Supporting Information for

A change in oxidation state of iron: scandium is not innocent

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Computational details

All calculations have been performed using the Amsterdam Density Functional (ADF, version 2012.01)[1, 2] and QUILD[3] programs. Here, a combination of density functionals was used that were chosen for the properties of interest: PBE-D[4, 5] for structures,[6] SSB-D[7] for spin-state energies and OPBE[5, 8, 9] for Mössbauer properties (for which Noodleman's parameterization[10] is used).[10] The frozen core approach[2] with a triple-ζ basis set with double polarization (TZ2P) was used for the geometry optimizations, all other calculations used all-electron TZ2P, except the Mössbauer calculations (all-electron TZP). Solvent effects were included in all calculations through the use of COSMO[11-13] with parameters corresponding to the different solvents used experimentally (see Supporting Information). Accurate numerical integration settings (accint 7.0, dishul 6.0) were used in all calculations.

Abbreviations of iron-ligands:

H_3buea	1,1,1-tris[(N'-tert-butylureaylato)-N-ethyl]aminato
N4Py	N,N-bis(2-pyridylmethyl)-N-bis(2-pyridyl)methylamine
TMC	1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane
TMC-Py	1-(2-pyridylmethyl)-4,8,11-trimethyl-1,4,8,11-tetraazacyclotetradecane
TMCS	1-(2-mercaptoethyl)-4,8,11-trimethyl-1,4,8,11-tetraazacyclotetradecane
$TMCSO_2$	1-(2-sulfinatoethyl)-4,8,11-trimethyl-1,4,8,11-tetraazacyclotetradecane
TMG_3tren	1,1,1-tris(2-[*N2*-(1,1,3,3-tetramethylguanidino)]ethyl)amine
tpa^{Ph}	tris(5-phenylpyrrol-2-ylmethyl)amine

Table S1. Validation of computational setup for Fe=O species[§]

complex		spin	Fe-O (Å)	Fe-N_{av} (Å)	*CCDC code*	δ ($mm \cdot s^{-1}$)	ΔE_Q ($mm \cdot s^{-1}$)	Ref.[a]
$[Fe^{III}(O)(H_3buea)]^{2-}$	exp.	5/2	1.813[b]	2.089[b]	*QASGUM*	0.30	0.71	[14]
	theory[c]	5/2	1.795	2.146		0.42	-1.61	t.w.
$[Fe^{III}(OH)(H_3buea)]^{-}$	exp.	5/2	2.048[b]	2.140[b]	*QASHAT*	0.32	0.92	[14]
	theory[c]	5/2	1.952	2.092		0.40	0.68	t.w.
$[Fe^{IV}(O)(H_3buea)]^{-}$	exp.	2	1.680[b]	2.007[b]	*UPICUS*	0.02	0.43	[15]
	theory[d]	2	1.679	2.026		0.15	0.65	t.w.
$[Fe^{IV}(O)(TMC)(NCCH_3)]^{2+}$	exp.	1	1.646[b]	2.084[b]	*WUSJOJ*	0.17	1.24	[16]
	theory[e]	1	1.645	2.085		0.18	0.96	t.w.
$[Fe^{IV}(O)(TMC^{i})(NCCH_3)]^{2+}$	exp.	1	1.64[f]	2.08[f]	-	0.14	0.78	[17]
inverted	theory[e]	1	1.634	2.088		0.18	1.21	t.w.
$[Fe^{III}(OO)(TMC^{i})]^{+}$	exp.	5/2	1.910[b]	2.225[b]	*POMKEI*	0.58	-0.92	[18, 19]
inverted	theory[e]	5/2	1.934	2.247		0.66	-1.24	t.w.
$[Fe^{III}(OOH)(TMC^{i})]^{2+}$	exp.	5/2	1.92[f]	2.15[f]	-	0.51	0.2	[19]
inverted	theory[e]	5/2	1.842	2.187		0.49	1.16	t.w.
$[Fe^{IV}(O)(TMC)(NCS)]^{+}$	exp.	1	1.65[f]	2.07[f]	-	0.18	0.55	[20, 21]
	theory[e]	1	1.660	2.075		0.17	0.40	t.w.
$[Fe^{IV}(O)(TMC)(none)]^{2+}$	theory[e]	1	1.621	2.050		0.15	3.61	t.w.
$[Fe^{IV}(O)(TMC^{i})(none)]^{2+}$	theory[e]	1	1.614	2.074		0.17	3.37	t.w.
$[Fe^{IV}(O)(TMC\text{-}Py)]^{2+}$	exp.	1	1.667[b]	2.090[b]	*YOHHEJ*	0.18	1.08	[22]
	theory[e]	1	1.649	2.095		0.19	1.00	t.w.
$[Fe^{IV}(O)(TMCS)]^{+}$	exp.	1	1.70[f]	2.09[f]	-	0.19	-0.22	[23]
	theory[g]	1	1.684	2.154		0.22	0.21	t.w.
$[Fe^{IV}(O)(TMCSO_2)]^{+}$	exp.	1	1.64[f]	2.05[f]	-	0.19	1.28	[24]
	theory[g]	1	1.663	2.081		0.22	0.61	t.w.
$[Fe^{IV}(O)(N4Py)]^{2+}$	exp.	1	1.639[b]	1.972[b]	*PASREH*	-0.04	0.93	[25, 26]
	theory[e]	1	1.649	1.988		0.03	0.80	t.w.
$[Fe^{IV}(O)(TMG_3tren)]^{2+}$	exp.	2	1.661[b]	2.032[b]	*ANEXAT*	0.09	-0.29	[27, 28]
	theory[e]	2	1.646	2.032		0.14	-0.22	t.w.
$[Fe^{IV}(O)(tpa^{Ph})]^{-}$	exp.	2	1.62[f]	1.99[f]	-	0.09	0.51	[29]
	theory[e]	2	1.630	2.034		0.13	0.43	t.w.

a) t.w. = this work; b) from X-ray; c) using COSMO parameters for N,N-dimethylacetamide (see Table S3); d) using COSMO parameters for N,N-dimethylformamide (see Table S3); e) using COSMO parameters for acetonitrile (see Table S3); f) from EXAFS; g) using COSMO parameters for methanol (see Table S3)

§ geometries obtained at (COSMO)PBE-D_2/TZ2P with COSMO parameters corresponding to the solvents used experimentally (see Table S3), and Mössbauer parameters obtained at (COSMO)OPBE/TZP (see refs. [10, 30, 31] for more details)

Table S2. Spin-state energies (kcal·mol^{-1})[a] for $Fe^{III/IV}$=O species

complex	exp.	l.s.	i.s.	h.s.	l.s.	i.s.	h.s.
			PBE-D[b]			SSB-D[c]	
$Fe^{III}(O)(H_3buea)^{2-}$	h.s.	11.2	1.9	0	32.6	14.6	0
$Fe^{III}(OH)(H_3buea)^{-}$	h.s.	1.5	0	2.2	20.1	9.6	0
$Fe^{IV}(O)(H_3buea)^{-}$	h.s.	13.3	6.3	0	30.9	16.2	0
$Fe^{IV}(O)(TMC)(NCCH_3)^{2+}$	i.s.	8.0	0	16.2	10.6	0	4.5
$Fe^{IV}(O)(TMC^{i})(NCCH_3)^{2+}$	i.s.	7.7	0	16.9	10.4	0	5.0
$[Fe^{III}(OO)(TMC^{i})]^{+}$	h.s.	0.5	0.9	0	20.5	8.6	0
$[Fe^{III}(OOH)(TMC^{i})]^{2+}$	h.s.	4.0	0	5.7	21.0	8.0	0
$Fe^{IV}(O)(TMC)(NCS)^{+}$	i.s.	7.8	0	13.8	10.3	0	1.7
$Fe^{IV}(O)(TMC)(none)^{2+}$	i.s.	8.0	0	18.8	11.3	0	8.7
$Fe^{IV}(O)(TMC^{i})(none)^{2+}$	i.s.	7.9	0	10.1	11.0	0	0.1
$Fe^{IV}(O)(TMC\text{-}Py)^{2+}$	i.s.	7.8	0	16.1	11.2	0	4.5
$Fe^{IV}(O)(TMCS)^{+}$	i.s.	7.7	0	13.7	10.0	0	1.0
$Fe^{IV}(O)(TMCSO_2)^{+}$	i.s.	9.4	0	13.7	32.5	0	1.7
$Fe^{IV}(O)(N4Py)^{2+}$	i.s.	8.2	0	22.4	31.7	0	9.8
$Fe^{IV}(O)(TMG_3tren)^{2+}$	h.s.	17.7	16.2	0	30.3	24.9	0
$Fe^{IV}(O)(tpa^{Ph})^{-}$	h.s.	12.6	19.8	0	24.1	28.5	0

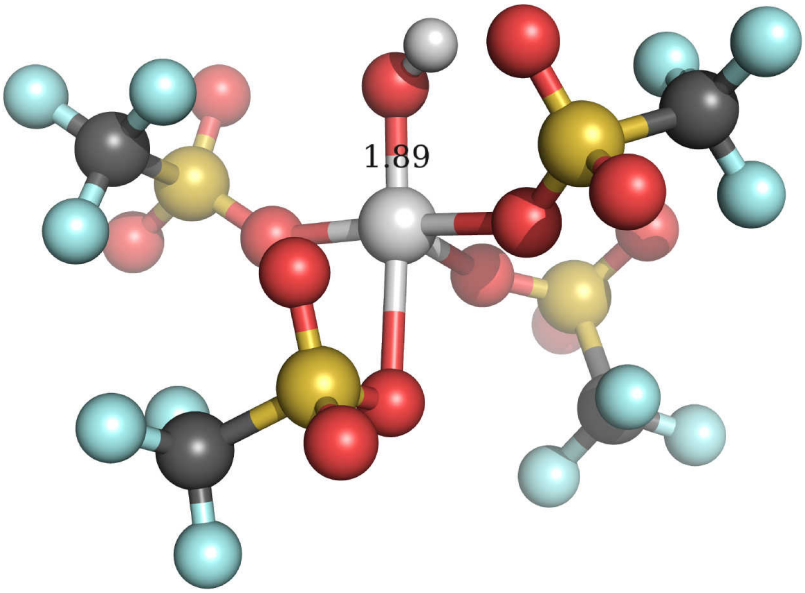
a) l.s. low spin, i.s. intermediate spin, h.s. high spin
b) obtained at (COSMO)PBE-D_2/TZ2P
c) obtained at (COSMO)SSB-D/TZ2P//(COSMO)PBE-D_2/TZ2P

