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Supporting Information for

DFT insight into axial ligand effects on electronic structure and mechanistic reactivity of oxoiron(IV) porphyrin

Zhifeng Ma[a], Naoki Nakatani[a], Hiroshi Fujii[b], and Masahiko Hada*[a],

a) Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University,

1-1 Minami-Osawa, Hachioji, Tokyo, 192-0397, Japan

b) Department of Chemistry, Graduate School of Humanities and Science, Nara Women's University, Kitauoyanishi, Nara, 630-8506, Japan

E-mail addresses:

ma-zhifeng@ed.tmu.ac.jp; naokin@tmu.ac.jp; fujii@cc.nara-wu.ac.jp; hada@tmu.ac.jp

*Corresponding Author:

E-mail: hada@tmu.ac.jp, Tel: +81-48-858-9113.

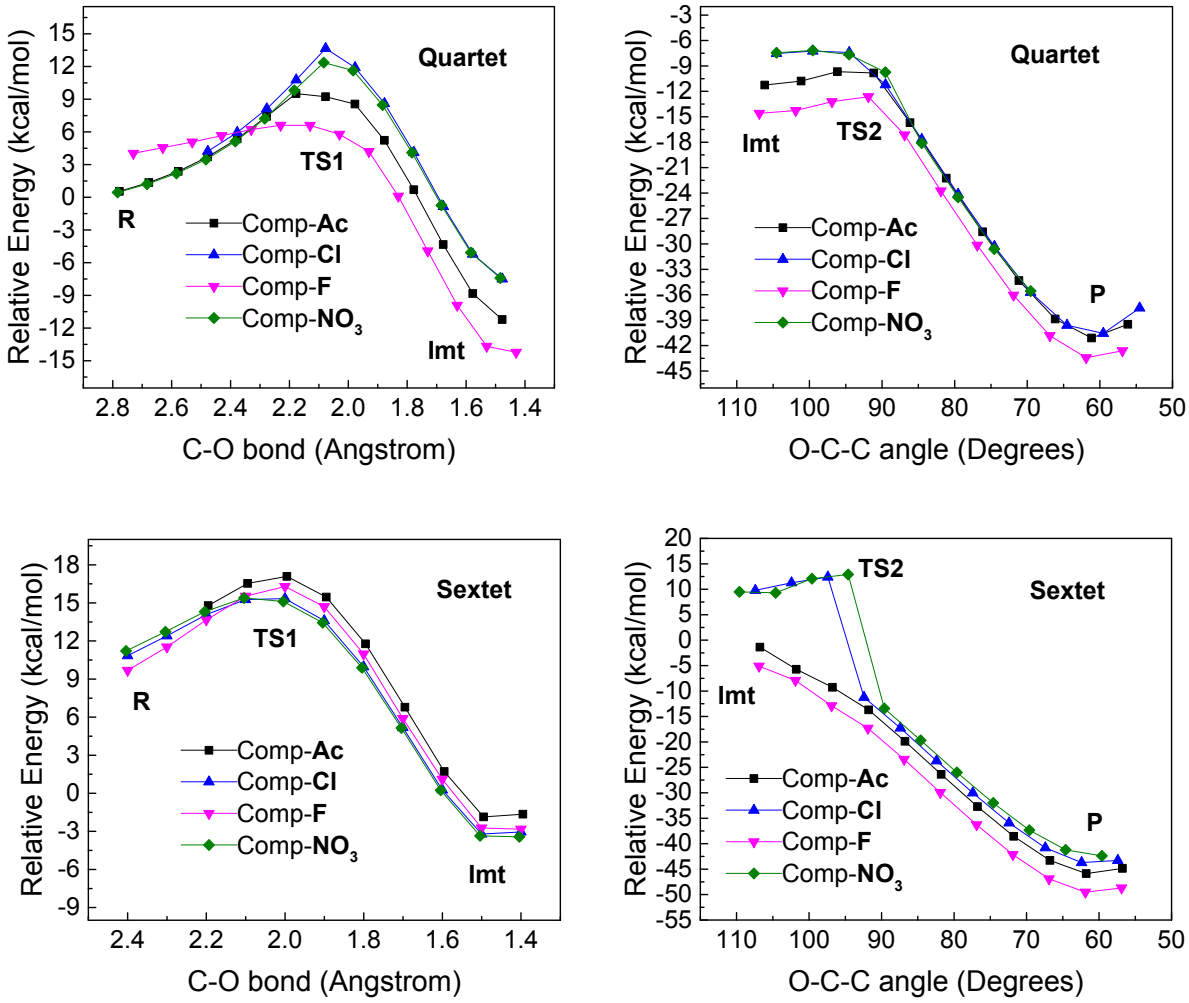

Figure S1. Geometry scans for the generation of radical complexes from reactants and epoxide formation scans starting from radical intermediates. Each point is a full geometry optimization.

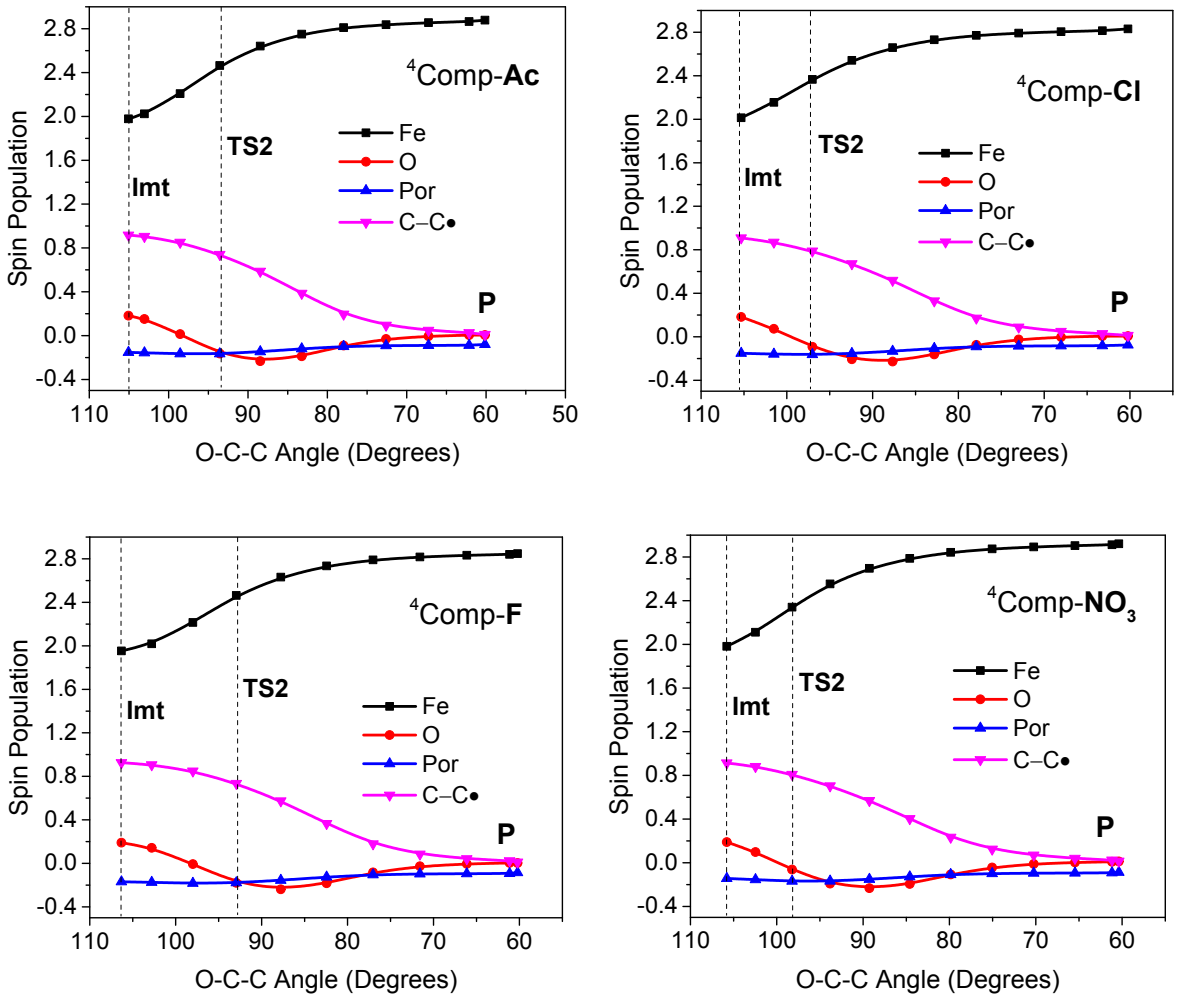

Figure S2. Change in spin population along ethylene oxidation by Fe(IV)OL-porphyrin complexes in the quartet ground spin state.

