Supporting Information

A T-shaped Cyanidometal-bridged Tetranuclear Fe_3Ru Complex With Oxidation-driven Intramolecular Charge Transfer Between Metal Centres

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Table S1. Crystallographic data of **1**$^{+}$.

	1^{+}
Empirical formula	$C_{109}H_{105}Cl_3F_{12}Fe_3N_7P_8Ru$
Color and Habit	Brown block
Crystal Size (mm)	0.1 × 0.1 × 0.1
Temperature(K)	100.0(10)
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	17.5721(3)
b (Å)	17.3121(2)
c (Å)	35.2530(5)
alpha (deg.)	90
beta (deg.)	100.2150(10)
gamma (deg.)	90
Volume (Å^3)	10554.3(3)
Z	4
Formula weight	2189.41
Density(cal.) (g/cm^3)	1.488
μ (mm^{-1})	6.834
F (000)	4836.0
Theta range (deg.)	5.094 to 134.152
Reflections collected / unique	74182 / 18785 [R(int) = 0.0487]
Index range	-20<=h<=20, -16<=k<=20, -40<=l<=42
Data/restraints/parameters (obs.)	18785/72/1461
Final R indices (obs.)	R_1 = 0.0540, wR_2 = 0.1414
R indices (all)	R_1 = 0.0640, wR_2 = 0.1477
Goodness-of-fit	1.012

$R_1 = \Sigma(||F_0| - |F_c||)/\Sigma|F_0|$;

$wR_2 = [\Sigma w(|F_0^2| - |F_c^2|)^2/\Sigma w|F_0^2|^2]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (deg.) for $\mathbf{1}^{+}$.

	$\mathbf{1}^{+}$**-100 K**	$\mathbf{1}^{+}$**-average**	
Ru(1)-Cl(1)	2.3513(10)		
Ru(1)-N(1)	2.008(4)		
Ru(1)-N(2)	2.012(3)	2.013(5)	
Ru(1)-N(3)	2.018(4)		
Ru(1)-N(4)	2.066(4)	2.070(4)	
Ru(1)-N(6)	2.074(3)		
Fe(1)-C(1)	1.847(4)		
Fe(2)-C(2)	1.846(4)	1.846(5)	
Fe(3)-C(3)	1.846(5)		
Fe(1)-P(1)	2.1875(12)	2.1875(12)	
Fe(1)-P(2)	2.1874(12)		
Fe(2)-P(3)	2.1935(11)	2.1879(11)	av.2.1905(25)
Fe(2)-P(4)	2.1822(11)		
Fe(3)-P(5)	2.1929(17)		
Fe(3)-P(6A)	2.062(2)	2.1960(32)	
Fe(3)-P(6B)	2.333(3)		
C(1)-N(1)	1.158(5)		
C(2)-N(2)	1.165(5)	1.157(6)	
C(3)-N(3)	1.149(5)		
N(1)-Ru(1)-N(2)	92.83(13)		
N(2)-Ru(1)-N(3)	90.44(13)		
N(1)-Ru(1)-N(3)	176.70(14)		
C(1)-N(1)-Ru(1)	163.5(3)		
C(2)-N(2)-Ru(1)	166.8(3)		
C(3)-N(3)-Ru(1)	165.1(3)		
N(1)-C(1)-Fe(1)	174.4(4)		
N(2)-C(2)-Fe(2)	173.4(3)		
N(3)-C(3)-Fe(3)	169.8(4)		

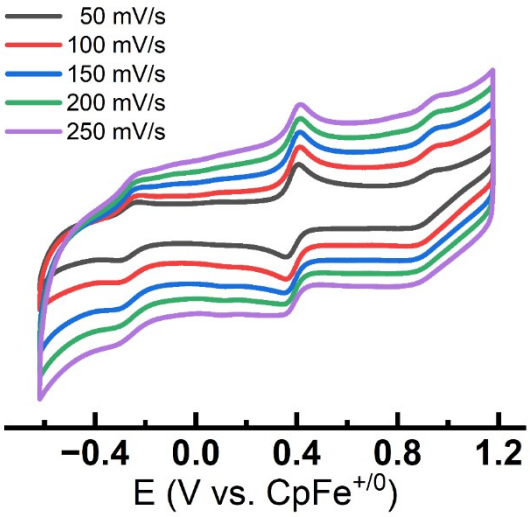

Figure S1. Cyclic voltammogram of **1**$^{+}$ recorded in a 1:1 mixture of CH_2Cl_2 and CH_3CN / 0.1 M $[TBA]PF_6$ at scan rate of 50, 100, 150, 200 and 250 mV/s.

