 0.0541$) of 5^{3+} .

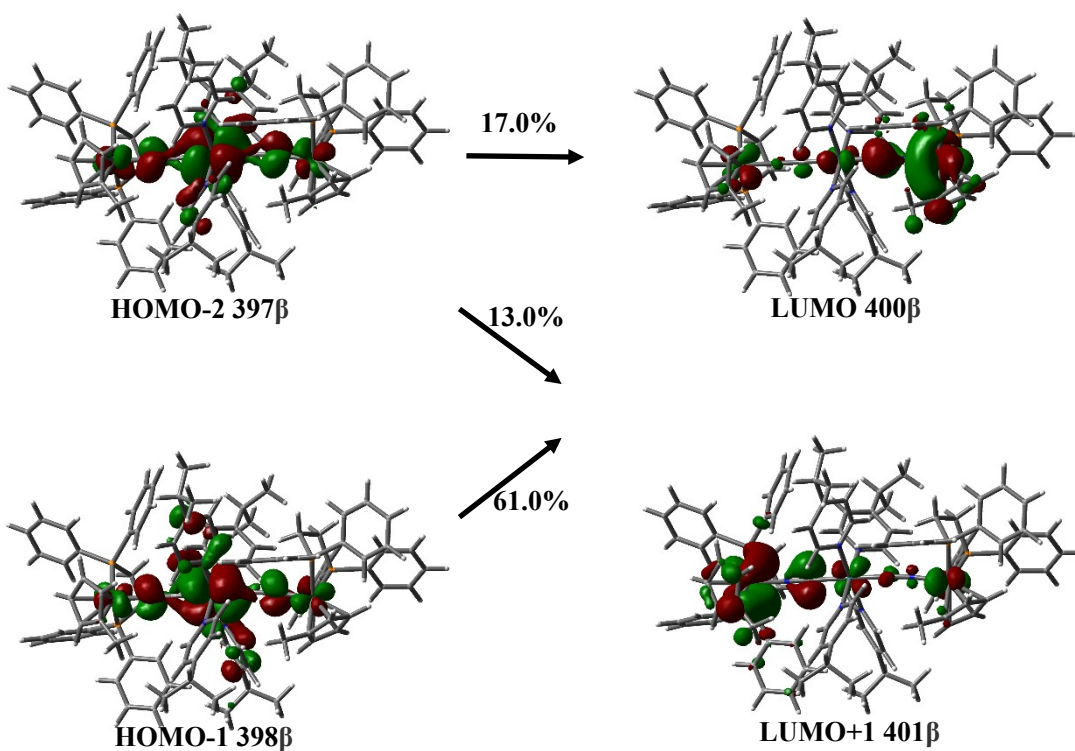


Figure S28. The major electronic transitions corresponding to the NIR band ($\lambda = 606$ nm, $f = 0.1741$) of 2^{4+} .

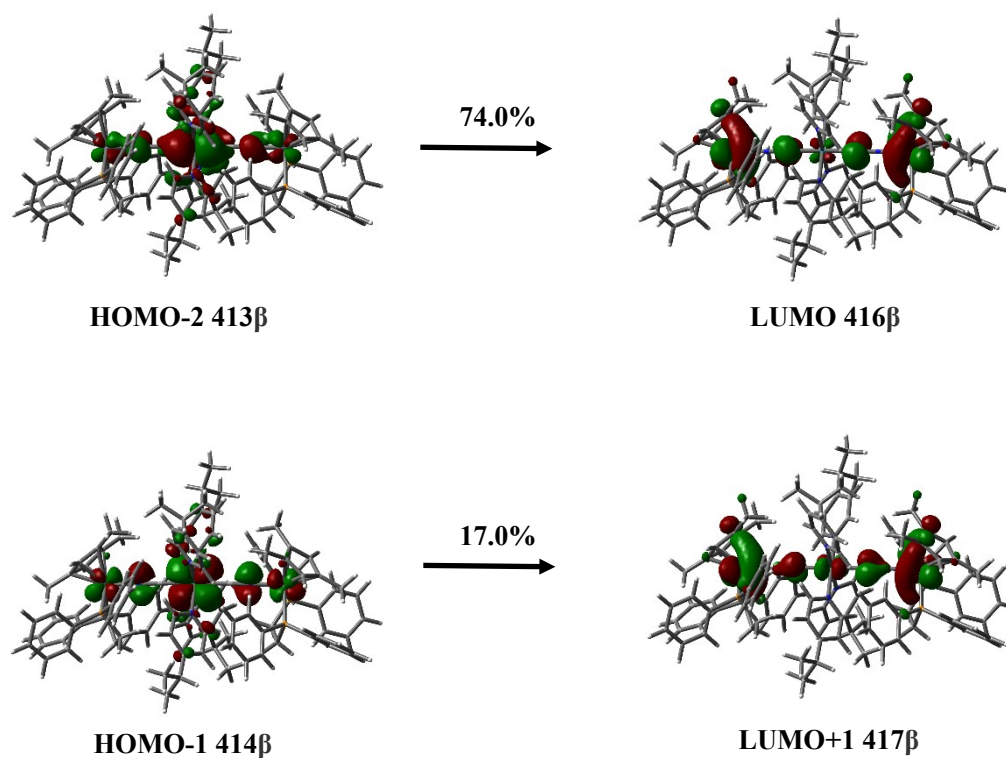


Figure S29. The major electronic transitions corresponding to the NIR band ($\lambda = 578$ nm, $f = 0.1898$) of 3^{4+} .

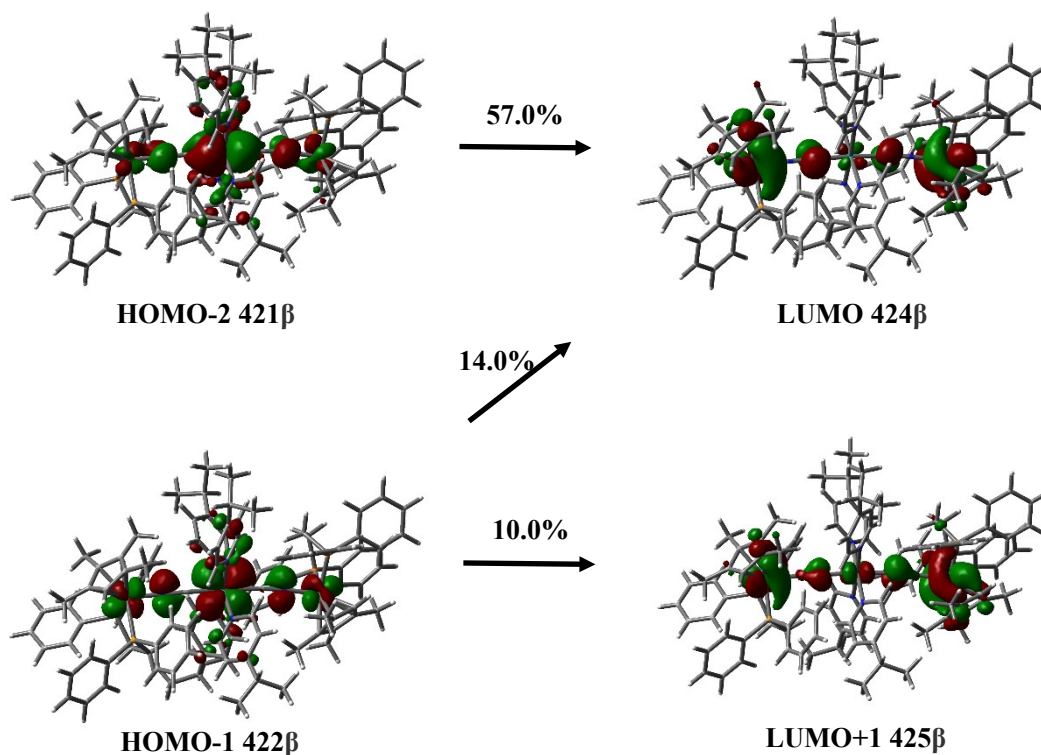


Figure S30. The major electronic transitions corresponding to the NIR band ($\lambda = 546$ nm, $f = 0.1482$) of 4^{4+} .

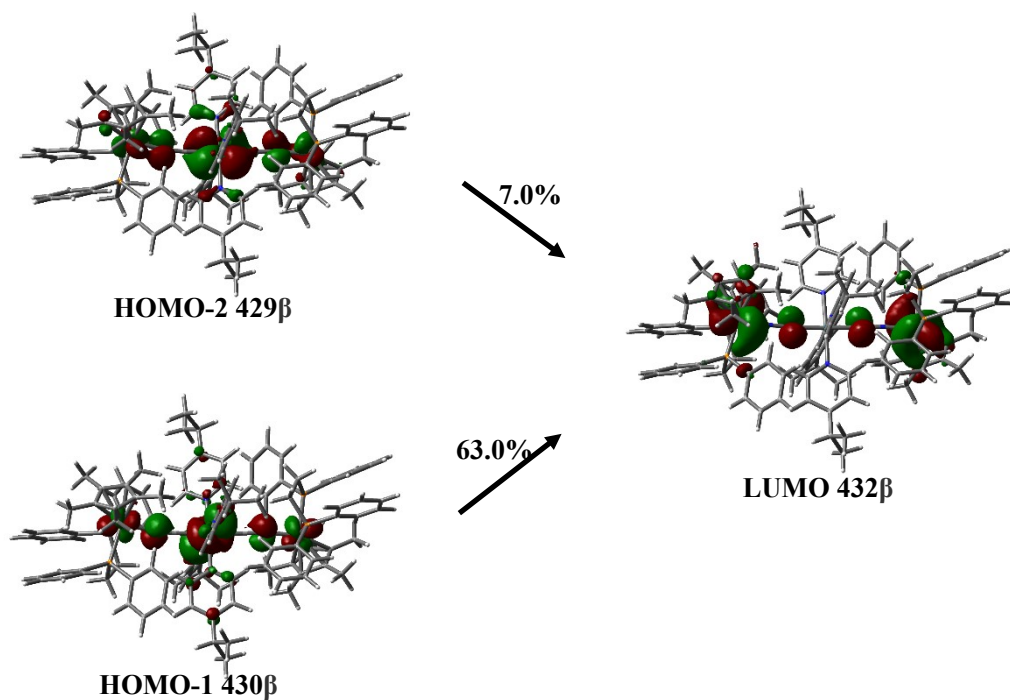


Figure S31. The major electronic transitions corresponding to the NIR band ($\lambda = 537$ nm, $f = 0.0391$) of 5^{4+} .

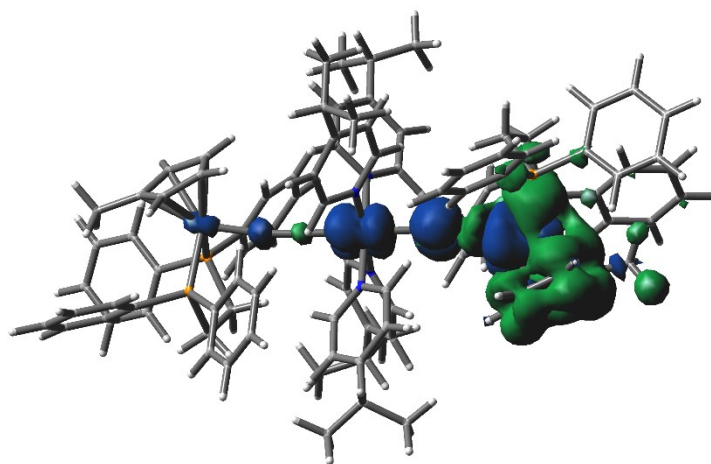


Figure S32. Computed spin densities of 2^{3+} .

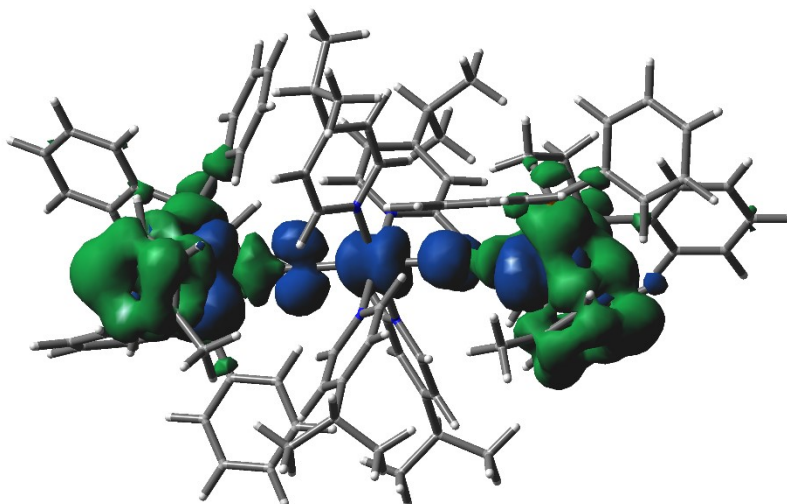


Figure S33. Computed spin densities of 2^{4+} .

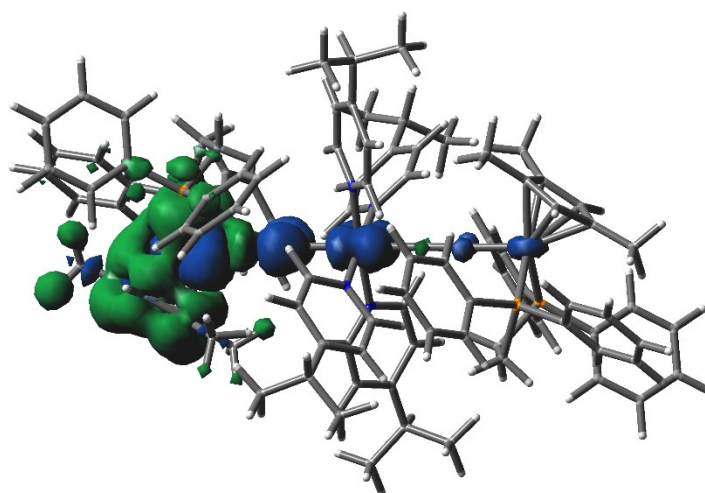


Figure S34. Computed spin densities of 3^{3+} .

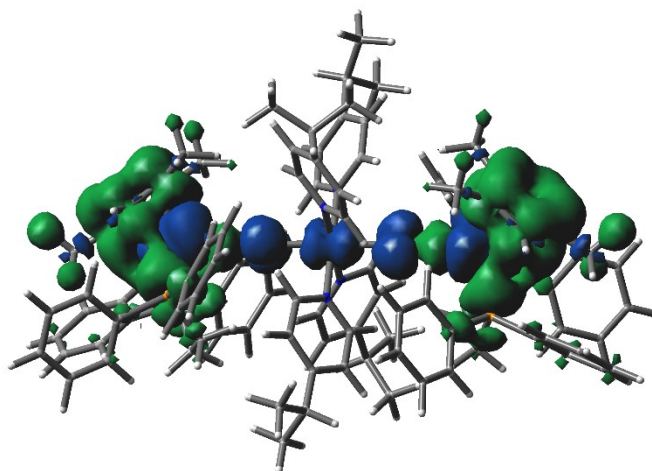


Figure S35. Computed spin densities of 3^{4+} .