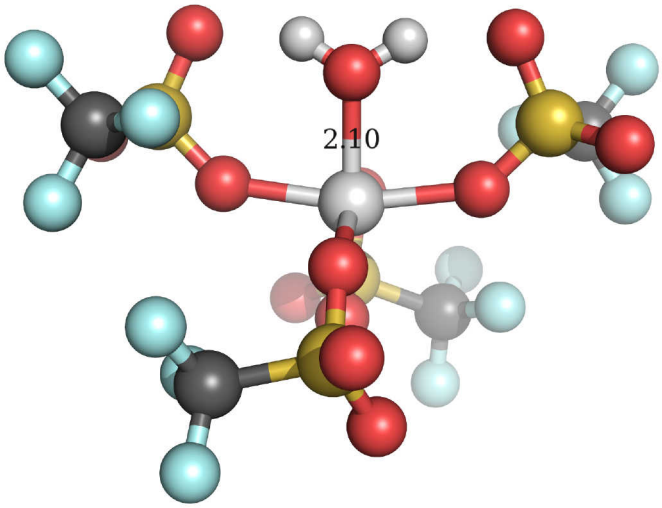
Table S3. COSMO parameters for different solvents

Solvent	Dielectric constant	Solvent radius (Å)
Acetonitrile[a]	37.5	2.76
Dimethylacetamide[b]	38.85	3.33
Dimethylformamide[b]	38.25	3.13
Methanol[a]	32.6	2.53
2,2,2-Trifluoroethanol[b]	26.5	3.05

a) see http://www.scm.com/Doc/Doc2012/ADF/ADFUsersGuide/page92.html#keyscheme%20SOLVATION
b) from CRC Handbook of Chemistry and Physics, 85th Edition, using formula from ref. [13] for obtaining solvent radius: R^3 (a.u.) = 2.6752 * M_m / ρ

Figure S1. Structures of $[Sc(OTf)_4(OH)]^{2-}$ and $[Sc(OTf)_4(OH_2)]^{-}$





Cartesian coordinates of all species considered here

$Fe^{III}(O)(H_3buea)^{2-}$, h.s.

Fe	0.27492665	0.85632138	-0.09049135
O	-0.04901838	-0.66768261	0.80040645
C	-1.14405788	3.52922010	0.24916359
N	0.74795347	2.86349999	-1.19410524
C	1.10802742	2.46018022	-2.55915387
C	-2.29323477	1.76057517	1.38313015
N	2.24102511	1.25927178	0.50773472
C	0.16542271	1.37885307	-3.08025314
O	-3.32939505	2.48009234	1.54082933
N	-2.18350172	0.51318865	1.99559358
N	-0.02295895	0.35179002	-2.06810541
C	-0.56178645	-0.81397551	-2.53695177
O	-0.78837425	-1.03637204	-3.77296497
N	-0.87367554	-1.73733224	-1.57212587
C	3.09828284	0.34086045	1.03952174
C	-1.14399675	-3.15316101	-1.81550013
C	-2.46067747	-3.34447473	-2.58466661
O	4.36221869	0.42373247	0.95478380
C	-3.32931217	-0.40980397	2.12281971
C	-3.95791580	-0.67266134	0.74226064
C	-1.27663172	-3.80577373	-0.43409959
N	2.47478544	-0.68095527	1.75529896
C	-0.49458465	3.64337643	-1.12820284
C	3.28264144	-2.58493077	0.39056522
C	0.01228780	-3.82206290	-2.58020985
C	-2.74333697	-1.72133584	2.66516165
C	3.02876625	-2.04862937	1.81096126
C	4.31097045	-2.11179423	2.64715964
C	1.86183226	3.46845825	-0.45412695
C	1.94494061	-2.90649689	2.47926707
N	-1.18655035	2.13651644	0.68037703
C	2.90264572	2.41446341	-0.08607262
C	-4.38441087	0.11252106	3.10301637
H	-2.15271464	3.96680509	0.19182336
H	-0.57626409	4.14386376	0.97505903
H	2.12344621	2.04409134	-2.52103846
H	1.11993294	3.32905413	-3.24739562
H	0.59926180	0.96885047	-4.00764451
H	-0.80066051	1.83286507	-3.37856249
H	-1.34925845	-0.00815922	1.61579346
H	-0.57585544	-1.47004291	-0.60325231
H	-2.67257689	-4.41822751	-2.71315971
H	-2.38818645	-2.86523640	-3.56914396
H	-3.28728529	-2.88388377	-2.02185125
H	-4.77349710	-1.41038659	0.81912329
H	-3.18926639	-1.05432458	0.05124757
H	-4.36468713	0.26679908	0.33722884
H	-1.45591024	-4.88535860	-0.54539864
H	-2.11413272	-3.35638342	0.11981481
H	-0.35845437	-3.64771541	0.15200373
H	1.45293903	-0.72737387	1.48723562
H	-1.18559397	3.22113993	-1.87005762
H	-0.31779455	4.70643541	-1.38850899
H	3.64538853	-3.62506816	0.42467021
H	4.03450767	-1.95856136	-0.11227472
H	2.34448252	-2.54894020	-0.18556626
H	0.94398920	-3.72906974	-2.00019896
H	0.14493221	-3.32676587	-3.55219739
H	-0.19965626	-4.89122611	-2.74299562
H	-3.52835448	-2.49100847	2.71579782
H	-2.33388520	-1.56409695	3.67536209
H	-1.92892787	-2.06602133	2.01029808
H	4.65324047	-3.15633558	2.72484896
H	4.11507936	-1.73120025	3.66186926
H	5.09392156	-1.49899802	2.18428721
H	1.44948407	3.89258220	0.47186343
H	2.33003053	4.29308536	-1.02781187
H	2.26084912	-3.96039922	2.50205601
H	1.00075218	-2.81349699	1.92031010
H	1.77221293	-2.56412778	3.51162017
H	3.62955736	2.87123436	0.60821147
H	3.48724928	2.12792544	-0.97984879
H	-5.17920069	-0.64084610	3.22629065
H	-4.81564034	1.04983890	2.73205058
H	-3.92327631	0.29938599	4.08553276

$Fe^{III}(OH)(H_3buea)^-$, h.s.

C	3.09376102	-2.75953088	0.87270570
H	2.15112925	-3.02414678	1.37521299
H	3.82409356	-3.56412042	1.03778304
H	2.89516397	-2.67985170	-0.20739211
C	-0.72509913	3.75855573	-0.89542112
H	-0.79548420	4.54805628	-1.66660334
H	-0.55283148	4.24459151	0.07540168
C	-2.01522035	2.95957857	-0.82035286
H	-2.82278676	3.62472946	-0.47815519
H	-2.31027139	2.61326819	-1.82715686
N	-1.83904392	1.82734757	0.09092598
C	-3.03224705	1.27731882	0.50820616
O	-4.15469204	1.66360110	0.08503958
N	-2.92129118	0.30088451	1.47911267
H	-1.96427793	-0.06055485	1.60091362
C	-3.95630884	-0.72094477	1.73011238
C	-5.20432721	-0.09663363	2.36554772
H	-4.93207017	0.41578195	3.30099388
H	-5.93453431	-0.88736737	2.59781773
H	-5.65689739	0.62905415	1.67897827
C	-4.32820078	-1.46099036	0.43411878
H	-4.74844481	-0.75466644	-0.29528030
H	-5.07074059	-2.24654285	0.64418685
H	-3.43211975	-1.93054404	-0.00074287
C	-3.33311117	-1.71484025	2.71756570
H	-3.07437363	-1.20718064	3.65948146
H	-2.41627472	-2.15199906	2.29319200
H	-4.04808644	-2.52131516	2.93427464
C	0.49398612	2.37234444	-2.53423187
H	1.00360279	3.10338047	-3.18891166
H	-0.53374557	2.23995714	-2.89860005
C	1.20355579	1.02198181	-2.57485557
H	1.16559414	0.62907410	-3.60064322
H	2.26959288	1.16202550	-2.31659923
N	0.58009621	0.08978170	-1.63664306
C	0.41675627	-1.20725063	-2.08303572
O	0.65931198	-1.58190517	-3.26305353
N	-0.02109618	-2.07941894	-1.12341821
H	-0.19844090	-1.68120657	-0.18980412
C	-0.43761834	-3.46824935	-1.34517175
C	-0.88353311	-4.00054147	0.02108690
H	-1.71334228	-3.39678938	0.41883299
H	-0.04974549	-3.96166681	0.73866491
H	-1.21888099	-5.04260425	-0.07707563
C	-1.61714416	-3.53380060	-2.32822257
H	-2.46898475	-2.96019866	-1.93162354
H	-1.93157597	-4.57906238	-2.47320539
H	-1.31803127	-3.10932635	-3.29606883
C	0.72827233	-4.32477781	-1.86190813
H	1.55847185	-4.30386944	-1.14047308
H	1.08120550	-3.93561281	-2.82509302
H	0.39530685	-5.36669849	-1.98811205
O	-0.29404073	-0.57789145	1.26537619
H	0.54516060	-0.75678197	1.73512514
N	0.41969533	2.86945136	-1.14743996
C	1.68686973	3.44176062	-0.65313834
H	1.72217523	4.53139069	-0.83326571
H	2.51520362	2.97216294	-1.19998735
Fe	-0.02303203	0.92931514	0.08293027
C	1.83336537	3.10139939	0.83158895
H	2.81700321	3.42336640	1.20211352
H	1.06608983	3.64008258	1.41232326
N	1.65442861	1.65944291	0.95587270
C	2.70791182	0.93180113	1.43020348
O	3.66702079	1.39321775	2.10013756
N	2.60595928	-0.42833893	1.13514568
H	2.09502483	-0.60544703	0.26644799
C	3.64289643	-1.43733912	1.41889592
C	4.96406477	-1.09819155	0.71042556
H	5.34431428	-0.13340491	1.07171609
H	4.80417093	-1.03810761	-0.37750578
H	5.71176053	-1.88115603	0.91121961
C	3.86089113	-1.56433820	2.93000595
H	4.23492507	-0.61875910	3.34122157
H	4.59395143	-2.36069033	3.12804023
H	2.91458565	-1.82586684	3.42769852

$Fe^{IV}(O)(H_3buea)^-$, h.s.