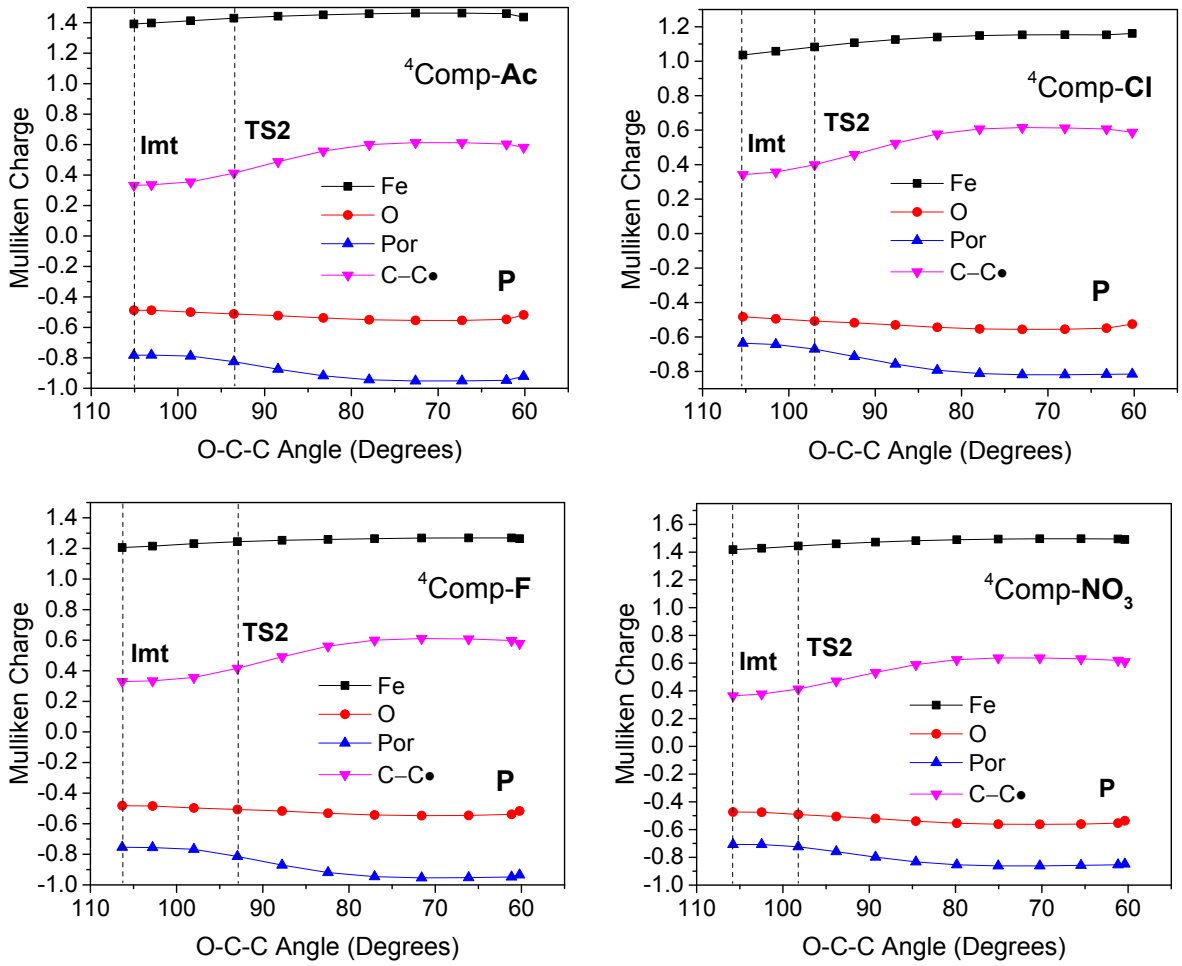

Figure S3. Change in Mulliken charge during ethylene oxidation by Fe(IV)OL-porphyrin complexes.

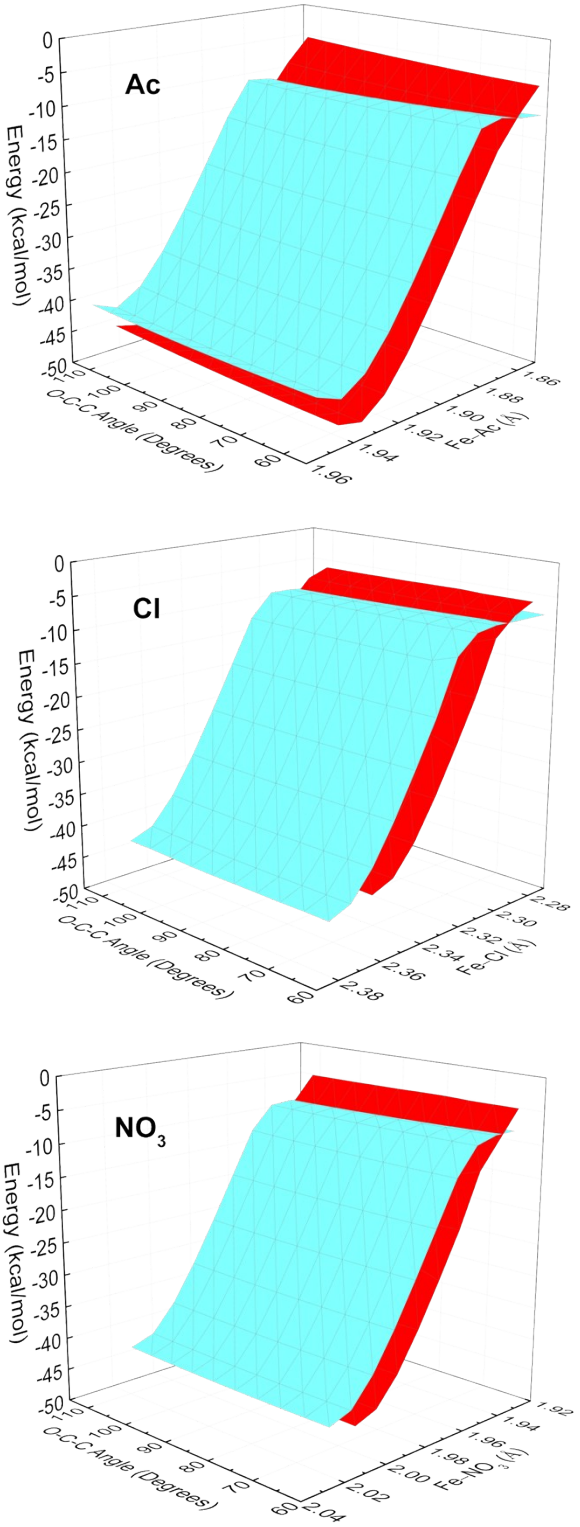

Figure S4. 2D potential energy surfaces of the quartet (blue) and sextet (red) spin states of the ring-closing reactions (from **Imt** to **P** through **TS2**) by the Fe(IV)OL-porphyrin complexes with Ac, Cl, and NO_3 as the axial ligands.

Table S1. Activation energies (kcal/mol) for optimized Comp-**Ac**, Comp-**Cl**, Comp-**F** and Comp-**NO_3** using various basis sets for other atoms, cc-pVTZ for iron atom in combination with PBE0 functional.

	Comp-**Ac**	Comp-**Cl**	Comp-**F**	Comp-**NO_3**
6-31G	9.5	13.7	6.6	12.3
6-31G(d)	12.1	14.1	9.2	14.2
6-31+G(d)	13.2	14.6	11.0	15.5
6-31++G(d,p)	13.2	14.6	10.9	15.4

Table S2. Bond lengths (Å) for optimized Comp-**Ac**, Comp-**Cl**, Comp-**F** and Comp-**NO_3** using various basis sets for other atoms, cc-pVTZ for iron atom in combination with PBE0 functional.

Reactants (R)								
	Fe–O				**Fe–L (L=Ligand)**			
	Comp-**Ac**	Comp-**Cl**	Comp-**F**	Comp-**NO_3**	Comp-**Ac**	Comp-**Cl**	Comp-**F**	Comp-**NO_3**
6-31G	1.637	1.630	1.642	1.626	1.966	2.404	1.867	2.019
6-31G(d)	1.627	1.623	1.633	1.618	1.974	2.362	1.850	2.022
6-31+G(d)	1.626	1.623	1.631	1.616	1.985	2.369	1.871	2.044
6-31++G(d,p)	1.626	1.623	1.631	1.616	1.984	2.369	1.871	2.045
Transition states (TS1)								
6-31G	1.759	1.702	1.770	1.712	1.873	2.329	1.793	1.952
6-31G(d)	1.716	1.691	1.758	1.689	1.900	2.294	1.775	1.962
6-31+G(d)	1.706	1.690	1.755	1.683	1.914	2.295	1.786	1.983
6-31++G(d,p)	1.707	1.691	1.755	1.684	1.913	2.294	1.786	1.982

Table S3. Mulliken spin population (*P*) of key atoms based on optimized structures during the epoxidation of ethylene in the quartet state.

	P_{Fe}	P_{Por}	P_N×4	P_O	P_L	P_{CH2}	P_{CH2}[a]
^{4}Ac+C_2H_4	1.17	0.89	0.76	0.87	0.03	0.00	0.00
^{4}Cl+C_2H_4	1.16	0.88	0.76	0.87	0.09	0.00	0.00
^{4}F+C_2H_4	1.19	0.91	0.75	0.84	0.06	0.00	0.00
$^4NO_3$+C_2H_4	1.16	0.93	0.73	0.89	0.01	0.00	0.00
^{4}Ac-TS1	1.68	0.04	-0.01	0.95	0.05	-0.11	0.38
^{4}Cl-TS1	1.47	0.28	0.25	0.81	0.11	-0.13	0.45
^{4}F-TS1	1.75	-0.03	-0.08	0.94	0.09	-0.11	0.36
$^4NO_3$-TS1	1.54	0.22	0.17	0.88	0.03	-0.10	0.42
^{4}Ac-Imt1	1.95	-0.15	-0.19	0.20	0.05	-0.04	0.97
^{4}Cl-Imt1	2.06	-0.15	-0.20	0.15	0.05	-0.04	0.94
^{4}F-Imt1	1.96	-0.17	-0.20	0.18	0.10	-0.04	0.97
$^4NO_3$-Imt1	2.04	-0.14	-0.20	0.16	0.02	-0.04	0.94
^{4}Ac-TS2	2.46	-0.16	-0.24	-0.16	0.10	-0.04	0.77
^{4}Cl-TS2	2.37	-0.16	-0.23	-0.09	0.10	-0.04	0.83
^{4}F-TS2	2.46	-0.18	-0.24	-0.18	0.16	-0.04	0.77
$^4NO_3$-TS2	2.34	-0.17	-0.24	-0.06	0.06	-0.03	0.84
^{4}Ac-P	2.87	-0.08	-0.18	0.02	0.15	0.00	0.00
^{4}Cl-P	2.82	-0.07	-0.18	0.02	0.22	0.00	0.00
^{4}F-P	2.84	-0.08	-0.17	0.02	0.22	0.00	0.00

$^4NO_3$-P	2.92	-0.08	-0.20	0.03	0.10	0.00	0.00

[a] Terminal CH_2 group in ethylene

Table S4. Mulliken spin population (*P*) of key atoms based on optimized structures during the epoxidation of ethylene in the sextet state.

	P_{Fe}	P_{Por}	P_N×4	P_O	P_L	P_{CH2}	P_{CH2}[a]
^{6}Ac+C_2H_4	3.21	1.18	1.02	0.59	0.01	0.00	0.00
^{6}Cl+C_2H_4	3.22	1.17	1.02	0.56	0.05	0.00	0.00
^{6}F+C_2H_4	3.22	1.18	1.00	0.55	0.05	0.00	0.00
$^6NO_3$+C_2H_4	3.22	1.21	1.00	0.56	0.01	0.00	0.00
^{6}Ac-TS1	3.98	1.20	1.02	0.01	0.09	0.17	-0.46
^{6}Cl-TS1	3.94	1.16	1.01	0.03	0.17	0.16	-0.48
^{6}F-TS1	3.98	1.18	1.01	-0.04	0.14	0.17	-0.44
$^6NO_3$-TS1	3.83	1.22	0.99	0.09	0.05	0.15	-0.34
^{6}Ac-Imt1	4.30	-0.42	-0.32	0.15	0.11	-0.05	0.89
^{6}Cl-Imt1	2.61	0.82	0.63	0.42	0.20	-0.06	1.00
^{6}F-Imt1	3.75	0.30	0.23	-0.03	0.11	-0.03	0.90
$^6NO_3$-Imt1	2.64	0.90	0.62	0.42	0.06	-0.06	1.00
^{6}Ac-TS2	4.31	-0.34	-0.26	0.04	0.12	-0.03	0.88
^{4}Cl-TS2	4.26	-0.64	-0.48	0.31	0.07	0.00	1.00
^{6}F-TS2	4.36	0.23	0.17	-0.62	0.23	-0.09	0.88
$^6NO_3$-TS2	4.29	-0.59	-0.42	0.27	0.05	-0.01	0.97
^{6}Ac-P	4.34	0.41	0.32	0.02	0.18	0.00	0.00
^{6}Cl-P	4.28	0.43	0.33	0.03	0.25	0.00	0.00
^{6}F-P	4.34	0.40	0.31	0.02	0.23	0.00	0.00
$^6NO_3$-P	4.36	0.43	0.32	0.03	0.13	0.00	0.00

[a] Terminal CH_2 group in ethylene

Table S5. Absolute energies (Hartree) in the 1-hexene solvent and the group Mulliken charges (*Q*) of optimized structures in the epoxidation in the quartet state.