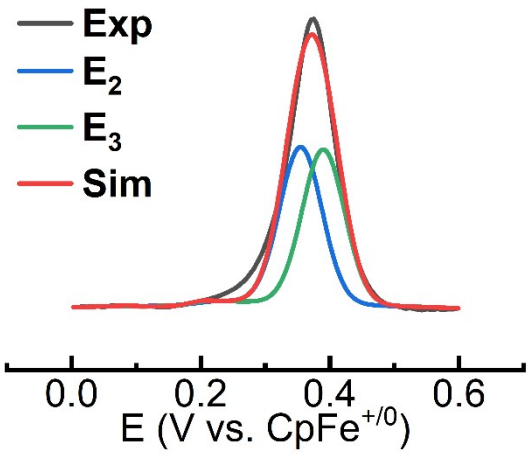

Figure S2. Peak distribution of the second redox peak of the DPV spectra.

Table S3. Redox potential according to the DPV sepctra for complexes **1**$^{+}$ in a 1:1 mixture of CH_2Cl_2 and CH_3CN / 0.1 M $[TBA]PF_6$(*vs*. Cp_2Fe).

Method	$E_{1/2}$(1)/V	$E_{1/2}$(2)/V	$E_{1/2}$(3)/V	$E_{1/2}$(4)/V
DPV	-0.27	0.35	0.39	0.91

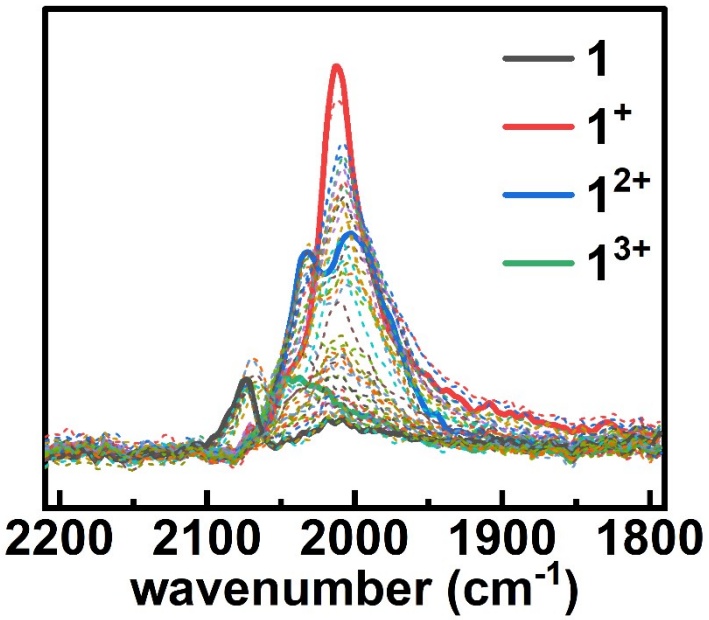

Figure S3. Liquid FTIR spectra of **1** – **1**$^{3+}$ in CH_2Cl_2.

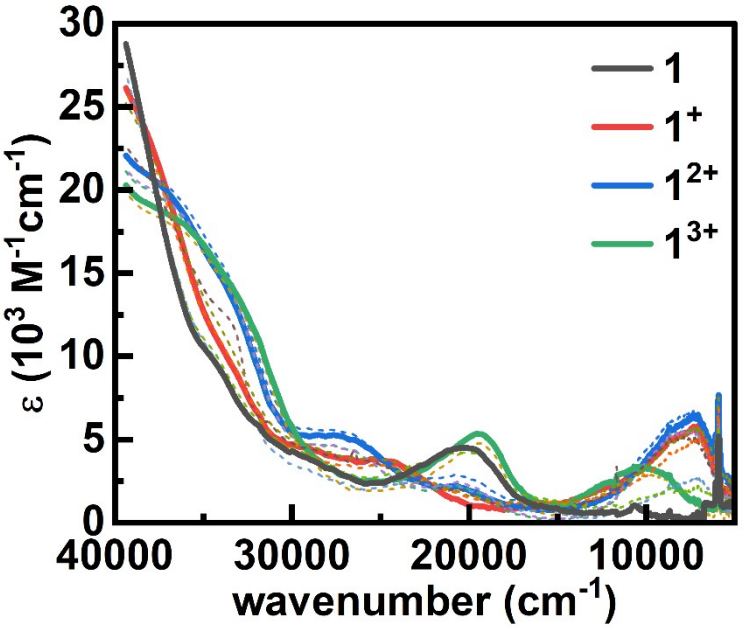

Figure S4. UV-vis-NIR spectra of **1** – **1**$^{3+}$ in CH_2Cl_2.