Fe	0.24223086	-0.99358313	0.30412719
C	-1.90267670	-1.53628364	-1.83544115
O	-0.18565617	0.55575658	-0.17964404
O	4.16401333	0.20784342	-0.64911995
O	-1.38564713	0.12453153	4.02775989
O	-2.35377571	-2.25825683	-2.76594643
C	-2.87437301	0.62397268	-2.69042062
C	-1.92743061	0.68517169	-3.90068534
N	0.78049630	-2.93409480	0.90871170
N	2.17678797	-0.89390365	-0.18895203
N	-0.25503324	-0.81277813	2.23326836
N	-0.99928348	-1.99607324	-0.90182825
N	2.16146650	1.06150320	-1.43386297
N	-0.57756991	1.48057637	2.33639728
N	-2.32836281	-0.24265648	-1.63048871
C	-4.26494049	0.14568710	-3.12246891
C	-2.98773231	2.01991536	-2.06570379
C	2.11432803	-3.23828555	0.31712093
C	2.97296788	-1.98989545	0.36327481
C	2.90781002	0.14099564	-0.73175064
C	2.58337706	2.45326427	-1.67459390
C	1.36159353	3.15646179	-2.27859190
C	3.74558196	2.50631889	-2.67261543
C	2.97172636	3.15006217	-0.35976048
C	0.83605602	-2.94410840	2.39804054
C	-0.29233505	-2.09133873	2.94309428
C	-0.79491981	0.25226703	2.92082525
C	-1.42527808	2.66466948	2.56664149
C	-2.90828974	2.34245302	2.31748651
C	-1.22739394	3.21035071	3.98511163
C	-0.95714917	3.71199799	1.54883261
C	-0.26149769	-3.87114410	0.40131025
C	-0.69939236	-3.42578510	-0.97989356
H	-1.11781923	-3.81327974	1.08459717
H	-0.29083814	1.37549292	1.35026671
H	1.15890917	0.97806233	-1.20301549
H	-1.08259640	3.33083611	0.52307337
H	-1.80807687	-0.31747550	-4.33534853
H	-0.94109345	1.05985788	-3.58496359
H	-2.33368282	1.36262391	-4.66794897
H	0.13223294	-4.90012558	0.40710282
H	0.08994297	-3.63393164	-1.72438994
H	-1.58197654	-4.00474113	-1.28784233
H	-4.94203440	0.12701165	-2.25488412
H	-4.20027591	-0.86384590	-3.54686069
H	-4.67633140	0.83490566	-3.87610734
H	-3.65641721	1.99587263	-1.19177241
H	-3.39019732	2.72918386	-2.80280572
H	-1.99714715	2.37383852	-1.73904183
H	1.95309531	-3.52461206	-0.72968172
H	2.57240586	-4.08495022	0.85313047
H	3.29466444	-1.77616293	1.39830379
H	3.88921942	-2.15210682	-0.22236051
H	0.51272059	3.11607871	-1.57782946
H	1.06322036	2.66721103	-3.21833557
H	1.59853052	4.20988755	-2.48499434
H	4.62057078	1.98805609	-2.26093815
H	4.00629894	3.55543792	-2.88156099
H	3.45304939	2.02112003	-3.61634237
H	3.82208353	2.62974958	0.10354002
H	2.11902262	3.13580619	0.33705941
H	3.25365827	4.19709577	-0.55190835
H	1.79510806	-2.50201618	2.69537517
H	0.79254258	-3.98284856	2.76261829
H	-1.26403918	-2.60025891	2.81110486
H	-0.15503334	-1.95276938	4.02511630
H	-1.69893823	0.25689632	-0.98250434
H	-3.24675798	1.56562184	3.01788777
H	-3.04425967	1.98063292	1.28625713
H	-3.52307570	3.24504781	2.45911825
H	-1.53741849	2.46082343	4.72376042
H	-1.82677189	4.12448710	4.11679426
H	-0.16727822	3.45752094	4.14798866
H	0.10575532	3.95089844	1.70591713
H	-1.54882640	4.63199167	1.65804174

$Fe^{IV}(O)(TMC)(NCCH_3)^{2+}$, i.s.

Fe	0.01854929	-0.00270235	-0.20626741
O	-0.01428943	-0.01632053	-1.85109329
N	1.39309523	-1.57017356	-0.33012572
N	-1.43722468	-1.54575360	-0.11043413
N	-1.43927879	1.54219258	-0.13699443
N	1.39237979	1.56368537	-0.35656641
C	0.60524828	-2.64472236	-1.01675609
H	1.18786500	-3.57871762	-1.02186313
H	0.44565082	-2.31477885	-2.04822205
C	-0.70598188	-2.85015180	-0.30881291
H	-0.53774975	-3.28764076	0.68121802
H	-1.34545256	-3.54458942	-0.87145786
C	-2.38581636	-1.32238244	-1.25496928
H	-3.10286452	-2.15996783	-1.24552915
H	-1.79356040	-1.37288706	-2.17511860
C	-3.16777544	-0.01203416	-1.19193959
H	-3.83994993	-0.01970793	-2.06238573
H	-3.83036064	-0.00494068	-0.31530111
C	-2.38701577	1.29778217	-1.27783529
H	-1.79439735	1.33249929	-2.19846057
H	-3.10485068	2.13465372	-1.28320930
C	-0.70748940	2.84257115	-0.35789461
H	-1.34679700	3.52730273	-0.93254446
H	-0.53957902	3.29665485	0.62467766
C	0.60388427	2.62530727	-1.06193169
H	1.18586081	3.55946998	-1.08364250
H	0.44450113	2.27721425	-2.08743430
C	2.57015850	1.24791349	-1.22457357
H	3.23263161	2.12749969	-1.19964376
H	2.18951805	1.12600512	-2.24604210
C	3.32677792	-0.00705324	-0.82852008
H	3.61607038	0.00190303	0.23162619
H	4.26578332	-0.01163473	-1.39920854
C	2.57085701	-1.26893900	-1.20327601
H	2.19061204	-1.16494400	-2.22688706
H	3.23362730	-2.14768855	-1.16287378
C	1.89706779	-2.07051971	0.97931091
H	2.54340832	-2.94375328	0.80100814
H	1.06341288	-2.35965694	1.62426590
H	2.47422327	-1.28409799	1.47544895
C	-2.23054491	-1.72668251	1.13818564
H	-2.88386040	-2.60381117	1.01146176
H	-2.85311739	-0.85723990	1.34443491
H	-1.55619161	-1.90175370	1.98060249
C	-2.23460810	1.74746599	1.10657483
H	-2.88052775	2.62779787	0.96496850
H	-1.56187843	1.92973824	1.94874333
H	-2.86576159	0.88665501	1.32275428
C	1.89613898	2.08711484	0.94387778
H	2.54198461	2.95752486	0.75041935
H	2.47366372	1.30943802	1.45319497
H	1.06254133	2.38707227	1.58403784
N	0.10392039	0.01520971	1.78900695
C	0.15023524	0.02908973	2.94638636
C	0.21179939	0.04766441	4.38476760
H	0.76364033	0.93844275	4.71656527
H	0.72768307	-0.85507577	4.74122220
H	-0.80638817	0.07293621	4.79771700

$Fe^{IV}(O)(TMC^{i})(NCCH_3)^{2+}$, i.s.

Fe	-0.00590845	-0.01948377	-0.42175759
H	-1.57869856	1.55904098	-2.64718989
H	-3.09886912	2.08802487	-1.84148515
C	2.40797280	1.51124176	0.61546535
H	2.03657985	1.48942131	1.64481179
H	3.01345300	2.42475739	0.50556920
O	-0.03001538	-0.10894166	-2.05351799
C	3.28377547	0.29244052	0.36455821
H	4.10969166	0.36030641	1.08709619
H	3.75506518	0.34313923	-0.62562595
C	-2.38588379	-1.42363300	0.84724066
H	-2.99270387	-2.34275889	0.85443569
H	-1.98482470	-1.29120145	1.85683129
C	-0.99655390	2.74549934	-0.41105225
H	-1.69817301	3.40637751	0.11569057
H	-0.86277277	3.13978436	-1.42374199
C	-3.27047861	-0.23728822	0.49293448
C	0.99023033	-2.76870606	-0.13519403

N	1.58022472	-1.41096289	-0.43186527
C	2.62796733	-1.06804526	0.58316672
H	3.40232049	-1.85003867	0.52625990
H	2.16722195	-1.12651687	1.57598898
H	1.70786744	-3.36661428	0.44289199
N	-1.22371531	-1.67339385	-0.07244895
H	0.83079569	-3.27530060	-1.09282051
N	-1.59392994	1.36457651	-0.53735089
C	-0.31656292	-2.65624187	0.60963295
H	-0.81275665	-3.63745194	0.65549210
N	1.21939505	1.66143793	-0.29170261
H	-0.15556236	-2.31178761	1.63510305
H	-4.07302882	-0.22436139	1.24453294
C	-1.73430142	-2.27463031	-1.33684757
H	-0.90724077	-2.43526842	-2.03281162
H	-2.45014037	-1.59399658	-1.80388216
H	-2.23277618	-3.22739737	-1.10012051
H	-3.77316156	-0.39385696	-0.47034821
C	0.33012796	2.71341066	0.30533265
H	0.19758988	2.48209261	1.36592524
C	1.69257556	2.11977085	-1.62838315
H	2.19447177	3.09300612	-1.51262244
H	0.84649375	2.20208876	-2.31508005
H	2.39823221	1.39220926	-2.03636942
H	0.82510656	3.69337845	0.23032581
C	-2.60906615	1.13732208	0.54124251
H	-3.38526997	1.91066512	0.42401786
H	-2.11783643	1.30350670	1.50710753
C	2.24160288	-1.52610189	-1.76579663
H	2.65536565	-0.56695559	-2.07852526
H	1.50132733	-1.84026791	-2.50529074
H	3.04815573	-2.27212664	-1.69252322
C	-2.29638777	1.33400244	-1.85478381
H	-2.72299710	0.34892504	-2.04588150
N	0.02547071	0.09223304	1.62842722
C	0.04646298	0.14818852	2.78626406
C	0.07277764	0.21512145	4.22349421
H	0.20939256	-0.79433380	4.63618363
H	-0.87526352	0.63429373	4.58865675
H	0.90345513	0.85836149	4.54662364

$Fe^{IV}(O)(TMC)(NCS)^{+}$, i.s.