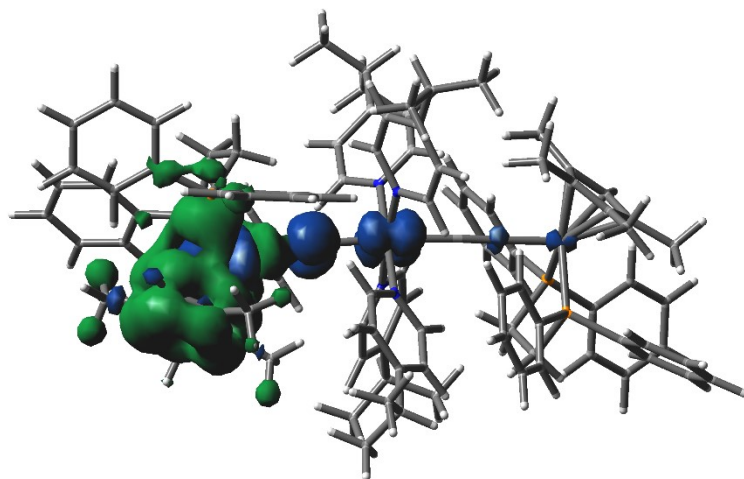


Figure S36. Computed spin densities of 4^{3+} .

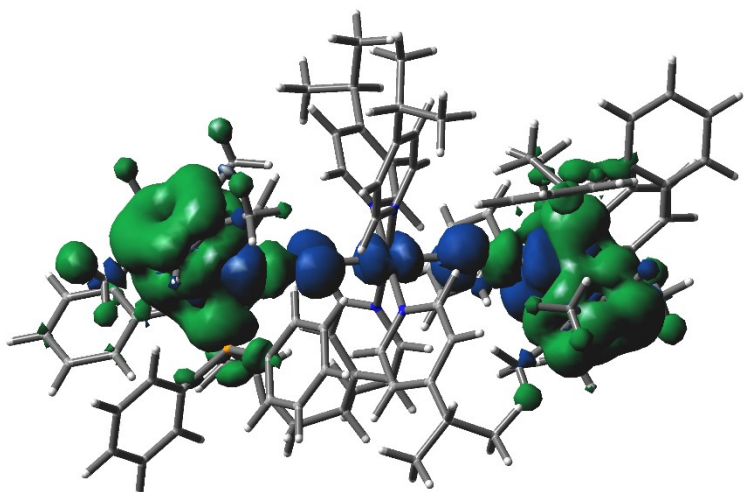


Figure S37. Computed spin densities of 4^{4+} .

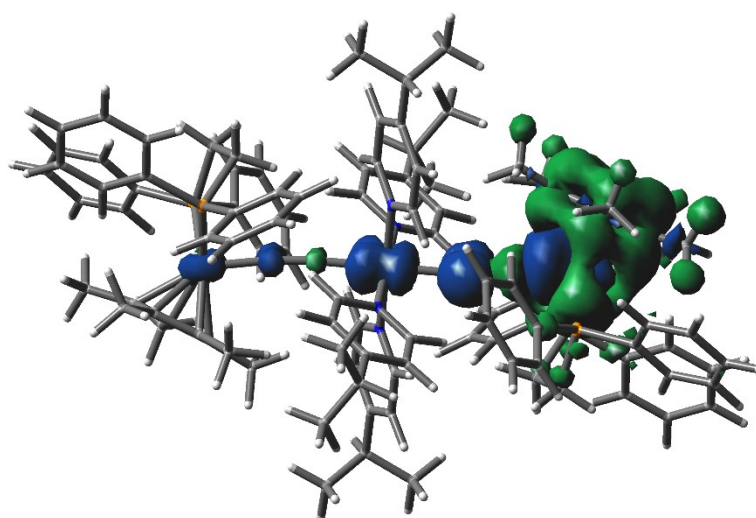


Figure S38. Computed spin densities of 5^{3+} .

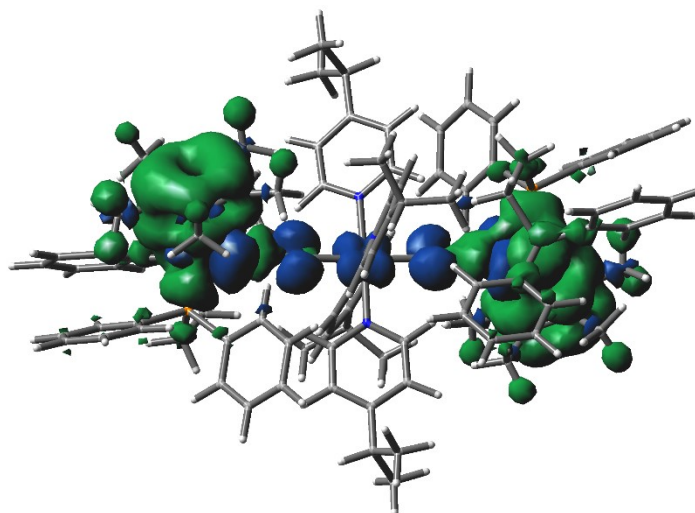


Figure S39. Computed spin densities of 5^{4+} .

Notes and references

1. Y.-Y. Yang, X.-Q. Zhu, J.-P. Launay, C.-B. Hong, S.-D. Su, Y.-H. Wen, X.-T. Wu and T.-L. Sheng, *Angew. Chem. Int. Ed.*, 2021, **60**, 4804-4814.

Table S8. Optimized Cartesian Coordinates of 1^{3+} .

Ru	-0.060597	0.483578	-0.1078	C	1.468234	3.771616	4.548804
Fe	-4.849595	-0.19113	1.423018	H	1.081946	3.382926	5.500591
Fe	4.934072	-0.28972	-1.40481	C	-1.53944	3.854281	-4.60433
P	-5.29993	1.834658	0.501224	H	-1.17538	3.503862	-5.57981
P	5.364119	1.787309	-0.47507	C	-4.29957	-0.05598	3.466938
P	-5.613369	-1.02691	-0.54576	H	-3.44616	0.46926	3.873457
P	5.57245	-1.07439	0.660661	C	8.271492	4.231318	-2.15042
N	0.427654	0.96221	1.395779	H	8.304105	5.07452	-2.83224
N	-0.298101	1.012219	-1.55869	C	-0.92886	-3.98987	-3.46555
N	0.276576	-2.03173	1.3308	C	-1.09631	2.072977	-1.25583
N	3.152577	-0.34907	-0.85217	H	-1.42484	2.154716	-0.22543
N	-3.086114	-0.24759	0.717216	C	3.164585	5.295433	-0.45673
N	-0.355005	-1.96414	-1.56292	H	3.191997	6.241481	0.074471
C	3.137658	2.868901	-1.87223	C	4.880606	-2.73435	1.137725
H	3.116663	1.923964	-2.41139	C	1.229716	2.035674	1.152286
C	0.230979	1.710285	3.684898	H	1.597912	2.141919	0.135955
H	-0.191038	1.544022	4.671867	C	-3.52664	-4.60648	-0.74489
C	1.989795	-0.45964	-0.56585	H	-2.82433	-5.15069	-0.11751
C	4.085764	3.080579	-0.86069	C	-9.2923	3.800691	1.949351
C	-6.862967	3.817285	1.858196	H	-10.2223	4.239185	2.295696
H	-5.919603	4.279082	2.143096	C	-3.97504	-5.17909	-1.94401

C	-6.882042	2.671954	1.044124	H	-3.62868	-6.16529	-2.24043
C	-4.022211	3.187053	0.68322	C	1.572352	2.953932	2.14023
C	7.036295	3.671053	-1.7967	H	2.211949	3.790184	1.869918
H	6.120453	4.092582	-2.20655	C	-8.2089	-1.95171	0.049262
C	-0.705238	-2.96685	1.44492	H	-7.72742	-2.43347	0.897571
H	-1.505253	-2.90801	0.714397	C	-5.50646	1.643359	-1.39216
C	6.99143	2.584527	-0.90441	H	-6.56507	1.812221	-1.62407
C	2.200342	3.86817	-2.17011	H	-4.92217	2.42564	-1.89103
H	1.472699	3.7031	-2.96055	C	5.867573	0.393893	-3.22548
C	-0.083406	0.827438	2.649733	H	6.133286	1.420245	-3.44346
H	-0.748931	-0.01523	2.811595	C	-2.02015	4.026243	1.777262
C	-1.95023	-0.36631	0.385334	H	-1.21213	3.88512	2.491767
C	-0.70685	-3.93319	2.449133	C	2.205003	5.075571	-1.4589
H	-1.530181	-4.64042	2.504932	H	1.479696	5.848074	-1.69618
C	6.699748	-0.55673	-2.52864	C	-1.76722	-2.8724	-3.29726
H	7.706629	-0.37556	-2.17852	H	-2.67191	-2.77127	-3.89115
C	0.139067	0.894981	-2.8414	C	-5.61361	0.482406	3.288601
H	0.781875	0.045996	-3.05476	H	-5.91994	1.499015	3.500261
C	5.980019	-1.80835	-2.4812	C	7.877049	-0.56086	2.281764
H	6.334738	-2.74449	-2.07143	H	7.225865	-0.01009	2.956656
C	-0.240675	1.787528	-3.84535	C	-3.17614	5.408026	0.147096
H	0.112949	1.631356	-4.8606	H	-3.27618	6.346084	-0.39064
C	-4.008772	-3.35204	-0.34489	C	-4.90544	-4.49653	-2.74371
H	-3.698472	-2.9011	0.598091	H	-5.27635	-4.95311	-3.65638
C	-4.935736	-2.66487	-1.14493	C	0.232586	-4.21037	5.889436
C	9.41537	2.621038	-0.73801	H	1.135024	-3.60693	6.054161
H	10.333594	2.215061	-0.32563	H	0.158145	-4.92623	6.714242
C	4.709773	-1.61039	-3.10867	H	-0.63824	-3.54699	5.934913
H	3.922306	-2.34666	-3.19704	C	-8.06702	4.378884	2.307386
C	-5.047284	0.247147	-1.83003	H	-8.04718	5.265319	2.93318
H	-3.950657	0.189876	-1.82816	C	3.938333	-3.37663	0.317826
H	-5.39992	-0.0084	-2.83689	H	3.593694	-2.88731	-0.59135
C	-7.447947	-1.19834	-0.86343	C	-2.11548	5.22122	1.050677
C	9.460507	3.709624	-1.62191	H	-1.38765	6.012555	1.207018
H	10.414153	4.148493	-1.895	C	-9.58913	-2.10155	-0.13143
C	1.091972	2.798009	3.45507	H	-10.1669	-2.68734	0.575929
C	5.356047	1.604409	1.420857	C	3.916967	-5.27038	1.837039
H	6.379162	1.786364	1.76971	H	3.565468	-6.26393	2.096098
H	4.711621	2.39054	1.831337	C	-0.93193	5.244142	-4.33041
C	8.18579	2.053306	-0.3825	H	-1.26338	5.957735	-5.0916
H	8.175717	1.202231	0.297877	H	0.164976	5.221206	-4.34742
C	1.370981	-3.04097	3.235956	H	-1.25774	5.62431	-3.35166
H	2.219072	-3.02722	3.914926	C	-10.2238	-1.49718	-1.22734
C	-5.661139	-1.74119	2.623234	H	-11.2938	-1.60998	-1.36651

H	-6.00132	-2.70709	2.272527	C	2.995938	3.913582	4.667264
C	1.312617	-2.09877	2.211574	H	3.419397	4.38583	3.769084
H	2.098322	-1.36024	2.085334	H	3.482843	2.941509	4.812984
C	4.639345	-0.2525	-3.56563	H	3.249406	4.551618	5.519732
H	3.799407	0.201936	-4.07252	C	-0.69671	-6.41952	-4.19973
C	-6.458144	-0.54131	2.739085	H	0.399622	-6.44355	-4.26025
H	-7.512038	-0.44063	2.520873	H	-1.07024	-7.14379	-4.93019
C	4.847422	0.218371	1.826909	H	-0.99624	-6.75937	-3.20054
H	3.759586	0.15611	1.700167	C	0.820328	5.146781	4.291716
H	5.08336	-0.01913	2.871285	H	1.125036	5.857679	5.06651
C	7.376279	-1.16788	1.11566	H	-0.27433	5.089944	4.301179
C	-9.469104	-0.75918	-2.14946	H	1.138015	5.552524	3.32039
H	-9.953933	-0.30173	-3.00586	C	4.857545	-4.62848	2.657195
C	0.211214	-4.05198	-2.64289	H	5.22783	-5.1227	3.549679
H	0.89711	-4.89093	-2.70954	C	8.246553	-1.90432	0.291157
C	-2.97224	3.012112	1.596489	H	7.871164	-2.42048	-0.58927
H	-2.905016	2.077931	2.152944	C	5.344158	-3.36197	2.308754
C	-1.092276	2.868272	-3.54962	H	6.102179	-2.88636	2.928758
C	-4.127406	4.394307	-0.03424	C	-1.24215	-5.02414	-4.52159
H	-4.968696	4.559544	-0.70631	H	-2.33818	-5.08354	-4.60535
C	-1.500135	3.002086	-2.20946	C	-3.07474	3.946666	-4.66267
H	-2.14523	3.816032	-1.88942	H	-3.47845	4.374197	-3.73383
C	0.309934	-4.96066	4.54582	H	-3.53462	2.964112	-4.81988
H	-0.592962	-5.57818	4.445214	H	-3.38112	4.60194	-5.48423
C	-8.112971	2.083749	0.69893	C	10.10626	-1.37682	1.760873
H	-8.150424	1.17929	0.091594	H	11.15908	-1.45678	2.00942
C	-4.336449	-1.44104	3.060357	C	9.605733	-2.00657	0.611
H	-3.495988	-2.12343	3.064224	H	10.26963	-2.58039	-0.02678
C	-1.464811	-1.89929	-2.35008	C	1.533398	-5.89177	4.521643
H	-2.116729	-1.04652	-2.19423	H	1.589829	-6.45657	3.583968
C	-9.312689	2.651787	1.144607	H	1.474197	-6.60785	5.347603
H	-10.258022	2.195647	0.867293	H	2.464498	-5.32097	4.642562
C	4.107541	4.302634	-0.16017	C	3.45609	-4.64399	0.670787
H	4.871853	4.49609	0.591723	H	2.738816	-5.15277	0.03244
C	0.331357	-3.97901	3.396317	C	9.238796	-0.66283	2.599455
C	-8.085456	-0.61392	-1.97157	H	9.618053	-0.19407	3.501361
H	-7.523453	-0.03834	-2.70414	C	-0.68908	-4.53268	-5.87754
C	0.46486	-3.03788	-1.72089	H	-1.1046	-3.55771	-6.15817
H	1.332655	-3.06873	-1.06927	H	-0.9346	-5.2498	-6.66738
C	-5.387124	-3.24184	-2.3449	H	0.404644	-4.44215	-5.83035
H	-6.141131	-2.73696	-2.94679				

Table S9. Optimized Cartesian Coordinates of 2^{3+} .

