SUPLEMENTARY INFORMATION

The effect of varying carboxylate ligation on the electronic environment of N_2O_x (x = 1-3) nonheme iron: A DFT analysis

Patrick J. Cappillino,[†] Joshua S. McNally,[†] Feng Wang[†] and John P. Caradonna[†]*

† Department of Chemistry, Boston University, Boston, MA 02215

* Corresponding author: Tel – (617) 353-1692 E-mail: caradonn@bu.edu

Table S1: AIM and NBO Charges

AIM

	$[Fe^{II}N_2O_1(H_2O)_3]^+$	$[Fe^{III}N_2O_1(H_2O)_3]^{2+}$	$[Fe^{II}N_2O_2(H_2O)_2]$	$[Fe^{III}N_2O_2(H_2O)_2]^+$	$[Fe^{II}N_2O_3(H_2O)]^-$	$[Fe^{III}N_2O_3(H_2O)]$
Fe	1.43	1.81	1.41	1.80	1.41	1.78
N1	-0.98	-1.00	-0.98	-0.99	-1.00	-1.00
N2	-0.99	-1.00	-0.98	-0.99	-0.99	-0.99
O1*	-1.22	-1.11	-1.23	-1.16	-1.23	-1.18
O2*	--	--	-1.23	-1.16	-1.23	-1.16
O3*	--	--	--	--	-1.23	-1.18
H2O1	-1.19	-1.20	-1.19	-1.20	-1.19	-1.20
H2O2	-1.19	-1.20	-1.18	-1.20	--	--
H2O3	-1.20	-1.21	--	--	--	--
sum	-5.34	-4.93	-5.37	-4.91	-5.46	-4.93

NBO

	$[Fe^{II}N_2O_1(H_2O)_3]^+$	$[Fe^{III}N_2O_1(H_2O)_3]^{2+}$	$[Fe^{II}N_2O_2(H_2O)_2]$	$[Fe^{III}N_2O_2(H_2O)_2]^+$	$[Fe^{II}N_2O_3(H_2O)]^-$	$[Fe^{III}N_2O_1(H_2O)_3]^{2+}$
Fe	1.48	1.78	1.46	1.77	1.46	1.76
N1	-0.62	-0.58	-0.62	-0.58	-0.62	-0.58
N2	-0.62	-0.58	-0.62	-0.58	-0.62	-0.59
O1*	-0.85	-0.78	-0.85	-0.81	-0.84	-0.82
O2*	--	--	-0.85	-0.81	-0.84	-0.81
O3*	--	--	--	--	-0.85	-0.82
H2O1	-0.99	-0.98	-0.99	-0.98	-0.98	-0.98
H2O2	-0.99	-0.98	-0.98	-0.98	--	--
H2O3	-0.99	-0.99	--	--	--	--
sum	-3.59	-3.11	-3.45	-2.97	-3.29	-2.82