Fe	-0.38492053	-0.12167597	-0.01610418
O	-1.98548180	-0.55605647	-0.08977011
N	-0.20267688	-1.50575573	1.54136947
N	-0.79332079	1.27783532	1.53112373
N	-0.66309225	1.32039134	-1.55190916
N	-0.07066741	-1.46183526	-1.59069050
C	-1.13306569	-0.95725132	2.57804259
H	-1.02240788	-1.53031546	3.51194194
H	-2.14973359	-1.08573453	2.19317002
C	-0.83372525	0.49787409	2.81954231
H	0.14523326	0.60651283	3.29938241
H	-1.58220653	0.94092950	3.49217910
C	-2.14637402	1.86284027	1.25093312
H	-2.38744699	2.53959030	2.08821814
H	-2.85803285	1.03009714	1.24917398
C	-2.24620468	2.65027061	-0.05574268
H	-3.27313020	3.04294970	-0.09405130
H	-1.59894168	3.53752375	-0.01609194
C	-2.03523912	1.89991325	-1.37094857
H	-2.74440770	1.06913048	-1.45375397
H	-2.20427079	2.60103666	-2.20585428
C	-0.59401936	0.57770945	-2.86099634
H	-1.28415840	1.04011459	-3.58137043
H	0.42149603	0.69927920	-3.25395863
C	-0.91076434	-0.88339058	-2.68648399
H	-0.72147488	-1.43000905	-3.62375842
H	-1.95627893	-1.02098599	-2.39257984
C	-0.59131378	-2.83749726	-1.32365805
H	-0.34113595	-3.45586558	-2.20105356
H	-1.68287070	-2.75571885	-1.25230903
C	-0.06458621	-3.47508256	-0.04955525
H	1.03330301	-3.45702141	-0.00329799
H	-0.35087446	-4.53583740	-0.07629494
C	-0.69678284	-2.87301162	1.19340697
H	-1.77883361	-2.78909125	1.03387263
H	-0.51934063	-3.51593234	2.07086831
C	1.17028219	-1.62949386	2.10329886

H	1.14122592	-2.31211684	2.96779123
H	1.54482639	-0.65083260	2.41261313
H	1.84342576	-2.02727032	1.33793410
C	0.17111786	2.38624295	1.77610933
H	-0.15816493	2.94511679	2.66669876
H	0.21058498	3.07267902	0.93146158
H	1.16763203	1.97146048	1.94929921
C	0.31837230	2.43311153	-1.68151455
H	0.06226415	3.02222914	-2.57663806
H	1.32532635	2.02115880	-1.78758528
H	0.29023617	3.09030451	-0.81360408
C	1.34492448	-1.57173627	-2.03797752
H	1.38974119	-2.23197419	-2.91899245
H	1.95214901	-1.98923074	-1.22929882
H	1.74239566	-0.58572111	-2.28999017
N	1.49694540	0.34300994	0.06990898
C	2.63948711	0.65298643	0.12324439
S	4.20276370	1.08136524	0.19690151

$Fe^{IV}(O)(TMC)(none)^{2+}$, i.s.

Fe	-0.03258186	-0.00071415	-0.03136917
O	-0.06007979	0.00022078	-1.65190172
N	-1.38186524	1.49124032	0.06181328
N	1.37754245	1.52051743	0.18749253
N	1.38547447	-1.51608308	0.18625871
N	-1.37441737	-1.49964240	0.06016277
C	-0.69834780	2.62778463	-0.63450767
H	-1.31090835	3.53624614	-0.53743558
H	-0.62717165	2.34853976	-1.69060143
C	0.66109535	2.84121783	-0.02233837
H	0.55901148	3.32181936	0.95601319
H	1.27686066	3.49377483	-0.65349800
C	2.39742545	1.31765762	-0.90213833
H	3.10969439	2.15571783	-0.83964493
H	1.85429716	1.38414758	-1.85157679
C	3.17733063	0.00727097	-0.81529174
H	3.86420604	0.00943949	-1.67385613
H	3.82761613	0.00838875	0.06981154
C	2.40317010	-1.30648100	-0.90411719
H	1.85913040	-1.37363512	-1.85295920
H	3.11924914	-2.14142238	-0.84417577
C	0.67446507	-2.83940516	-0.02488912
H	1.29393025	-3.48932946	-0.65515437
H	0.57270076	-3.32050988	0.95327681
C	-0.68501531	-2.63125455	-0.63850407
H	-1.29344727	-3.54290517	-0.54456298
H	-0.61319277	-2.34850576	-1.69352891
C	-2.67393837	-1.26975883	-0.64481065
H	-3.29815264	-2.15859684	-0.46498096
H	-2.43693661	-1.21650855	-1.71487878
C	-3.40705270	-0.00874578	-0.22787715
H	-3.65747649	-0.00903833	0.84144310
H	-4.36952027	-0.01099278	-0.75708320
C	-2.67968085	1.25556453	-0.64448015
H	-2.44173382	1.20372988	-1.71443190
H	-3.30802165	2.14158043	-0.46494655
C	-1.62386524	1.81247223	1.49706038
H	-2.15477510	2.77382644	1.57057731
H	-0.67463947	1.89185978	2.03847576
H	-2.23317389	1.03026586	1.95761733
C	2.07302629	1.65065326	1.50611593
H	2.59323820	2.61908253	1.53260363
H	2.81278498	0.86646866	1.64747432
H	1.34333567	1.61775415	2.32364454
C	2.08373531	-1.64679113	1.50349448
H	2.60592093	-2.61430244	1.52778873
H	1.35592125	-1.61641148	2.32284812
H	2.82286500	-0.86188023	1.64433452
C	-1.61388120	-1.82403915	1.49518148
H	-2.12721587	-2.79484333	1.56885115
H	-2.23827235	-1.05218174	1.95266157
H	-0.66470850	-1.88544411	2.03929095

$Fe^{IV}(O)(TMC^{i})(none)^{2+}$, i.s.

Fe	-0.00001614	0.00108891	0.24585985
H	-1.97123443	-1.28842996	2.27419620
H	-3.29245844	-2.02345063	1.29454529
C	1.97460710	-1.37900164	-1.44062607

H	1.30977442	-1.07237184	-2.26387561
H	2.43807167	-2.33514018	-1.73062207
O	0.00087578	0.00042627	1.85997655
C	3.03383984	-0.31571830	-1.23045640
H	3.64895447	-0.30449444	-2.14019719
H	3.71194576	-0.57571615	-0.40789033
C	-1.97226972	1.37883551	-1.43847793
H	-2.43281400	2.33539852	-1.73125419
H	-1.30623146	1.06955134	-2.25988792
C	-1.08972324	-2.65918026	0.19745409
H	-1.86259912	-3.37475351	-0.11530783
H	-0.80768740	-2.88307871	1.23279697
C	-3.03468478	0.31916442	-1.22689495
C	1.08950704	2.66081690	0.20030417
N	1.65976587	1.27263003	0.18252647
C	2.45627772	1.08086585	-1.07389728
H	3.25948391	1.83432875	-1.06864735
H	1.80126468	1.29603727	-1.93014271
H	1.86154738	3.37813813	-0.11185039
N	-1.09280031	1.66830703	-0.25309744
H	0.80872780	2.88128963	1.23655890
N	-1.66100747	-1.27147028	0.18388228
C	-0.10954111	2.71682683	-0.69892605
H	-0.59169895	3.70321254	-0.66925477
N	1.09312532	-1.66734157	-0.25660976
H	0.16423552	2.50876460	-1.74011505
H	-3.65223861	0.30995759	-2.13505144
C	-1.88711385	2.22480639	0.87771744
H	-1.20908947	2.49669104	1.69194405
H	-2.59362315	1.48286370	1.24812866
H	-2.43171820	3.11221429	0.52185269
H	-3.71010753	0.58204953	-0.40308907
C	0.10789911	-2.71328430	-0.70405675
H	-0.16746057	-2.50223918	-1.74441875
C	1.88579581	-2.22732323	0.87367863
H	2.41730370	-3.12392292	0.52069034
H	1.20878146	-2.48507228	1.69325051
H	2.60438785	-1.49276257	1.23585832
H	0.58867749	-3.70023080	-0.67853531
C	-2.46089299	-1.07887845	-1.07064944
H	-3.26593112	-1.83029958	-1.06291894
H	-1.80821175	-1.29644378	-1.92793493
C	2.57024205	1.19270965	1.36056223
H	3.11056521	0.24640819	1.38101991
H	1.97452533	1.29205527	2.27181087
H	3.29966955	2.01380965	1.28782649
C	-2.56954790	-1.19624855	1.36380121
H	-3.11842677	-0.25478562	1.38333240

$Fe^{IV}(O)(TMC\text{-}Py)^{2+}$, i.s.

Fe	-0.47721090	-0.16795059	0.07696880
O	-1.76314017	-0.91842912	0.78574212
N	0.70417368	-1.07207760	1.49464144
C	0.28352801	-2.49829018	1.74659731
C	3.75398669	0.62031282	0.13770802
C	2.15824947	-1.01070164	1.16556382
C	0.31611185	-3.39403293	0.51302040
C	4.02602404	1.63370271	-0.77551863
C	2.45107866	0.13972504	0.25786892
C	-0.57549908	-3.00252308	-0.66261845
C	2.97223961	2.14119043	-1.53527951
N	-0.65849738	1.40191917	1.44684081
N	-0.20107776	-1.70492361	-1.32442296
C	-1.15368297	-1.42738619	-2.45903535
C	1.69735800	1.62773117	-1.34319371
C	0.10169312	2.66413996	1.15996908
C	-2.34964006	-0.65268990	-1.97969384
N	1.41869084	0.63804768	-0.46534134
C	1.14123101	-1.86354924	-1.95736245
C	-2.10207557	1.77157347	1.67863153
C	-3.10105678	1.15459794	-0.57302411
C	-1.43880778	1.58549331	-2.27483046
C	-0.13902621	0.85797544	2.68974229
C	-2.80668774	2.26130013	0.42404308
C	0.49150228	-0.30526877	2.71616179
N	-1.89657776	0.59172682	-1.27196908
H	-0.73222787	-2.44231473	2.15134488
H	0.95710854	-2.90544796	2.51576749
H	4.53748582	0.19060254	0.76000767

H	2.45071781	-1.94695574	0.67441519
H	2.75363325	-0.94586437	2.08709988
H	-0.03430048	-4.37911216	0.85267966
H	1.34728163	-3.56053753	0.17173686
H	5.03681017	2.02292697	-0.88729434
H	-1.61812548	-2.90998437	-0.34030326
H	-0.50549646	-3.78695319	-1.43347466
H	3.12211695	2.93670769	-2.26199551
H	-1.46186550	-2.37787010	-2.91707982
H	-0.60418955	-0.85789813	-3.21729291
H	0.86830535	2.03685339	-1.90271794
H	-0.16462872	3.03624887	0.16601175
H	1.17650300	2.46975924	1.20790946
H	-0.16697152	3.41853953	1.91427406
H	-2.92769521	-1.24103133	-1.25995701
H	-2.99880789	-0.37905052	-2.82480443
H	1.08678222	-2.69009928	-2.68274527
H	1.90561507	-2.10096286	-1.21684244
H	1.41319572	-0.94257286	-2.48114445
H	-2.11176000	2.55459893	2.45246915
H	-2.60133802	0.87528698	2.06437766
H	-3.57992571	0.32191422	-0.04627037
H	-3.78557814	1.51771217	-1.35598759
H	-0.61895247	1.17618420	-2.87197672
H	-1.11675659	2.50211745	-1.76973512
H	-2.27429575	1.83170620	-2.94842054
H	-0.28691343	1.46619098	3.58353305
H	-2.27360401	3.10342603	-0.03846112
H	-3.77822791	2.66222551	0.74482037
H	0.90574358	-0.73538294	3.62874145

$Fe^{IV}(O)(TMCS)^{+}$, i.s.