Ru	0.053904	-0.31649	0.017457	H	-2.40174	-2.38498	-4.07106
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Fe	-4.93218	-0.26664	1.334242	C	-0.59686	-2.95973	1.361889
Fe	4.937773	-0.26792	-1.2996	H	-1.3175	-2.95118	0.550775
P	5.452215	1.713682	-0.23226	C	-2.64919	5.382557	1.256721
P	-5.68522	-1.26136	-0.55814	H	-2.03798	6.243056	1.512726
P	5.789663	-1.22564	0.639808	C	0.74464	-4.5802	5.801865
P	-5.31976	1.678315	0.221552	H	0.643484	-5.40586	6.513083
N	3.184742	-0.23362	-0.60274	H	0.084823	-3.76923	6.129467
C	7.613886	-1.25398	1.011159	H	1.783646	-4.2306	5.862669
N	-0.29806	1.266261	-1.34113	C	1.17026	2.094075	1.543428
C	8.10657	-0.80059	2.249189	H	1.699532	2.215277	0.601773
H	7.439034	-0.41295	3.01453	C	0.399693	-5.06673	4.388175
C	-4.26196	3.16939	0.627579	H	-0.59298	-5.53757	4.412707
N	0.296285	1.053495	1.617275	C	-1.06838	2.318679	-0.95306
N	-3.14361	-0.26849	0.670035	H	-1.39217	2.333064	0.080833
C	-5.75478	-1.78652	2.564989	C	10.37153	-1.36535	1.571269
H	-6.12521	-2.74455	2.219607	H	11.43385	-1.40653	1.786697
C	-4.41662	-1.49301	2.969912	C	-5.68289	0.435483	3.19427
H	-3.58205	-2.18237	2.973767	H	-5.9767	1.450905	3.427954
N	-0.2475	-1.71322	-1.5521	C	-10.1425	-2.68996	-0.50136
C	-7.46207	-1.84259	-0.60436	H	-11.176	-3.01818	-0.46613
C	3.195576	2.960487	-1.45866	C	-7.76952	-3.18627	-0.32304
H	3.123013	2.065454	-2.07366	H	-6.97523	-3.9119	-0.156
C	-1.98538	-0.3156	0.402292	C	9.88237	-1.84893	0.348613
C	4.661344	-1.7374	-2.85791	H	10.56421	-2.27271	-0.38112
H	4.041496	-2.61615	-2.74695	C	-0.24698	2.208921	-3.56412
N	0.270277	-1.91098	1.398167	H	0.093321	2.121465	-4.59199
C	-8.50402	-0.92504	-0.82009	C	7.077759	3.596257	-1.57627
H	-8.29494	0.128728	-0.99781	H	6.153032	3.94389	-2.0333
C	-0.22744	1.742071	3.874242	C	-7.01829	2.453041	0.093479
H	-0.80264	1.564452	4.779547	C	2.287397	4.013077	-1.64293
C	-0.56514	-3.49782	-3.74301	H	1.52875	3.937546	-2.41809
C	9.472555	2.753267	-0.38018	C	-9.83856	-1.34917	-0.77697
H	10.39666	2.430207	0.088365	H	-10.6359	-0.63322	-0.94991
C	-5.15021	-3.35346	-2.4174	C	-1.46171	3.326274	-1.8279
H	-5.95975	-2.92135	-3.00373	H	-2.0926	4.123317	-1.44085
C	-4.77756	-2.77166	-1.19139	C	-7.68782	2.621368	-1.13095
C	-5.5557	-0.02299	-2.01676	H	-7.23433	2.302533	-2.06733
H	-5.00255	-0.51138	-2.82757	C	4.243257	-5.54635	1.482824
H	-6.57226	0.167589	-2.38123	H	3.880851	-6.55262	1.669129
C	0.35614	-3.95401	3.366187	C	3.844117	-3.26998	0.738113
C	4.184894	3.05745	-0.46937	H	3.169679	-2.50702	0.354604
C	8.263891	2.139965	-0.0255	C	-9.56751	3.649268	0.017035
H	8.280821	1.332707	0.705425	H	-10.5505	4.107453	-0.01227
C	-4.52117	-4.52251	-2.86184	C	1.195794	-1.89401	2.395125

H	-4.84214	-4.98925	-3.78851	H	1.875038	-1.0469	2.400822
C	-7.62716	2.910756	1.276059	C	2.275252	4.359513	5.07903
H	-7.10838	2.821508	2.228687	H	2.423305	5.083093	4.265673
C	-3.77618	-3.37102	-0.41381	H	3.074583	3.609956	5.030974
H	-3.52361	-2.92377	0.547678	H	2.384783	4.909265	6.018875
C	-8.89454	3.50464	1.239719	C	-0.57959	-3.97612	2.314658
H	-9.35377	3.855744	2.158002	H	-1.30781	-4.7811	2.249958
C	-0.40416	0.901344	2.777741	C	5.054962	-0.07832	1.943197
H	-1.10707	0.074416	2.808744	H	3.969433	-0.19608	1.854595
C	-0.20106	4.821541	4.971511	H	5.351032	-0.39255	2.950078
H	-0.09406	5.483232	5.836918	C	3.360957	5.263428	0.142089
H	-1.21395	4.401023	4.990884	H	3.441736	6.162069	0.745323
H	-0.0928	5.433241	4.06403	C	3.370162	-4.56134	0.995218
C	-3.13596	-4.53593	-0.86666	H	2.323889	-4.79995	0.814337
H	-2.37018	-5.01401	-0.25951	C	-8.95917	3.213431	-1.16781
C	0.699558	2.801522	3.821495	H	-9.46812	3.339045	-2.11823
C	2.006567	-0.26556	-0.36167	C	2.362278	5.159307	-0.84014
C	9.480276	-0.8512	2.524008	H	1.660522	5.974357	-0.989
H	9.850499	-0.50132	3.481871	C	-6.55838	-0.59355	2.695622
C	7.061648	2.564815	-0.61812	C	1.420133	-6.12778	3.923905
C	0.527899	-3.59304	-2.85643	H	2.424599	-5.68462	3.860813
H	1.279526	-4.36594	-2.99673	H	1.158264	-6.53849	2.940233
C	6.06706	-3.93827	1.479224	H	1.456997	-6.95427	4.640833
H	7.11074	-3.706	1.676969	C	0.658312	-2.70249	-1.79745
C	-3.50795	-5.11255	-2.08863	H	1.500101	-2.76169	-1.11498
H	-3.03178	-6.02868	-2.42704	C	0.883047	3.721962	5.007883
C	6.055217	-1.65425	-2.56022	H	0.722942	3.125018	5.917147
H	6.666866	-2.48548	-2.2357	C	-9.10562	-3.60628	-0.27134
C	5.192998	-2.95438	0.98477	H	-9.33612	-4.645	-0.05761
C	-3.23529	3.04502	1.575831	C	-4.37002	-0.1042	3.362792
H	-3.07555	2.082447	2.06198	H	-3.5102	0.427941	3.746595
C	-0.64275	-4.42444	-4.93814	C	5.470651	1.365331	1.642882
H	-0.48844	-5.44924	-4.5656	H	6.480092	1.582334	2.011162
C	-4.49513	4.411213	0.008805	H	4.780758	2.07333	2.115544
H	-5.32102	4.525351	-0.69201	C	7.920958	0.183104	-2.81222
C	9.489208	3.779966	-1.33546	H	7.960668	1.275391	-2.87088
H	10.4262	4.253812	-1.60804	H	8.450707	-0.21265	-3.68752
C	5.35947	0.439809	-3.26582	H	8.477181	-0.12644	-1.92099
H	5.382205	1.476351	-3.57792	C	-1.97543	-4.36923	-5.68726
C	8.510072	-1.79634	0.072908	H	-2.82873	-4.57211	-5.02913
H	8.146856	-2.20094	-0.86807	H	-1.98325	-5.11449	-6.48851
C	-1.33287	-1.64565	-2.36995	H	-2.12345	-3.38722	-6.15653
H	-2.06399	-0.8787	-2.13435	C	8.290653	4.20035	-1.93184
C	6.512714	-0.30994	-2.81663	H	8.299803	5.001277	-2.66359

C	0.120756	1.234849	-2.63376	C	-1.04907	5.737947	-3.7313
H	0.7366	0.386864	-2.91768	H	-1.47158	6.017559	-2.75619
C	4.2747	4.217731	0.324338	H	-1.376	6.486986	-4.45975
H	5.07178	4.323347	1.059065	H	0.044415	5.790058	-3.66319
C	1.267711	-2.88151	3.375066	C	-1.06999	3.283912	-3.1791
H	2.027848	-2.80565	4.146206	C	0.513021	-4.09939	-5.91129
C	-3.68932	5.515238	0.321098	H	0.402165	-3.07989	-6.30284
H	-3.88623	6.477562	-0.14148	H	0.492453	-4.7903	-6.76004
C	4.23175	-0.44318	-3.30541	H	1.496604	-4.18168	-5.4338
H	3.220951	-0.17958	-3.58488	C	-3.06459	4.315783	-4.28695
C	-2.42637	4.148236	1.884826	H	-3.53892	4.577229	-3.33013
H	-1.63441	4.046161	2.624098	H	-3.42912	3.32873	-4.59442
C	5.588087	-5.23311	1.72379	H	-3.39195	5.048535	-5.03158
H	6.263718	-5.9931	2.101752	C	-1.52942	4.33895	-4.15869
C	-4.86121	1.272032	-1.5736	C	-8.03939	-0.49967	2.512714
H	-5.08848	2.114504	-2.24026	H	-8.33586	0.424406	2.000673
H	-3.76997	1.147108	-1.55706	H	-8.54478	-0.51724	3.486064
C	1.390627	2.968508	2.607585	H	-8.42264	-1.34309	1.927826
H	2.108885	3.772381	2.477962	H	-1.09673	4.108491	-5.14192
C	-1.51432	-2.50175	-3.45789				

Table S10. Optimized Cartesian Coordinates of $\mathbf{3}^{3+}$.

Ru	-0.04634	0.109874	0.099367	C	5.192659	-0.6313	-2.01865
Fe	4.986616	-0.07907	1.356568	H	6.162013	-0.64335	-2.53125
Fe	-4.94952	-0.078	-1.32039	H	4.495592	-1.21838	-2.62899
P	5.404378	1.525136	-0.20582	C	-10.3867	2.46116	-0.22681
P	5.412628	-1.53442	-0.3387	H	-11.4424	2.686551	-0.33342
P	-5.83906	1.472629	0.17176	C	-3.60185	4.762173	-1.00507
P	-5.314	-1.55369	0.427035	H	-2.92108	5.013029	-1.81306
N	-3.15576	0.106942	-0.69567	C	8.196871	-0.4395	2.151639
C	0.314814	3.129258	3.252479	H	8.422897	-1.44017	1.768525
H	0.921652	3.199139	4.152471	H	8.82749	-0.27621	3.034468
N	-0.44434	-1.03933	1.830944	H	8.499056	0.289447	1.389466
N	3.129127	-0.00496	0.875682	C	1.292109	-1.77753	-1.89922
C	4.611667	-0.86907	3.298828	H	2.04721	-0.99967	-1.83951
C	5.832166	-1.39611	2.775303	C	2.784053	-5.39877	-0.68333
H	6.045849	-2.44712	2.612383	H	2.207077	-6.31796	-0.73048
C	1.972281	0.036609	0.594244	C	-2.58731	-4.53323	1.465496
C	7.123218	-2.28729	-0.45272	H	-1.86835	-4.71985	2.25918
N	-0.26377	1.859472	1.278014	C	-3.76	-5.26085	-0.53107
C	6.064591	0.893094	2.900764	H	-3.96008	-6.01809	-1.28265
H	6.47635	1.895155	2.870163	C	-9.56617	-3.21675	1.459612
C	-1.99189	0.131048	-0.39378	H	-10.5477	-3.61238	1.697729
C	6.753615	-0.31235	2.521875	C	7.138791	2.036879	-0.69172
C	-0.77156	-2.48294	4.254504	C	-9.42588	3.322093	-0.77849

C	-7.02015	-2.18986	0.843888	H	-9.73758	4.215064	-1.31001
C	0.073217	-2.94228	3.225612	C	-1.15122	2.838855	0.956937
H	0.646315	-3.85859	3.344489	H	-1.71261	2.700669	0.037259
C	-7.47064	-2.21545	2.176479	C	-7.84257	-2.70566	-0.17186
H	-6.84726	-1.85325	2.990492	H	-7.50413	-2.7184	-1.20502
N	0.46428	1.310382	-1.57316	C	4.285159	5.515533	-0.71814
C	4.579607	-3.9994	-1.53306	H	4.593295	6.360143	-1.32638
H	5.398229	-3.84235	-2.23393	C	7.637673	1.88751	-1.99745
C	-5.01708	3.142691	0.12546	H	7.024757	1.456542	-2.78654
C	3.302515	-3.28891	0.40682	C	4.685286	0.8021	-1.80892
H	3.135677	-2.55436	1.193534	H	3.597357	0.820918	-1.65571
C	-8.09092	-0.10744	-2.53695	H	4.906739	1.451497	-2.66606
H	-8.44754	-0.71865	-1.70143	C	8.94235	2.297565	-2.31048
H	-8.5811	-0.47258	-3.44806	H	9.317727	2.17677	-3.32178
H	-8.43246	0.918745	-2.3694	C	-0.61806	-3.73258	-1.93584
C	-8.61645	1.021826	0.61038	H	-1.39259	-4.49414	-1.88413
H	-8.32847	0.112583	1.136871	C	-0.71207	-2.6344	-1.08835
C	4.558176	3.190497	-0.05274	H	-1.55189	-2.52705	-0.40663
C	7.377609	-3.54084	0.134185	C	1.208728	2.435443	-1.38366
H	6.568613	-4.11625	0.580966	H	1.459772	2.686449	-0.36043
C	8.184969	-1.56699	-1.02461	C	0.444211	-3.29473	6.290711
H	8.027685	-0.57654	-1.4479	H	1.183181	-3.85875	5.705883
C	8.675534	-4.06872	0.135869	H	0.32829	-3.80178	7.253909
H	8.862485	-5.03751	0.587893	H	0.847962	-2.29331	6.478286
C	3.417704	-1.64004	3.759442	C	9.756291	2.869828	-1.32351
H	2.482632	-1.20287	3.376401	H	10.76489	3.18776	-1.56588
H	3.356257	-1.64257	4.855875	C	0.426931	6.312572	3.559703
H	3.467625	-2.68681	3.432706	H	0.408796	6.647971	2.512823
C	0.21552	-2.20918	2.050464	H	1.396932	5.840307	3.758026
H	0.881089	-2.53376	1.256975	H	0.347553	7.197417	4.19922
C	4.935312	4.28074	-0.85704	C	-3.98368	5.742515	-0.07762
H	5.752173	4.178171	-1.56978	H	-3.60687	6.756176	-0.17152
C	3.537833	3.347695	0.897671	C	1.653405	3.228077	-2.43608
H	3.258888	2.497396	1.519087	H	2.249643	4.110268	-2.20856
C	-9.97927	1.31411	0.469715	C	-8.06127	3.038716	-0.63563
H	-10.7188	0.648262	0.902896	H	-7.32754	3.725468	-1.05376
C	-1.45902	-1.27948	4.011305	C	-5.58204	0.792664	1.93321
H	-2.1198	-0.86456	4.767387	H	-5.04148	1.556607	2.503448
C	-0.6173	4.13889	2.940781	H	-6.5718	0.669457	2.388134
C	4.329708	-3.05643	-0.51912	C	-4.45172	0.4999	-3.36119
C	9.256586	3.043663	-0.02409	C	-4.46995	-4.05465	-0.55016
H	9.876088	3.501107	0.740358	H	-5.21985	-3.89334	-1.32296
N	0.218814	-1.63866	-1.0747	C	-2.08186	6.094836	3.670244
C	-7.65241	1.887604	0.063986	H	-2.1618	6.884823	4.423306