	Energy	Q_{Fe}	Q_{Por}	Q_N×4	Q_O	Q_X	Q_{CH2}	Q_{CH2}[a]
^{4}Ac+C_2H_4	-2632.28493	1.06	-0.24	-2.76	-0.27	-0.58	0.0	0.0
^{4}Cl+C_2H_4	-2864.17171	0.78	-0.12	-2.69	-0.26	-0.40	0.0	0.0
^{4}F+C_2H_4	-2503.87022	0.86	-0.19	-2.68	-0.29	-0.38	0.0	0.0
$^4NO_3$+C_2H_4	-2684.02848	1.11	-0.16	-2.79	-0.24	-0.42	0.0	0.0
^{4}Ac-TS1	-2632.26976	1.24	-0.68	-2.95	-0.29	-0.56	0.12	0.07
^{4}Cl-TS1	-2864.14995	0.87	-0.48	-2.83	-0.30	-0.30	0.15	0.07
^{4}F-TS1	-2503.85971	1.07	-0.66	-2.91	-0.28	-0.31	0.11	0.07
$^4NO_3$-TS1	-2684.00879	1.28	-0.56	-2.93	-0.28	-0.41	0.14	0.08
^{4}Ac-Imt1	-2632.30281	1.39	-0.78	-3.03	-0.48	-0.56	0.25	0.08
^{4}Cl-Imt1	-2864.18366	1.04	-0.63	-2.96	-0.49	-0.25	0.25	0.10
^{4}F-Imt1	-2503.89290	1.21	-0.75	-2.98	-0.48	-0.30	0.25	0.08
$^4NO_3$-Imt1	-2684.04028	1.15	-0.71	-3.06	-0.47	-0.41	0.26	0.10
^{4}Ac-TS2	-2632.30035	1.43	-0.82	-3.06	-0.51	-0.58	0.26	0.16
^{4}Cl-TS2	-2864.18352	1.08	-0.67	-2.98	-0.51	-0.30	0.25	0.17
^{4}F-TS2	-2503.89035	1.24	-0.81	-3.00	-0.51	-0.34	0.26	0.15
$^4NO_3$-TS2	-2684.03990	1.44	-0.72	-3.08	-0.49	-0.41	0.26	0.15
^{4}Ac-P	-2632.35050	1.43	-0.91	-3.11	-0.50	-0.62	0.29	0.29
^{4}Cl-P	-2864.23693	1.15	-0.81	-3.07	-0.51	-0.41	0.29	0.29

^{4}F-P	-2503.93972	1.25	-0.93	-3.04	-0.50	-0.39	0.28	0.28
^{4}NO$_3$-P	-2684.09384	1.49	-0.84	-3.14	-0.52	-0.45	0.30	0.30

[a] Terminal CH_2 group in ethylene

Table S6. Absolute energies (Hartree) in the 1-hexene solvent and group Mulliken charges (Q) of optimized structures in the epoxidation in the sextet state.

	Energy	Q_{Fe}	Q_{Por}	Q_N×4	Q_O	Q_X	Q_{CH2}	Q_{CH2}[a]
^{6}Ac+C$_2$H$_4$	-2632.27542	1.22	-0.39	-2.89	-0.29	-0.58	0.0	0.0
^{6}Cl+C$_2$H$_4$	-2864.16140	0.94	-0.28	-2.82	-0.28	-0.38	0.00	0.00
^{6}F+C$_2$H$_4$	-2503.86280	1.03	-0.36	-2.83	-0.30	-0.37	0.00	0.00
^{6}NO$_3$+C$_2$H$_4$	-2684.01733	1.27	-0.31	-2.92	-0.26	-0.43	0.00	0.00
^{6}Ac-TS1	-2632.25771	1.36	-0.49	-2.93	-0.43	-0.60	0.12	0.04
^{6}Cl-TS1	-2864.14727	1.14	-0.42	-2.88	-0.44	-0.47	0.13	0.06
^{6}F-TS1	-2503.84426	1.16	-0.47	-2.87	-0.42	-0.40	0.11	0.02
^{6}NO$_3$-TS1	-2684.00395	1.36	-0.40	-2.95	-0.36	-0.43	0.10	0.03
^{6}Ac-Imt1	-2632.28790	1.54	-0.68	-3.06	-0.58	-0.61	0.23	0.10
^{6}Cl-Imt1	-2864.17683	1.12	-0.27	-2.79	-0.60	-0.48	0.20	0.03
^{6}F-Imt1	-2503.87473	1.39	-1.01	-3.17	-0.47	-0.30	0.27	0.13
^{6}NO$_3$-Imt1	-2684.03394	1.34	-0.25	-2.87	-0.60	-0.41	0.21	0.03
^{6}Ac-TS2	-2632.28711	1.54	-0.72	-3.08	-0.58	-0.61	0.25	0.10
^{6}Cl-TS2	-2864.15196	1.29	-0.45	-2.94	-0.63	-0.48	0.25	0.02
^{6}F-TS2	-2503.87837	1.41	-1.04	-3.17	-0.41	-0.38	0.30	0.12
^{6}NO$_3$-TS2	-2684.00792	1.54	-0.50	-3.05	-0.61	-0.42	0.26	0.05
^{6}Ac-P	-2632.35829	1.61	-1.14	-3.24	-0.51	-0.63	0.29	0.29
^{6}Cl-P	-2864.24198	1.30	-1.04	-3.21	-0.51	-0.34	0.29	0.29
^{6}F-P	-2503.94950	1.46	-1.15	-3.21	-0.51	-0.38	0.29	0.29
^{6}NO$_3$-P	-2684.09614	1.67	-1.07	-3.28	-0.52	-0.45	0.30	0.30

[a] Terminal CH_2 group in ethylene

Figure S5. Cartesian coordinates of representative stationary structures and an estimated structure of the minimum energy point as follows.

Reactant (^{4}R) for Comp-F

Fe	0.00000000	0.00000000	0.08294900
O	0.00000000	0.00000000	1.72517300
N	1.42315900	-1.42318600	0.01366900
N	-1.42318600	-1.42315900	0.01366900
N	-1.42315900	1.42318600	0.01366900
N	1.42318600	1.42315900	0.01366900
C	1.23531100	-2.78465600	0.00455700
C	0.00000000	-3.41677100	0.00205500
C	-1.23531400	-2.78456800	0.00468600
C	-2.50578900	-3.46949300	-0.00800000
C	-3.46951900	-2.50580800	-0.00787000
C	-2.78465600	-1.23531100	0.00455700
C	-3.41677100	0.00000000	0.00205500
C	-2.78456800	1.23531400	0.00468600

C	-3.46949300	2.50578900	-0.00800000
C	-2.50580800	3.46951900	-0.00787000
C	-1.23531100	2.78465600	0.00455700
C	0.00000000	3.41677100	0.00205500
C	1.23531400	2.78456800	0.00468600
C	2.50578900	3.46949300	-0.00800000
C	3.46951900	2.50580800	-0.00787000
C	2.78465600	1.23531100	0.00455700
C	3.41677100	0.00000000	0.00205500
C	2.78456800	-1.23531400	0.00468600
C	3.46949300	-2.50578900	-0.00800000
C	2.50580800	-3.46951900	-0.00787000
H	-2.62846500	-4.54223200	-0.01872900
H	-4.54223200	2.62846500	-0.01872900
H	-2.62853800	4.54225200	-0.01855900
H	4.54225200	2.62853800	-0.01855900
H	2.62853800	-4.54225200	-0.01855900
H	2.62846500	4.54223200	-0.01872900
H	4.54223200	-2.62846500	-0.01872900
H	-4.54225200	-2.62853800	-0.01855900
F	0.00000000	0.00000000	-1.78413900
H	4.50175000	-0.00006000	-0.00616500
H	0.00006000	4.50175000	-0.00616500
H	-0.00006000	-4.50175000	-0.00616500
H	-4.50175000	0.00006000	-0.00616500

Reactant (^{4}R) for Comp-Ac

Fe	-0.11718700	0.00004700	-0.40698400
O	-0.21884900	0.00035500	-2.04059600
N	1.30084700	1.41395800	-0.42750600
N	-1.53536200	1.41906200	-0.24843900
N	-1.53395300	-1.42035200	-0.24874800
N	1.30218200	-1.41248100	-0.42838200
C	1.12176200	2.77373300	-0.30191700
C	-0.10342200	3.40366800	-0.15070700
C	-1.34274100	2.77523700	-0.14821800
C	-2.61051500	3.46057800	-0.08665000
C	-3.57780400	2.50210500	-0.16317300
C	-2.89795500	1.23307600	-0.25336100
C	-3.53083400	-0.00163500	-0.28008600
C	-2.89670400	-1.23571200	-0.25278600
C	-3.57526100	-2.50536500	-0.16153600
C	-2.60699400	-3.46287500	-0.08540600
C	-1.33993000	-2.77632000	-0.14804100
C	-0.10003800	-3.40356200	-0.15139200
C	1.12446700	-2.77241600	-0.30334800
C	2.38959100	-3.45645300	-0.42576800
C	3.33219000	-2.49912900	-0.65126400
C	2.64710800	-1.22937400	-0.64210000
C	3.26922300	0.00177700	-0.77622300

C	2.64597200	1.23228800	-0.64094400
C	3.32987900	2.50266600	-0.64906500
C	2.38627100	3.45900400	-0.42353800
H	-2.73038900	4.53044200	-0.00302200
H	-4.64748400	-2.63218100	-0.14681300
H	-2.72569600	-4.53284200	-0.00139000
H	4.39491900	-2.62365800	-0.79511600
H	2.51643400	4.52855600	-0.35325300
H	2.52078500	-4.52591800	-0.35607300
H	4.39254800	2.62830500	-0.79237600
H	-4.65016400	2.62786200	-0.14923700
O	-0.13000400	-0.00069400	1.55857500
O	2.07211700	0.00038000	2.17968800
C	0.35956700	-0.00100700	3.87740000
H	-0.26300300	-0.88311300	4.05748500
H	-0.26475100	0.87977000	4.05785400
H	1.20660300	-0.00035500	4.56451400
C	0.84951300	-0.00028400	2.44369900
H	4.34002100	0.00232300	-0.95018200
H	-0.09234900	-4.48527000	-0.06621200
H	-4.61598700	-0.00216900	-0.28231400
H	-0.09680600	4.48539000	-0.06556700