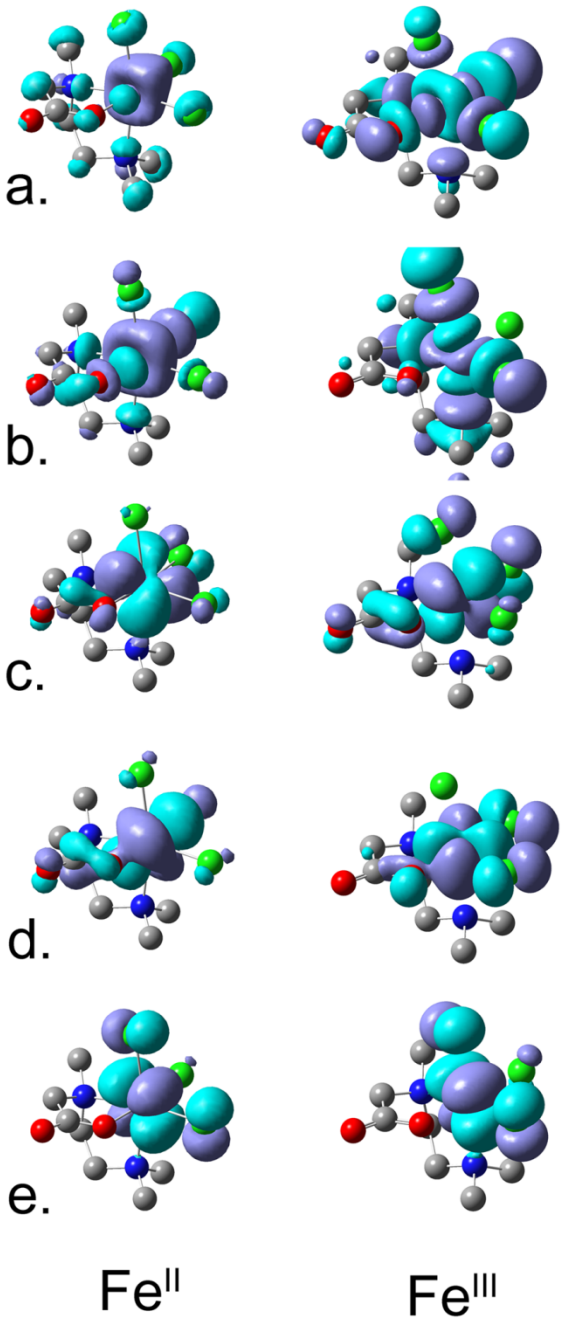

Figure S1. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_1 with L = Cl

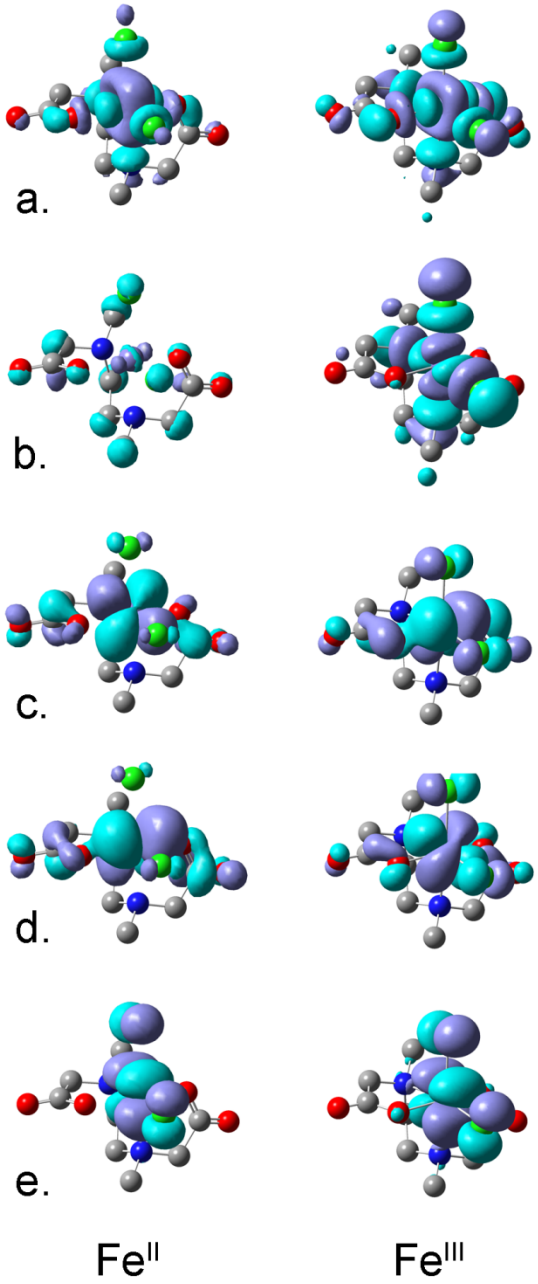

Figure S2. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_2 with L = Cl

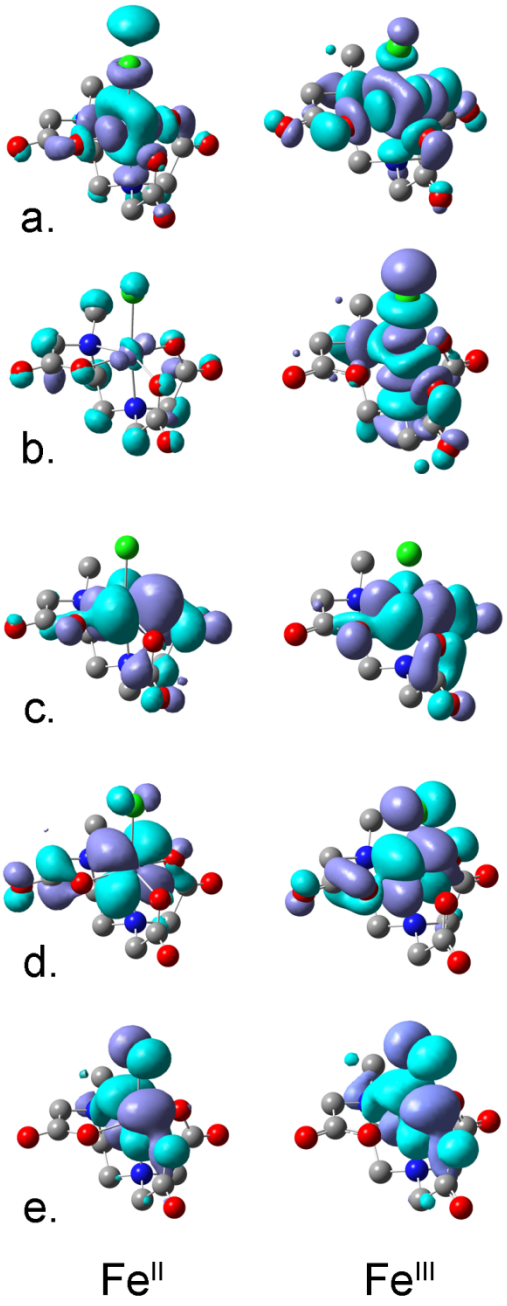

Figure S3. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_3 with L = Cl

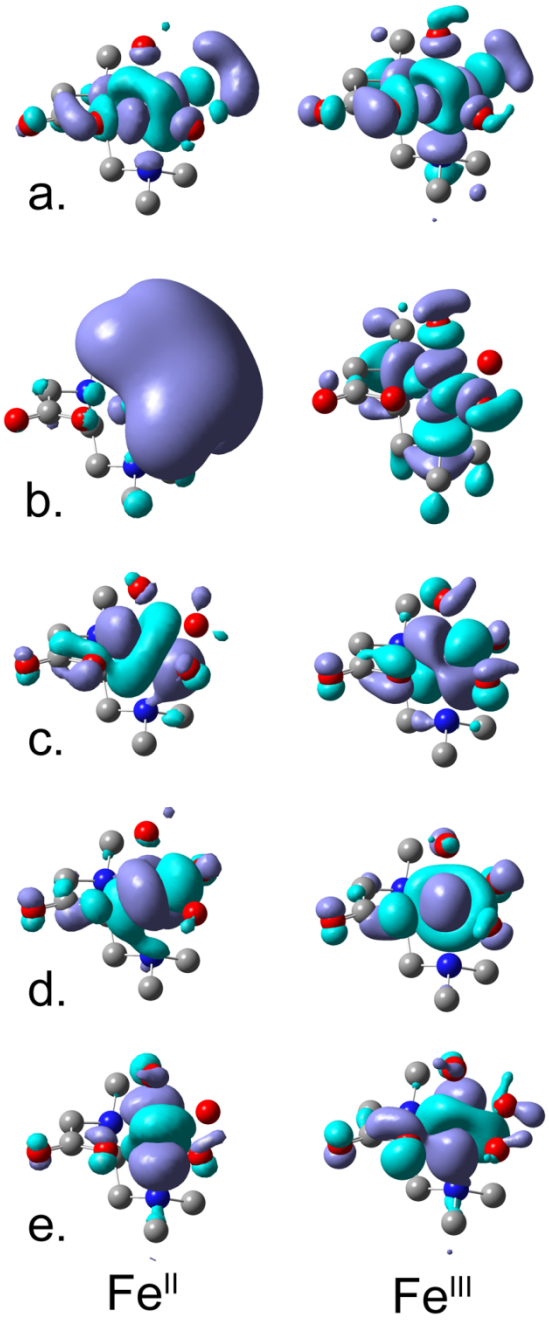

Figure S4. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_1 with L = H_2O

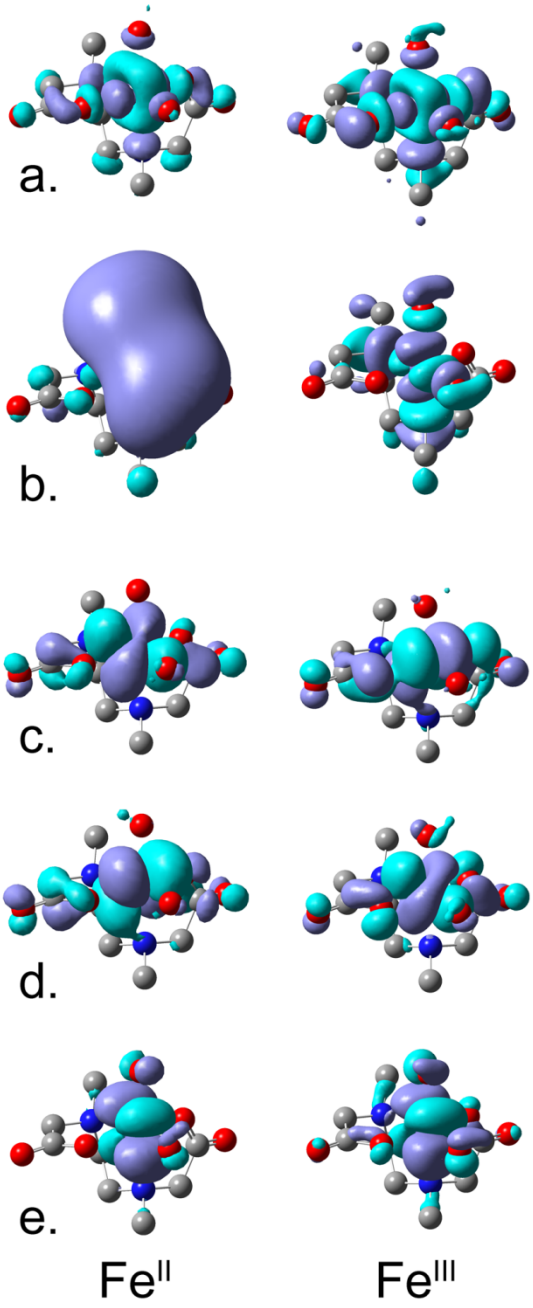

Figure S5. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_2 with L = H_2O

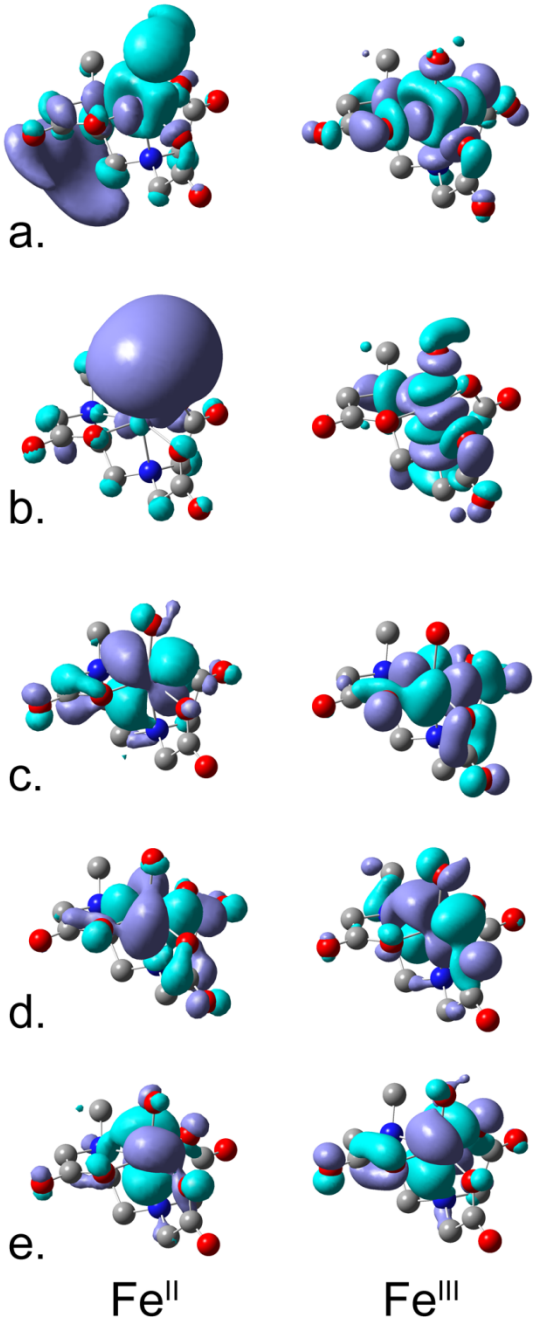

Figure S6. RAMO+4 (a), RAMO+3 (b), RAMO+2 (c), RAMO +1 (d), and RAMO (e) of Fe^{II} (left) and Fe^{III} (right) complexes of N_2O_3 with L = H_2O

Mulliken Population Analyses

Table 3.1 Mulliken Population Analyses for β HOMO to LUMO -3 for $[Fe^{II}(N_2O_1)(Cl)_3]^{2-}$

Frag.	0	(Fe-d):
Frag.	1	(Fe-s):
Frag.	2	(N1):
Frag.	3	(N2):
Frag.	4	(O7):