C	-1.2783	-0.59591	2.808753	H	-2.9443	5.426409	3.785089
H	-1.78125	0.347955	2.619722	H	-2.14489	6.578932	2.685223
C	-0.91007	-3.23263	5.559078	C	1.347058	2.885633	-3.76754
H	-1.61874	-2.68311	6.193963	C	-5.78507	-1.33526	-2.8606
C	3.814108	-5.1703	-1.60982	H	-6.12128	-2.36032	-2.77117
H	4.042201	-5.91725	-2.36463	C	3.257451	5.667048	0.227239
C	2.525899	-4.45508	0.319659	H	2.768576	6.629473	0.347644
H	1.740949	-4.6508	1.048911	C	0.56465	1.731242	-3.95307
C	-8.7418	-2.72121	2.480242	H	0.276854	1.408155	-4.94844
H	-9.08273	-2.73826	3.510081	C	9.730136	-3.3506	-0.4476
C	7.955533	2.630308	0.287781	H	10.73404	-3.76209	-0.44822
H	7.574793	2.785941	1.295204	C	-0.7524	5.352417	3.833807
C	0.464156	2.025289	2.418536	H	-0.66661	5.007903	4.874775
H	1.169362	1.234314	2.649574	C	-4.46744	-0.9422	-3.25657
C	0.447759	-3.84696	-2.85089	C	-3.28905	1.326542	-3.79927
C	-3.30231	-3.32521	1.453184	H	-3.58912	2.359269	-4.00255
H	-3.12234	-2.59938	2.245112	H	-2.85823	0.919839	-4.72264
C	0.488079	-5.00627	-3.82684	H	-2.49284	1.337846	-3.04272
H	0.484135	-5.9307	-3.22684	C	1.200766	3.485926	-6.24653
C	-4.11725	3.461542	-0.90177	H	1.391244	2.472737	-6.62566
H	-3.82436	2.695502	-1.61614	H	1.588998	4.1848	-6.99369
C	-1.35143	3.967052	1.752955	H	0.116659	3.636261	-6.17958
H	-2.09087	4.697449	1.435283	C	-9.11072	-3.21666	0.133408
C	-5.38759	4.121642	1.066958	H	-9.73768	-3.61625	-0.6569
H	-6.1083	3.891734	1.850065	C	3.412756	3.423201	-5.03778
C	4.758548	0.569964	3.381936	H	3.951937	3.641792	-4.10668
C	1.424463	-2.83885	-2.79506	H	3.846607	4.034707	-5.83545
H	2.293397	-2.86969	-3.44336	H	3.572644	2.366702	-5.29298
C	-6.60982	-0.16291	-2.71313	C	-1.46645	-4.64933	5.32838
C	-2.81561	-5.5018	0.479522	H	-1.59672	-5.16217	6.286588
H	-2.27929	-6.44479	0.508199	H	-0.77252	-5.25303	4.727392
C	9.481051	-2.09951	-1.02859	H	-2.43909	-4.62834	4.820993
H	10.29237	-1.53393	-1.47613	C	-5.75317	0.969827	-3.0003
C	3.791866	1.508306	4.026342	H	-6.07976	2.003499	-3.01786
H	3.89527	2.529922	3.640558	C	1.724158	-5.01617	-4.72944
H	3.968233	1.549298	5.109163	H	1.734171	-4.13838	-5.3899
H	2.754983	1.176455	3.883765	H	1.712765	-5.90445	-5.36863
C	-3.31257	-1.84559	-3.52509	H	2.658565	-5.02909	-4.15599
H	-2.36666	-1.39732	-3.19533	C	0.145432	0.982059	-2.85218
H	-3.22888	-2.05555	-4.59918	H	-0.44786	0.082131	-2.98495
H	-3.42334	-2.80492	-3.00523	C	1.901233	3.715252	-4.90494
C	-4.24682	-3.0828	0.442673	H	1.789999	4.772985	-4.62396
C	2.885837	4.581424	1.034178	C	-0.78555	-5.00411	-4.69957
H	2.099184	4.696436	1.778039	H	-1.70396	-5.05878	-4.10173

C	-4.801	-0.52544	1.915036	H	-0.77684	-5.86247	-5.37895
H	-4.93102	-1.08142	2.851103	H	-0.82251	-4.09188	-5.30992
H	-3.73153	-0.33749	1.776406				

Table S11. Optimized Cartesian Coordinates of 4^{3+} .

Ru	-0.06938	-0.20967	0.311643	H	-4.83411	1.913754	2.308147
Fe	-4.927	-0.21191	-1.32071	H	-6.48175	1.285058	2.145606
Fe	5.054337	-0.16996	1.218291	C	7.627959	-2.92954	-1.33236
P	5.454267	-1.11763	-0.82861	H	6.932642	-3.73301	-1.09851
P	-5.46739	1.694614	-0.07423	C	6.065953	-1.72042	2.32546
P	5.163328	1.802665	0.061186	C	2.852066	5.513067	1.757587
P	-5.63337	-1.32294	0.593813	H	2.329204	6.369432	2.173253
N	3.153799	-0.20005	0.891753	C	-1.31755	2.164512	1.79834
N	-3.14874	-0.19055	-0.6147	H	-1.90183	2.200449	0.882876
N	-0.37691	1.181427	1.881665	C	-5.20971	-5.44418	0.681899
N	-0.26647	-1.78821	1.720273	H	-5.85423	-6.30985	0.570938
C	1.975878	-0.21936	0.712575	C	0.529015	-3.41677	-3.42054
N	0.245923	-1.61584	-1.24386	C	-8.25549	2.190538	0.323108
N	0.297054	1.41084	-1.00617	H	-8.25547	1.348921	1.012924
C	-0.59616	-2.67216	-1.4056	C	-0.95334	4.048038	5.107278
H	-1.38489	-2.77402	-0.66598	H	-0.22729	3.825125	5.900849
C	0.997948	3.547107	-2.74304	C	-2.85148	-0.50344	-3.80654
C	1.259817	-1.48045	-2.14434	H	-2.50875	0.537708	-3.83978
H	1.947797	-0.65855	-1.97352	H	-2.79309	-0.90119	-4.82812
C	-6.50275	-0.14538	-2.87656	H	-2.15941	-1.08665	-3.18335
C	0.52612	-3.90201	2.585003	C	-5.13686	1.786854	-3.95426
H	1.195189	-4.74891	2.458245	H	-5.81038	2.503117	-3.46881
C	4.303385	1.389602	-1.5806	H	-5.41349	1.751131	-5.01624
H	3.254741	1.204636	-1.31489	H	-4.11724	2.182985	-3.89654
H	4.31981	2.245817	-2.26702	C	-5.25907	0.428234	-3.34688
C	3.298328	3.124152	1.731773	C	3.14062	-5.04329	-1.92396
H	3.114978	2.12011	2.111675	H	2.651812	-5.98697	-2.14876
C	4.245403	3.304367	0.711613	C	8.240609	3.518419	-2.20868
C	0.287488	2.42223	-3.20324	H	8.417562	3.788792	-3.24484
H	-0.00928	2.337526	-4.24417	C	-4.17005	-3.11606	-2.5872
C	-8.45153	-1.12141	0.185073	H	-3.2466	-3.00929	-2.00499
H	-8.20953	-0.7064	-0.78878	H	-3.89866	-3.54282	-3.56289
C	0.969192	2.503205	-0.55005	H	-4.81246	-3.8362	-2.07014
H	1.236228	2.508519	0.498896	C	-10.1125	-1.76435	1.834317
C	1.410054	-2.33528	-3.23236	H	-11.1503	-1.87326	2.131271
H	2.225613	-2.16832	-3.93129	C	0.690842	4.760045	-4.96883
C	2.946912	-4.42944	-0.6789	H	0.987626	5.660847	-5.51461
H	2.302076	-4.90368	0.058488	H	-0.39723	4.797431	-4.8288
C	-2.01781	-0.19269	-0.20847	H	0.930846	3.901797	-5.61068
C	-4.93304	-0.23455	1.967517	C	-8.32863	4.362229	-1.45028

H	-5.23506	-0.63353	2.942414	H	-8.35267	5.209811	-2.12716
H	-3.84181	-0.2675	1.888907	C	8.985416	3.420354	0.097309
C	1.442195	4.684102	-3.63734	H	9.739302	3.61597	0.852869
H	1.273451	5.620068	-3.0833	C	9.873471	-2.23239	-1.95225
C	3.61993	-3.23789	-0.36847	H	10.90277	-2.48078	-2.18906
H	3.499686	-2.7557	0.601815	C	-0.70486	5.485631	4.614257
C	-4.85048	-1.80086	-2.76433	H	-1.42694	5.766065	3.835192
C	-4.92819	-3.03135	0.774669	H	0.305196	5.607505	4.204933
C	-1.08834	-1.69918	2.800806	H	-0.82105	6.191745	5.442702
H	-1.70858	-0.81022	2.859613	C	0.646258	-4.29166	-4.64683
C	-1.13165	-2.67253	3.797692	H	1.71684	-4.38756	-4.88313
H	-1.80169	-2.54268	4.642215	C	-7.84074	0.513477	-2.97619
C	-6.22999	-1.50294	-2.50586	H	-8.65287	-0.19419	-2.78448
H	-6.95773	-2.21466	-2.13094	H	-7.98283	0.894323	-3.99522
C	7.198481	-1.58976	-1.33982	H	-7.95609	1.368237	-2.29804
C	-3.22231	3.048645	-1.20764	C	-4.33539	4.190321	0.629451
H	-3.11923	2.179142	-1.8549	H	-5.13456	4.238486	1.367776
C	0.530423	-2.89055	1.628154	C	-2.45811	5.243786	-0.49558
H	1.190575	-2.93187	0.76709	H	-1.78564	6.087881	-0.61119
C	-7.42566	-1.49463	1.06467	C	8.958964	-3.2473	-1.63648
C	1.325172	3.56575	-1.37411	H	9.278568	-4.28452	-1.62925
H	1.870082	4.403214	-0.941	C	9.229531	3.753894	-1.2431
C	-1.52436	3.092558	2.815559	H	10.17496	4.202691	-1.52935
H	-2.29038	3.851036	2.675202	C	3.996357	-4.45449	-2.86834
C	-0.74968	3.049378	3.991321	H	4.16843	-4.93975	-3.8248
C	-0.31086	-3.81155	3.713937	C	0.049934	-5.69167	-4.47211
C	-0.47834	-3.58225	-2.45411	H	0.447256	-6.20419	-3.58777
H	-1.17556	-4.4135	-2.50842	H	0.27535	-6.30637	-5.34901
C	0.218337	2.032976	4.066833	H	-1.04464	-5.64913	-4.38428
H	0.853338	1.940364	4.943842	C	-9.46576	2.850569	0.070728
C	-3.54903	-3.20233	0.978808	H	-10.3701	2.523569	0.574073
H	-2.8955	-2.338	1.080081	C	-0.34815	-4.89733	4.76356
C	8.122504	-0.57594	-1.65112	H	-0.95486	-4.53568	5.604995
H	7.830503	0.472709	-1.63474	C	-9.50645	3.93267	-0.82006
C	-9.79381	-1.25736	0.567824	H	-10.4434	4.444448	-1.01223
H	-10.5836	-0.96873	-0.11892	C	-7.74759	-2.00882	2.337174
C	-2.34934	4.136781	-1.34797	H	-6.96339	-2.32717	3.022184
H	-1.59165	4.119949	-2.12736	C	-3.45293	5.269863	0.495346
C	-0.04681	1.393471	-2.32005	H	-3.55703	6.136309	1.141114
H	-0.58875	0.51784	-2.66026	C	-1.02893	-6.15462	4.185624
C	-5.75954	-4.15624	0.623342	H	-2.04918	-5.9401	3.844546
H	-6.83051	-4.03621	0.472908	H	-1.08046	-6.93914	4.947346
C	4.485555	-2.65308	-1.3048	H	-0.4542	-6.55097	3.336948
C	4.957539	0.144676	-2.19293	C	-9.08763	-2.13888	2.719154

H	5.871452	0.405776	-2.74031	H	-9.334	-2.53726	3.697622
H	4.286081	-0.36001	-2.89885	C	-2.36976	3.921825	5.698943
C	-7.07465	2.613534	-0.3121	H	-2.4908	4.617189	6.535698
C	-4.21698	3.072368	-0.21915	H	-2.56713	2.908891	6.066709
C	4.504042	4.598117	0.224839	H	-3.13127	4.172292	4.947673
H	5.268691	4.754981	-0.53399	C	-0.04204	-3.56953	-5.82658
C	7.018369	2.938803	-1.83859	H	-1.11427	-3.44633	-5.61382
H	6.26924	2.772795	-2.61003	H	0.054871	-4.16051	-6.743
C	-3.83333	-5.61446	0.894416	H	0.391208	-2.57888	-6.00921
H	-3.413	-6.61375	0.949039	C	1.057089	-5.23539	5.288182
C	4.859098	-1.34064	2.994026	H	1.684215	-5.67093	4.499157
C	-4.25028	-0.6038	-3.30316	H	0.988074	-5.97432	6.092802
C	2.6012	4.22409	2.251197	H	1.566441	-4.34921	5.682995
H	1.879103	4.074382	3.052369	C	6.203629	0.535708	2.838704
C	3.806681	5.698585	0.744503	H	6.571465	1.54661	2.97139
H	4.024971	6.697283	0.379484	C	8.323725	-0.51613	1.722505
C	2.962054	4.559735	-3.88554	H	8.536289	-1.32307	1.01224
H	3.184081	3.620309	-4.41046	H	9.013109	-0.63307	2.568473
H	3.528487	4.578055	-2.94439	H	8.568296	0.428967	1.223106
H	3.311496	5.388256	-4.51003	C	3.73184	-2.23882	3.388743
C	6.776508	2.576221	-0.50102	H	3.74065	-2.41635	4.472663
C	4.945692	0.065449	3.327416	H	3.801165	-3.21865	2.898766
C	6.907438	-0.5437	2.202403	H	2.756643	-1.79682	3.13354
C	7.765506	2.837129	0.463892	C	3.99213	0.807498	4.204888
H	7.58578	2.595881	1.50878	H	2.948882	0.570659	3.955681
C	9.449923	-0.89581	-1.96224	H	4.132251	1.892052	4.130372
H	10.15053	-0.10232	-2.20346	H	4.146427	0.527753	5.255568
C	4.663385	-3.26137	-2.56097	C	6.452461	-3.11483	1.947829
H	5.353783	-2.8284	-3.28353	H	6.782965	-3.6637	2.838957
C	-7.11633	3.707382	-1.19921	H	7.284264	-3.12387	1.236242
H	-6.20634	4.067815	-1.67596	H	5.621069	-3.67815	1.50505
C	-3.00521	-4.49226	1.047432	C	0.377071	1.132212	3.013603
H	-1.938	-4.62024	1.225453	H	1.118063	0.340514	3.055464
C	-5.45686	1.191626	1.768228				

Table S12. Optimized Cartesian Coordinates of 5^{3+} .