Reactant (^{4}R) for Comp-Cl

Fe	0.00000000	0.00000000	0.21114500
O	0.00000000	0.00000000	1.84088800
N	0.72283200	-1.87196800	0.12359800
N	-1.87196800	-0.72283200	0.12359800
N	-0.72283200	1.87196800	0.12359800
N	1.87196800	0.72283200	0.12359800
C	0.00000000	-3.04320200	0.11303500
C	-1.38358700	-3.12375200	0.11000100
C	-2.25381300	-2.04520400	0.11210800
C	-3.69148900	-2.15538900	0.09395200
C	-4.18214700	-0.88431800	0.09468000
C	-3.04320200	0.00000000	0.11303500
C	-3.12375200	1.38358700	0.11000100
C	-2.04520400	2.25381300	0.11210800
C	-2.15538900	3.69148900	0.09395200
C	-0.88431800	4.18214700	0.09468000
C	0.00000000	3.04320200	0.11303500
C	1.38358700	3.12375200	0.11000100
C	2.25381300	2.04520400	0.11210800
C	3.69148900	2.15538900	0.09395200
C	4.18214700	0.88431800	0.09468000
C	3.04320200	0.00000000	0.11303500
C	3.12375200	-1.38358700	0.11000100
C	2.04520400	-2.25381300	0.11210800
C	2.15538900	-3.69148900	0.09395200
C	0.88431800	-4.18214700	0.09468000

H	-4.23677300	-3.08705900	0.07887300
H	-3.08705900	4.23677300	0.07887300
H	-0.56066600	5.21207000	0.08015800
H	5.21207000	0.56066600	0.08015800
H	0.56066600	-5.21207000	0.08015800
H	4.23677300	3.08705900	0.07887300
H	3.08705900	-4.23677300	0.07887300
H	-5.21207000	-0.56066600	0.08015800
H	4.11568500	-1.82289600	0.09940300
H	1.82289600	4.11568500	0.09940300
H	-1.82289600	-4.11568500	0.09940300
H	-4.11568500	1.82289600	0.09940300
Cl	0.00000000	0.00000000	-2.19305700

Reactant (^{4}R) for Comp-NO_3

Fe	-0.11588800	0.00382400	-0.40244600
O	-0.21486100	0.00950100	-2.02586800
N	1.29139200	1.42756800	-0.40614100
N	-1.54052800	1.41407700	-0.22759500
N	-1.52525800	-1.42352500	-0.23954600
N	1.30702500	-1.40406400	-0.41385200
C	1.10600100	2.78615100	-0.28635300
C	-0.12314300	3.41046400	-0.13509200
C	-1.35660200	2.77299400	-0.12789000
C	-2.62730100	3.44974900	-0.05715000
C	-3.58895700	2.48533100	-0.12691700
C	-2.90215100	1.22158000	-0.22317400
C	-3.53016700	-0.01555100	-0.25028200
C	-2.88892500	-1.24595100	-0.23374800
C	-3.56183900	-2.51789300	-0.14684400
C	-2.58964700	-3.47210200	-0.08354500
C	-1.32645300	-2.78080300	-0.14884600
C	-0.08588100	-3.40443900	-0.15774800
C	1.13646900	-2.76560100	-0.30272000
C	2.40448500	-3.44171600	-0.42024400
C	3.34508500	-2.47690200	-0.62686000
C	2.65319400	-1.21255500	-0.61338500
C	3.27102300	0.02364400	-0.73176600
C	2.63958200	1.25206400	-0.60764800
C	3.31736600	2.52422700	-0.61431700
C	2.36633200	3.47717100	-0.40114900
H	-2.75288500	4.51842900	0.03083100
H	-4.63329800	-2.64832500	-0.12341000
H	-2.70339000	-4.54269600	-0.00294700
H	4.40979300	-2.59476700	-0.76071300
H	2.49064000	4.54737600	-0.33247200
H	2.54072000	-4.51085500	-0.35777100
H	4.38055900	2.65475400	-0.74841100
H	-4.66179800	2.60372500	-0.10267600
O	-0.20365400	-0.00872700	1.61463300

N	0.78920700	-0.02430400	2.50647900
O	1.98593600	0.01281000	2.11532600
O	0.45850300	-0.07466400	3.71644500
H	-0.12304100	4.49188900	-0.04876600
H	4.34370900	0.02983500	-0.89355800
H	-0.07395600	-4.48627600	-0.07787900
H	-4.61505100	-0.02130400	-0.24428000

Transition state (^{4}TS1) for Comp-F

Fe	0.14970100	0.00088500	-0.21691700
O	0.15277900	-0.03282400	1.55310500
N	-0.44106300	-1.91615200	-0.30316300
N	-1.75961900	0.58195100	-0.33022900
N	0.73276300	1.91703200	-0.20859900
N	2.02343500	-0.57056300	-0.01644700
C	-1.72408100	-2.38601400	-0.50700100
C	-2.85731800	-1.60529400	-0.61097400
C	-2.86603900	-0.22555100	-0.51173400
C	-4.05558000	0.58066900	-0.58553600
C	-3.66399500	1.88240100	-0.45961000
C	-2.23204800	1.87884800	-0.31980900
C	-1.45994900	3.02393800	-0.24858400
C	-0.08202100	3.03338400	-0.21699600
C	0.72230100	4.23068100	-0.19619500
C	2.02447600	3.83452300	-0.17228200
C	2.02516400	2.39180800	-0.16565200
C	3.16134900	1.61366100	-0.06296300
C	3.14885100	0.23806200	0.03386100
C	4.32468700	-0.57079600	0.20701100
C	3.91617300	-1.87064600	0.26483300
C	2.48691200	-1.87451300	0.11419300
C	1.72132000	-3.01858200	0.04632500
C	0.35676100	-3.03101800	-0.17474700
C	-0.43675600	-4.22697700	-0.31254500
C	-1.72197900	-3.82835200	-0.52575200
H	-5.05205300	0.18931700	-0.72793100
H	0.32394400	5.23443400	-0.20195100
H	2.91430800	4.44595400	-0.14995500
H	4.51883900	-2.75889900	0.38289700
H	-2.59985800	-4.43927800	-0.67552900
H	5.32905700	-0.17939300	0.27146600
H	-0.04442600	-5.23145500	-0.25530200
H	-4.27437300	2.77309100	-0.48129500
F	0.21556400	0.00853300	-2.00835800
H	2.22826700	-3.97148900	0.14418100
H	4.12106600	2.11552400	-0.02465400
H	-3.80652400	-2.10634100	-0.76225900
H	-1.97329800	3.97861700	-0.25160700
C	-1.52430800	-0.62179200	2.81291000
H	-0.78201300	-0.98146400	3.51578300

H	-1.87205100	-1.33414400	2.07342600
C	-2.13489900	0.57852700	2.98412900
H	-2.92048200	0.91718100	2.31645900
H	-1.82767600	1.26344900	3.76826400

Transition state (^{4}TS1) for Comp-Ac

Fe	-0.02526400	0.11839700	-0.11955400
O	0.19358400	0.14313300	-1.86491100
N	-0.31452200	-1.85841100	-0.12755000
N	1.93239000	-0.18608400	0.22512900
N	0.27839200	2.09401400	-0.03510200
N	-1.90759900	0.42201100	-0.51580000
C	0.59661000	-2.83927400	0.22048800
C	1.92225200	-2.62625700	0.54093000
C	2.54482300	-1.38890700	0.51061400
C	3.95109600	-1.18242100	0.73706000
C	4.18603000	0.15498000	0.58596200
C	2.91974600	0.77219300	0.29031500
C	2.72729300	2.13929300	0.17949000
C	1.49507100	2.74558100	0.06011900
C	1.28686900	4.17312200	0.07299100
C	-0.05703800	4.38106800	-0.00039200
C	-0.67878700	3.08204800	-0.08531300
C	-2.03108200	2.86990300	-0.27844300
C	-2.58690500	1.63102700	-0.52067400
C	-3.96348100	1.41601000	-0.87772400
C	-4.11810700	0.08154700	-1.10910000
C	-2.84829500	-0.54428400	-0.86484500
C	-2.64115800	-1.90390800	-0.88914600
C	-1.46362000	-2.51554400	-0.49615600
C	-1.28111700	-3.93969400	-0.37220900
C	-0.01354300	-4.13959700	0.08751500
H	4.65442000	-1.96497900	0.98114200
H	2.07820500	4.90516800	0.13941300
H	-0.59356600	5.31816700	-0.01441300
H	-5.01331800	-0.44963300	-1.39597300
H	0.48295300	-5.07350200	0.30621800
H	-4.70416700	2.19895800	-0.94541100
H	-2.03817100	-4.67581800	-0.59800400
H	5.11940100	0.68862400	0.68846800
O	-0.22442300	0.12965200	1.74322000
O	-2.21166700	-0.93021100	2.16800300
C	-0.83720900	-0.17960300	4.00657300
H	-0.70094300	0.88437900	4.22162500
H	0.10531700	-0.68306200	4.24303100
H	-1.63803100	-0.58383300	4.62629900
C	-1.16776700	-0.37218600	2.54712000
H	-3.47503800	-2.53782700	-1.16714200
H	-2.68519600	3.73353400	-0.30475800
H	3.60022100	2.77838800	0.24980200

H	2.52934300	-3.49045100	0.78552600
C	2.65133500	-0.44687600	-3.00959700
H	2.82484500	0.30239100	-3.77571500
H	3.41391100	-0.55303700	-2.24487300
C	1.50389800	-1.17418500	-2.97731400
H	1.35881500	-1.97039800	-2.25621100
H	0.77580700	-1.11091400	-3.77745100