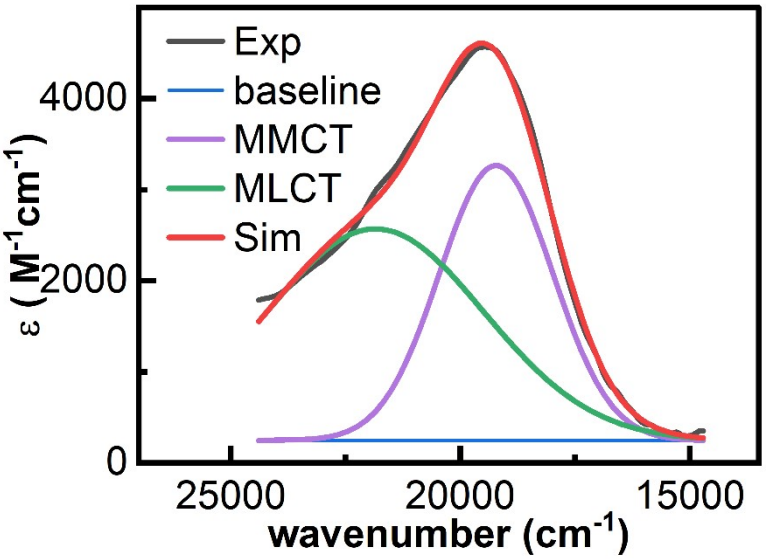

Figure S5. Gaussian peak fitting of the second absorption band in the vis-NIR region of $\mathbf{1}^{3+}$.

Table S4. Selected absorption bands of **1** – $\mathbf{1}^{3+}$ in CH_2Cl_2.

Complex	ν_{exp} (cm^{-1}) (ε ($M^{-1}\,cm^{-1}$))
1	20161 (4243)
$\mathbf{1}^{+}$	7321 (5192)
$\mathbf{1}^{2+}$	7310 (5921)
$\mathbf{1}^{3+}$	10504 (2567); 19217 (3020)

Table S5. Calculated electronic absorption of **1** – $\mathbf{1}^{3+}$ in CH_2Cl_2.

Complex	ν_{cal}	Excitation (percentage)
1	20654	HOMO-2 (208α) → LUMO (211α) (45%) HOMO-1 (209α) → LUMO (211α) (27%)
$\mathbf{1}^{+}$	7755	HOMO-1 (208β) → LUMO (210β) (89%)
$\mathbf{1}^{2+}$	5617	HOMO-1 (207β) → LUMO (209β) (44%) HOMO (208β) → LUMO (209β) (43%)
$\mathbf{1}^{3+}$	8659	HOMO-1 (206β) → LUMO (208β) (29%) HOMO (207β) → LUMO (208β) (56%)
	11911	HOMO (207β) → LUMO+1 (209β) (67%)