Ru	0.000029	-4.8E-05	-0.00028	Fe	5.003243	-0.05478	1.096501
Fe	-5.00344	0.054843	-1.09622	P	5.314463	1.62985	-0.45624
P	-5.31458	-1.62975	0.456537	P	5.672987	-1.45128	-0.63714
P	-5.67247	1.451303	0.637706	N	0.080973	-1.72887	-1.26222
N	-0.08078	1.728818	1.261585	N	3.196319	-0.09677	0.504932
N	-3.19637	0.096705	-0.50514	N	0.151657	1.36017	-1.64222
N	-0.15167	-1.36033	1.641573	C	6.064756	0.961381	2.729976
C	-6.06551	-0.96126	-2.72941	C	2.024498	-0.06928	0.257785
C	-2.0245	0.069195	-0.25825	C	-0.4136	3.485727	-2.64357

C	0.413388	-3.48598	2.642855	H	-0.93839	4.433852	-2.55199
H	0.938113	-4.43414	2.551264	C	0.321882	3.201185	-3.80617
C	-0.32204	-3.2014	3.805482	C	-0.99248	-2.56296	-1.33964
C	0.992678	2.562937	1.338779	H	-1.882	-2.26557	-0.79574
H	1.882108	2.265545	0.794724	C	0.167201	-4.13518	-2.7822
C	-0.16669	4.135136	2.781595	C	0.852401	1.069714	-2.77152
C	-0.85238	-1.06985	2.770891	H	1.330801	0.100303	-2.81028
H	-1.33067	-0.10039	2.8097	C	7.016131	2.258656	-0.90641
C	-7.01622	-2.2582	0.907273	C	-0.48054	2.563064	-1.59985
C	0.480407	-2.56329	1.599163	H	-1.05155	2.780215	-0.70327
H	1.051389	-2.78045	0.702559	C	1.270256	-3.26633	-2.7067
C	-1.26975	3.266285	2.706329	H	2.195905	-3.50299	-3.2243
H	-2.19529	3.502926	3.22414	C	4.341402	3.225229	-0.3598
C	-4.3419	-3.22533	0.359475	C	6.644813	-0.32943	2.498793
C	-6.64528	0.329671	-2.49815	C	4.741141	0.833791	-2.07572
C	-4.74041	-0.83395	2.075834	H	4.925239	1.52613	-2.90733
H	-4.92429	-1.52628	2.907503	H	3.661561	0.662743	-1.98551
H	-3.66083	-0.66314	1.985181	C	1.204203	-2.10902	-1.93693
C	-1.20387	2.108986	1.936522	H	2.084239	-1.48579	-1.8103
H	-2.08395	1.485786	1.810052	C	8.152129	1.649417	-0.35587
C	-8.15232	-1.64908	0.356798	H	8.033639	0.827074	0.344446
H	-8.03397	-0.82691	-0.34375	C	4.665154	0.781383	3.016929
C	-4.66595	-0.78154	-3.01667	C	4.398219	-0.63881	3.051096
C	-4.39875	0.638613	-3.05097	C	5.609629	-1.32561	2.714303
C	-5.60997	1.325644	-2.71396	C	4.637038	-2.99563	-0.88861
C	-4.63643	2.995671	0.888699	C	3.684299	-3.3783	0.066886
C	-3.68397	3.378137	-0.06716	H	3.473204	-2.71047	0.901712
H	-3.47314	2.710137	-0.90191	C	4.801641	4.228462	0.515917
C	-4.80294	-4.22851	-0.51587	H	5.698578	4.062204	1.108094
H	-5.70038	-4.06219	-1.10726	C	7.395735	-2.19134	-0.74755
C	-7.39516	2.191384	0.748601	C	0.955266	1.944049	-3.85042
C	-0.95532	-1.94421	3.849758	H	1.529811	1.64104	-4.72091
H	-1.52986	-1.64117	4.72025	C	-0.97762	-3.75302	-2.06336
C	0.977961	3.752997	2.062479	H	-1.87354	-4.36948	-2.05513
H	1.87388	4.369457	2.054041	C	3.224586	3.484868	-1.17163
C	-3.22437	-3.48503	1.170313	H	2.856793	2.738625	-1.87546
H	-2.85596	-2.73883	1.873856	C	6.812804	2.251753	2.834184
C	-6.81381	-2.2515	-2.83348	H	6.132696	3.095086	2.99116
H	-6.13387	-3.09497	-2.99044	H	7.478488	2.211577	3.706024
H	-7.47952	-2.21124	-3.7053	H	7.442976	2.463218	1.962845
H	-7.44397	-2.4628	-1.9621	C	5.495011	-0.4831	-2.27783
C	-5.4939	0.48312	2.278314	H	4.984403	-1.128	-3.00259
H	-4.9828	1.127913	3.002819	H	6.502739	-0.28905	-2.66231
H	-6.50148	0.289275	2.663298	C	8.104945	-0.63592	2.36754

C	-8.10531	0.63648	-2.36648	H	8.708072	0.276782	2.312007
H	-8.70867	-0.2761	-2.31148	H	8.445308	-1.1904	3.251854
H	-8.44566	1.19168	-3.25034	H	8.337907	-1.25808	1.493021
H	-8.33797	1.258092	-1.49149	C	3.038345	5.722037	-0.22874
C	-3.03896	-5.72212	0.227068	H	2.549269	6.690737	-0.19433
H	-2.5499	-6.69081	0.192149	C	5.864814	-2.79515	2.805651
C	-5.86495	2.795219	-2.80531	H	6.759538	-3.07809	2.241449
H	-6.75926	3.078386	-2.24056	H	6.043769	-3.07343	3.852761
H	-6.04453	3.07342	-3.85234	H	5.026691	-3.40236	2.445135
H	-5.02649	3.402318	-2.44541	C	4.153238	5.467347	0.58582
C	-4.1546	-5.46739	-0.58646	H	4.533937	6.238997	1.247584
H	-4.53588	-6.23898	-1.24796	C	7.63737	-3.46911	-0.20578
C	-7.63701	3.469114	0.20683	H	6.818717	-4.06229	0.19725
H	-6.8185	4.062306	-0.19648	C	2.581113	4.731134	-1.10635
C	-2.58096	-4.73129	1.104357	H	1.734486	4.928928	-1.75871
H	-1.7337	-4.92911	1.755905	C	3.026471	-4.61233	-0.05155
C	-3.02606	4.612168	0.05084	H	2.308637	-4.92297	0.704349
H	-2.30848	4.922641	-0.70537	C	0.395597	4.174167	-4.95898
C	-0.39601	-4.17441	4.958252	H	-0.02762	5.131126	-4.62179
H	0.02821	-5.13107	4.621449	C	3.106526	-1.26723	3.454976
C	-3.10705	1.266791	-3.45522	H	3.089623	-2.33874	3.220024
H	-3.08984	2.338265	-3.22013	H	2.961263	-1.16682	4.538764
H	-2.9622	1.166494	-4.53907	H	2.247338	-0.79501	2.959325
H	-2.24778	0.794325	-2.95993	C	8.46659	-1.47321	-1.30787
C	-8.46583	1.473225	1.309248	H	8.319251	-0.48797	-1.74393
H	-8.31832	0.488002	1.745292	C	3.691113	1.859421	3.356521
C	-3.69218	-1.85979	-3.35637	H	2.658567	1.514326	3.224398
H	-2.65954	-1.51486	-3.22454	H	3.804601	2.180169	4.400863
H	-3.80597	-2.18063	-4.40066	H	3.831824	2.743429	2.719141
H	-3.83291	-2.7437	-2.71887	C	4.245214	-5.0727	-2.09967
C	-4.24418	5.072956	2.09924	H	4.479377	-5.73372	-2.92833
H	-4.47808	5.73413	2.92785	C	4.907095	-3.84372	-1.98015
C	-4.90614	3.843972	1.980151	H	5.66999	-3.57342	-2.70859
H	-5.66884	3.573831	2.70887	C	7.16557	3.316804	-1.82268
C	-7.16551	-3.31607	1.823904	H	6.290955	3.808939	-2.24558
H	-6.29081	-3.8081	2.246757	C	9.43482	2.089772	-0.7128
C	-9.43495	-2.08931	0.714128	H	10.30952	1.613824	-0.27815
H	-10.3097	-1.61348	0.279521	C	0.203692	-5.38609	-3.62673
C	-0.203	5.386019	3.626178	H	1.257364	-5.61271	-3.84741
H	-1.25663	5.612676	3.847031	C	3.310974	-5.46368	-1.12722
C	-3.31021	5.463717	1.126445	H	2.823292	-6.43108	-1.20271
H	-2.82246	6.431112	1.201621	C	9.582426	3.142948	-1.62519
C	-9.58239	-3.1422	1.626869	H	10.57296	3.490228	-1.90009
H	-10.5729	-3.48937	1.902073	C	8.44642	3.753904	-2.18111

C	-8.44629	-3.75302	2.182741	H	8.56118	4.570726	-2.88609
H	-8.56093	-4.56962	2.887996	C	9.759562	-2.01505	-1.31288
C	-9.75883	2.015011	1.314612	H	10.57434	-1.45213	-1.75746
H	-10.5735	1.452075	1.759443	C	9.997197	-3.27881	-0.75584
C	-9.99667	3.278743	0.757596	H	10.99783	-3.69783	-0.76053
H	-10.9973	3.697731	0.762557	C	-0.52062	-5.1149	-4.96226
C	0.5215	5.114701	4.961579	H	-0.06685	-4.27946	-5.50732
H	0.067811	4.279198	5.506612	H	-0.48347	-6.0029	-5.6017
H	0.484437	6.002628	5.601113	H	-1.57719	-4.87315	-4.78015
H	1.578039	4.872976	4.779284	C	-0.42149	-6.59511	-2.91545
C	0.422118	6.595043	2.914864	H	-1.50529	-6.46513	-2.791
H	1.505879	6.464974	2.790109	H	-0.27111	-7.50104	-3.51127
H	0.271996	7.500925	3.510829	H	0.01914	-6.75739	-1.92375
H	-0.01876	6.757477	1.923311	C	8.930477	-4.00697	-0.20851
C	-8.93013	4.006919	0.209915	H	9.102648	-4.9946	0.206896
H	-9.10247	4.994522	-0.20548	C	-0.46192	3.655795	-6.13129
C	0.459955	-3.65548	6.131423	H	-1.50678	3.508252	-5.8336
H	1.505108	-3.50766	5.834914	H	-0.43971	4.370743	-6.95998
H	0.437037	-4.37025	6.960234	H	-0.07167	2.699261	-6.50346
H	0.068988	-2.699	6.502958	C	1.843526	4.416941	-5.41555
C	-1.84425	-4.41821	5.413341	H	2.28171	3.507989	-5.84781
H	-2.28356	-3.50949	5.844953	H	1.866198	5.187663	-6.19245
H	-1.86717	-5.18882	6.190353	H	2.482982	4.748901	-4.58838
H	-2.48258	-4.75078	4.585549				

Table S13. Optimized Cartesian Coordinates of $\mathbf{1}^{4+}$.

Ru	-0.01594	0.137377	0.680754	C	-10.2693	2.336529	-0.3109
Fe	-5.07392	-0.59053	0.782151	H	-11.3252	2.581193	-0.27051
Fe	5.08036	0.548616	0.969293	C	3.301184	-3.8763	2.49202
P	-5.73397	1.260791	-0.46944	H	2.661942	-3.73849	3.361326
P	5.404018	-1.45581	-0.13477	C	8.145331	-2.02768	0.264192
P	-5.12057	-1.66927	-1.26265	H	7.970772	-1.74996	1.300455
P	5.37161	1.453599	-1.15346	C	3.405236	4.515169	-3.11373
N	-0.12997	1.450675	-0.98485	H	3.417336	4.946749	-4.11006
N	-0.26578	1.778025	2.004997	C	1.134942	-2.5032	-0.32332
N	3.19466	0.412449	0.782676	H	1.656708	-2.41411	0.62348
N	0.24967	-1.51376	-0.63065	C	7.014373	0.961767	1.699076
N	0.092437	-1.1626	2.365932	H	7.936276	0.81202	1.153291
N	-3.21179	-0.26047	0.604484	C	-1.17358	2.318343	-1.12407
C	-2.02537	-0.11092	0.618281	H	-1.88643	2.361198	-0.30511
C	-4.06011	2.906269	1.145626	C	-8.47308	0.897613	-1.09097
H	-3.95233	2.038152	1.793044	H	-8.16043	0.01734	-1.65272
C	-3.42959	4.113168	1.480546	C	7.300776	3.501537	-1.49787
H	-2.8486	4.180611	2.397443	H	6.497021	4.197287	-1.2628

C	4.67815	-2.93422	0.728528	C	-9.83563	1.214713	-1.03378
C	-7.53655	1.715573	-0.43004	H	-10.5552	0.590238	-1.55324
C	2.00149	0.343826	0.745822	C	0.873354	-0.85932	3.442123
C	3.438858	3.445823	-0.51698	H	1.451433	0.056989	3.371833
H	3.465372	3.034712	0.490426	C	-2.27199	-4.57866	-0.46204
C	4.2124	2.858441	-1.52926	H	-1.58261	-4.82703	0.341646
C	-4.09114	-3.98508	-2.52068	C	-7.97068	2.835316	0.303324
H	-4.81884	-3.78274	-3.30442	H	-7.2579	3.476781	0.818105
C	-0.42422	-1.62255	-1.80588	C	6.377486	0.02399	2.594076
H	-1.13332	-0.83141	-2.02839	H	6.717928	-0.97312	2.838609
C	2.652685	4.571248	-0.80336	C	1.027124	-4.84043	-3.33338
H	2.078545	5.051885	-0.01598	H	0.964828	-5.7654	-2.73848
C	2.637152	5.106571	-2.09775	C	-6.00526	-2.21183	1.813435
H	2.055449	5.998972	-2.30658	H	-6.05984	-3.2356	1.468481
C	4.448796	-1.17479	-1.73707	C	-6.95646	-1.15656	1.54655
H	4.511474	-2.05498	-2.38856	H	-7.87013	-1.23952	0.973895
H	3.398704	-1.06052	-1.43974	C	-9.33697	3.143286	0.356888
C	-5.32027	0.914591	-2.29404	H	-9.67141	4.012449	0.913085
H	-6.27132	0.81502	-2.82941	C	-4.33382	5.151938	-0.52177
H	-4.80047	1.793071	-2.69095	H	-4.46491	6.026022	-1.15119
C	1.378325	-3.58081	-1.16739	C	-7.58557	-3.05165	-1.27668
H	2.097197	-4.33583	-0.85475	H	-7.30396	-3.39688	-0.28462
C	-0.22292	-2.67606	-2.69898	C	-7.09761	-1.82582	-3.31947
H	-0.79845	-2.70029	-3.61841	H	-6.44981	-1.19981	-3.92885
C	-4.00166	-3.15009	-1.39235	C	3.60138	-5.16865	2.035588
C	4.989201	-4.22939	0.274479	H	3.201576	-6.03568	2.552066
H	5.671579	-4.37442	-0.56117	C	4.447061	-5.34448	0.928631
C	-4.82278	2.820153	-0.02894	H	4.70206	-6.34393	0.592281
C	0.672271	2.173883	-3.15132	C	-8.31189	-2.26262	-3.86723
H	1.427895	2.070372	-3.92345	H	-8.58461	-1.96914	-4.87535
C	8.626274	-2.83176	-2.37819	C	2.484461	-4.7039	-3.82884
H	8.807706	-3.15627	-3.39734	H	2.600972	-3.78132	-4.41319
C	-3.09796	-3.45202	-0.36031	H	2.739667	-5.54735	-4.47782
H	-3.05685	-2.81173	0.519289	H	3.20292	-4.68835	-2.99871
C	-1.34123	3.106978	-2.25853	C	0.914712	-1.65216	4.586502
H	-2.20386	3.767917	-2.31356	H	1.539219	-1.35106	5.423631
C	0.705321	-3.6905	-2.40207	C	-0.65582	3.862638	-4.57595
C	9.668984	-2.84701	-1.44041	H	-1.72606	3.777494	-4.81934
H	10.65909	-3.17833	-1.73427	C	8.110318	1.234845	-1.88841
C	7.059648	2.115744	-1.56935	H	7.954468	0.15802	-1.938
C	-6.5255	0.011464	2.277246	C	-0.64395	-2.30533	2.433069
H	-7.04243	0.96202	2.303488	H	-1.24154	-2.53796	1.556645
C	7.101418	-1.98863	-0.67824	C	-8.79682	-3.48772	-1.82729
C	-5.3051	-0.30737	2.945161	H	-9.44489	-4.14445	-1.25694