Transition state (^{4}TS1) for Comp-Cl

Fe	0.16190600	0.01211000	-0.05502100
O	0.03444100	0.00607900	1.65134200
N	2.01212500	-0.61186800	0.10348400
N	-0.48650400	-1.89265000	-0.17778200
N	-1.75246500	0.64465200	-0.25577100
N	0.78426000	1.89549100	-0.04270000
C	2.44254300	-1.92987100	0.23566800
C	1.64258200	-3.04728000	0.18136500
C	0.27263500	-3.02714700	-0.04202700
C	-0.54547500	-4.20166600	-0.20738600
C	-1.81357900	-3.76678000	-0.45763800
C	-1.77592800	-2.32625200	-0.43077000
C	-2.88229600	-1.51296500	-0.57915700
C	-2.86862200	-0.13128000	-0.48001800
C	-4.03986200	0.70275100	-0.57431500
C	-3.62173100	1.99168500	-0.40680300
C	-2.19349100	1.94539200	-0.22512400
C	-1.38220000	3.06340600	-0.10514000
C	-0.00637500	3.03486900	-0.04270100
C	0.82665300	4.21161600	-0.00904300
C	2.11924700	3.78542100	-0.00091400
C	2.08622400	2.34384500	-0.01246300
C	3.20496600	1.53457200	0.05100900
C	3.16209300	0.15865900	0.13357300
C	4.32063900	-0.68322300	0.29364800
C	3.87654600	-1.96725300	0.36810400
H	-0.18170100	-5.21666500	-0.14856700
H	-5.04084600	0.33837200	-0.75227100
H	-4.21003200	2.89712900	-0.42378600
H	3.02287300	4.37618300	0.01861400
H	4.45400400	-2.87202100	0.48633000
H	0.45251000	5.22461700	-0.00294400
H	5.33601900	-0.31919700	0.34366900
H	-2.70160100	-4.35334300	-0.64094000
Cl	0.24922200	0.01393600	-2.37238600
C	-1.53770800	-0.66438400	2.84555200
H	-0.79151400	-0.88517600	3.60021900
H	-1.76555100	-1.46317800	2.14935400
C	-2.35912700	0.42102900	2.96991900
H	-3.17795300	0.59750400	2.28024200
H	-2.18467600	1.17471600	3.73122100

H	2.12232800	-4.01460600	0.27948300
H	4.17709600	2.01337800	0.07441900
H	-1.86466900	4.03452300	-0.10034400
H	-3.83645100	-1.99288900	-0.76697300

Transition state (^{4}TS1) for Comp-NO_3

Fe	-0.03597100	0.14157700	-0.14386300
O	0.18913200	0.18824500	-1.84080600
N	-0.25030500	-1.84287400	-0.13401000
N	1.93637900	-0.09021600	0.20844600
N	0.18568200	2.11102900	-0.01808000
N	-1.94153500	0.36992500	-0.45526000
C	0.69492800	-2.78899500	0.22760000
C	2.00922000	-2.52219800	0.55564500
C	2.59101200	-1.26380900	0.51173700
C	3.99238700	-1.00716400	0.71644100
C	4.18126400	0.33344400	0.52837400
C	2.88996200	0.89925400	0.23818700
C	2.63761000	2.25782600	0.11916200
C	1.37910600	2.81358000	0.03820100
C	1.11221900	4.22992700	0.08418400
C	-0.24088200	4.38227700	0.08022100
C	-0.81195100	3.06090900	-0.00132600
C	-2.16190000	2.79598500	-0.14219400
C	-2.67594700	1.54255500	-0.40303400
C	-4.05059800	1.27871600	-0.74380700
C	-4.14835500	-0.04900200	-1.02810200
C	-2.84539300	-0.62595000	-0.82702500
C	-2.57582300	-1.97131700	-0.88723000
C	-1.36781000	-2.54371200	-0.50941400
C	-1.13390100	-3.95844200	-0.38459400
C	0.13621700	-4.10995000	0.09151800
H	4.72373600	-1.75913300	0.97305200
H	1.87412900	4.99365000	0.13131000
H	-0.81529300	5.29595000	0.11364000
H	-5.02335100	-0.60874000	-1.32296300
H	0.66242200	-5.02452100	0.32149600
H	-4.82650900	2.02917300	-0.76845800
H	-1.86047100	-4.72342100	-0.61403300
H	5.09724700	0.89996300	0.60780700
O	-0.11931700	0.13954100	1.80614800
N	-1.00764300	-0.49566600	2.59991900
O	-2.03046500	-1.02118500	2.10039200
O	-0.73838500	-0.49895900	3.82164300
H	2.64505000	-3.36142100	0.81422600
H	-3.38212300	-2.63649500	-1.17396300
H	-2.85042100	3.63253000	-0.11893500
H	3.48450400	2.93320400	0.16536200
C	2.64926200	-0.48358400	-2.94898900
H	2.90701600	0.29155200	-3.66366700

H	3.38798400	-0.71884800	-2.19007300
C	1.42441900	-1.08823400	-2.97064600
H	1.19995200	-1.92584300	-2.32032400
H	0.73532600	-0.91781900	-3.78961000

Intermediate (^{4}Imt) for Comp-F

Fe	0.06624300	0.00008700	-0.21170700
O	0.02595700	0.00121100	1.55509800
N	-1.34374900	-1.40932500	-0.28822200
N	-1.34131800	1.41214200	-0.28820000
N	1.48568500	1.41182100	-0.18139400
N	1.48310000	-1.41436800	-0.18159500
C	-2.70357800	-1.21878500	-0.45347300
C	-3.34156300	0.00323000	-0.54401300
C	-2.70146500	1.22414000	-0.45329200
C	-3.37145700	2.49835500	-0.47581000
C	-2.41469200	3.45694000	-0.31777400
C	-1.14877300	2.77885000	-0.21274300
C	0.07015800	3.41953000	-0.10256500
C	1.29210700	2.77643200	-0.10761700
C	2.56524100	3.45216700	-0.07798000
C	3.52799800	2.49061000	-0.14589400
C	2.85136300	1.21856700	-0.20193400
C	3.49464600	-0.00312700	-0.23087800
C	2.84913000	-1.22363400	-0.20210700
C	3.52342500	-2.49696000	-0.14631600
C	2.55901600	-3.45673500	-0.07838200
C	1.28713900	-2.77863700	-0.10798200
C	0.06400800	-3.41944200	-0.10301400
C	-1.15372700	-2.77645500	-0.21314600
C	-2.42088800	-3.45214400	-0.31842000
C	-3.37590500	-2.49172700	-0.47618100
H	-4.43713200	2.62598000	-0.59563700
H	2.68738500	4.52371600	-0.02228900
H	4.60104300	2.61231500	-0.15226300
H	2.67922100	-4.52854100	-0.02282800
H	-4.44182700	-2.61733600	-0.59610000
H	4.59623100	-2.62067500	-0.15276900
H	-2.54532200	-4.52447300	-0.28788200
H	-2.53713500	4.52949000	-0.28691600
F	0.12831200	0.00010200	-1.99922500
H	0.06021600	-4.50197100	-0.04977700
H	4.57835000	-0.00412200	-0.24617400
H	-4.41754600	0.00414900	-0.67401000
H	0.06834900	4.50208600	-0.04920300
C	-1.14200700	-0.00375400	2.43725200
H	-1.73794000	-0.89845900	2.22539200
H	-1.74724500	0.88412800	2.22244500
C	-0.61652300	0.00134200	3.82126000
H	-0.31891700	0.93366700	4.28916000

H	-0.32046200	-0.92729900	4.29738700

Intermediate (^{4}Imt) for Comp-Ac

Fe	0.08832500	0.05931700	-0.10737600
O	0.28864200	-0.00960700	-1.86429700
N	-1.10904100	-1.51841900	-0.13896600
N	1.66282000	-1.14312900	0.15236000
N	1.30172600	1.65460700	-0.04284900
N	-1.47435700	1.26676800	-0.32816700
C	-0.76972000	-2.83044300	0.14046900
C	0.50252100	-3.29325700	0.41783400
C	1.63726100	-2.50393700	0.39431500
C	2.98055900	-2.99649000	0.55373900
C	3.81870300	-1.93179500	0.39449200
C	2.99442200	-0.77425700	0.16139100
C	3.47754100	0.51545300	0.04233100
C	2.68140100	1.64265400	-0.02185100
C	3.18256900	2.99455500	-0.00134200
C	2.09913300	3.82129000	0.01178100
C	0.92755500	2.98157600	-0.02657000
C	-0.36969200	3.45219900	-0.10002200
C	-1.47787000	2.64597400	-0.27482800
C	-2.81071600	3.14035700	-0.51431800
C	-3.60440200	2.05618400	-0.74033600
C	-2.77103500	0.88824000	-0.61076400
C	-3.23053700	-0.40974100	-0.70102900
C	-2.45863000	-1.52309100	-0.43520600
C	-2.96985700	-2.86560300	-0.35459200
C	-1.93315600	-3.66927800	0.01865300
H	3.23442000	-4.02724000	0.75272500
H	4.22978600	3.25823900	0.01527500
H	2.07728700	4.90087400	0.03289400
H	-4.66163200	2.03072000	-0.95869100
H	-1.93764000	-4.73551800	0.19035800
H	-3.08214700	4.18562300	-0.51956800
H	-3.99780900	-3.13912400	-0.54055000
H	4.89742500	-1.91334200	0.44484500
O	-0.02095000	0.16789200	1.74901400
O	-2.22306700	-0.11041100	2.33107800
C	-0.56529300	0.27825300	4.04460400
H	-0.09866700	1.26195900	4.15467900
H	0.19251400	-0.47135700	4.29136700
H	-1.41042100	0.19139500	4.72819100
C	-1.03381600	0.08964500	2.62276500
H	-4.27980900	-0.56236200	-0.92502700
H	-0.52269500	4.52492900	-0.07689400
H	4.55227700	0.65538200	0.06106900
H	0.62377700	-4.35117300	0.61982200
C	0.59445700	-0.70731400	-4.09488600
H	-0.31308200	-0.53042600	-4.66219200

H	1.52814100	-0.32180200	-4.49029100
C	0.51739800	-1.19091600	-2.69777100
H	1.44719500	-1.67228300	-2.37431600
H	-0.31320200	-1.89006100	-2.54807900

Intermediate (^{4}Imt) for Comp-Cl

Fe	-0.06125400	0.00001300	-0.10086100
O	-0.01270000	0.00072600	1.67645500
N	-1.47862800	1.40941200	-0.06462400
N	1.34567400	1.40957600	-0.18319100
N	1.34771100	-1.40737000	-0.18305600
N	-1.47648400	-1.41159300	-0.06480500
C	-1.28506500	2.77528300	0.00383000
C	-0.06403700	3.41903200	-0.00103100
C	1.15382400	2.77756600	-0.11231000
C	2.41832500	3.45509500	-0.22510400
C	3.37484600	2.49623800	-0.38401700
C	2.70614800	1.22256300	-0.35453800
C	3.34624300	0.00260100	-0.44943500
C	2.70795500	-1.21827400	-0.35427400
C	3.37860200	-2.49090100	-0.38351700
C	2.42354900	-3.45123800	-0.22462000
C	1.15798800	-2.77569000	-0.11211600
C	-0.05889800	-3.41906200	-0.00115300
C	-1.28090700	-2.77718600	0.00339400
C	-2.55187800	-3.45484900	0.03822000
C	-3.51681300	-2.49494200	-0.02126300
C	-2.84358900	-1.22209500	-0.07754300
C	-3.48987500	-0.00260500	-0.10445800
C	-2.84543400	1.21786800	-0.07715200
C	-3.52055700	2.48967800	-0.02045200
C	-2.55704100	3.45101500	0.03915300
H	2.54029100	4.52776200	-0.19815100
H	4.44390600	-2.61664100	-0.50824900
H	2.54718300	-4.52371200	-0.19757900
H	-4.58962000	-2.61847700	-0.02168200
H	-2.67814300	4.52274300	0.09314500
H	-2.67137000	-4.52677600	0.09187600
H	-4.59354900	2.61160800	-0.02064600
H	4.43994000	2.62361500	-0.50886800
Cl	-0.14888800	0.00005900	-2.39482400
C	1.17024600	-0.00261800	2.54222400
H	1.77045500	0.88716300	2.32484100
H	1.76329300	-0.89785700	2.32773100
C	0.62754200	0.00181400	3.91788700
H	0.32046100	-0.92687300	4.38659800
H	0.32760300	0.93443500	4.38339900
H	-0.06230200	4.50175300	0.04645400
H	-4.57351000	-0.00342000	-0.11618100
H	-0.05549800	-4.50177700	0.04629000