Frag.	5	(Cl28):
Frag.	6	(Cl29):
Frag.	7	(Cl30):
Frag.	8	(else):

MO	Energy(eV)	0	1	2	3	4	5	6	7	8	% Fe	% L	sum
81	-4.868	90.58	0.02	0.22	0.23	0.02	3.47	4.49	0.5	0.47	91	9	100
82	-0.807	91.8	1.65	-0.62	-0.13	0.47	0.62	0.62	2.07	3.51	93	4	98
83	-0.739	94.32	0.16	0.15	-0.09	0.74	0.05	0.9	1.57	2.2	94	3	98
84	-0.234	68.73	16.28	2.3	0.5	1.77	2.19	2.48	3.34	2.42	85	13	98
85	-0.129	10.96	132.8	2.08	-0.06	2.47	-3.12	0.6	-0.63	-45.11	78	9	87

Table 3.2 Mulliken Population Analyses for β HOMO to LUMO -3 for $[Fe^{II}(N_2O_2)(Cl)_2]^{2-}$

Frag.	0	(Fe-d):	Orbitals										
Frag.	1	(Fe-s):	Orbitals										
Frag.	2	(N26):	Orbitals										
Frag.	3	(N27):	Orbitals										
Frag.	4	(O28):	Orbitals										
Frag.	5	(O29):	Orbitals										
Frag.	6	(Cl23):	Orbitals										
Frag.	7	(Cl24):	Orbitals										
Frag.	8	(else):	Orbitals										
MO	Energy(eV)	0	1	2	3	4	5	6	7	8	% Fe	% L	sum
83	-4.744	91.21	0.28	0.24	0.23	0.07	0.06	3.73	3.73	0.47	91	8	99
84	-0.613	87.1	0	0.11	0.1	0.6	0.45	0.54	0.41	10.69	87	2	89