H	-4.72357	0.366669	3.558719	C	0.156122	3.399143	-5.78837
C	0.363743	3.994702	2.724432	H	1.231584	3.561356	-5.63054
H	0.950537	4.892103	2.542904	H	-0.12754	3.980722	-6.67059
C	0.788789	1.413108	-1.98783	H	-0.00636	2.340039	-6.02013
H	1.623114	0.732606	-1.84741	C	-9.16678	-3.0853	-3.11991
C	-1.07999	1.698299	3.092566	H	-10.1046	-3.42419	-3.54658
H	-1.63128	0.769723	3.210205	C	-0.54353	5.082994	4.825051
C	-3.5626	5.233866	0.649346	H	0.453014	5.545328	4.874406
H	-3.09095	6.172754	0.921938	C	8.583493	3.99994	-1.75964
C	-4.45552	-0.34133	-2.42186	H	8.765395	5.068365	-1.71469
H	-3.43061	-0.14376	-2.08587	C	0.134307	-2.82316	4.676961
H	-4.41298	-0.71082	-3.45341	C	-0.36852	5.351997	-4.28653
C	-3.26371	-5.11175	-2.61708	H	-0.91003	5.717593	-3.40584
H	-3.34983	-5.77134	-3.47482	H	-0.66166	5.963359	-5.14552
C	5.139997	1.989296	2.616157	H	0.706325	5.501559	-4.12095
H	4.366885	2.711644	2.840219	C	-0.64569	-3.14205	3.548726
C	3.842981	-2.75846	1.844301	H	-1.26603	-4.03322	3.540416
H	3.614858	-1.75583	2.204562	C	0.081272	-4.96171	-4.5301
C	-2.3536	-5.40747	-1.5906	H	-0.96874	-5.04597	-4.22151
H	-1.73466	-6.29731	-1.6591	H	0.330516	-5.85292	-5.11373
C	-4.98545	-1.67716	2.661224	H	0.179073	-4.09844	-5.20205
H	-4.11115	-2.20737	3.013849	C	9.628106	3.123215	-2.08671
C	0.436789	2.931826	1.828421	H	10.61891	3.513089	-2.29332
H	1.060296	2.977426	0.940323	C	9.388763	1.742591	-2.15159
C	4.988021	0.085029	-2.42363	H	10.19412	1.062671	-2.40966
H	4.262111	0.491378	-3.13696	C	-1.51584	6.131032	4.236124
H	5.915669	-0.11933	-2.97081	H	-1.21838	6.446888	3.227797
C	9.424095	-2.45308	-0.11609	H	-1.54022	7.018632	4.875375
H	10.22321	-2.48587	0.616619	H	-2.53637	5.724448	4.194004
C	4.19677	3.394894	-2.83145	C	-1.08344	-4.50695	6.155239
H	4.829983	2.974873	-3.61165	H	-1.98318	-3.88064	6.157086
C	-0.42528	3.035759	-3.32838	H	-1.02386	-5.00642	7.126584
C	-6.73566	-2.20554	-2.01338	H	-1.20343	-5.29532	5.400135
C	7.344564	-2.40845	-1.99985	C	1.412411	-4.63111	5.812461
H	6.553907	-2.41843	-2.74688	H	1.307815	-5.29771	4.943951
C	5.219442	0.656782	3.141922	H	1.476272	-5.25724	6.707458
H	4.516747	0.202122	3.826734	H	2.354891	-4.07584	5.723743
C	6.251801	2.188997	1.742485	C	0.19066	-3.68982	5.914563
H	6.493202	3.098235	1.207698	C	-0.97851	4.699691	6.242948
C	-1.19028	2.72474	4.031079	H	-2.02521	4.367931	6.265316
H	-1.8358	2.587323	4.892613	H	-0.91029	5.572125	6.899321
C	-4.96601	3.948723	-0.86078	H	-0.35112	3.909809	6.671305
H	-5.59769	3.907526	-1.74692	H	0.351577	-3.02595	6.775864
C	-0.45228	3.91282	3.87161				

Table S14. Optimized Cartesian Coordinates of **2⁴⁺**.

Ru	-0.06272	-0.01874	0.418909	H	-4.68269	0.294321	4.935322
Fe	-5.13827	0.697401	0.777656	H	-3.32641	0.373943	3.798789
Fe	5.003819	-0.88744	0.602172	C	4.000649	3.885856	3.995993
P	-5.71962	-1.36822	-0.06332	H	3.628811	4.479154	4.8253
P	-5.46175	1.367227	-1.41778	C	0.138215	0.529079	-4.51319
P	5.619284	1.330998	0.445309	C	-5.20077	-0.16455	-2.522
P	5.472418	-0.86806	-1.67334	H	-6.14012	-0.35536	-3.05353
N	-0.17115	-2.12602	0.145761	H	-4.43956	0.0914	-3.26746
N	-0.08209	-0.27252	2.529646	C	-5.22853	0.889002	2.955702
N	-0.02321	0.224883	-1.69012	C	-2.539	4.717328	-2.82874
N	3.148359	-0.42824	0.444895	H	-1.89872	5.530484	-3.15606
N	0.056866	2.087578	0.652368	C	1.040739	-0.28586	-3.80192
N	-3.27137	0.339958	0.530537	H	1.830678	-0.83272	-4.31149
C	1.968835	-0.22637	0.43796	C	2.767552	-3.6474	-4.2652
C	-2.08907	0.174121	0.452048	H	2.176463	-4.32349	-4.87434
C	-6.94589	1.507208	1.503815	C	-7.47428	-1.78352	-0.51979
H	-7.88441	1.53311	0.965952	C	-7.2961	3.476881	-1.83587
C	7.388841	-2.76288	-2.51265	H	-6.46269	4.139591	-1.60807
H	6.562046	-3.47147	-2.5162	C	2.642364	-3.66612	-2.86849
C	-3.40912	3.306555	-1.05033	H	1.947429	-4.35328	-2.39293
H	-3.42128	3.011524	-0.00234	C	-3.29982	-3.98233	2.052942
C	-1.01758	-1.04762	3.143995	H	-2.23189	-4.1357	2.203596
H	-1.75504	-1.51761	2.500221	C	-8.55016	4.028235	-2.12612
C	-5.94589	2.549982	1.482639	H	-8.68398	5.104481	-2.10415
H	-6.00888	3.471697	0.920261	C	-5.59975	-4.63547	2.482477
C	0.934274	-0.41267	-2.42261	H	-6.31754	-5.28851	2.967147
H	1.622229	-1.04576	-1.87426	C	8.670525	-3.20532	-2.86152
C	0.904605	4.234671	-0.07339	H	8.831229	-4.24853	-3.11175
H	1.518099	4.781866	-0.78162	C	7.666575	3.039988	-0.47795
C	0.462869	-4.36595	0.806868	H	6.864039	3.644229	-0.89532
H	1.012501	-4.99427	1.501721	C	4.465492	-1.91695	-4.09478
C	-6.4995	0.495144	2.429112	H	5.200268	-1.27155	-4.57371
H	-7.02519	-0.41005	2.707978	C	8.249553	-0.49943	-2.23714
C	-0.85294	1.174722	-3.75245	H	8.118026	0.554222	-1.99615
H	-1.58433	1.821342	-4.23102	C	-7.70964	-2.6792	-1.58165
C	-4.23938	2.654902	-1.97579	H	-6.88629	-3.11998	-2.13912
C	0.203282	4.911166	0.942521	C	-3.37046	4.066657	-3.75524
C	-0.90921	1.006953	-2.3666	H	-3.37749	4.37896	-4.79445
H	-1.66849	1.517209	-1.77868	C	-4.22599	-4.82208	2.691958
C	4.66336	-2.71245	1.691951	H	-3.88153	-5.62146	3.340403
H	3.73152	-3.26296	1.674803	C	-8.19921	1.242774	-2.20517

C	-5.12293	-2.76934	1.000649	H	-8.09269	0.159331	-2.23876
C	7.39232	1.848514	0.222645	C	-9.8733	-1.63372	-0.13448
C	4.756739	1.835905	-1.15502	H	-10.7083	-1.23947	0.43481
H	3.684291	1.699031	-0.98085	C	4.123922	-1.1672	3.73599
H	4.938853	2.891549	-1.38248	H	4.262153	-0.08766	3.882923
C	-0.88518	-2.67147	-0.8768	H	4.363907	-1.6637	4.683993
H	-1.39349	-1.97133	-1.53199	H	3.065342	-1.3546	3.519159
C	5.243021	0.922299	-2.28671	C	0.290005	6.405204	1.15314
H	6.202318	1.264308	-2.69169	H	-0.68259	6.743307	1.540388
H	4.519877	0.898077	-3.11013	C	-0.05973	-0.80057	6.852417
C	-0.11092	-0.60465	5.355444	H	0.2764	0.145801	7.299864
C	7.173845	-1.40541	-2.20162	C	-9.44957	1.803152	-2.49697
C	-0.28063	-4.94059	-0.24382	H	-10.2788	1.154529	-2.76018
C	0.849514	0.200114	4.709001	C	-8.56343	-1.2739	0.209336
H	1.608061	0.721357	5.28932	H	-8.41062	-0.59801	1.043679
C	0.807633	2.848707	-0.18903	C	10.04401	2.737694	-0.07624
H	1.33042	2.315026	-0.97675	H	11.06641	3.081312	-0.19098
C	-0.96153	-4.04618	-1.0921	C	-1.49301	-6.96281	0.534757
H	-1.55335	-4.42474	-1.92062	H	-1.63086	-8.03866	0.389324
C	4.971086	2.37523	1.837968	H	-2.45742	-6.46612	0.369805
C	0.495653	-2.98221	0.969999	H	-1.19224	-6.80126	1.579845
H	1.05754	-2.52528	1.779127	C	9.528276	-0.94997	-2.59166
C	6.298282	-1.19434	2.30359	H	10.35209	-0.24471	-2.63098
H	6.824757	-0.42062	2.849044	C	-0.4029	-6.43536	-0.42475
C	5.755391	-2.87622	0.786691	H	-0.7386	-6.62345	-1.45419
H	5.830704	-3.6041	-0.0095	C	-9.02076	-3.02936	-1.92932
C	-0.57671	4.113998	1.80542	H	-9.19568	-3.71799	-2.74895
H	-1.14199	4.578554	2.609635	C	9.772785	1.566149	0.644527
C	-6.05158	-3.61334	1.635445	H	10.58505	1.00227	1.090595
H	-7.11898	-3.49236	1.463669	C	0.243835	0.682069	-6.01207
C	-0.63044	2.732396	1.636778	H	-0.53628	1.38056	-6.34337
H	-1.22784	2.106931	2.293327	C	-10.1046	-2.5039	-1.20932
C	-2.56194	4.33838	-1.47902	H	-11.1187	-2.78208	-1.47533
H	-1.93964	4.859001	-0.75557	C	9.742231	-2.3005	-2.90052
C	6.770625	-1.91261	1.146944	H	10.73281	-2.64438	-3.17791
H	7.732496	-1.81064	0.661375	C	-9.62831	3.193339	-2.45572
C	-4.22398	3.039559	-3.33064	H	-10.5969	3.623717	-2.68592
H	-4.90089	2.573693	-4.04525	C	0.611638	7.191474	-0.12233
C	3.587691	2.577072	1.988687	H	1.641031	7.007857	-0.45708
H	2.885837	2.152401	1.272586	H	0.528118	8.264601	0.07249
C	3.679309	-2.77161	-4.87864	H	-0.0718	6.947177	-0.94603
H	3.79693	-2.77504	-5.95754	C	8.988682	3.475623	-0.63429
C	-3.74469	-2.9524	1.214215	H	9.193897	4.392434	-1.17643
H	-3.02046	-2.30084	0.728129	C	1.353561	6.690414	2.238279

C	4.99652	-1.68103	2.642539	H	1.112024	6.197008	3.188174
C	-4.77213	-1.38236	-1.69468	H	1.418874	7.766977	2.423437
H	-3.71071	-1.32228	-1.43171	H	2.340802	6.341667	1.905153
H	-4.94027	-2.31784	-2.23844	C	0.916958	-7.18479	-0.19375
C	-7.11647	2.080282	-1.87849	H	1.22307	-7.14495	0.859674
C	0.843598	0.337068	3.324249	H	1.732635	-6.787	-0.8095
H	1.589652	0.944859	2.821512	H	0.791332	-8.24181	-0.44673
C	-4.88766	2.153049	2.354818	C	0.014696	-0.67226	-6.71082
H	-3.97328	2.701035	2.54265	H	0.793224	-1.39485	-6.42783
C	4.336561	-1.93544	-2.69188	H	0.060146	-0.54582	-7.79699
C	5.86825	2.929194	2.769208	H	-0.96073	-1.10277	-6.4591
H	6.941804	2.798201	2.650728	C	1.615304	1.26096	-6.40848
C	-1.05386	-1.23892	4.524732	H	1.807112	2.225632	-5.9256
H	-1.83015	-1.87266	4.943874	H	1.659671	1.409506	-7.49187
C	5.379773	3.679132	3.848239	H	2.42629	0.568892	-6.13849
H	6.073997	4.110658	4.561292	C	-1.40467	-1.19025	7.473639
C	3.107095	3.33813	3.062285	H	-1.70713	-2.20155	7.170746
H	2.036889	3.513943	3.164986	H	-2.20373	-0.48847	7.204517
C	8.45208	1.121654	0.792681	H	-1.32148	-1.19763	8.564301
H	8.269274	0.209161	1.349507	C	1.006031	-1.87589	7.166818
C	3.428762	-2.8129	-2.07943	H	1.089714	-2.01538	8.248827
H	3.334485	-2.82979	-0.99367	H	1.995082	-1.59571	6.782706
C	-4.38389	0.101739	3.89777	H	0.718942	-2.83833	6.722794
H	-4.48494	-0.97713	3.719127				

Table S15. Optimized Cartesian Coordinates of 3^{4+} .