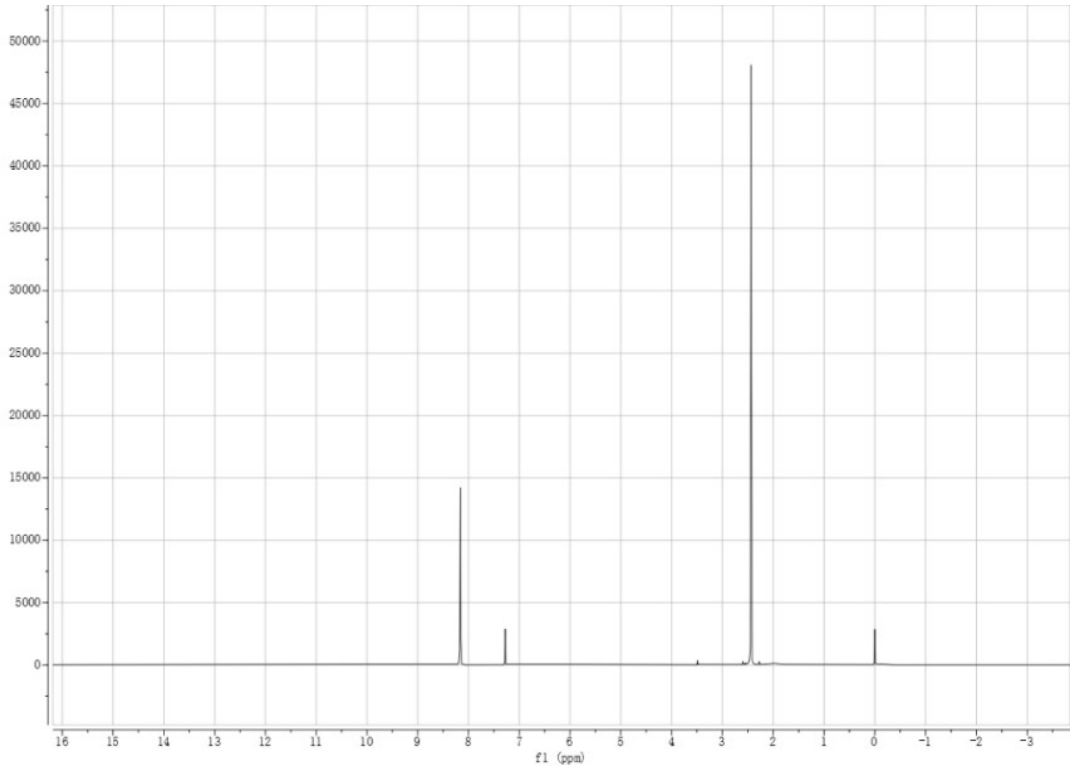

Figure S6. ^{1}H NMR of $[Ru(DMPZ)_4Cl_2]$ in $CDCl_3$.

Table S6. Optimized Cartesian Coordinates of **1**.

Ru	-0.32307	-0.30661	-0.27428	C	-1.3863	1.70133	1.672184
Fe	1.177615	4.369134	-0.73862	H	-1.83071	2.08991	0.762386
Fe	4.27127	-2.14054	0.404584	C	-0.11789	5.731874	0.211177
Fe	-5.30688	-0.69924	-0.33961	H	-0.53702	5.637076	1.202993
Cl	-0.79268	-2.56778	0.763466	C	-3.50097	-0.31214	-0.61635
P	2.071677	3.509633	1.137893	C	1.077985	-0.87505	-2.8663
P	2.996128	3.621264	-1.80503	H	1.723271	-0.09141	-2.48551
P	2.820186	-3.86657	0.523695	C	-0.2598	0.690867	3.929464
P	4.109481	-2.0014	2.632198	C	-0.82578	-2.17599	-2.57087
P	-4.62058	-2.71971	0.388	H	-1.67325	-2.43574	-1.94894
P	-4.94825	0.025706	1.753063	C	-0.716	5.267683	-1.00255
N	0.002686	-1.20722	-2.10556	H	-1.6302	4.69637	-1.07953
N	-0.62583	0.576653	1.552666	C	1.277632	6.325433	-1.54835
N	-2.32102	-0.16694	-0.64864	H	2.10455	6.732322	-2.11428
N	1.662693	-0.58875	0.141523	C	2.505577	-1.15286	-4.94044
N	-1.01257	1.815165	4.046479	H	3.126685	-2.03597	-5.12301
N	0.092027	1.535075	-0.99023	H	3.119225	-0.37432	-4.47468
N	0.502863	-2.48731	-4.54868	H	2.16549	-0.79555	-5.9178
C	-1.57594	2.317815	2.918279	C	1.124881	6.397622	-0.13087
C	0.46311	2.664728	-1.00033	H	1.793607	6.893793	0.5577
C	1.32733	-1.5147	-4.08776	C	2.733275	-1.09876	0.25463