H	4.42119800	0.00336900	-0.58685700

Intermediate (^{4}Imt) for Comp-NO_3

Fe	-0.08666400	0.05638500	0.11003000
O	-0.29881800	-0.02276100	1.85526200
N	0.93316700	-1.63587700	0.09775800
N	-1.77257900	-0.95867700	-0.19530200
N	-1.11648600	1.77013800	0.04731000
N	1.59465300	1.08458400	0.32349500
C	0.45872300	-2.90053700	-0.21008000
C	-0.85213900	-3.21746600	-0.50868400
C	-1.89342900	-2.31029800	-0.46953800
C	-3.28048500	-2.65219000	-0.63518900
C	-4.00113000	-1.50965600	-0.44341200
C	-3.06004100	-0.45215900	-0.18748000
C	-3.40409400	0.87751000	-0.03873600
C	-2.49025000	1.90973900	0.03549400
C	-2.84122000	3.30713700	0.02665500
C	-1.67472300	4.01134000	0.00787600
C	-0.60134300	3.05056800	0.03482900
C	0.73807700	3.37959900	0.10475300
C	1.75068700	2.45696300	0.27884700
C	3.12612500	2.80050100	0.53136500
C	3.79404000	1.63514700	0.76307600
C	2.84095700	0.56619500	0.62121900
C	3.15611700	-0.77449500	0.70377700
C	2.27109400	-1.79359200	0.41430500
C	2.63393000	-3.18106200	0.31575400
C	1.52233200	-3.86072700	-0.08921200
H	-3.64242200	-3.64407900	-0.86156700
H	-3.85354100	3.68287900	0.01601200
H	-1.53578100	5.08196900	-0.01286300
H	4.83992900	1.49450000	0.99156100
H	1.41555100	-4.91765700	-0.28314500
H	3.51135300	3.80921700	0.54018300
H	3.62255600	-3.56862200	0.51185100
H	-5.07179500	-1.37639400	-0.48879100
O	-0.03362400	0.21016100	-1.82141000
N	1.02201200	0.11446600	-2.66626100
O	2.13459300	-0.26399300	-2.23919600
O	0.78233000	0.41726300	-3.85476700
H	-1.08591100	-4.25062300	-0.73683400
H	4.17918700	-1.04276300	0.93953600
H	1.00579400	4.42934600	0.08306900
H	-4.45738900	1.13222900	-0.05068700
C	-0.70964400	-0.69364300	4.05211000
H	0.19858200	-0.61877000	4.64002800
H	-1.60358500	-0.20491500	4.42389500
C	-0.65880200	-1.19533200	2.66295800
H	-1.62476100	-1.57556600	2.31521300

H	0.10559300	-1.96580900	2.51952200

Transition state (^{4}TS2) for Comp-F

Fe	-0.05855400	0.00000300	-0.25473000
O	-0.03147900	0.00000500	1.63313200
N	1.35828700	1.41332500	-0.26988600
N	1.35888000	-1.41272500	-0.26983600
N	-1.47790400	-1.41550600	-0.18636800
N	-1.47849000	1.41492200	-0.18632600
C	2.72265900	1.22381000	-0.39255500
C	3.36373200	0.00071700	-0.45821300
C	2.72317700	-1.22264400	-0.39247900
C	3.39430000	-2.49680400	-0.41241300
C	2.43277000	-3.45759600	-0.30019000
C	1.16410800	-2.78026100	-0.22026100
C	-0.05766500	-3.42147800	-0.13924800
C	-1.28192500	-2.78046500	-0.13559100
C	-2.55423900	-3.45859400	-0.10524000
C	-3.51896900	-2.49700000	-0.14641200
C	-2.84390400	-1.22340500	-0.19161700
C	-3.48761700	-0.00070700	-0.20817100
C	-2.84441200	1.22225600	-0.19151200
C	-3.52000100	2.49556900	-0.14617400
C	-2.55566800	3.45756100	-0.10500000
C	-1.28307800	2.77995900	-0.13547500
C	-0.05908500	3.42148500	-0.13920200
C	1.16294900	2.78078100	-0.22032300
C	2.43132700	3.45864300	-0.30031800
C	3.39325300	2.49824900	-0.41255700
H	4.46303000	-2.62391700	-0.50281600
H	-2.67549800	-4.53106700	-0.06573700
H	-4.59185800	-2.62088900	-0.14396900
H	-2.67736200	4.52998500	-0.06542400
H	4.46193000	2.62579900	-0.50300400
H	-4.59293900	2.61901800	-0.14365300
H	2.55313800	4.53166300	-0.28341400
H	2.55502500	-4.53056600	-0.28326300
F	-0.11450400	-0.00005600	-2.07454100
H	-0.05768100	4.50501000	-0.10510100
H	-4.57158800	-0.00093600	-0.21327300
H	4.44328100	0.00094400	-0.55613900
H	-0.05580100	-4.50500600	-0.10519500
C	1.15448300	-0.00003500	2.48283500
H	1.75749900	0.89767600	2.32660900
H	1.75741700	-0.89780500	2.32663400
C	0.36003200	0.00001100	3.72150500
H	-0.03334900	-0.93137000	4.11254600
H	-0.03324900	0.93143100	4.11255600

Transition state (^{4}TS2) for Comp-Ac

Fe	0.08848000	0.05374800	-0.07872700
O	0.30426300	-0.00569200	-1.94785500
N	-1.12249100	-1.52318600	-0.17452800
N	1.65676700	-1.17351500	0.13317000
N	1.32145800	1.63765900	-0.03560200
N	-1.46191000	1.27971200	-0.33755600
C	-0.79009600	-2.84680700	0.05370200
C	0.48150400	-3.32654800	0.30685500
C	1.62095500	-2.54324300	0.32223200
C	2.95860700	-3.04865600	0.48814400
C	3.80442000	-1.98227700	0.39059800
C	2.99036700	-0.81281400	0.18299700
C	3.48380400	0.47626800	0.10353100
C	2.70017000	1.61186800	0.02319900
C	3.21550800	2.95826900	0.04209900
C	2.14124500	3.79694600	0.01001100
C	0.96205200	2.96958400	-0.04762800
C	-0.32875300	3.45400900	-0.14714000
C	-1.44828800	2.65981600	-0.30763700
C	-2.77831900	3.16754600	-0.53413300
C	-3.59035300	2.08930700	-0.72170800
C	-2.76833100	0.91340200	-0.58899000
C	-3.24381500	-0.38030000	-0.66770200
C	-2.47845800	-1.50698400	-0.44030200
C	-3.00097900	-2.84714200	-0.39198100
C	-1.96273400	-3.67241000	-0.07350800
H	3.20423700	-4.08744400	0.65312200
H	4.26461200	3.21141900	0.08578000
H	2.13139000	4.87693800	0.01575900
H	-4.65216300	2.07368400	-0.91793500
H	-1.97355600	-4.74384400	0.06214400
H	-3.03729100	4.21585900	-0.55341700
H	-4.03559000	-3.10578200	-0.56215400
H	4.88187200	-1.97165200	0.46541900
O	-0.04046800	0.15596600	1.82174800
O	-2.23672100	-0.11048200	2.41139800
C	-0.57951400	0.26675500	4.12580800
H	-0.11503500	1.25113100	4.24135300
H	0.17953800	-0.48190500	4.37236900
H	-1.42590400	0.17601600	4.80769900
C	-1.04148600	0.08318200	2.69910500
H	-4.30028400	-0.51933200	-0.86588400
H	-0.46817800	4.52896000	-0.14184200
H	4.55880200	0.60756000	0.15296900
H	0.59677200	-4.39180100	0.47071200
C	0.54933600	-0.46433500	-4.01972300
H	-0.38700600	-0.21807300	-4.50750400
H	1.45128800	0.03860100	-4.34968200
C	0.54225400	-1.20370300	-2.74706800
H	1.49460800	-1.67155000	-2.48577200

H	-0.27655500	-1.91964700	-2.64152700

Transition state (^{4}TS2) for Comp-Cl

Fe	-0.05727700	0.00000000	-0.12039600
O	-0.01583800	-0.00000800	1.72491200
N	-1.47363300	1.41137500	-0.06593000
N	1.35519500	1.40921600	-0.17021000
N	1.35505600	-1.40935900	-0.17021500
N	-1.47377400	-1.41123600	-0.06592400
C	-1.27887000	2.77756200	-0.01010000
C	-0.05668000	3.42008800	-0.01908600
C	1.16248300	2.77787000	-0.11369600
C	2.42866200	3.45465000	-0.21243400
C	3.38795900	2.49435300	-0.34553700
C	2.71843500	1.22098300	-0.31740500
C	3.35899700	-0.00017100	-0.39820400
C	2.71831300	-1.22126300	-0.31741500
C	3.38771000	-2.49469900	-0.34555400
C	2.42831800	-3.45490100	-0.21244900
C	1.16220700	-2.77799400	-0.11370200
C	-0.05702000	-3.42008800	-0.01907900
C	-1.27914600	-2.77744200	-0.01008000
C	-2.55051700	-3.45449500	0.02413900
C	-3.51515000	-2.49313600	-0.02145100
C	-2.84097600	-1.22060700	-0.07128000
C	-3.48581000	0.00016900	-0.09212100
C	-2.84085500	1.22088200	-0.07129700
C	-3.51490200	2.49347900	-0.02149200
C	-2.55017500	3.45474200	0.02409600
H	2.55052900	4.52754300	-0.19378100
H	4.45466600	-2.62160000	-0.45427000
H	2.55007800	-4.52780600	-0.19379800
H	-4.58802800	-2.61628200	-0.01816600
H	-2.67064000	4.52702300	0.06843200
H	-2.67108800	-4.52676300	0.06849000
H	-4.58776800	2.61673100	-0.01821900
H	4.45492800	2.62114600	-0.45424800
Cl	-0.13973000	0.00000800	-2.44623500
C	1.17664100	0.00003300	2.57034100
H	1.77609900	0.89621500	2.38885800
H	1.77618000	-0.89609000	2.38883000
C	0.47743900	-0.00002400	3.86818800
H	0.11377700	-0.93111100	4.28848200
H	0.11366600	0.93101000	4.28850000
H	-0.05474500	4.50332900	0.01733600
H	-4.56956200	0.00022300	-0.09937300
H	-0.05519300	-4.50333000	0.01734700
H	4.43615400	-0.00022400	-0.51777600