Ru	-0.00997	0.008694	0.756074	C	4.748078	0.306005	3.8493
Fe	5.134076	-0.53573	0.646437	H	5.058472	-0.02428	4.848818
Fe	-5.16074	0.503752	0.693885	H	3.671891	0.111023	3.761111
P	-5.37107	-1.43575	-0.55877	H	4.920702	1.385682	3.793876
P	-5.17832	1.558112	-1.39335	C	1.098173	2.270204	4.357736
P	5.132193	-1.59474	-1.43753	H	1.74686	2.056935	5.201742
P	5.346455	1.399505	-0.61387	C	-9.51416	-3.00301	-2.04471
N	3.207292	-0.33368	0.678511	H	-10.4763	-3.37798	-2.37654
N	-0.16814	-1.47524	2.263624	C	1.381044	5.684274	4.827258
N	0.168031	1.497854	2.260006	H	1.383973	6.519829	5.533653
N	-3.23211	0.317952	0.715294	H	1.056384	6.065521	3.850558
N	0.16453	1.502683	-0.73902	H	2.414954	5.320738	4.740775
C	-2.04032	0.220755	0.74589	C	-4.75219	-0.32899	3.894477
N	-0.20201	-1.48849	-0.73265	H	-4.92553	-1.40895	3.84735
C	6.631238	0.063743	2.061072	H	-5.05208	0.007107	4.895256
H	7.063328	1.050264	2.171788	H	-3.67688	-0.13503	3.79371
C	-3.96128	2.960948	-1.57017	C	-7.03659	3.668191	-1.71798
C	2.017754	-0.21549	0.721322	H	-6.30406	4.285178	-1.20001
C	-5.5361	0.403082	2.860284	C	-8.59733	-2.49865	-2.97716

C	-4.67207	0.274422	-2.71082	H	-8.84491	-2.49388	-4.0336
H	-5.49803	0.199229	-3.42689	C	0.943177	4.068508	6.713643
H	-3.81415	0.692057	-3.25058	H	1.995767	3.757017	6.675507
C	3.909918	-2.99448	-1.59966	H	0.344149	3.232907	7.093266
C	-6.64775	-0.10054	2.117393	H	0.880446	4.881768	7.442563
H	-7.07394	-1.08909	2.232565	C	0.351267	-2.42866	-2.88564
C	-8.46281	0.926983	0.524825	H	0.969788	-2.38197	-3.77884
H	-8.57674	1.81496	-0.10328	C	0.548869	-1.49812	-1.87005
H	-9.30143	0.915854	1.232165	H	1.308868	-0.72674	-1.9513
H	-8.56189	0.037213	-0.10925	C	-9.19255	3.472829	-2.8237
C	4.617956	-0.31257	-2.75333	H	-10.1277	3.920508	-3.14213
H	5.437631	-0.24113	-3.47696	C	-3.05276	4.754425	-2.93762
H	3.753807	-0.72873	-3.28424	H	-3.02329	5.294783	-3.87853
C	8.431811	-0.97715	0.461156	C	-0.59549	1.509668	-1.87027
H	8.534299	-0.08627	-0.17074	H	-1.35745	0.739562	-1.94374
H	8.534986	-1.8641	-0.17026	C	-3.4174	-4.07853	1.987572
H	9.274451	-0.97505	1.163794	H	-2.87401	-4.02385	2.928638
C	7.151309	-0.99434	1.224702	C	-0.63376	-3.43007	-2.75999
C	-1.13601	-2.46533	-0.59151	C	-0.36335	-3.45523	4.293848
H	-1.71288	-2.4545	0.327003	C	7.301048	1.976963	-2.63068
C	6.710387	-2.35846	-2.06759	H	6.584433	1.624528	-3.37033
C	0.528768	-2.64257	2.18053	C	-0.966	-1.29885	3.35104
H	1.145016	-2.76302	1.294515	H	-1.49982	-0.35413	3.397676
C	-6.76288	2.317936	-2.01273	C	0.365697	3.471109	4.299075
C	7.918402	2.513041	-0.34136	C	-7.71304	1.549601	-2.70595
H	7.670647	2.583717	0.71633	H	-7.54167	0.497099	-2.91994
C	-7.02001	-2.02988	-1.18434	C	-8.92102	2.128816	-3.11616
C	-7.17818	0.952569	1.28133	H	-9.64737	1.532689	-3.65853
C	-3.93301	-2.90691	1.414233	C	0.581117	3.438539	-2.77499
H	-3.7664	-1.9445	1.895397	C	-0.88779	-4.39458	-3.89614
C	-4.6516	-2.97482	0.210391	H	0.091871	-4.69603	-4.29891
C	-7.35151	-2.01526	-2.55029	C	6.29228	-2.14167	1.447877
H	-6.64668	-1.65778	-3.2988	H	6.428581	-3.11725	0.995545
C	-1.37048	-3.43699	-1.56319	C	-2.35124	4.512915	-0.62396
H	-2.13263	-4.18628	-1.37035	H	-1.76745	4.86867	0.222182
C	1.327659	3.448209	-1.58432	C	4.325485	5.35046	0.124726
H	2.091743	4.197435	-1.39917	H	4.502431	6.31296	-0.34435
C	-8.24851	4.240641	-2.12382	C	8.542276	2.457595	-3.07354
H	-8.45252	5.283146	-1.90381	H	8.774557	2.456137	-4.13345
C	-5.32672	1.77793	2.467594	C	-9.17542	-3.04504	-0.68288
C	3.139808	-3.41836	-0.50724	H	-9.87204	-3.46057	0.037321
H	3.209535	-2.8809	0.436686	C	2.296792	-4.53231	-0.63573
C	6.989495	1.987274	-1.25993	H	1.714786	-4.87925	0.215324
C	-4.28398	2.684102	3.028352	C	-3.6179	-5.31698	1.360289

H	-3.30144	2.193936	3.068004	H	-3.23767	-6.2265	1.813895
H	-4.5479	2.971586	4.053936	C	-0.40494	2.436977	-2.89027
H	-4.19662	3.607152	2.444851	H	-1.02978	2.387672	-3.77887
C	-3.18831	3.395808	-0.48413	C	0.977505	1.324156	3.339149
H	-3.2511	2.86462	0.463717	H	1.516248	0.38198	3.37914
C	4.637228	2.939095	0.162968	C	3.603385	5.274536	1.326954
C	-3.88981	3.64013	-2.80186	H	3.222929	6.18092	1.787578
H	-4.51482	3.332556	-3.63878	C	3.400557	4.031803	1.944495
C	5.302151	-1.80679	2.423361	H	2.851996	3.969627	2.882521
C	2.22402	-5.22256	-1.85303	C	-1.64393	-4.47281	6.254384
H	1.597138	-6.1047	-1.94254	H	-1.67826	-3.56869	6.876395
C	4.846007	4.186041	-0.45652	H	-1.64215	-5.32682	6.937938
H	5.43424	4.257151	-1.37001	H	-2.56522	-4.5241	5.660321
C	-0.53732	2.661077	2.187999	C	9.132397	-3.51763	-2.89486
H	-1.16771	2.777635	1.311416	H	10.06456	-3.96701	-3.21966
C	3.917631	2.864477	1.365473	C	8.191834	-4.28371	-2.18846
H	3.749727	1.899546	1.840435	H	8.395538	-5.32654	-1.96971
C	5.521234	-0.4322	2.811444	C	-1.08629	-2.24904	4.364935
C	-4.32454	-1.08464	-2.09298	H	-1.73971	-2.04268	5.207061
H	-3.28614	-1.10559	-1.73642	C	-0.38449	-4.50277	5.383062
H	-4.44069	-1.90413	-2.81489	H	-0.31138	-5.48752	4.898393
C	6.983693	-3.7091	-1.77439	C	8.86131	-2.17312	-3.1856
H	6.253688	-4.32463	-1.2512	H	9.585015	-1.57833	-3.73296
C	-0.46007	3.645503	3.169083	C	2.986396	-4.79229	-2.95102
H	-1.05393	4.551151	3.065397	H	2.949982	-5.33863	-3.88822
C	3.829031	-3.68084	-2.82669	C	9.474353	2.954806	-2.15239
H	4.45077	-3.38108	-3.66885	H	10.43288	3.327766	-2.49665
C	-4.85876	-4.21797	-0.41723	C	0.826571	4.400053	-3.91541
H	-5.44691	-4.2838	-1.3312	H	-0.15556	4.689936	-4.32052
C	0.454858	-3.62971	3.158924	C	-1.64803	-3.65092	-5.01724
H	1.036986	-4.54158	3.044195	H	-2.63061	-3.32211	-4.64968
C	-7.93333	-2.5636	-0.25475	H	-1.81277	-4.31802	-5.86903
H	-7.66984	-2.63875	0.798823	H	-1.09997	-2.77126	-5.37426
C	4.257967	-2.70581	2.993588	C	9.155931	2.991804	-0.78553
H	3.278266	-2.2102	3.039288	H	9.864751	3.401246	-0.07381
H	4.527636	-2.99198	4.018215	C	-1.66173	-5.6496	-3.48285
H	4.161061	-3.62992	2.413191	H	-1.19003	-6.1736	-2.64229
C	-4.33734	-5.38549	0.156226	H	-1.72087	-6.34706	-4.32369
H	-4.51206	-6.34502	-0.31967	H	-2.69465	-5.40026	-3.19859
C	-6.32418	2.105069	1.497118	C	1.587884	5.664588	-3.50729
H	-6.46845	3.078874	1.043466	H	1.110432	6.187307	-2.66925
C	1.100317	2.479202	-0.60838	H	1.640276	6.35895	-4.35114
H	1.684684	2.469811	0.305211	H	2.623125	5.42736	-3.22139
C	4.280376	1.048473	-2.1345	C	0.874599	-4.31728	6.261945

H	3.24687	1.071642	-1.76412	H	1.798476	-4.38802	5.674281
H	4.388773	1.866312	-2.85935	H	0.906106	-5.08787	7.038094
C	7.65718	-1.59175	-2.76729	H	0.850962	-3.33808	6.757973
H	7.486089	-0.53889	-2.98002	C	1.595317	3.657872	-5.03165
C	-2.28702	5.195185	-1.84618	H	2.580577	3.340759	-4.66089
H	-1.6643	6.079329	-1.94452	H	1.754658	4.321915	-5.88686
C	0.457246	4.558643	5.346487	H	1.056058	2.770992	-5.38429
H	-0.54991	4.985232	5.46222				

Table S16. Optimized Cartesian Coordinates of 4⁴⁺.

Ru	0.031106	-0.31116	0.253305	H	-4.42392	2.180599	-2.11213
Fe	4.978613	-0.20585	-1.30988	C	-3.48235	2.941838	1.578221
Fe	-5.06436	-0.3692	1.159784	H	-3.38515	1.987951	2.095771
P	5.391191	1.90397	-0.35987	C	-7.22367	2.403257	0.026102
P	5.792255	-0.96425	0.744405	C	-1.6033	3.798912	-4.46531
P	-5.51281	1.65851	0.03897	H	-1.22064	3.412972	-5.41973
P	-5.36758	-1.27899	-0.97683	C	6.856682	3.851161	-1.80416
N	-0.12499	-1.94406	-1.11338	H	5.919963	4.055654	-2.31999
N	3.169902	-0.2297	-0.60058	C	8.007253	4.562968	-2.16616
N	0.253423	1.277108	1.647861	H	7.958236	5.297336	-2.96316
N	-0.3855	1.082992	-1.28966	C	9.272148	3.40324	-0.44852
N	0.338786	-1.68074	1.855436	H	10.20153	3.237473	0.086724
N	-3.14851	-0.33254	0.827301	C	9.934716	-0.55112	0.690405
C	5.068607	-2.00856	-2.47891	H	10.70666	-0.31182	-0.03427
C	1.385762	3.274773	2.400122	C	-4.5085	0.007856	-2.06091
H	2.101358	4.060217	2.170319	H	-3.45646	-0.0008	-1.75202
C	4.020346	3.130274	-0.67972	H	-4.55918	-0.28278	-3.11786
C	-1.58752	3.042968	-2.03295	C	3.061018	5.333085	-0.28522
H	-2.22285	3.879631	-1.75221	H	3.093703	6.294261	0.217703
C	6.412367	-1.54804	-2.27488	C	-6.9405	-0.60425	2.204069
H	7.198972	-2.12281	-1.7978	C	-2.67219	4.027818	1.94197
C	0.769035	-2.97406	-1.06121	H	-1.96719	3.92309	2.763166
H	1.505404	-2.93482	-0.26399	C	1.337401	3.656496	6.065527
C	1.132494	2.294776	1.438323	H	0.483248	3.102808	6.476256
H	1.643295	2.310016	0.479041	H	1.590528	4.439601	6.786799
C	1.373452	-2.28072	3.960638	H	2.190277	2.972487	5.995052
H	2.091121	-2.02002	4.731405	C	7.842765	0.499163	-3.07886
C	-1.06144	-1.98769	-2.09785	H	8.713471	-0.0926	-2.78232
H	-1.78068	-1.17575	-2.11215	H	7.876378	1.459233	-2.5487
C	6.16491	-3.73139	1.247681	H	7.957725	0.722617	-4.14681
H	7.227075	-3.53907	1.112501	C	-3.7065	5.386462	0.21315
C	2.031416	-0.2462	-0.23507	H	-3.81212	6.336956	-0.29998
C	4.370221	-0.9719	-3.20174	C	-7.04547	-1.50275	-1.75813
C	0.761685	-4.02043	-1.97664	C	-4.53705	-2.92391	-1.2816
H	1.493921	-4.81852	-1.87304	C	9.278497	-1.13492	2.956012

C	-0.41299	1.261064	2.838223	H	9.545751	-1.35115	3.984835
H	-1.11986	0.449725	2.97738	C	-2.78165	5.248351	1.261656
C	1.219841	-1.43463	2.863118	H	-2.16947	6.094409	1.557969
H	1.802744	-0.52253	2.778084	C	-3.57657	-3.40697	-0.3771
C	5.72665	-5.03901	1.500581	H	-3.29038	-2.79673	0.476127
H	6.448259	-5.84719	1.554549	C	-7.36715	-0.92952	-3.00245
C	-0.30288	-3.70357	3.01371	H	-6.65317	-0.31297	-3.54345
H	-0.92819	-4.59378	3.033167	C	-8.22225	1.830134	-0.78337
C	-1.18449	2.157177	-1.03757	H	-8.01174	0.968256	-1.41432
H	-1.50503	2.293418	-0.00999	C	-7.54047	3.498188	0.85256
C	-4.40644	3.077141	0.532151	H	-6.78138	3.965174	1.476491
C	-0.33129	1.75405	-3.61158	C	10.27938	-0.82198	2.021015
H	0.029867	1.553516	-4.61672	H	11.319	-0.79631	2.32957
C	-1.17744	2.851581	-3.36748	C	-6.29192	-1.88759	2.083152
C	3.027861	2.87094	-1.63608	H	-6.70534	-2.76704	1.605704
H	3.009391	1.914753	-2.15704	C	-3.13663	3.889608	-4.55925
C	5.233057	-2.67926	1.184061	H	-3.56209	4.331192	-3.6462
C	-1.96876	-0.35313	0.631102	H	-3.59219	2.904479	-4.71866
C	0.602026	-3.45317	4.065731	H	-3.42395	4.533604	-5.39609
C	5.283963	0.127069	-3.41518	C	-9.8357	3.443199	0.050179
C	0.734673	3.24393	3.646171	H	-10.8419	3.848308	0.056653
C	-0.19553	2.202245	3.840215	C	-9.52099	2.352843	-0.77436
H	-0.74475	2.115184	4.773899	H	-10.2832	1.909601	-1.4071
C	-0.41094	-2.81559	1.946782	C	-0.23033	5.217568	4.84307
H	-1.10313	-2.9924	1.129118	H	-0.47594	5.710495	3.89392
C	-1.10713	-2.99507	-3.06303	H	-0.02856	5.996749	5.584481
H	-1.87843	-2.95678	-3.82547	H	-1.11068	4.656624	5.186465
C	3.433609	-4.24948	1.630832	C	-0.09901	-5.13916	-4.0756
H	2.374757	-4.4484	1.792955	H	0.010523	-6.09539	-3.54119
C	4.039576	4.368987	-0.00916	C	1.720329	-5.56128	4.749082
H	4.837646	4.60108	0.694512	H	1.367783	-6.07185	3.843508
C	0.046735	0.90918	-2.56646	H	1.819922	-6.30862	5.542242
H	0.693252	0.056108	-2.73973	H	2.716843	-5.14231	4.550535
C	4.51883	-3.34518	-2.11494	C	-5.05067	-1.85673	2.783778
H	5.117846	-3.83386	-1.339	C	-4.88709	-0.52718	3.320956
H	4.514107	-4.00355	-2.99392	C	1.174861	-4.92761	-4.9261
H	3.487166	-3.26683	-1.75035	H	1.275342	-5.7339	-5.65905
C	-4.51833	4.304367	-0.15096	H	2.084475	-4.91317	-4.31228
H	-5.25574	4.428803	-0.94289	H	1.107699	-3.97867	-5.4754
C	2.978605	-1.08583	-3.72319	C	-6.05367	0.243713	2.989301
H	2.56949	-0.10603	-3.99705	C	-8.62576	-1.15428	-3.57823
H	2.312193	-1.5648	-2.99193	H	-8.86524	-0.71162	-4.53938
H	2.971227	-1.70757	-4.62803	C	-3.00531	-4.67167	-0.56725
C	0.993499	4.289138	4.706325	H	-2.28459	-5.05919	0.149959