Fe	-0.10901966	0.05961067	-0.19533131
C	1.16606509	2.63959167	0.99624824
C	-1.04939632	-2.81000731	0.51390237
C	1.44160289	2.32436704	-1.39401515
C	-3.23341885	-1.01973003	-0.81322622
N	-1.98255502	0.82789646	0.39565989
N	0.53832293	2.07478314	-0.22496204
C	1.59411456	-2.18498960	-0.87110168
C	-2.54803384	0.41437710	1.71237772
C	2.46596619	-0.03304128	-1.64503260
N	1.78643602	-0.73478195	-0.50748334
C	2.69522269	1.46317399	-1.44134162
N	-0.83577312	-1.87531576	-0.61926155
S	0.36058325	-0.33877359	2.07986415
C	-0.74783472	2.79246239	-0.49634905
C	2.68636298	-0.68107337	0.69371471
C	0.24545318	-2.40779187	-1.50810147
C	-1.81166807	2.32109529	0.46186433
C	-2.09083927	-1.80885250	-1.43623319
C	1.98905642	-1.16297512	1.94537753
C	-2.98710208	0.47934318	-0.66138288
H	1.34088312	3.71831462	0.84311732
H	2.11897020	2.13936056	1.19140894
H	0.52151309	2.47619749	1.86388292
H	-0.13754713	-2.89808368	1.11083459
H	-1.33885587	-3.79731908	0.11513814
H	-1.84452284	-2.43215234	1.16269651
H	1.72516763	3.39013084	-1.37124029
H	0.84752367	2.13325377	-2.29330345
H	-4.08801624	-1.12618589	-1.49768487
H	-3.55848514	-1.46558121	0.13701825
H	1.68274733	-2.78240996	0.04175363
H	2.39856339	-2.49945477	-1.55145706
H	-1.90401272	0.77521173	2.52044535
H	-2.61993279	-0.67236671	1.78170003
H	-3.55109979	0.85856358	1.82254107
H	3.43990047	-0.52790178	-1.79734727
H	1.83856545	-0.19557974	-2.52973372
H	3.26890183	1.80275513	-2.31643082
H	3.34430020	1.65706710	-0.57652839
H	-0.59707504	3.87920948	-0.39595673
H	-1.03519136	2.56132041	-1.52713127
H	2.99011393	0.35724845	0.84189491
H	3.58940850	-1.27506511	0.46779429
H	0.08143821	-3.48085751	-1.69569470
H	0.18073365	-1.86019365	-2.45373870
H	-1.52937551	2.57318970	1.49052546

H	-2.77293819	2.81239875	0.24777533
H	-2.41535594	-2.84551402	-1.62791770
H	-1.81960610	-1.33993345	-2.38754466
H	1.85826673	-2.25536234	1.95456184
H	2.60333454	-0.90289225	2.81735751
H	-3.93299760	0.97535345	-0.38404028
H	-2.62020280	0.89692276	-1.60614337
O	-0.38415304	0.32071082	-1.83557686

$Fe^{IV}(O)(TMCSO_2)^+$, i.s.

Fe	-0.41610822	-0.09139210	-0.15759261
O	-1.58600311	-0.60505079	-1.22229190
N	-0.84084268	-1.81513850	0.94771045
N	-1.87685493	0.82873932	1.10278838
N	-0.15664659	1.68838021	-1.30405116
N	1.00062720	-0.93174377	-1.43628496
C	-2.26872382	-1.61123151	1.34515909
C	-2.42952833	-0.25919675	1.98335442
C	-2.96915843	1.35086272	0.21972671
C	-2.53926463	2.44253374	-0.75775731
C	-1.50895128	2.08473585	-1.82651198
C	0.73174251	1.33617629	-2.47112828
C	0.79395349	-0.15396823	-2.70669842
C	0.68227343	-2.36219676	-1.78127801
C	0.51567576	-3.29605923	-0.59398758
C	-0.79349292	-3.06976989	0.13975025
C	-0.00058830	-1.99598658	2.16229644
C	-1.44037366	1.90276279	2.03763198
C	0.46463406	2.87591850	-0.65579902
C	2.44697963	-0.93317532	-1.01685372
S	2.47442422	0.50805178	1.35933915
C	3.03907042	0.30791852	-0.38348010
H	-2.57227071	-2.40539103	2.04564468
H	-2.86992626	-1.68270235	0.43276795
H	-1.88640196	-0.22149901	2.93413316
H	-3.48842542	-0.05340380	2.19850753
H	-3.75489146	1.75914127	0.87844225
H	-3.37243863	0.49066375	-0.32602889
H	-3.44851136	2.73705856	-1.30270738
H	-2.22636361	3.34306499	-0.21136836
H	-1.86799096	1.24836189	-2.43578419
H	-1.35942580	2.96459489	-2.47539313
H	0.35284907	1.82966189	-3.37803447
H	1.72518347	1.74913408	-2.28021601
H	1.59892430	-0.39411451	-3.41855006
H	-0.16048303	-0.49257546	-3.12072879
H	1.48415132	-2.72044272	-2.44620269
H	-0.25808863	-2.34907273	-2.34269842
H	1.37392457	-3.26756966	0.09148358
H	0.48691956	-4.31744783	-0.99875659
H	-1.60491669	-3.00456281	-0.59528444
H	-1.00295484	-3.90816467	0.82430791
H	-0.38499004	-2.85677488	2.73404674
H	-0.02366372	-1.09231019	2.77545201
H	1.03950505	-2.15951666	1.86956215
H	-2.27610134	2.13563547	2.71699799
H	-1.17155487	2.81223950	1.50145938
H	-0.57535345	1.55213263	2.60658033
H	0.60697802	3.65941034	-1.41707260
H	1.42953006	2.60600384	-0.22184790
H	-0.17181515	3.27048657	0.13452446
H	3.03163768	-1.19077782	-1.91571502
H	2.57697031	-1.74950519	-0.29473437
H	4.12671589	0.16806961	-0.31105597
H	2.85422949	1.24685234	-0.91198430
O	0.91951102	0.51524597	1.13831894
O	2.93855766	-0.78123263	2.00542086

$Fe^{IV}(O)(N4Py)^{2+}$, i.s.

O	0.15211313	2.30381473	0.00000000
Fe	0.04604424	0.65865309	0.00000000
N	-0.10814791	-1.40817524	0.00000000
C	-1.61511264	-1.48193973	0.00000000
C	3.39186205	-0.36584882	-3.18427624
C	-2.06501569	-0.69212854	-1.21079343
C	-3.08154366	-1.04660577	-2.08397766
C	-3.39679854	-0.16445689	3.12276834
C	-3.39679854	-0.16445689	-3.12276834

C	3.24139474	0.95796770	-2.76728814
C	-2.68662638	1.02946063	-3.25077979
C	0.52715135	-1.94058646	-1.24311912
C	-1.66933340	1.31865098	-2.34403930
C	2.24415990	1.26713429	-1.85108162
N	-1.37486506	0.46766767	-1.34797902
C	0.52715135	-1.94058646	1.24311912
N	-1.37486506	0.46766767	1.34797902
N	1.41359004	0.32013291	-1.36934811
C	1.54343694	-0.96681277	1.77348448
C	2.53268243	-1.33996846	2.67813583
C	-1.66933340	1.31865098	2.34403930
C	3.39186205	-0.36584882	3.18427624
C	2.53268243	-1.33996846	-2.67813583
C	3.24139474	0.95796770	2.76728814
C	-2.68662638	1.02946063	3.25077979
C	2.24415990	1.26713429	1.85108162
C	1.54343694	-0.96681277	-1.77348448
N	1.41359004	0.32013291	1.36934811
C	-2.06501569	-0.69212854	1.21079343
C	-3.08154366	-1.04660577	2.08397766
H	-1.99426323	-2.50865296	0.00000000
H	4.17219818	-0.63858969	-3.89286943
H	-3.60747323	-1.99066261	-1.95452663
H	-4.18925489	-0.41263887	3.82653176
H	-4.18925489	-0.41263887	-3.82653176
H	3.89126349	1.74870633	-3.13565955
H	-2.91004375	1.73850901	-4.04492691
H	-0.25140417	-2.08379601	-2.00489311
H	0.97676085	-2.92235027	-1.05570887
H	-1.07784421	2.23048931	-2.38721349
H	2.07966654	2.27464401	-1.47607686
H	0.97676085	-2.92235027	1.05570887
H	-0.25140417	-2.08379601	2.00489311
H	2.61678249	-2.38357092	2.97686592
H	-1.07784421	2.23048931	2.38721349
H	4.17219818	-0.63858969	3.89286943
H	2.61678249	-2.38357092	-2.97686592
H	3.89126349	1.74870633	3.13565955
H	-2.91004375	1.73850901	4.04492691
H	2.07966654	2.27464401	1.47607686
H	-3.60747323	-1.99066261	1.95452663

$Fe^{IV}(O)(TMG_3tren)^{2+}$, h.s.