C	-0.57457	-2.81553	-3.79473	H	-2.29988	-4.09767	-3.62637
C	0.153244	5.605819	-2.09807	C	0.344633	0.136753	5.183634
H	-0.02976	5.403538	-3.14248	H	-0.44126	-0.08681	5.912218
C	5.85121	-3.2577	-0.46501	H	1.006095	0.876876	5.64605
H	6.006858	-4.3238	-0.37834	H	0.91292	-0.77849	4.98659
C	3.802021	2.290768	-0.70808	C	-5.8334	-0.06524	-2.28537
H	3.194663	1.38076	-0.81501	H	-5.10213	0.191652	-3.03756
H	4.821558	2.081438	-1.04883	C	-6.35212	-1.37571	-2.03812
C	5.07388	-2.58986	-1.49006	H	-6.14024	-2.26217	-2.61831
H	4.557888	-3.06364	-2.31283	C	-7.2602	-1.28792	-0.91045
C	3.782545	2.754006	0.751346	H	-7.84126	-2.09892	-0.49503
H	4.532252	3.533715	0.93111	C	-4.21547	-2.63262	2.249706
H	3.979631	1.914604	1.427332	H	-5.12122	-2.91231	2.800754
C	-0.064	0.073348	2.686215	H	-3.42088	-3.34884	2.478824
H	0.517088	-0.83481	2.57616	C	-6.37862	0.834043	-1.30466
C	3.234388	-3.56015	3.294276	H	-6.19241	1.895466	-1.23975
H	4.004516	-4.33534	3.386586	C	-7.27694	0.069325	-0.47084
H	2.818185	-3.37525	4.289849	H	-7.85875	0.457548	0.354
C	5.164566	-1.18105	-1.25167	C	-3.77063	-1.20768	2.59157
H	4.663273	-0.41813	-1.8318	H	-2.77036	-1.02492	2.173518
C	5.953659	-0.96285	-0.07086	H	-3.7401	-1.04026	3.673077
H	6.23311	-0.00797	0.349854	H	-6.0147	0.150845	2.713192
C	6.391462	-2.25975	0.39726	H	-4.28162	1.279455	1.979308
H	7.019605	-2.44232	1.258395	H	-3.4051	-3.26305	-0.14597
C	2.148786	-3.97649	2.298762	H	-5.48497	-3.86494	0.308213
H	1.2808	-3.30216	2.316411	H	5.252886	-1.89663	3.496687
H	1.784359	-4.98777	2.501841	H	3.298962	-0.94658	3.186762
C	-2.40997	3.554969	3.060263	H	1.392431	2.403974	1.758013
H	-3.25137	3.368586	3.736778	H	2.345889	4.315587	2.295759
H	-2.7999	3.892041	2.093989	H	2.869745	2.933678	-3.05923
H	-1.81829	4.359962	3.509757	H	4.108211	4.479744	-2.11992
C	-1.48264	-3.88384	-4.32152	H	3.274193	-5.203	0.249574
H	-0.91748	-4.80405	-4.50041	H	1.609651	-3.81368	-0.24375
H	-1.90528	-3.57622	-5.28362				

Table S7. Optimized Cartesian Coordinates of **1**$^{+}$.

Ru	0.101245	-0.29925	0.014654	P	-3.36981	-3.65104	0.522691
Fe	-1.18153	4.518349	0.544574	P	-5.51755	-1.41898	0.483939
Fe	4.856196	-1.31445	-0.16003	N	0.532002	0.075914	-1.98934
Fe	-4.21049	-2.31719	-1.10047	N	-0.36038	-0.69724	2.013857
Cl	0.385745	-2.72209	-0.39165	N	-1.84297	-0.56706	-0.43107
P	0.709513	5.237121	1.536693	N	2.080208	-0.25012	0.379896
P	-0.20438	5.019338	-1.41493	N	-1.10528	-1.31806	4.634441
P	4.221524	-3.15504	0.968198	N	-0.17004	1.666002	0.309685
P	5.818822	-0.62635	1.750649	N	1.12529	0.596936	-4.66519