Transition state (^{4}TS2) for Comp-NO_3

Fe	-0.09937300	0.06394800	0.07117600
O	-0.39590400	0.07188000	1.86119300
N	-0.01604300	-1.92159400	0.05845700
N	-2.05043300	-0.01057700	-0.30584300
N	-0.17777600	2.06459100	0.07231900
N	1.87079500	0.14436700	0.34954900
C	-1.03719900	-2.79604000	-0.27357600
C	-2.33144200	-2.43815500	-0.59589400
C	-2.80281200	-1.13950100	-0.58591500
C	-4.17473300	-0.76950400	-0.80480300
C	-4.25738700	0.58265400	-0.64023400
C	-2.93295800	1.05566300	-0.34069400
C	-2.60134600	2.38577000	-0.16975700
C	-1.31163100	2.84924100	-0.00228000
C	-0.94955700	4.24288100	0.05284500
C	0.40908400	4.29823300	0.14043800
C	0.88624000	2.93879500	0.16066700
C	2.21354300	2.58148400	0.29185000
C	2.65958000	1.28055800	0.41029000
C	4.02191800	0.91597000	0.69282800
C	4.05366700	-0.43953500	0.83744400
C	2.71529400	-0.91935900	0.62233300
C	2.35011600	-2.25003300	0.64657900
C	1.08338800	-2.71040500	0.34685300
C	0.73584800	-4.09986500	0.21698900
C	-0.56785200	-4.15247000	-0.17985900
H	-4.96404200	-1.46573800	-1.04650400
H	-1.65445100	5.05988000	0.01083700
H	1.04490800	5.16955600	0.19029300
H	4.90105800	-1.07175200	1.05680800
H	-1.17000400	-5.02300000	-0.39332500
H	4.83689100	1.61948800	0.77559900
H	1.41939700	-4.91828200	0.38710700
H	-5.12706700	1.21703000	-0.72620300
O	0.13096100	0.12622000	-1.87577700
N	1.32079400	-0.14733700	-2.47292500
O	1.66457300	-1.34421100	-2.58300700
O	1.97813300	0.82186700	-2.90686300
H	-3.03110200	-3.22956000	-0.83804600
H	3.11907900	-2.98360300	0.85806000
H	2.94936300	3.37489700	0.34724700
H	-3.40013700	3.11642200	-0.22207600
C	-1.05896800	-0.27790900	3.95317800
H	-0.19051200	-0.56485700	4.53569200
H	-1.63304700	0.58385200	4.27506300
C	-1.26409800	-0.84284900	2.60705900
H	-2.29292400	-0.76175600	2.24538200
H	-0.90935400	-1.87118800	2.50019400

Product (^{4}P) for Comp-F

Fe	0.08139200	-0.00223000	-0.36943800
O	0.07977300	-0.01175300	2.03676800
N	-0.00656800	-2.00309500	-0.19801300
N	-1.93078000	0.07452600	-0.27960600
N	0.14582700	1.99988500	-0.19511100
N	2.07130500	-0.07808500	-0.13072300
C	-1.13950400	-2.79389100	-0.25363100
C	-2.44214100	-2.33265800	-0.32368600
C	-2.80463000	-0.99736500	-0.34302200
C	-4.16181800	-0.52296500	-0.42707400
C	-4.10992000	0.84039900	-0.42511700
C	-2.72059600	1.20997600	-0.34023500
C	-2.25788300	2.51385700	-0.31782800
C	-0.92384000	2.87460700	-0.24861700
C	-0.45016900	4.23534200	-0.21915500
C	0.91103200	4.18242900	-0.15444800
C	1.27909000	2.78930800	-0.14455200
C	2.58141000	2.32693200	-0.09489700
C	2.94268900	0.99211800	-0.08783700
C	4.30301000	0.51898600	-0.01943200
C	4.25113500	-0.84309400	-0.01945200
C	2.85878600	-1.21136400	-0.08782900
C	2.39700300	-2.51463700	-0.09576800
C	1.06324800	-2.87649500	-0.14669000
C	0.59030500	-4.23761600	-0.15868900
C	-0.77085000	-4.18673400	-0.22532800
H	-5.03161500	-1.16058500	-0.48697800
H	-1.08706800	5.10714900	-0.25019000
H	1.61347600	5.00224600	-0.12154400
H	5.06986700	-1.54625800	0.02257500
H	-1.47225000	-5.00748900	-0.25828300
H	5.17286900	1.15779200	0.02258300
H	1.22822900	-5.10856600	-0.12591100
H	-4.92872000	1.54249800	-0.48307300
F	0.14499200	-0.00283600	-2.22559200
H	3.13331200	-3.30974700	-0.06113300
H	3.37596900	3.06383100	-0.06027200
H	-3.23514900	-3.07033500	-0.37510000
H	-2.99281100	3.30956600	-0.36690000
C	-0.94208500	-0.70954100	2.86345800
H	-0.52395000	-1.26715600	3.69362400
H	-1.70797100	-1.21320700	2.28515400
C	-0.88635700	0.76269300	2.86248000
H	-1.61323600	1.31865700	2.28211000
H	-0.42622500	1.28478100	3.69318200

Product (^{4}P) for Comp-Ac

Fe	0.12729100	0.05085100	0.01784200
O	0.38003900	-0.00797000	-2.35635000

N	-1.20160900	-1.44248300	-0.17632900
N	1.61511800	-1.30193000	0.02931500
N	1.48492700	1.52335100	-0.10566300
N	-1.33126500	1.37850800	-0.33317300
C	-0.95377200	-2.79864200	-0.03704300
C	0.29495200	-3.37819400	0.09737400
C	1.48751900	-2.67712700	0.11763600
C	2.78736100	-3.28731800	0.22487400
C	3.70494600	-2.27799500	0.20479700
C	2.97245200	-1.04355600	0.09031100
C	3.55683200	0.20916200	0.06121800
C	2.85882100	1.39915600	-0.02661400
C	3.47426800	2.70182400	-0.04920300
C	2.46759700	3.61704000	-0.13962900
C	1.23048500	2.87954600	-0.17846500
C	-0.01931900	3.45955900	-0.29410300
C	-1.20652300	2.75565400	-0.37273300
C	-2.50331900	3.36448500	-0.52034400
C	-3.41604100	2.35249000	-0.56898200
C	-2.68500500	1.11831900	-0.44473700
C	-3.26906100	-0.13395400	-0.43438200
C	-2.57572300	-1.32073300	-0.29136600
C	-3.19217200	-2.61988700	-0.24013700
C	-2.19122100	-3.53260800	-0.07868100
H	2.96062300	-4.35031200	0.30650300
H	4.53883000	2.87741700	-0.00022100
H	2.54045900	4.69384000	-0.18073000
H	-4.48936500	2.42081100	-0.66735100
H	-2.26996300	-4.60618300	0.01003300
H	-2.67771400	4.42901300	-0.57434800
H	-4.25566800	-2.79578300	-0.30663500
H	4.78096600	-2.34817500	0.26716100
O	0.04234000	0.15043600	1.96566700
O	-2.13557900	0.05569100	2.64256500
C	-0.39376000	0.24917600	4.30081800
H	0.17129200	1.17926600	4.41997800
H	0.29441200	-0.57653500	4.50833400
H	-1.22150400	0.22730900	5.01080400
C	-0.91303500	0.14200200	2.88482700
H	-4.34869600	-0.18741200	-0.51549700
H	-0.07112600	4.54165100	-0.33622700
H	4.63816100	0.26205000	0.11963100
H	0.34256600	-4.45740700	0.18994000
C	-0.73083700	-0.23868200	-3.32070200
H	-1.69384100	-0.40071200	-2.85077200
H	-0.71584200	0.43662200	-4.16823900
C	0.32504900	-1.25357200	-3.17010400
H	1.11650400	-1.32471500	-3.90698800
H	0.12279300	-2.14711700	-2.59116600

Product (^{4}P) for Comp-Cl

Fe	-0.07632800	0.00042600	-0.23153400
O	-0.06074300	0.00153100	2.13045200
N	-2.06319600	0.01589200	-0.00516200
N	-0.05031800	1.99780100	-0.07497600
N	1.93187900	-0.01505000	-0.16548700
N	-0.08127000	-1.99689900	-0.07418300
C	-2.88714100	1.12511700	0.03984000
C	-2.46778900	2.44144800	0.02906200
C	-1.14619800	2.84111300	-0.02445800
C	-0.71468900	4.21420800	-0.04349800
C	0.64720400	4.20435100	-0.11443000
C	1.05806700	2.82487300	-0.13846100
C	2.37324800	2.40597200	-0.21747500
C	2.77415800	1.08287500	-0.23797900
C	4.14263100	0.64984500	-0.33713500
C	4.13208000	-0.71444400	-0.33537100
C	2.75706000	-1.12599700	-0.23534700
C	2.33580000	-2.44272200	-0.21305300
C	1.01421700	-2.84120000	-0.13551600
C	0.58181000	-4.21409600	-0.11194600
C	-0.78020700	-4.20266200	-0.04378200
C	-1.19025500	-2.82300400	-0.02560800
C	-2.50557000	-2.40299800	0.02663600
C	-2.90445300	-1.08032300	0.03834900
C	-4.27663100	-0.64839800	0.10897400
C	-4.26592000	0.71468300	0.11000700
H	-1.37892700	5.06522200	-0.01300600
H	4.99154000	1.31383900	-0.40751700
H	4.97059800	-1.39170300	-0.40403500
H	-1.45776600	-5.04316100	-0.01452400
H	-5.10517300	1.39297200	0.15338500
H	1.24481600	-5.06579100	-0.15039500
H	-5.12645700	-1.31344000	0.15137600
H	1.32340800	5.04554800	-0.15433000
Cl	-0.14113100	-0.00014300	-2.60700900
C	0.93359200	0.73072700	2.96643600
H	0.48803300	1.27617300	3.78996500
H	1.68839500	1.25531400	2.39240200
C	0.92264300	-0.74149200	2.96706900
H	1.66965900	-1.27760900	2.39350000
H	0.46907800	-1.27942100	3.79117200
H	-3.22772500	3.21371900	0.06250200
H	-3.27734200	-3.16348800	0.05888200
H	3.09341500	-3.21588900	-0.27138800
H	3.14254500	3.16735700	-0.27779800