Fe	-0.00827748	-0.00396183	0.37935886
O	-0.03035014	0.00839032	-1.26727296
N	0.02073348	-0.01976215	2.51108939
N	1.95262572	-0.30228543	0.62659546
N	-1.23745489	-1.55494280	0.66142424
N	-0.72773869	1.83575967	0.67907461
N	4.10378173	-0.01539699	-0.32740901
N	2.54437595	-1.41007586	-1.34044789
N	-2.08562910	-3.56379728	-0.26975450
N	-2.54420381	-1.51748788	-1.27157609
N	-2.06870352	3.57231744	-0.21929648
N	-0.09112453	2.94947221	-1.27009982
C	1.35074681	-0.54420602	2.93838237
C	-3.02025967	-0.15614392	-1.07706841
C	-0.18378026	1.38415732	2.97360084
C	2.41233583	-0.01109641	1.99288529
C	-3.34825932	3.13308694	0.32601968
C	-2.05123752	4.94524829	-0.72125231
C	2.85464354	-0.55769364	-0.33408974
C	4.37943077	1.31317113	0.20774780
C	5.26949288	-0.72137073	-0.85629215
C	2.97960806	-1.18934153	-2.71504855
C	1.60186321	-2.50401417	-1.16041054
C	-1.08615469	-0.90933132	2.96922527
C	-1.19009690	2.05735108	2.05744145
C	-0.51635536	3.24028297	-2.63483731
C	-1.17957113	-2.09668353	2.02738434
C	1.33029349	2.68083225	-1.11111276
C	-0.97245829	2.76553948	-0.25775244
C	-1.93234533	-2.21074191	-0.28131476
C	-1.06013289	-4.46689150	0.24079046
C	-3.28899864	-4.22169447	-0.77629204
C	-2.59610970	-2.00043971	-2.64697214
H	1.31961325	-1.63795270	2.86864452
H	1.54982844	-0.26035975	3.98277677

H	-2.34005481	0.56765621	-1.55072532
H	-3.07142670	0.05077973	-0.00326950
H	-4.02460502	-0.06873237	-1.51902243
H	0.77798106	1.90580997	2.90153656
H	-0.51408083	1.39131952	4.02339963
H	2.54893800	1.06980825	2.15535269
H	3.37742453	-0.49554893	2.19904152
H	-4.14465702	3.40191511	-0.38333972
H	-3.55998169	3.61756264	1.29165181
H	-3.34774129	2.04918224	0.45818680
H	-1.01982310	5.26155244	-0.90843016
H	-2.49861076	5.60068757	0.04044662
H	-2.63402178	5.03915839	-1.65071754
H	4.99282389	1.86552223	-0.51910031
H	4.92918643	1.25584337	1.15974971
H	3.44470432	1.85605177	0.36245273
H	5.62288888	-0.26455790	-1.79377096
H	5.01967929	-1.77175442	-1.03848686
H	6.07819580	-0.66490187	-0.11279239
H	2.08693505	-1.13702856	-3.35735410
H	3.62261729	-2.01120755	-3.06570886
H	3.52754150	-0.24483237	-2.79174951
H	0.63570717	-2.26814125	-1.63110927
H	1.44683230	-2.66434462	-0.08886734
H	2.02594661	-3.41301719	-1.61377085
H	-2.01981290	-0.33613534	2.92397088
H	-0.91204468	-1.22264113	4.00978490
H	-2.19201986	1.63161544	2.22541625
H	-1.25020810	3.13054609	2.28785815
H	-0.12955550	4.21396631	-2.97246951
H	-1.60913005	3.24398861	-2.69843527
H	-0.12335619	2.45239957	-3.29588716
H	-0.30801255	-2.75534325	2.16897491
H	-2.07614221	-2.68986805	2.25739771
H	1.60467177	1.73018151	-1.59277433
H	1.56173513	2.61983633	-0.04279650
H	1.89683830	3.50709430	-1.56699893
H	-0.90273063	-5.27214885	-0.49169834
H	-1.36399487	-4.91782579	1.19801455
H	-0.11972033	-3.92923790	0.37761455
H	-3.09259243	-4.74027792	-1.72777005
H	-4.08347079	-3.48283736	-0.92498679
H	-3.61745947	-4.96346036	-0.03355674
H	-2.12145300	-1.24902340	-3.29681137
H	-3.63547891	-2.15119606	-2.97664045
H	-2.04827668	-2.94375608	-2.73803830

$Fe^{IV}(O)(tpa^{Ph})^{-}$, h.s.

Fe	0.00000000	0.00000000	1.02924975
N	1.94537805	0.00000000	1.29153658
N	-0.97268902	-1.68474681	1.29153658
N	0.00000000	0.00000000	3.27769850
C	-0.72108886	-1.24896254	3.73124498
C	-0.72108886	1.24896254	3.73124498
C	1.44217772	0.00000000	3.73124498
C	-1.20642464	-2.08958877	2.58715183
C	-1.20642464	2.08958877	2.58715183
C	2.41284928	0.00000000	2.58715183
C	-1.90064808	-3.29201903	2.58982931
C	-2.09950483	-3.63644903	1.21676596
C	-1.51917176	-2.63128267	0.44795345
C	-1.90064808	3.29201903	2.58982931
C	-2.09950483	3.63644903	1.21676596
C	-1.51917176	2.63128267	0.44795345
C	3.80129615	0.00000000	2.58982931
C	4.19900965	0.00000000	1.21676596
C	3.03834351	0.00000000	0.44795345
H	-1.56641525	-0.95892852	4.37036399
H	-0.04724883	-1.83601966	4.37036399
H	-0.04724883	1.83601966	4.37036399
H	-1.56641525	0.95892852	4.37036399
H	1.61366408	-0.87709114	4.37036399
H	1.61366408	0.87709114	4.37036399
H	-2.22511406	-3.85401060	3.46270799
H	-2.60815271	-4.51745301	0.83035805
H	-3.30485615	-1.42875534	-1.19525195
H	-2.22511406	3.85401060	3.46270799
H	-2.60815271	4.51745301	0.83035805
H	0.41508965	3.57646706	-1.19525195

H	4.45022811	0.00000000	3.46270799
H	5.21630542	0.00000000	0.83035805
H	2.88976650	-2.14771171	-1.19525195
O	0.00000000	0.00000000	-0.60132014
C	2.92014199	0.00000000	-1.02768261
C	2.87741311	1.20497273	-1.74412827
C	2.79984547	1.20816106	-3.13841121
C	2.76302909	0.00000000	-3.84068700
C	2.79984547	-1.20816106	-3.13841121
C	2.87741311	-1.20497273	-1.74412827
H	2.88976650	2.14771171	-1.19525195
H	2.75680616	2.15539303	-3.67721335
H	2.69712522	0.00000000	-4.92969610
H	2.75680616	-2.15539303	-3.67721335
C	-1.46007099	2.52891714	-1.02768261
C	-2.48224355	1.88942648	-1.74412827
C	-2.44622091	1.82065677	-3.13841121
C	-1.38151455	2.39285339	-3.84068700
C	-0.35362456	3.02881784	-3.13841121
C	-0.39516956	3.09439922	-1.74412827
H	-3.30485615	1.42875534	-1.19525195
H	-3.24502820	1.30976765	-3.67721335
H	-1.34856261	2.33577895	-4.92969610
H	0.48822204	3.46516068	-3.67721335
C	-1.46007099	-2.52891714	-1.02768261
C	-0.39516956	-3.09439922	-1.74412827
C	-0.35362456	-3.02881784	-3.13841121
C	-1.38151455	-2.39285339	-3.84068700
C	-2.44622091	-1.82065677	-3.13841121
C	-2.48224355	-1.88942648	-1.74412827
H	0.41508965	-3.57646706	-1.19525195
H	0.48822204	-3.46516068	-3.67721335
H	-1.34856261	-2.33577895	-4.92969610
H	-3.24502820	-1.30976765	-3.67721335
N	-0.97268902	1.68474681	1.29153658

$[Sc(OTf)_4(OH)]^{2-}$

F	-3.77822674	-0.95560351	2.63292361
Sc	-0.13211717	0.34854992	-0.36185038
S	-1.18039011	-0.81995546	2.06599435
S	2.28913489	2.04854653	1.34695289
S	-3.11335420	0.43491158	-2.08030283
S	2.30340017	-1.57659653	-1.93487925
O	3.38450272	-0.60477919	-2.01993523
O	1.58235554	0.81795159	0.86261235
O	-1.94876476	-0.15841586	-1.33747979
O	0.98127091	-0.97871662	-1.53289465
O	-1.41120248	0.54514283	1.48370103
O	2.74794588	1.93388348	2.72644066
O	1.62545520	3.29852373	0.96097151
F	-2.74543740	-2.88894276	2.58438928
F	2.86078324	-1.89251659	0.66511814
C	-2.85781500	-1.68941609	1.98380067
O	-0.07256014	2.08978789	-1.10603065
H	0.44558200	2.78545029	-0.65306353
C	3.86975122	2.04591422	0.32082526
C	2.73650196	-2.64246027	-0.44071794
F	3.91068982	-3.26384517	-0.68138225
O	-4.11688113	-0.57059212	-2.41597626
F	-5.01788786	2.12010353	-1.33636879
O	2.15117684	-2.53513126	-3.02558732
O	-0.32137394	-1.57280561	1.11796174
F	-3.11040651	2.44206741	-0.30756683
F	-3.24596248	-1.87165481	0.71472683
O	-2.72444992	1.37919150	-3.12279934
C	-3.95527020	1.50687948	-0.77397202
F	3.58330781	2.23443275	-0.97950680
F	1.78685665	-3.57466514	-0.23636863
F	-4.38720631	0.75610400	0.25587055
F	4.53186664	0.88657865	0.46547813
O	-0.83607051	-0.85704489	3.47670454
F	4.66060472	3.05625698	0.74029738

$[Sc(OTf)_4(OH_2)]^{-}$

F	-4.18378755	1.07158145	0.86755525
Sc	0.08464835	0.00848968	-0.27772937
S	-1.84302398	2.14836652	1.54956692
S	2.70480179	1.83150035	-1.48444908

S	-2.17460617	-2.14496475	-1.67847589
S	1.30448898	-1.80624084	1.45395892
O	1.49701683	-1.69961757	-0.03223586
O	1.75102560	1.25903025	-0.45686298
O	-1.47046235	-1.36252837	-0.59391551
O	0.34904181	-0.69789610	1.80329566
O	-1.21178208	1.43683532	0.35975577
O	2.99190443	3.23703881	-1.26495564
O	2.36771237	1.40081548	-2.84901285
F	-3.93674668	1.45870694	3.00928195
F	3.17874725	0.02536899	1.93097211
C	-3.32036667	1.02829442	1.89577720
O	0.09745171	0.07323480	-2.37299263
H	0.88239999	0.45324027	-2.84709832
C	4.31845122	0.92322625	-1.10199442
C	2.94763206	-1.26221451	2.21859785
F	3.93469751	-2.02067547	1.72285643
O	-2.51193296	-3.49829780	-1.27788904
F	-4.52540601	-1.71619461	-2.81910299
O	1.03864679	-3.11860796	1.99700492
O	-1.01974527	2.08263325	2.74596988
F	-3.58271414	0.08584138	-2.00019806
F	-2.91033657	-0.23949472	2.07622012
O	-1.54777318	-1.95387412	-2.99454270
C	-3.81507221	-1.22221191	-1.79340410
F	4.09441257	-0.39881971	-1.01265710
F	2.87668710	-1.42009556	3.54604093
F	-4.50836675	-1.37874672	-0.65527311
F	4.83729230	1.36659566	0.05314500
O	-2.41610882	3.42488172	1.15150775
F	5.18714560	1.15928054	-2.09716990
H	-0.35906863	-0.63535374	-2.89582135

$Fe^{IV}(O)(Sc^{3+}(OTf)_4OH)^0$, h.s.