85	-0.595	91.98	0.14	0.02	0.05	0.31	0.44	0.38	0.51	6.17	92	2	94
86	-0.155	0.78	158.23	-0.28	-0.37	-0.24	-0.26	6.63	6.76	-71.3	0	11	11
87	0.046	68.28	9.97	-2.46	-2.51	3.8	3.83	-5.47	-5.44	30	52	22	74

Table 3.3 Mulliken Population Analyses for β HOMO to LUMO -3 for $[Fe^{II}(N_2O_3)(Cl)]^{2-}$

Frag.	0	(Fe-d):	Orbitals										
Frag.	1	(Fe-s):	Orbitals										
Frag.	2	(N4):	Orbitals										
Frag.	3	(N18):	Orbitals										
Frag.	4	(O1):	Orbitals										
Frag.	5	(O5):	Orbitals										
Frag.	6	(O6):	Orbitals										
Frag.	7	(Cl3):	Orbitals										
Frag.	8	(else):	Orbitals										
MO	Energy(eV)	0	1	2	3	4	5	6	7	8	% Fe	% L	sum
85	-4.57	90.09	-0.02	0.07	1.06	0.17	2.42	0.05	4.41	1.75	90	8	98
86	-0.589	90.64	0.35	0.53	-0.05	0.42	0.13	-0.04	1.63	6.38	90	3	93
87	-0.533	85.49	0.02	0.07	0.26	-0.15	-0.14	0.83	0.01	13.6	85	1	86
88	-0.164	1.42	205.7	-8.04	-5.31	-3.88	-3.48	-4.47	24.08	-106.05	0	32	32
89	0.189	61.81	4.96	0.94	0.23	3.29	0.9	3.07	-8.17	32.98	53	15	69