C	-1.72403	-0.32198	3.954493	C	6.321541	-0.40029	-1.38473
C	-0.51941	2.803195	0.407869	H	7.019293	0.368815	-1.08447
C	1.669259	1.347071	-3.6768	C	6.555809	-1.82405	-1.32453
C	-1.3514	-0.01161	2.636134	H	7.468998	-2.30902	-1.01306
H	-1.8358	0.778385	2.072835	C	4.405459	-2.78811	2.825017
C	-2.61261	4.304988	2.078087	H	3.541987	-2.1742	3.1147
H	-2.47972	3.806908	3.026985	H	4.38301	-3.71388	3.407456
C	-2.83974	-1.1721	-0.69865	C	-2.80833	0.427441	4.665343
C	1.37397	1.08383	-2.32991	H	-3.4894	-0.27339	5.158042
H	1.805591	1.660639	-1.5191	H	-3.37901	1.066709	3.982865
C	-0.10668	-1.9944	4.018298	H	-2.37897	1.05466	5.454205
C	-0.00923	-0.67636	-2.97555	C	-0.28671	-1.23342	-5.43634
H	-0.65824	-1.49157	-2.67749	H	0.515419	-1.63252	-6.06439
C	-3.11012	3.717101	0.860467	H	-0.91007	-0.60672	-6.08274
H	-3.34595	2.672639	0.703734	H	-0.88884	-2.06554	-5.06069
C	-2.73002	5.977353	0.4579	C	0.576506	-3.07921	4.791159
H	-2.69999	6.943553	-0.02464	H	-0.16438	-3.71059	5.28931
C	2.59047	2.454988	-4.0862	H	1.202201	-2.64572	5.579469
H	3.422681	2.054782	-4.67432	H	1.203157	-3.7038	4.146796
H	2.994314	2.992168	-3.22067	C	-4.05757	-1.85001	-3.15322
H	2.063133	3.164036	-4.73324	H	-3.49984	-1.00243	-3.52667
C	-2.40767	5.709045	1.821324	C	-3.53252	-3.16798	-2.90439
H	-2.0594	6.437246	2.540758	H	-2.5289	-3.51304	-3.10877
C	3.215501	-0.60338	0.2445	C	-4.6142	-3.97219	-2.39038
C	0.2921	-0.41448	-4.32585	H	-4.55085	-5.01787	-2.12354
C	-3.16381	4.733714	-0.14482	C	-4.28328	-3.29936	2.158624
H	-3.51536	4.604896	-1.15821	H	-5.13731	-3.98457	2.207159
C	5.391491	-2.47094	-1.86083	H	-3.63151	-3.51329	3.011863
H	5.255686	-3.53786	-1.97211	C	-5.43071	-1.82817	-2.75147
C	1.650494	5.303287	-1.09554	H	-6.1042	-0.9882	-2.83954
H	2.111563	4.308107	-1.02962	C	-5.77697	-3.1552	-2.28381
H	2.110123	5.840774	-1.93005	H	-6.75185	-3.47859	-1.94816
C	4.43227	-1.4676	-2.2222	C	-4.7546	-1.84209	2.172085
H	3.447712	-1.6496	-2.63098	H	-3.90305	-1.15939	2.301073
C	1.813253	6.06388	0.223783	H	-5.47026	-1.65898	2.97913
H	1.4726	7.100749	0.122719	H	-6.87908	-1.85144	0.626061
H	2.856147	6.082166	0.552337	H	-5.7049	-0.00032	0.575406
C	0.268042	-1.6813	2.699235	H	-1.98561	-3.45473	0.846053
H	1.037265	-2.23393	2.172892	H	-3.4245	-5.07984	0.430418
C	5.712649	-2.01972	3.043982	H	7.20479	-0.26204	1.783162
H	6.580147	-2.67137	2.887778	H	5.256538	0.492153	2.450746
H	5.775871	-1.61107	4.056276	H	1.591522	4.260873	2.108554
C	5.020565	-0.18048	-1.93625	H	0.692659	6.202769	2.595564
H	4.551907	0.781317	-2.08883	H	-0.19087	4.057914	-2.48106

H	-0.59103	6.194158	-2.14394	H	2.867409	-3.60668	0.831051
H	4.943777	-4.38541	0.812342				

Table S8. Optimized Cartesian Coordinates of $\mathbf{1}^{2+}$.