Fe	0.00026303	-2.61406175	-0.04964075
Sc	0.00452265	1.25506447	0.06370245
S	2.28897616	1.41174186	-2.54683388
S	-2.10316779	1.41057202	-2.83967026
S	2.15555898	1.29231494	2.84153158
S	-2.28194540	1.31406001	2.63172447
O	0.02002533	-0.92448230	-0.14575477
O	-1.24571348	1.13966715	-1.64782031
O	1.31104611	0.81954667	1.70192474
O	-1.73061734	0.81920452	1.32653426
O	1.78712884	1.34399239	-1.13401729
O	-2.47540387	0.18954024	-3.55141656
O	-1.65989294	2.54897567	-3.63626105
C	2.38732618	-2.84854804	-1.60182460
H	3.44158009	-3.13640551	-1.71662408
H	2.25845711	-1.82855538	-1.98501817
O	-0.17608138	3.12001430	0.44984737
H	-0.70285928	3.40174626	1.22132210
N	-2.07376256	-2.78966569	0.04012196
C	-2.51987288	-4.12513642	-0.49389137
H	-3.59553737	-4.18951755	-0.26864050
H	-2.00997948	-4.91126321	0.07837754
F	4.52369212	2.49017235	2.86653312
N	-0.07291908	-3.27505818	2.01151937
O	1.99731976	0.20667753	-3.32280223
N	2.07351024	-2.81406095	-0.12809891
F	4.49680608	0.17538332	-1.67898558
O	1.58104424	2.39697665	3.59963159
N	0.05845162	-3.41555959	-2.06363073
F	-3.49522196	3.05681759	-1.25891879
F	-4.47637350	-0.01909988	1.88752786
F	4.25022647	1.09268643	1.20101464
F	-4.23291181	0.99305848	-1.28541809
O	2.06097495	2.70048025	-3.18926449
F	-4.59526622	2.30871175	-2.99916065
F	4.56785632	2.35891173	-1.50627682
O	-2.02304124	2.73018737	2.88599213
F	4.77137110	1.40782557	-3.46827972
C	-0.28244485	-2.30349960	-3.00282513
H	-0.18390361	-2.68241872	-4.03240831
H	0.39595162	-1.46004457	-2.84543596
H	-1.30281582	-1.95461482	-2.84583569
F	-4.79819108	1.47721328	3.45637804
O	2.71601850	0.17076429	3.59504156
O	-2.05883776	0.37410355	3.72738713

F	3.26795139	3.05105484	1.16155632
C	-2.83471406	-1.68797504	-0.61368112
H	-2.65269846	-1.65614795	-1.68782178
H	-2.53094632	-0.74163217	-0.16496719
H	-3.90617191	-1.86992484	-0.43725232
C	2.84311546	-1.67138801	0.43854953
H	2.69339680	-1.58211978	1.51483795
H	2.51571898	-0.75165753	-0.04957645
H	3.90999217	-1.85451998	0.23847096
C	-0.81930068	-4.59663399	-2.30799665
H	-0.43062426	-5.42309928	-1.69555240
H	-0.70990615	-4.87673251	-3.36797128
C	-2.27950192	-4.35633351	-1.97418806
H	-2.82086850	-5.27542778	-2.23411766
H	-2.71575561	-3.56118631	-2.59143641
C	0.79483917	-4.44612937	2.32989304
H	0.67776293	-4.66159844	3.40376870
H	0.40187832	-5.30382126	1.76513222
C	4.15217723	1.33710317	-2.27377403
C	-2.39304077	-2.71697586	1.51092296
H	-3.45175559	-2.98068647	1.64321769
H	-2.24957693	-1.67412463	1.81752016
C	-1.49722387	-3.64288847	2.28809606
H	-1.69351351	-3.55684979	3.36623034
H	-1.64808811	-4.69060204	2.00818936
C	3.64230611	2.03285581	1.95532773
C	0.27989507	-2.10907777	2.87688585
H	-0.40619384	-1.27862844	2.68485256
H	1.29533115	-1.76554615	2.68151073
H	0.19999385	-2.42585943	3.92897521
C	-3.70853270	1.98196116	-2.03950181
C	1.47899418	-3.81593257	-2.31072245
H	1.61765277	-4.84248425	-1.95563638
H	1.67692247	-3.80831402	-3.39187094
C	2.51575378	-4.10812106	0.50104858
H	3.59396059	-4.18779387	0.29188399
H	2.01112130	-4.93078673	-0.02209556
C	2.25941393	-4.23850731	1.99164894
H	2.79054660	-5.14256799	2.31765782
H	2.69655272	-3.40780022	2.55975577
F	-4.50751884	2.11236155	1.38180173
C	-4.13772269	1.21714525	2.31268132

$Fe^{III}(O)(Sc^{3+}(OTf)_4OH_2)^0$, h.s.

Fe	0.02052723	-2.51887301	-0.41648157
Sc	-0.03417681	1.07340605	0.15938926
S	2.26485501	2.06978996	-2.27206189
S	-2.23249495	2.03340405	-2.35041810
S	2.01877401	1.13019712	2.90186549
S	-2.21195485	0.84366909	2.86531313
O	-0.05365179	-0.84015549	0.12279265
O	-1.66052649	1.17020091	-1.26778354
O	1.60812752	1.36043101	1.47110440
O	-1.45990468	1.38377937	1.68026020
O	1.47074366	1.10540722	-1.43812381
O	-2.14386981	1.43722522	-3.67528401
O	-1.84250977	3.44608501	-2.21526689
C	2.45192247	-2.30443886	-2.07270366
H	3.49011244	-2.52884547	-2.36504657
H	2.30264962	-1.22077091	-2.14833871
O	-0.02356532	3.32133744	-0.11604269
H	-0.72873554	3.57353096	-0.76380525
N	-2.15916016	-2.99200764	-0.38313479
C	-2.60779752	-4.01959812	-1.36829707
H	-3.69829477	-4.14273712	-1.24728949
H	-2.13405232	-4.97565953	-1.10682595
F	4.42397751	1.15785614	4.00178355
N	0.05098767	-3.89785856	1.26340468
O	2.15226241	1.81690319	-3.70078392
N	2.23478712	-2.68042014	-0.64458408
F	4.30308936	0.34628422	-2.19588560
O	1.61763589	2.21352396	3.79223428
N	0.07032405	-2.71907803	-2.58808807
F	-4.28812306	2.65217802	-0.76925980
F	-4.35672672	0.60277691	1.29117218
F	4.40497216	0.35061898	1.96730511
F	-4.51779089	0.75340375	-1.83895451
O	2.13701632	3.46258391	-1.81670684
F	-4.74581036	2.65123913	-2.91047714

F	4.24617923	1.75260744	-0.51832265
O	-1.95640594	1.60079720	4.08411602
F	4.87570978	2.43836122	-2.50029651
C	-0.30610278	-1.39805003	-3.16868085
H	-0.29982589	-1.47007691	-4.26904119
H	0.40707975	-0.63418619	-2.84234737
H	-1.29985466	-1.09654876	-2.82813611
F	-4.80271615	0.91801185	3.41134057
O	1.80431153	-0.24059901	3.35283688
O	-2.20192841	-0.61319291	2.95324461
F	4.22823269	2.51094390	2.29046380
C	-2.97073957	-1.75946781	-0.54116959
H	-2.83899678	-1.33616637	-1.53995350
H	-2.64350395	-1.02418281	0.19880526
H	-4.03679791	-2.00109397	-0.39138567
C	2.94655830	-1.68581124	0.19893717
H	2.79242849	-1.89471266	1.26096477
H	2.55629196	-0.68826031	-0.01773372
H	4.02653050	-1.72536675	-0.02267160
C	-0.79891861	-3.79885446	-3.15370937
H	-0.40776327	-4.75697713	-2.77956132
H	-0.66280223	-3.78643282	-4.24851208
C	-2.27715606	-3.69506756	-2.81774589
H	-2.78782136	-4.44770303	-3.43438294
H	-2.69299281	-2.72593926	-3.12380409
C	1.03820789	-5.01881349	1.17447121
H	0.93801263	-5.61519701	2.09732544
H	0.72891668	-5.65406361	0.33077381
C	4.04262949	1.61960939	-1.83857785
C	-2.37678415	-3.50223244	1.00340858
H	-3.37545321	-3.96110398	1.07804510
H	-2.34639441	-2.63865381	1.67898079
C	-1.31075128	-4.50826832	1.37245398
H	-1.46613481	-4.87375523	2.39909953
H	-1.34472193	-5.37691701	0.70396448
C	3.89101674	1.30105448	2.77189108
C	0.30959947	-3.06995665	2.47662675
H	-0.46462886	-2.30124706	2.57027867
H	1.27240077	-2.56043514	2.39316745
H	0.30947845	-3.72258947	3.36543596
C	-4.07060463	2.01966211	-1.93433770
C	1.48186727	-3.03254787	-2.97446068
H	1.61794364	-4.11799115	-2.90253594
H	1.64546975	-2.74795197	-4.02495878
C	2.79785692	-4.04022247	-0.39387165
H	3.89011662	-3.98053990	-0.54318012
H	2.39490585	-4.72510783	-1.15229016
C	2.48863752	-4.60649031	0.98459257
H	3.08645710	-5.52245370	1.09043525
H	2.82486180	-3.93495457	1.78556689
F	-4.11442742	2.59262601	2.17762842
C	-3.98646568	1.27289153	2.40009185
H	0.81155562	3.57841122	-0.58192384

Fe^{III}(OO)(TMC)+, h.s.