X, Y, Z Coordinates of the Geometry Optimized Structures

Table S5. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_1)(Cl)_3]^{2-}$

#	Z	X (Å)	Y (Å)	Z (Å)
1	7	0.6425	1.9770	-0.1125
2	7	-1.4240	0.1487	1.1245
3	6	-2.5576	-0.0556	0.1991
4	1	-3.3847	0.6343	0.4129
5	1	-2.9377	-1.0705	0.3432
6	6	-2.1945	0.0318	-1.2899
7	8	-0.9596	-0.0644	-1.5915
8	8	-3.1274	0.1495	-2.1059
9	6	0.9104	2.5001	-1.4644
10	1	0.1754	2.0983	-2.1606
11	1	1.8996	2.1739	-1.7849
12	1	0.8697	3.6005	-1.4811
13	6	1.6905	2.4672	0.8005
14	1	2.6566	2.0775	0.4790
15	1	1.5139	2.1122	1.8136
16	1	1.7274	3.5679	0.8007
17	6	-1.6311	-0.6393	2.3556
18	1	-2.5472	-0.3314	2.8809
19	1	-0.7745	-0.5057	3.0148
20	1	-1.6984	-1.6947	2.0933
21	6	-1.2451	1.5765	1.4801
22	1	-2.2018	2.0090	1.8125
23	1	-0.5626	1.6143	2.3315
24	6	-0.6943	2.4231	0.3383
25	1	-0.6611	3.4748	0.6643
26	1	-1.3696	2.3838	-0.5176
27	26	0.4689	-0.4555	-0.1178
28	17	-0.2863	-2.9775	-0.1543
29	17	2.4055	-0.7264	-1.7393
30	17	1.8572	-0.7482	1.9135

Table S6. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_1)(Cl)_3]^-$

#	Z	X (Å)	Y (Å)	Z (Å)
1	7	0.8670	1.8152	-0.0404
2	7	-1.3704	0.2017	1.1281
3	6	-2.5297	0.2048	0.2027
4	1	-3.2405	0.9991	0.4580
5	1	-3.0562	-0.7478	0.3031
6	6	-2.1411	0.3156	-1.2715
7	8	-0.9011	0.0918	-1.5463
8	8	-3.0093	0.5727	-2.1070
9	6	1.1578	2.3736	-1.3823
10	1	0.3726	2.0843	-2.0777
11	1	2.1063	1.9769	-1.7393
12	1	1.2208	3.4687	-1.3305
13	6	2.0007	2.1498	0.8523
14	1	2.8967	1.6387	0.5014
15	1	1.7993	1.8220	1.8690
16	1	2.1753	3.2338	0.8465
17	6	-1.6908	-0.6240	2.3181
18	1	-2.5656	-0.2170	2.8403
19	1	-0.8370	-0.6327	2.9924
20	1	-1.8969	-1.6447	2.0006
21	6	-1.0150	1.5758	1.5781
22	1	-1.9111	2.0847	1.9592
23	1	-0.3187	1.4737	2.4123
24	6	-0.3930	2.4134	0.4736
25	1	-0.2001	3.4249	0.8566
26	1	-1.0848	2.5231	-0.3627
27	26	0.4168	-0.5362	-0.1574
28	17	-0.5166	-2.7346	-0.2526
29	17	2.1605	-0.8516	-1.6862
30	17	1.6606	-0.9687	1.7946

Table S7. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_2)(Cl)_2]^{2-}$

#	Z	X (Å)	Y (Å)	Z (Å)
1	6	-0.2623	-2.2466	-0.6869
2	1	0.5911	-2.2731	-1.3674
3	1	-0.8329	-3.1727	-0.8553
4	6	0.2229	-2.2279	0.7545
5	1	-0.6303	-2.2190	1.4358
6	1	0.7785	-3.1574	0.9517
7	6	-1.1818	-0.9783	-2.5147
8	1	-1.6601	-1.8732	-2.9383
9	1	-0.1806	-0.8751	-2.9342
10	1	-1.7567	-0.0941	-2.7845
11	6	1.1665	-0.9188	2.5407
12	1	1.6300	-1.8083	2.9911
13	1	0.1681	-0.7856	2.9585
14	1	1.7573	-0.0370	2.7825
15	6	-2.4330	-1.1218	-0.4362
16	1	-2.7910	-2.1555	-0.3521
17	1	-3.1262	-0.5979	-1.1007
18	6	-2.5814	-0.4233	0.9302
19	6	2.4108	-1.1479	0.4653
20	1	2.7487	-2.1902	0.4083
21	1	3.1159	-0.6204	1.1142
22	6	2.5695	-0.4904	-0.9204
23	17	1.1967	2.4037	1.4366
24	17	-1.1436	2.3603	-1.4963
25	26	0.0031	0.7224	-0.0122
26	7	-1.0834	-1.0648	-1.0424
27	7	1.0637	-1.0492	1.0718
28	8	-1.7109	0.4468	1.2460
29	8	1.7064	0.3754	-1.2672
30	8	-3.5858	-0.7253	1.6071
31	8	3.5749	-0.8196	-1.5830