Ru	0.168427	-0.29107	0.06285	C	3.300082	-0.31256	0.505055
Fe	-1.56293	4.376654	0.380714	C	0.546598	-0.61035	-4.26962
Fe	5.10637	-0.74218	0.281351	C	-3.48457	4.248701	-0.4811
Fe	-3.98174	-2.56235	-1.11644	H	-3.72429	4.029771	-1.51143
Cl	0.636752	-2.73227	-0.21101	C	6.805043	-0.416	-1.08299
P	0.069849	5.420653	1.54165	H	7.14001	-1.06469	-1.88049
P	-0.51717	5.09491	-1.48008	C	1.145252	5.88828	-0.99283
P	4.37303	-2.57507	-0.91676	H	1.879138	5.074658	-0.92037
P	5.22151	-2.2024	2.061147	H	1.480688	6.581503	-1.76913
P	-3.21189	-3.77695	0.659558	C	5.813803	0.620543	-1.19722
P	-5.45535	-1.64479	0.343033	H	5.288856	0.897217	-2.10055
N	0.639082	0.025906	-1.95592	C	0.982708	6.59388	0.356624
N	-0.36439	-0.61715	2.066372	H	0.365888	7.494202	0.25793
N	-1.69296	-0.71725	-0.44447	H	1.948402	6.893319	0.773359
N	2.125304	-0.12715	0.476361	C	0.293795	-1.51563	2.837787
N	-1.20279	-1.14428	4.676242	H	1.129178	-2.03896	2.386867
N	-0.20154	1.66818	0.274372	C	5.051319	-3.97326	1.420703
N	1.246057	0.488165	-4.63918	H	6.039219	-4.28798	1.066692
C	-1.84915	-0.22962	3.914186	H	4.760626	-4.64257	2.235365
C	-0.66292	2.770148	0.324	C	5.701603	1.269277	0.085995
C	1.644927	1.358684	-3.68077	H	5.053927	2.099344	0.325655
C	-1.42712	0.035922	2.599197	C	6.578319	0.596307	0.99974
H	-1.92284	0.771422	1.974914	H	6.759678	0.871718	2.028791
C	-3.07748	3.999444	1.801106	C	7.266753	-0.4453	0.264148
H	-2.96062	3.570689	2.785439	H	8.029819	-1.10375	0.655767
C	-2.6768	-1.33777	-0.72661	C	4.016081	-3.98335	0.294597
C	1.341265	1.125885	-2.32889	H	2.995622	-3.80629	0.661328
H	1.64565	1.809349	-1.54386	H	4.020091	-4.93835	-0.23811
C	-0.1263	-1.77991	4.154795	C	-3.01113	0.483241	4.532693
C	0.241523	-0.84454	-2.91426	H	-3.65327	-0.22868	5.060277
H	-0.29341	-1.72982	-2.58926	H	-3.60466	1.02749	3.789826
C	-3.36425	3.293723	0.57894	H	-2.65763	1.196907	5.285003
H	-3.41865	2.218931	0.456128	C	0.114509	-1.55016	-5.35019
C	-3.31369	5.566778	0.093426	H	0.977972	-1.86818	-5.94219
H	-3.39398	6.506946	-0.43335	H	-0.56385	-1.04109	-6.04298
C	2.402639	2.570285	-4.12709	H	-0.38516	-2.4368	-4.94889
H	3.268905	2.277089	-4.72842	C	0.585242	-2.76098	5.031589
H	2.740864	3.179003	-3.28167	H	-0.13046	-3.456	5.479976
H	1.773815	3.186928	-4.77833	H	1.071719	-2.23833	5.862162
C	-3.07786	5.407921	1.48961	H	1.338913	-3.33224	4.481488
H	-2.92387	6.211009	2.197069	C	-3.65533	-2.35739	-3.18667

H	-3.02065	-1.59284	-3.61238	H	-5.5396	-1.72425	2.839148
C	-3.2389	-3.667	-2.76102	H	-6.79254	-2.1517	0.407593
H	-2.24659	-4.08638	-2.8477	H	-5.70165	-0.23753	0.287579
C	-4.40648	-4.35608	-2.26487	H	-1.85955	-3.48074	1.029889
H	-4.43449	-5.37259	-1.89808	H	-3.19341	-5.20621	0.626671
C	-4.25183	-3.36438	2.196046	H	6.353586	-2.20547	2.931622
H	-5.08028	-4.08058	2.231651	H	4.141866	-2.03924	2.983237
H	-3.65463	-3.50036	3.103175	H	1.140174	4.63048	2.078769
C	-5.05499	-2.21749	-2.90189	H	-0.22134	6.248461	2.672835
H	-5.67124	-1.36311	-3.14069	H	-0.12712	4.161072	-2.49957
C	-5.51683	-3.47061	-2.34421	H	-1.13828	6.100676	-2.29212
H	-6.53308	-3.70385	-2.05915	H	5.247062	-3.13206	-1.90166
C	-4.77193	-1.92813	2.087105	H	3.146691	-2.39367	-1.62721
H	-3.95552	-1.20507	2.219638				

Table S9. Optimized Cartesian Coordinates of $\mathbf{1}^{3+}$.