Fe	0.00131040	-0.00011624	-0.47700717
N	1.72584928	-1.34311744	-0.07292790
N	-1.72179902	1.34871475	-0.08628908
N	-1.12416384	-1.73185155	0.46654643
N	1.12963235	1.74382442	0.44255958
C	2.00195858	1.38860187	1.59645284
H	2.49033045	2.31245019	1.95738311
H	1.34599040	1.02425325	2.40250250
C	-2.51030250	1.10258995	1.15549756
H	-3.34491204	1.82763183	1.17327584
H	-1.86607919	1.32030308	2.01818103
C	-1.99503465	-1.36296180	1.61738210
H	-1.33792704	-0.98954358	2.41823774
H	-2.48330323	-2.28238463	1.98959431
C	0.09533511	2.70505461	0.91705150
H	-0.20157783	2.41199940	1.93167592
H	0.51947045	3.72072875	0.98411099
C	1.10815776	-2.69685430	0.02229504
H	1.85547420	-3.42999615	0.36963715
H	0.79696701	-2.98108501	-0.99104215
C	3.06112630	0.33375973	1.30555932
H	3.73746932	0.31986507	2.17232710
H	3.68294401	0.61717057	0.44572404
C	-0.08888958	-2.68702546	0.95158289

H	-0.51289400	-3.70175780	1.03222989
H	0.20949084	-2.38108771	1.96213427
C	-1.10351261	2.70316283	-0.01013186
H	-0.79403816	2.97412910	-1.02765035
H	-1.84945248	3.44156403	0.32933816
C	2.62717450	-1.33337202	-1.25142621
H	3.40273620	-2.11049925	-1.13618979
H	3.10875517	-0.35583243	-1.35069775
H	2.02992332	-1.52540043	-2.14949757
C	2.51817903	-1.08191246	1.16325618
H	3.35324891	-1.80615760	1.18664860
H	1.87656429	-1.29032732	2.03024490
C	-1.93366728	-2.40021567	-0.58150421
H	-1.27434023	-2.76933752	-1.37435594
H	-2.63416240	-1.69016215	-1.03110902
H	-2.49252579	-3.24509178	-0.14041054
C	1.93766234	2.39878815	-0.61489755
H	1.27676519	2.76016657	-1.40996567
H	2.63575948	1.68257223	-1.05834700
H	2.49902025	3.24766398	-0.18473266
C	-2.62657958	1.32444425	-1.26185054
H	-3.10818067	0.34569180	-1.34787058
H	-2.03214196	1.50560663	-2.16400491
H	-3.40200674	2.10279339	-1.15373263
C	-3.05399285	-0.31091778	1.31629443
H	-3.67879570	-0.60403652	0.46191493
H	-3.72729883	-0.28547249	2.18512877
O	0.38561419	0.60099197	-2.27454083
O	-0.38741645	-0.62042444	-2.26661618

Fe^{III}(OO)(TMC)+, h.s.

Fe	-0.00107134	-0.00060946	0.30886769
N	2.01104404	0.91783826	0.01403380
N	-1.99645421	-0.94924996	0.06714291
N	-0.66380660	1.79210375	-0.66682334
N	0.70961752	-1.92888403	-0.31070154
C	1.70028736	-1.91535734	-1.43392664
H	1.95819072	-2.96550953	-1.64952213
H	1.18025532	-1.50992950	-2.31468307
C	-2.68861286	-0.64019819	-1.22126290
H	-3.66523085	-1.15354226	-1.20517978
H	-2.09781830	-1.07373841	-2.03903544
C	-1.59707949	1.58803967	-1.82113285
H	-1.03599472	1.03974826	-2.59238654
H	-1.83532113	2.58694844	-2.22242539
C	-0.48050286	-2.72323198	-0.75202610
H	-0.67608522	-2.47361818	-1.80146081
H	-0.24020632	-3.79546647	-0.70262581
C	1.69963261	2.36105232	-0.21132924
H	2.59026829	2.88053599	-0.59792197
H	1.45337714	2.80276593	0.76255464
C	2.96693921	-1.11574476	-1.17505633
H	3.64488047	-1.33482685	-2.01139038
H	3.48553163	-1.46215606	-0.27125439
C	0.54533819	2.51276043	-1.17662596
H	0.30137625	3.57549760	-1.32111225
H	0.79423943	2.09210928	-2.15783608
C	-1.67999326	-2.40855871	0.11484202
H	-1.48202420	-2.66938580	1.16206559
H	-2.55366941	-2.99030776	-0.21706044
C	2.85785681	0.82020311	1.23138104
H	3.77376618	1.41685829	1.08835820
H	3.14068810	-0.21950234	1.41848453
H	2.29677633	1.20055357	2.09171696
C	2.76302477	0.39159726	-1.16658240
H	3.73960970	0.90512119	-1.19241235
H	2.21421123	0.67372610	-2.07505200
C	-1.31365124	2.62232895	0.38767809
H	-0.59179316	2.85097697	1.17831188
H	-2.15377407	2.08327602	0.83336855
H	-1.67805408	3.55943971	-0.06301443
C	1.30327832	-2.57402920	0.89674756
H	0.54307936	-2.66146730	1.67988868
H	2.12927611	-1.97095619	1.28182247
H	1.67241009	-3.57567469	0.62468306
C	-2.90019782	-0.64220721	1.20705811
H	-3.20420921	0.40815904	1.18459188
H	-2.37487282	-0.84634237	2.14580234
H	-3.80363229	-1.26990117	1.13680400

C	-2.88161978	0.84258645	-1.49936226
H	-3.44686780	1.33868989	-0.69936333
H	-3.51029456	0.91325734	-2.39741999
O	0.05446799	-0.10291151	2.14721233
O	-0.25655108	1.05272684	2.93315332
H	-0.00492713	0.73571963	3.82647621

References

1. E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Berger, A. Bérces, F. M. Bickelhaupt, C. Bo, P. L. de Boeij, P. M. Boerrigter, S. Borini, R. E. Bulo, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, A. C. T. van Duin, D. E. Ellis, M. v. Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, T. Heine, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, E. S. Kadantsev, J. W. Kaminski, G. van Kessel, R. Klooster, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, J. N. Louwen, D. A. McCormack, E. McGarrity, A. Michalak, M. Mitoraj, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Romaniello, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, D. G. Skachkov, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo and A. L. Yakovlev, *ADF2012.01*, (2012) SCM, Amsterdam.
2. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931-967.
3. M. Swart and F. M. Bickelhaupt, *J. Comput. Chem.*, 2008, **29**, 724-734.
4. S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787-1799.
5. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
6. M. Swart, *J. Chem. Theory Comp.*, 2008, **4**, 2057-2066.
7. M. Swart, M. Solà and F. M. Bickelhaupt, *J. Chem. Phys.*, 2009, **131**, 094103.
8. N. C. Handy and A. J. Cohen, *Molec. Phys.*, 2001, **99**, 403-412.
9. M. Swart, A. W. Ehlers and K. Lammertsma, *Molec. Phys.*, 2004, **102**, 2467-2474.
10. W. G. Han and L. Noodleman, *Inorg. Chim. Acta*, 2008, **361**, 973-986.
11. A. Klamt and G. Schüürmann, *J. Chem. Soc. Perkin Trans. 2*, 1993, 799-805.
12. C. C. Pye and T. Ziegler, *Theor. Chem. Acc.*, 1999, **101**, 396-408.
13. M. Swart, E. Rösler and F. M. Bickelhaupt, *Eur. J. Inorg. Chem.*, 2007, 3646-3654.
14. C. E. MacBeth, A. P. Golombek, V. G. Young Jr., C. Yang, K. Kuczera, M. P. Hendrich and A. S. Borovik, *Science*, 2000, **289**, 938-941.
15. D. C. Lacy, R. Gupta, K. L. Stone, J. Greaves, J. W. Ziller, M. P. Hendrich and A. S. Borovik, *J. Am. Chem. Soc.*, 2010, **132**, 12188-12190.
16. J. U. Rohde, J. H. In, M. H. Lim, W. W. Brennessel, M. R. Bukowski, A. Stubna, E. Münck, W. Nam and L. Que Jr., *Science*, 2003, **299**, 1037-1039.
17. K. Ray, J. England, A. T. Fiedler, M. Martinho, E. Münck and L. Que Jr., *Angew. Chem. Int. Ed.*, 2008, **47**, 8068-8071.
18. J. Cho, S. Jeon, S. A. Wilson, L. V. Liu, E. A. Kang, J. J. Braymer, M. H. Lim, B. Hedman, K. O. Hodgson, J. S. Valentine, E. I. Solomon and W. Nam, *Nature*, 2011, **478**, 502-505.
19. F. Li, K. K. Meier, M. A. Cranswick, M. Chakrabarti, K. M. Van Heuvelen, E. Münck and L. Que Jr., *J. Am. Chem. Soc.*, 2011, **133**, 7256-7259.
20. C. V. Sastri, M. J. Park, T. Ohta, T. A. Jackson, A. Stubna, M. S. Seo, J. Lee, J. Kim, T. Kitagawa, E. Münck, L. Que Jr. and W. Nam, *J. Am. Chem. Soc.*, 2005, **127**, 12494-12495.
21. T. A. Jackson, J.-U. Rohde, M. S. Seo, C. V. Sastri, R. DeHont, A. Stubna, T. Ohta, T. Kitagawa, E. Münck, W. Nam and L. Que Jr., *J. Am. Chem. Soc.*, 2008, **130**, 12394-12407.
22. A. Thibon, J. England, M. Martinho, V. G. Young, Jr., J. R. Frisch, R. Guillot, J. J. Girerd, E. Münck, L. Que Jr. and F. Banse, *Angew. Chem. Int. Ed.*, 2008, **47**, 7064-7067.
23. M. R. Bukowski, K. D. Koehntop, A. Stubna, E. L. Bominaar, J. A. Halfen, E. Münck, W. Nam and L. Que Jr., *Science*, 2005, **310**, 1000-1002.
24. A. R. McDonald, M. R. Bukowski, E. R. Farquhar, T. A. Jackson, K. D. Koehntop, M. S. Seo, R. F. De Hont, A. Stubna, J. A. Halfen, E. Münck, W. Nam and L. Que Jr., *J. Am. Chem. Soc.*, 2010, **132**, 17118-17129.
25. E. J. Klinker, J. Kaizer, W. W. Brennessel, N. L. Woodrum, C. J. Cramer and L. Que, Jr., *Angew. Chem. Int. Ed.*, 2005, **44**, 3690-3694.
26. J. Kaizer, E. J. Klinker, N. Y. Oh, J.-U. Rohde, W. J. Song, A. Stubna, J. Kim, E. Münck, W. Nam and L. Que Jr., *J. Am. Chem. Soc.*, 2004, **126**, 472-473.
27. J. England, M. Martinho, E. R. Farquhar, J. R. Frisch, E. L. Bominaar, E. Münck and L. Que Jr., *Angew. Chem. Int. Ed.*, 2009, **48**, 3622-3626.
28. J. England, Y. Guo, E. R. Farquhar, V. G. Young Jr., E. Münck and L. Que Jr., *J. Am. Chem. Soc.*, 2010, **132**, 8635-8644.
29. J. P. Bigi, W. H. Harman, B. Lassalle-Kaiser, D. M. Robles, T. A. Stich, J. Yano, R. D. Britt and C. J. Chang, *J. Am. Chem. Soc.*, 2012, **134**, 1536-1542.
30. W.-g. Han, T. Liu, T. Lovell and L. Noodleman, *J. Comput. Chem.*, 2006, **27**, 1292-1306.
31. M. Güell, M. Solà and M. Swart, *Polyhedron*, 2010, **29**, 84-93.