H	1.847862	4.89756	4.379549	C	-8.84348	4.014131	0.86111
C	2.053863	3.839943	-1.91365	H	-9.08084	4.863601	1.492836
H	1.295242	3.638433	-2.66565	C	-4.11856	-2.99931	2.996463
C	0.751475	-4.4431	5.197833	H	-4.20805	-3.35957	4.029552
H	-0.23287	-4.90172	5.370569	H	-3.0719	-2.70371	2.846016
C	7.58863	-0.90303	1.221882	H	-4.35117	-3.83913	2.334312
C	3.865527	-2.94299	1.369178	C	-0.99792	5.197321	-4.23165
H	3.137575	-2.13657	1.304723	H	-1.30214	5.87747	-5.03331
C	8.590426	-0.58986	0.292031	H	0.098453	5.170894	-4.21434
H	8.329576	-0.35583	-0.73571	H	-1.35152	5.623163	-3.28223
C	8.124732	2.686069	-0.08379	C	-7.9849	-2.33263	-1.11931
H	8.199054	1.962017	0.725178	H	-7.7363	-2.83166	-0.18525
C	4.361887	-5.30032	1.692976	C	-3.74801	-0.08587	4.175824
H	4.02806	-6.31278	1.897868	H	-3.96324	-0.30503	5.229774
C	5.045308	1.35922	-4.22397	H	-3.57166	0.994093	4.101938
H	5.335832	1.187126	-5.26868	H	-2.82456	-0.6183	3.912929
H	5.645956	2.199907	-3.85714	C	-9.56844	-1.95811	-2.92152
H	3.993157	1.665106	-4.22519	H	-10.5409	-2.13231	-3.36927
C	4.995637	0.260662	1.940662	C	-1.32259	-5.22133	-4.99074
H	3.909974	0.141769	1.864003	H	-1.40319	-4.32892	-5.62603
H	5.31171	0.031048	2.964482	H	-2.25658	-5.33319	-4.42607
C	6.911479	2.905671	-0.76035	H	-1.22963	-6.08251	-5.65903
C	6.568353	-0.25026	-2.8667	C	-8.34375	-0.28956	1.811573
C	-0.17383	-4.04586	-3.03264	H	-8.61553	-0.73777	0.848916
C	2.064139	5.067675	-1.23851	H	-8.52716	0.787445	1.744692
H	1.316694	5.820878	-1.46958	H	-9.0317	-0.6927	2.566069
C	9.21776	4.337737	-1.49271	C	-6.37438	1.598919	3.525182
H	10.10604	4.894415	-1.77122	H	-6.70165	1.512284	4.569248
C	5.428159	1.67323	1.534047	H	-7.18913	2.073879	2.971279
H	6.448497	1.879094	1.87712	H	-5.50882	2.27234	3.510707
H	4.769381	2.427934	1.977527	C	-3.38088	-5.4536	-1.66901
C	7.936977	-1.17946	2.560232	H	-2.95567	-6.44329	-1.80722
H	7.175231	-1.45034	3.289723	C	-4.91525	-3.7084	-2.3866
C	1.241102	-3.81758	6.508287	C	-9.24173	-2.55647	-1.69493
H	2.285702	-3.48891	6.428393	H	-9.95802	-3.20122	-1.19691
H	1.204316	-4.5615	7.309525	C	-4.3312	-4.96787	-2.58017
H	0.627633	-2.96294	6.815768	H	-4.64185	-5.58048	-3.42074
C	-5.11961	1.388126	-1.81064	H	-5.68195	-3.36119	-3.07623
H	-6.05368	1.531454	-2.36534				

Table S17. Optimized Cartesian Coordinates of 5^{4+} .

Ru	-0.03053	-0.03707	0.239475	Fe	5.099241	0.01231	1.00317
Fe	-4.9929	0.002978	-1.19676	P	5.392401	1.652776	-0.65929
P	-5.50947	-1.64055	0.384905	P	5.659812	-1.44475	-0.76611
P	-5.97622	1.461051	0.419117	N	0.140729	-1.76404	-1.02083

N	-0.2525	1.613664	1.599163	N	3.196896	-0.02216	0.578644
N	-3.20495	-0.00519	-0.41606	N	0.129612	1.383487	-1.37332
N	-0.15032	-1.40555	1.868141	C	6.359686	1.180602	2.454463
C	-5.89431	-1.09424	-2.94424	C	2.006095	-0.02529	0.461057
C	-2.04984	-0.03488	-0.10709	C	-0.23713	3.606981	-2.25135
C	0.619252	-3.42048	2.957383	H	-0.65667	4.598455	-2.09893
H	1.257333	-4.30093	2.922861	C	0.469818	3.323679	-3.43249
C	-0.19963	-3.19634	4.080503	C	-0.88515	-2.66009	-1.0527
C	0.817919	2.363738	1.9836	H	-1.76426	-2.41635	-0.46588
H	1.783906	2.06811	1.591141	C	0.295796	-4.16629	-2.54882
C	-0.54386	3.875741	3.315943	C	0.776212	1.088332	-2.53492
C	-0.94752	-1.18275	2.946612	H	1.14291	0.076037	-2.64209
H	-1.55466	-0.28606	2.924095	C	7.044816	2.152229	-1.35817
C	-7.24574	-2.27981	0.596263	C	-0.38935	2.635771	-1.2602
C	0.621264	-2.52715	1.888715	H	-0.93058	2.85878	-0.34551
H	1.247431	-2.69888	1.019004	C	1.359637	-3.24666	-2.50029
C	-1.64196	3.082616	2.939703	H	2.281331	-3.44311	-3.04262
H	-2.64357	3.327119	3.283512	C	4.512199	3.267389	-0.37023
C	-4.46984	-3.1841	0.456292	C	6.892465	-0.14741	2.280685
C	-6.48924	0.209878	-2.82457	C	4.565258	0.819219	-2.13982
C	-5.19149	-0.74805	2.0199	H	4.648528	1.476508	-3.0142
H	-5.43319	-1.42331	2.850112	H	3.505261	0.692857	-1.89425
H	-4.12531	-0.49429	2.059116	C	1.260418	-2.09231	-1.72899
C	-1.46799	1.99117	2.092999	H	2.110286	-1.42289	-1.63529
H	-2.32898	1.419865	1.761437	C	8.242276	1.641206	-0.83887
C	-8.30671	-1.67033	-0.08938	H	8.22113	0.92929	-0.01856
H	-8.10944	-0.84723	-0.77141	C	4.99416	1.062164	2.886055
C	-4.47463	-0.92193	-3.07173	C	4.695543	-0.34262	3.057205
C	-4.1891	0.50141	-3.10205	C	5.861708	-1.09427	2.664234
C	-5.42884	1.20208	-2.93233	C	4.644652	-3.015	-0.81658
C	-4.92002	2.963457	0.77508	C	3.768504	-3.34699	0.227061
C	-3.83685	3.305975	-0.04879	H	3.601534	-2.6368	1.036858
H	-3.52794	2.629649	-0.84561	C	5.260063	4.413509	-0.03525
C	-4.80465	-4.2611	-0.3879	H	6.347149	4.377915	-0.02027
H	-5.66042	-4.18633	-1.05594	C	7.385306	-2.12672	-0.99478
C	-7.67032	2.229529	0.226492	C	0.962127	2.010308	-3.56072
C	-0.99537	-2.03555	4.048278	H	1.495155	1.701415	-4.45534
H	-1.65314	-1.792	4.876739	C	-0.83654	-3.84574	-1.78106
C	0.708801	3.475274	2.816002	H	-1.69629	-4.50963	-1.7414
H	1.608407	4.035605	3.058084	C	3.108721	3.3426	-0.41947
C	-3.41151	-3.32446	1.369276	H	2.511643	2.466732	-0.67665
H	-3.14975	-2.5184	2.052167	C	7.108385	2.466937	2.367747
C	-6.629	-2.38628	-3.07789	H	6.437323	3.315914	2.198474
H	-5.94578	-3.241	-3.06058	H	7.617726	2.645119	3.324584

H	-7.14597	-2.40795	-4.0462	H	7.877859	2.470022	1.590028
H	-7.39414	-2.53113	-2.30686	C	5.255437	-0.52655	-2.39355
C	-6.06185	0.507852	2.0643	H	4.626794	-1.18857	-3.00104
H	-5.74804	1.182162	2.868573	H	6.195572	-0.37785	-2.93677
H	-7.10874	0.240001	2.245665	C	8.321512	-0.50538	2.028706
C	-7.949	0.521428	-2.86992	H	8.952708	0.383452	1.934046
H	-8.56393	-0.38331	-2.84065	H	8.708612	-1.08275	2.877996
H	-8.17816	1.035416	-3.81296	H	8.458543	-1.13033	1.135849
H	-8.27189	1.191958	-2.06221	C	3.210375	5.692669	0.209536
C	-3.02476	-5.5957	0.588194	H	2.708865	6.6306	0.426001
H	-2.48324	-6.53419	0.654273	C	6.088876	-2.5593	2.838755
C	-5.65999	2.667872	-3.09572	H	6.883661	-2.92068	2.178024
H	-6.61867	2.971776	-2.66378	H	6.40972	-2.7641	3.86869
H	-5.69553	2.917353	-4.16439	H	5.189895	-3.15698	2.653272
H	-4.8705	3.279445	-2.64503	C	4.610531	5.620432	0.253412
C	-4.0844	-5.46062	-0.32362	H	5.195323	6.50013	0.500646
H	-4.36856	-6.29513	-0.95671	C	7.72712	-3.33989	-0.36205
C	-7.7879	3.501904	-0.36848	H	6.97817	-3.91198	0.182621
H	-6.90194	4.068901	-0.6481	C	2.465073	4.555119	-0.13167
C	-2.69365	-4.52834	1.434289	H	1.379425	4.609809	-0.17282
H	-1.89085	-4.63376	2.160395	C	3.125449	-4.59402	0.23167
C	-3.16468	4.521471	0.150943	H	2.470197	-4.8678	1.054785
H	-2.35111	4.806643	-0.51185	C	0.713556	4.368556	-4.49416
C	-0.16046	-4.12961	5.267	H	0.196084	5.289487	-4.19283
H	0.148392	-5.12085	4.904839	C	3.436106	-0.90356	3.628146
C	-2.85822	1.114634	-3.37624	H	3.322131	-1.96803	3.390273
H	-2.82919	2.170414	-3.08041	H	3.451244	-0.81438	4.722103
H	-2.6401	1.070742	-4.45133	H	2.544693	-0.37744	3.262471
H	-2.0504	0.590655	-2.84917	C	8.357664	-1.44124	-1.74314
C	-8.8314	1.545444	0.630809	H	8.127447	-0.50955	-2.25444
H	-8.77874	0.569013	1.106356	C	4.100322	2.207809	3.222997
C	-3.47887	-2.01565	-3.25184	H	3.095981	1.862514	3.489152
H	-2.45831	-1.66334	-3.06458	H	4.497964	2.762068	4.082884
H	-3.51523	-2.40563	-4.27771	H	4.017659	2.919177	2.387065
H	-3.67533	-2.85593	-2.57173	C	4.212583	-5.17044	-1.86165
C	-4.62626	5.035434	2.020637	H	4.404911	-5.88224	-2.6581
H	-4.94691	5.709782	2.807982	C	4.860214	-3.92848	-1.86702
C	-5.3083	3.828946	1.816967	H	5.566979	-3.69615	-2.66201
H	-6.17136	3.593447	2.437359	C	7.078374	3.044208	-2.44967
C	-7.50215	-3.33872	1.488217	H	6.157464	3.463615	-2.85305
H	-6.6875	-3.82577	2.021456	C	9.471778	2.021995	-1.39622
C	-9.62182	-2.11491	0.106388	H	10.3961	1.62559	-0.9869
H	-10.4392	-1.6417	-0.43072	C	0.352786	-5.39856	-3.41829
C	-0.69597	5.084292	4.207744	H	1.409153	-5.60667	-3.64252

H	-1.77091	5.262682	4.354859	C	3.350916	-5.50815	-0.80569
C	-3.56076	5.389181	1.177381	H	2.878984	-6.48555	-0.78435
H	-3.06093	6.343525	1.310428	C	9.504836	2.910561	-2.47885
C	-9.87701	-3.17111	0.992088	H	10.45512	3.209829	-2.90802
H	-10.8926	-3.52159	1.142271	C	8.30611	3.417698	-3.00792
C	-8.81689	-3.77925	1.683836	H	8.33181	4.106049	-3.84595
H	-9.01602	-4.59557	2.369951	C	9.65893	-1.95306	-1.84586
C	-10.0937	2.120888	0.43192	H	10.39807	-1.4219	-2.437
H	-10.9823	1.592071	0.76112	C	9.999973	-3.14982	-1.20109
C	-10.2082	3.378825	-0.17637	H	11.00626	-3.5459	-1.2845
H	-11.1858	3.82374	-0.32715	C	-0.36922	-5.09671	-4.74999
C	-0.05672	4.816286	5.58501	H	0.081705	-4.24646	-5.27452
H	-0.50048	3.94498	6.078485	H	-0.32556	-5.9684	-5.41042
H	-0.19428	5.683954	6.237718	H	-1.42798	-4.86675	-4.5632
H	1.023126	4.643289	5.484653	C	-0.26365	-6.63409	-2.74683
C	-0.07619	6.336823	3.563186	H	-1.35263	-6.53018	-2.644
H	1.015723	6.245506	3.490721	H	-0.08488	-7.52228	-3.36052
H	-0.28639	7.217964	4.177278	H	0.159482	-6.81522	-1.75108
H	-0.47388	6.517716	2.556488	C	9.028424	-3.84554	-0.46489
C	-9.05207	4.070056	-0.56936	H	9.280927	-4.78441	0.01659
H	-9.1344	5.054131	-1.01863	C	0.16207	3.925831	-5.86111
C	0.921073	-3.6243	6.248412	H	-0.90874	3.696459	-5.81387
H	1.909021	-3.57476	5.773184	H	0.304172	4.723273	-6.59694
H	0.990091	-4.29502	7.110292	H	0.68913	3.038858	-6.2357
H	0.662269	-2.62308	6.618393	C	2.222529	4.673093	-4.59042
C	-1.51042	-4.26676	5.981746	H	2.777209	3.786295	-4.92727
H	-1.78616	-3.33903	6.499706	H	2.397851	5.469033	-5.32086
H	-1.44911	-5.04882	6.744275	H	2.633866	4.994898	-3.62565
H	-2.31818	-4.53423	5.289064				