Table S8. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_2)(Cl)_2]^-$

#	Z	X (Å)	Y (Å)	Z (Å)
1	6	0.0000	0.0000	0.0000
2	1	0.0000	0.0000	1.0912
3	1	1.0514	0.0000	-0.3184
4	6	-0.6781	-1.2510	-0.5303
5	1	-0.6347	-1.2754	-1.6205
6	1	-0.1326	-2.1340	-0.1702
7	6	-0.2054	2.3720	0.4029
8	1	0.8845	2.4827	0.3403
9	1	-0.4909	2.1752	1.4356
10	1	-0.6847	3.2933	0.0791
11	6	-2.7800	-2.3466	-0.9922
12	1	-2.3003	-3.3278	-0.8868
13	1	-2.7213	-2.0250	-2.0314
14	1	-3.8280	-2.4208	-0.7097
15	6	-0.4081	1.5398	-1.8787
16	1	0.5891	1.2049	-2.1863
17	1	-0.4468	2.6229	-2.0267
18	6	-1.4608	0.9539	-2.8237
19	6	-2.2724	-1.6812	1.2971
20	1	-1.4674	-2.3345	1.6526
21	1	-3.2116	-2.2281	1.4206
22	6	-2.3788	-0.4572	2.2107
23	17	-5.1585	0.0166	-0.3325
24	17	-3.4533	3.1149	-0.3765
25	26	-2.9563	0.8243	-0.3356
26	7	-0.6670	1.2507	-0.4495
27	7	-2.1089	-1.3409	-0.1349
28	8	-2.5790	0.5991	-2.2772
29	8	-2.6345	0.6680	1.6263
30	8	-1.2229	0.8853	-4.0282
31	8	-2.2584	-0.5983	3.4267

Table S9. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_3)(Cl)]^{2-}$

#	Z	X (Å)	Y (Å)	Z (Å)
1	8	0.0000	0.0000	0.0000
2	26	0.0000	0.0000	2.0852
3	17	2.4942	0.0000	2.3261
4	7	-2.2317	-0.0855	1.6471
5	8	-0.4935	-2.0971	2.3806
6	8	-0.4653	0.4254	4.0842
7	6	-0.6054	1.6232	4.5036
8	6	-2.3721	-0.3709	0.2042
9	1	-3.1911	0.2087	-0.2376
10	1	-2.6330	-1.4251	0.0691
11	6	-0.4070	2.7520	3.4795
12	1	-1.1106	3.5662	3.6988
13	1	0.5984	3.1404	3.6695
14	8	-0.8490	1.9471	5.6792
15	6	-1.0996	-0.1475	-0.6325
16	8	-1.2205	-0.1634	-1.8696
17	8	-2.1792	-3.4725	2.9201
18	7	-0.4821	2.3237	2.0711
19	6	-2.7311	-1.1928	2.4805
20	1	-3.6925	-1.5824	2.1247
21	1	-2.8806	-0.8255	3.4991
22	6	-2.7664	1.2408	2.0224
23	1	-2.8640	1.2703	3.1084
24	1	-3.7719	1.3968	1.6037
25	6	-1.7225	-2.3601	2.5890
26	6	0.4152	3.1338	1.2268
27	1	0.3900	2.7515	0.2060
28	1	1.4361	3.0429	1.5988
29	1	0.1277	4.1958	1.2198
30	6	-1.8661	2.3803	1.5392
31	1	-1.7999	2.3524	0.4492
32	1	-2.3417	3.3377	1.8022

Table S10. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_3)(Cl)]^-$

#	Z	X (Å)	Y (Å)	Z (Å)
1	8	0.9953	1.6023	0.8823
2	26	-0.0764	-0.0796	0.7519
3	17	-1.1508	0.1639	2.7830
4	7	1.1161	-0.1577	-1.1879
5	8	1.3655	-1.4007	1.1491
6	8	-1.2244	-1.5419	-0.0211
7	6	-2.3158	-1.2984	-0.6695
8	6	2.1969	0.8488	-1.0544
9	1	2.3763	1.3651	-2.0028
10	1	3.1302	0.3440	-0.7872
11	6	-2.6523	0.1810	-0.8631
12	1	-3.0969	0.3357	-1.8523
13	1	-3.4211	0.4126	-0.1199
14	8	-3.0883	-2.1582	-1.0893
15	6	1.9438	1.8825	0.0484
16	8	2.6544	2.8832	0.1086
17	8	2.7311	-2.9810	0.3507
18	7	-1.4927	1.0781	-0.6393
19	6	1.6492	-1.5344	-1.2282
20	1	2.5380	-1.6166	-1.8621
21	1	0.8848	-2.2044	-1.6294
22	6	0.1685	0.1595	-2.2843
23	1	-0.4236	-0.7329	-2.4904
24	1	0.7084	0.4119	-3.2061
25	6	1.9706	-2.0308	0.1895
26	6	-1.9430	2.3710	-0.0657
27	1	-1.0744	2.9912	0.1498
28	1	-2.4778	2.1839	0.8647
29	1	-2.6036	2.8975	-0.7652
30	6	-0.7298	1.3289	-1.8971
31	1	-0.1289	2.2272	-1.7432
32	1	-1.4227	1.5457	-2.7202