Ru	0.027656	-0.21986	-0.00037	C	-0.03671	-0.84689	-2.97297
Fe	-0.96244	4.702831	0.514363	H	-0.67154	-1.65029	-2.6216
Fe	4.875498	-1.39892	-0.16997	C	-2.93237	4.110819	1.004753
Fe	-4.57035	-2.12577	-0.78753	H	-3.29936	3.107646	0.839041
Cl	0.245003	-2.70988	-0.19383	C	-2.36992	6.34473	0.66524
P	1.07391	5.431129	1.329824	H	-2.29716	7.332122	0.230988
P	-0.15622	5.357718	-1.53125	C	2.497768	2.237886	-4.32912
P	4.002244	-3.2806	0.874007	H	3.322621	1.81475	-4.91128
P	6.022805	-1.06181	1.814228	H	2.909488	2.844183	-3.51482
P	-3.20929	-3.98434	-1.16327	H	1.947667	2.888077	-5.01748
P	-4.47849	-2.77728	1.427822	C	-1.98516	5.985317	1.992769
N	0.471274	-0.00365	-2.04384	H	-1.53366	6.647206	2.719452
N	-0.43602	-0.46157	2.036249	C	3.184625	-0.5949	0.228657
N	-1.94201	-0.5404	-0.39559	C	0.274082	-0.69663	-4.34021
N	2.050777	-0.25225	0.301337	C	-2.96317	5.179925	0.045074
N	-1.18347	-0.86703	4.700028	H	-3.42865	5.149252	-0.92987
N	-0.19565	1.746133	0.163521	C	5.342706	-2.7054	-1.9005
N	1.092323	0.298784	-4.75278	H	5.136308	-3.76074	-2.01769
C	-1.83249	0.041182	3.930993	C	1.690567	5.750077	-1.37111
C	-0.42449	2.911941	0.280534	H	2.230815	4.797781	-1.43952
C	1.603745	1.146569	-3.82733	H	2.011832	6.38467	-2.20173
C	-1.45831	0.241358	2.590939	C	4.470285	-1.63339	-2.28128
H	-1.97416	0.952075	1.955278	H	3.482658	-1.74263	-2.70852
C	-2.29799	4.598461	2.199437	C	1.938574	6.432477	-0.02363
H	-2.1325	4.043956	3.112225	H	1.518669	7.444232	-0.00296
C	-2.99435	-1.06269	-0.56318	H	3.00758	6.515392	0.191573
C	1.29428	0.993539	-2.46506	C	0.218724	-1.35583	2.815093
H	1.699923	1.654936	-1.70689	H	1.01123	-1.92922	2.348868
C	-0.15658	-1.56215	4.157728	C	5.703824	-2.52921	2.964519

H	6.448974	-3.29814	2.732597	H	-4.84399	-2.38085	-3.67295
H	5.853252	-2.22911	4.005368	C	-6.16041	-3.04871	-1.95965
C	5.149293	-0.39305	-2.00671	H	-6.31764	-4.1001	-2.15782
H	4.764527	0.597271	-2.20311	C	-2.95665	-4.90793	0.46857
C	6.424778	-0.70254	-1.42319	H	-3.75754	-5.64867	0.566546
H	7.197641	0.006296	-1.16044	H	-2.00198	-5.44048	0.429339
C	6.533986	-2.14101	-1.33706	C	-6.34449	-0.93435	-1.02717
H	7.397673	-2.69517	-0.99697	H	-6.65808	-0.12153	-0.38723
C	4.278612	-3.0386	2.730268	C	-6.76743	-2.30244	-0.90708
H	3.538044	-2.30621	3.074938	H	-7.43774	-2.69759	-0.15604
H	4.107058	-3.98032	3.260052	C	-2.97036	-3.89925	1.61929
C	-2.94704	0.80784	4.571214	H	-2.07958	-3.25757	1.576524
H	-3.6324	0.125651	5.083227	H	-2.9985	-4.40452	2.588918
H	-3.50987	1.405193	3.846102	H	-5.57222	-3.51592	1.975648
H	-2.54991	1.472504	5.346282	H	-4.31122	-1.7327	2.387595
C	-0.27617	-1.61494	-5.38336	H	-1.88746	-3.62398	-1.56905
H	0.538686	-2.08314	-5.94421	H	-3.60102	-4.9726	-2.11603
H	-0.86304	-1.04743	-6.11275	H	7.438464	-0.88636	1.789182
H	-0.90372	-2.40011	-4.95188	H	5.590605	0.090475	2.538316
C	0.548665	-2.54509	5.0375	H	1.983354	4.371742	1.630278
H	-0.17804	-3.11206	5.625452	H	1.162227	6.231391	2.50833
H	1.184493	-2.01998	5.759311	H	-0.25449	4.402491	-2.58822
H	1.16588	-3.24346	4.463765	H	-0.72923	6.521698	-2.13122
C	-5.49913	-0.8263	-2.18666	H	4.581803	-4.55538	0.58827
H	-5.04168	0.077777	-2.55974	H	2.597523	-3.47136	0.659637
C	-5.36133	-2.13642	-2.75616				