Table S11. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_1)(H_2O)_3]^+$

#	Z	X (Å)	Y (Å)	Z (Å)
1	7	0.0000	0.0000	0.0000
2	7	0.0000	0.0000	2.9903
3	6	1.3737	0.0000	3.5567
4	1	1.7306	-1.0199	3.7398
5	1	1.3499	0.5070	4.5256
6	6	2.4153	0.7601	2.7204
7	8	1.9587	1.5717	1.8331
8	8	3.6118	0.5835	2.9729
9	6	0.9836	0.2515	-1.0761
10	1	1.9508	0.4944	-0.6361
11	1	0.6481	1.0948	-1.6807
12	1	1.0914	-0.6277	-1.7260
13	6	-1.3226	-0.2561	-0.6113
14	1	-1.6297	0.6197	-1.1858
15	1	-2.0718	-0.4455	0.1565
16	1	-1.2806	-1.1205	-1.2875
17	6	-1.0022	0.0987	4.0750
18	1	-0.9358	-0.7543	4.7627
19	1	-2.0038	0.1227	3.6438
20	1	-0.8376	1.0211	4.6319
21	6	-0.2599	-1.2144	2.1716
22	1	0.0625	-2.1168	2.7093
23	1	-1.3405	-1.2938	2.0354
24	6	0.4362	-1.1658	0.8160
25	1	0.2412	-2.1037	0.2770
26	1	1.5181	-1.0970	0.9475
27	26	-0.0387	1.7212	1.5026
28	8	-0.0522	3.2860	3.1216
29	8	-0.0036	3.2411	-0.0731
30	8	-2.1994	1.9784	1.4957
31	1	0.7741	3.7995	3.2051
32	1	-0.7728	3.9351	3.2362
33	1	-0.5233	4.0614	0.0408
34	1	0.8624	3.5307	-0.4221
35	1	-2.6638	2.4145	2.2377
36	1	-2.7542	2.1510	0.7091

Table S12. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_1)(H_2O)_3]^{2+}$

#	Z	X (Å)	Y (Å)	Z (Å)
1	7	-1.3445	-1.2560	0.0395
2	7	1.0983	-0.1038	1.1954
3	6	2.3130	-0.4594	0.4011
4	1	2.7847	-1.3681	0.7877
5	1	3.0432	0.3509	0.4916
6	6	2.0372	-0.6133	-1.0927
7	8	0.8979	-0.0745	-1.4951
8	8	2.8283	-1.1480	-1.8384
9	6	-1.7306	-1.8771	-1.2594
10	1	-0.8671	-1.9167	-1.9218
11	1	-2.5175	-1.2845	-1.7231
12	1	-2.1015	-2.8923	-1.0830
13	6	-2.5630	-1.1418	0.8883
14	1	-3.2875	-0.4928	0.3940
15	1	-2.3179	-0.7286	1.8649
16	1	-3.0114	-2.1319	1.0209
17	6	1.4665	0.8366	2.2894
18	1	2.2013	0.3694	2.9535
19	1	0.5789	1.0873	2.8701
20	1	1.8915	1.7427	1.8603
21	6	0.4353	-1.3151	1.7755
22	1	1.1861	-1.9533	2.2561
23	1	-0.2485	-0.9739	2.5549
24	6	-0.3085	-2.1028	0.7123
25	1	-0.7873	-2.9782	1.1667
26	1	0.3759	-2.4747	-0.0531
27	26	-0.3514	0.6902	-0.2887
28	8	0.7003	2.5177	-0.3861
29	8	-1.7416	1.2178	-1.7297
30	8	-1.4621	1.6985	1.1807
31	1	1.3356	2.6738	-1.1203
32	1	0.3058	3.3924	-0.1708
33	1	-2.3588	1.9787	-1.6323
34	1	-1.5161	1.1594	-2.6867
35	1	-1.1262	2.4776	1.6807
36	1	-2.4400	1.8150	1.1632

Table S13. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_2)(H_2O)_2]$

#	Z	X (Å)	Y (Å)	Z (Å)
1	6	0.1563	-2.0391	0.8374
2	1	-0.7791	-2.0144	1.4016
3	1	0.6857	-2.9547	1.1389
4	6	-0.1371	-2.1096	-0.6566
5	1	0.7989	-2.1280	-1.2198
6	1	-0.6574	-3.0542	-0.8724
7	6	0.8547	-0.6196	2.6739
8	1	1.2674	-1.4685	3.2361
9	1	-0.1898	-0.4827	2.9573
10	1	1.4061	0.2830	2.9379
11	6	-0.8449	-0.8751	-2.6169
12	1	-1.2417	-1.7799	-3.0976
13	1	0.1977	-0.7466	-2.9108
14	1	-1.4119	-0.0123	-2.9683
15	6	2.3535	-0.9312	0.7738
16	1	2.6699	-1.9744	0.6597
17	1	2.9946	-0.4932	1.5445
18	6	2.6855	-0.1670	-0.5196
19	6	-2.3450	-1.0231	-0.6993
20	1	-2.6508	-2.0537	-0.4849
21	1	-2.9896	-0.6700	-1.5099
22	6	-2.6889	-0.1406	0.5126
23	26	0.0013	0.8461	-0.0356
24	7	0.9410	-0.8363	1.2142
25	7	-0.9328	-0.9544	-1.1439
26	8	1.8128	0.6739	-0.9441
27	8	-1.8250	0.7455	0.8569
28	8	3.7852	-0.3760	-1.0470
29	8	-3.7888	-0.3063	1.0542
30	8	-0.5092	2.5084	-1.4619
31	8	0.5801	2.4971	1.3651
32	1	-0.0493	2.6973	2.0833
33	1	0.7747	3.3579	0.9490
34	1	-0.1853	2.5692	-2.3793
35	1	-1.3776	2.9523	-1.4485

Table S14. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_2)(H_2O)_2]^+$

#	Z	X (Å)	Y (Å)	Z (Å)
1	6	-0.1339	0.7663	-2.0430
2	1	0.8040	1.3252	-2.0476
3	1	-0.6825	1.0499	-2.9494
4	6	0.1331	-0.7290	-2.0570
5	1	-0.8046	-1.2881	-2.0701
6	1	0.6806	-0.9958	-2.9691
7	6	-0.7792	2.6540	-0.6458
8	1	-1.1787	3.1822	-1.5184
9	1	0.2711	2.9132	-0.5160
10	1	-1.3307	2.9535	0.2436
11	6	0.7861	-2.6415	-0.6972
12	1	1.1875	-3.1513	-1.5798
13	1	-0.2631	-2.9074	-0.5723
14	1	1.3393	-2.9560	0.1860
15	6	-2.3348	0.7785	-0.9100
16	1	-2.6624	0.6708	-1.9488
17	1	-2.9510	1.5607	-0.4574
18	6	-2.6477	-0.5078	-0.1418
19	6	2.3350	-0.7565	-0.9272
20	1	2.6601	-0.6252	-1.9640
21	1	2.9539	-1.5472	-0.4931
22	6	2.6464	0.5125	-0.1303
23	26	-0.0001	-0.0108	0.8362
24	7	-0.9036	1.1834	-0.8319
25	7	0.9052	-1.1671	-0.8552
26	8	-1.7027	-0.9165	0.6676
27	8	1.7015	0.9007	0.6893
28	8	-3.7256	-1.0607	-0.2729
29	8	3.7223	1.0714	-0.2511
30	8	0.5856	-1.4327	2.2498
31	8	-0.5892	1.3926	2.2707
32	1	0.0686	1.9656	2.7214
33	1	-1.3111	1.2166	2.9126
34	1	-0.0640	-2.0254	2.6868
35	1	1.3118	-1.2719	2.8907

Table S15. Geometry optimized atomic coordinates for $[Fe^{II}(N_2O_3)(H_2O)]^-$

#	Z	X (Å)	Y (Å)	Z (Å)
1	8	-1.1835	-1.5240	1.0790
2	26	0.0498	0.1472	0.8065
3	7	-0.9668	0.0900	-1.1938
4	8	-1.4803	1.6109	1.0179
5	8	1.5660	1.4908	0.3894
6	6	2.6301	1.1738	-0.2438
7	6	-2.0559	-0.9091	-1.0906
8	1	-2.0984	-1.5364	-1.9879
9	1	-3.0170	-0.3893	-1.0339
10	6	2.8240	-0.3120	-0.5876
11	1	3.1856	-0.3892	-1.6197
12	1	3.6395	-0.6609	0.0526
13	8	3.5323	1.9618	-0.5704
14	6	-2.0023	-1.8292	0.1469
15	8	-2.7875	-2.7916	0.1662
16	8	-2.7220	3.0728	-0.1406
17	7	1.6318	-1.1592	-0.3626
18	6	-1.4812	1.4576	-1.3889
19	1	-2.2966	1.4990	-2.1205
20	1	-0.6710	2.0888	-1.7663
21	6	0.0854	-0.3066	-2.1568
22	1	0.7231	0.5621	-2.3367
23	1	-0.3494	-0.5954	-3.1246
24	6	-1.9510	2.1010	-0.0645
25	6	1.9875	-2.4073	0.3440
26	1	1.0782	-2.9629	0.5740
27	1	2.4859	-2.1616	1.2829
28	1	2.6555	-3.0416	-0.2558
29	6	0.9203	-1.4736	-1.6282
30	1	0.2715	-2.3315	-1.4389
31	1	1.6340	-1.7818	-2.4059
32	8	0.6057	-0.0191	2.9263
33	1	0.5938	0.7832	3.4816
34	1	0.1547	-0.7101	3.4467

Table S16. Geometry optimized atomic coordinates for $[Fe^{III}(N_2O_3)(H_2O)]$

#	Z	X (Å)	Y (Å)	Z (Å)
1	8	-1.0380	-1.5042	1.0094
2	26	0.0467	0.1310	0.7999
3	7	-0.9796	0.1268	-1.1735
4	8	-1.3329	1.5236	1.0428
5	8	1.4390	1.4454	0.3800
6	6	2.5513	1.1717	-0.2380
7	6	-2.1020	-0.8433	-1.0442
8	1	-2.2216	-1.4236	-1.9642
9	1	-3.0364	-0.2959	-0.8895
10	6	2.7445	-0.2912	-0.6378
11	1	3.0654	-0.3320	-1.6835
12	1	3.5769	-0.6694	-0.0377
13	8	3.4236	1.9930	-0.4861
14	6	-1.9640	-1.8006	0.1465
15	8	-2.7253	-2.7541	0.2443
16	8	-2.6041	3.0868	0.0700
17	7	1.5428	-1.1366	-0.4072
18	6	-1.4705	1.5134	-1.3460
19	1	-2.3109	1.5684	-2.0446
20	1	-0.6622	2.1341	-1.7440
21	6	0.0231	-0.2891	-2.1922
22	1	0.6689	0.5675	-2.3981
23	1	-0.4717	-0.5617	-3.1323
24	6	-1.8675	2.1122	0.0110
25	6	1.9073	-2.3835	0.3157
26	1	1.0048	-2.9526	0.5318
27	1	2.3933	-2.1252	1.2566
28	1	2.5905	-2.9937	-0.2862
29	6	0.8402	-1.4676	-1.6802
30	1	0.1935	-2.3267	-1.4921
31	1	1.5635	-1.7750	-2.4454
32	8	0.7245	-0.1924	2.7354
33	1	1.1919	0.4937	3.2577
34	1	0.2293	-0.7607	3.3631