Product (^{4}P) for Comp-NO_3

Fe	0.12220900	0.04852400	-0.00320200
O	0.42415600	-0.06842300	-2.28677300

N	-0.50868000	-1.85175600	-0.03667300
N	2.00967000	-0.59162900	0.15698500
N	0.78260500	1.92827400	-0.20441500
N	-1.73766100	0.66655700	-0.37124300
C	0.24925100	-2.98495400	0.21875000
C	1.61826800	-3.00999400	0.40771000
C	2.43357600	-1.89390800	0.36708000
C	3.86317900	-1.92829000	0.51959100
C	4.30926300	-0.64419500	0.40124200
C	3.15519700	0.18585300	0.18324100
C	3.20126100	1.55959300	0.04076000
C	2.09208300	2.36509000	-0.12948900
C	2.14096400	3.80036200	-0.23642000
C	0.85544200	4.23501700	-0.36559000
C	0.01259600	3.06768600	-0.34684400
C	-1.36310600	3.09852000	-0.47186500
C	-2.17082000	1.97777900	-0.49391700
C	-3.59676500	2.01038700	-0.67526800
C	-4.03121900	0.71715300	-0.67069600
C	-2.87644500	-0.11653900	-0.47535900
C	-2.91773500	-1.49492300	-0.39252000
C	-1.81517800	-2.29557400	-0.16437900
C	-1.86850700	-3.72399300	-0.00808000
C	-0.59504100	-4.14909000	0.23503800
H	4.43870900	-2.82481000	0.69649500
H	3.04794700	4.38563100	-0.20554500
H	0.49549100	5.24840900	-0.46329500
H	-5.04078400	0.34851400	-0.77544500
H	-0.24678300	-5.15525000	0.41593800
H	-4.17846800	2.91319500	-0.78775500
H	-2.77271600	-4.31187700	-0.06311000
H	5.32328500	-0.27788800	0.46305300
O	0.04382000	0.28846800	2.01427300
N	-1.05006900	0.32571600	2.78317300
O	-1.99557600	-0.46759300	2.53547400
O	-1.06315100	1.14815300	3.72961400
H	2.08514700	-3.97007700	0.59540100
H	-3.88452000	-1.97754800	-0.47691200
H	-1.84048900	4.06647700	-0.57103200
H	4.17213300	2.03938100	0.08668600
C	-0.46860600	-0.77280900	-3.25140000
H	-1.30365900	-1.28191200	-2.78463700
H	-0.69218700	-0.18665600	-4.13475700
C	0.89724100	-1.27357300	-3.02609100
H	1.67947800	-1.05648200	-3.74356100
H	1.04553200	-2.14329500	-2.39674800

***a* point for Comp-F**

Fe	-0.27767700	0.00903400	-0.30122800
O	0.08860100	-0.00471100	1.43052600

N	0.70945300	1.74345000	-0.53228700
N	1.41157800	-0.98212600	-0.50862700
N	-1.27804400	-1.72670700	-0.13731300
N	-1.90178900	0.99781700	0.20670600
C	2.05127200	1.90647000	-0.80571800
C	2.97874900	0.88977600	-0.88788800
C	2.67508400	-0.44777000	-0.73624700
C	3.63349100	-1.50480400	-0.86898500
C	2.95441000	-2.68469500	-0.74688400
C	1.57483600	-2.36285700	-0.53703700
C	0.57101100	-3.30476200	-0.44443600
C	-0.76212800	-2.99887500	-0.26931400
C	-1.81047000	-3.97723300	-0.11272900
C	-2.95715500	-3.29127400	0.14836700
C	-2.61690400	-1.88961200	0.15109800
C	-3.49431000	-0.87356200	0.46590500
C	-3.15055200	0.46264000	0.50221400
C	-4.07932300	1.51825800	0.77881600
C	-3.40845000	2.69900300	0.62766000
C	-2.06114700	2.37847500	0.25943300
C	-1.10299700	3.32152000	-0.05286700
C	0.18760700	3.01611100	-0.43110300
C	1.21270200	3.99490700	-0.69949100
C	2.36555500	3.30866800	-0.92912900
H	4.68638800	-1.35383300	-1.05486500
H	-1.66523800	-5.04509000	-0.18069500
H	-3.94614400	-3.68073000	0.33875000
H	-3.78869200	3.70399300	0.73437200
H	3.34845000	3.69768900	-1.14890600
H	-5.11739200	1.36493400	1.03304700
H	1.05503700	5.06306300	-0.69216600
H	3.34189900	-3.69033000	-0.81253000
F	-0.65023000	0.02647300	-2.04023800
H	-1.38332200	4.36618400	0.01067700
H	-4.51930700	-1.13724200	0.69819300
H	4.01073400	1.15507100	-1.08394700
H	0.85123500	-4.34963200	-0.50650300
C	2.84654600	0.24781200	3.36814600
H	1.95421600	0.18106300	2.75173700
H	2.80615300	0.93426600	4.21069100
C	3.94398200	-0.46342900	3.10098800
H	4.84212000	-0.39183700	3.70951600
H	3.98747300	-1.14866300	2.25833600

***a* point for Comp-Ac**

Fe	-0.05349600	0.12294200	-0.13495300
O	0.13800100	0.17278600	-1.76553600
N	-0.11975900	-1.88339400	-0.09620700
N	1.93099700	0.03612000	0.27751600
N	0.03675600	2.12542400	-0.03473000

N	-1.97283800	0.20084600	-0.50742100
C	0.88543100	-2.75412000	0.27999800
C	2.17262700	-2.37945100	0.61691700
C	2.66701600	-1.07925400	0.58561000
C	4.04180900	-0.72539800	0.83762900
C	4.13355900	0.62594700	0.66983300
C	2.80940400	1.09048100	0.33912900
C	2.45807600	2.42614100	0.20639200
C	1.16646100	2.90651700	0.06208700
C	0.81196400	4.30442400	0.04054600
C	-0.54646800	4.36416000	-0.06065800
C	-1.01606900	3.00156300	-0.12389200
C	-2.33253900	2.62180200	-0.34918100
C	-2.76300800	1.32394700	-0.57633800
C	-4.09716100	0.96651900	-0.99774900
C	-4.09614500	-0.37545300	-1.21740300
C	-2.77209500	-0.85405400	-0.90187800
C	-2.39841500	-2.18189200	-0.91221200
C	-1.16842600	-2.67026200	-0.48308800
C	-0.83482500	-4.06653700	-0.34396100
C	0.43563700	-4.11848700	0.14865100
H	4.82062400	-1.42446800	1.10400100
H	1.51771300	5.11945400	0.10206800
H	-1.17932300	5.23781700	-0.10606800
H	-4.91216900	-1.00231400	-1.54365700
H	1.02929300	-4.98864500	0.38647800
H	-4.91078200	1.66609200	-1.11639300
H	-1.49723900	-4.88555600	-0.58076100
H	5.00113400	1.25957400	0.77884400
O	-0.25867600	0.12264800	1.79659000
O	-2.15435800	-1.11133600	2.13729700
C	-0.93111800	-0.24323100	4.02973300
H	-0.91042100	0.82804100	4.25210600
H	0.04656900	-0.65118500	4.30436700
H	-1.71191200	-0.72794300	4.61664900
C	-1.17387500	-0.45360300	2.55154400
H	-3.14219400	-2.90650700	-1.22633900
H	-3.07477900	3.41003100	-0.41973800
H	3.25549900	3.15909000	0.27291300
H	2.86879400	-3.16876500	0.88109000
C	2.89803500	-0.25598400	-3.04735500
H	2.95763900	0.58543400	-3.73253600
H	3.65820900	-0.29915200	-2.27276500
C	1.92555500	-1.16336400	-3.13486500
H	1.84564800	-1.98982800	-2.43675500
H	1.15018600	-1.10589700	-3.89255400

***a* point for Comp-Cl**

Fe	0.15907600	0.02170100	-0.03244100
O	0.06226300	0.05156800	1.60735500

N	2.01056100	-0.65937300	0.09308800
N	-0.53664900	-1.87266500	-0.15431400
N	-1.73202400	0.69551900	-0.27165700
N	0.82769400	1.88193500	-0.02303100
C	2.40470100	-1.97743900	0.23601000
C	1.56344300	-3.07249500	0.21398100
C	0.19073000	-3.02482500	0.00137000
C	-0.65299600	-4.18196700	-0.15573700
C	-1.90611800	-3.71761000	-0.42855100
C	-1.82675300	-2.27913800	-0.41982500
C	-2.90743400	-1.43183500	-0.60618600
C	-2.86466700	-0.04924600	-0.52171300
C	-4.01426700	0.81159700	-0.63550200
C	-3.57087900	2.08690400	-0.44217200
C	-2.14874400	2.00137200	-0.22828100
C	-1.30789900	3.09639300	-0.06788500
C	0.06993700	3.03864500	0.00682200
C	0.92872500	4.19564700	0.06039000
C	2.21010700	3.73851100	0.04500500
C	2.13935600	2.29933400	0.00277700
C	3.23833700	1.45797500	0.03352700
C	3.17380700	0.07688000	0.10432500
C	4.31722300	-0.78848600	0.25184400
C	3.84005000	-2.05913800	0.34617700
H	-0.31728200	-5.20537000	-0.08054300
H	-5.02048200	0.47320800	-0.83255600
H	-4.13886000	3.00501400	-0.45569800
H	3.12713000	4.30774300	0.06772200
H	4.39451400	-2.97770100	0.46665700
H	0.58021800	5.21703700	0.09221900
H	5.34222100	-0.45122400	0.28515600
H	-2.80617900	-4.28405600	-0.61516800
Cl	0.28161400	-0.02823900	-2.37373000
C	-1.64517900	-0.68870400	2.79979300
H	-0.90871800	-0.94395900	3.55494200
H	-1.78707300	-1.41425600	2.00529700
C	-2.40585400	0.40583000	2.89877800
H	-3.15472200	0.65202800	2.15120700
H	-2.27460000	1.12326400	3.70397200
H	2.01727000	-4.05154600	0.32607200
H	4.22141600	1.91609300	0.04545700
H	-1.76715200	4.07906500	-0.04541400
H	-3.87005400	-1.88917700	-0.80958200

***a* point for Comp-NO_3**

Fe	-0.03856500	0.14213300	-0.15565000
O	0.13993100	0.22400300	-1.78375500
N	-0.19233300	-1.85286300	-0.13137400
N	1.93808100	-0.03103300	0.21957900
N	0.12303100	2.12330800	-0.01692200

N	-1.97145100	0.30654600	-0.45125700
C	0.77381500	-2.76925900	0.23553300
C	2.08008000	-2.45255700	0.56730000
C	2.63059800	-1.17630500	0.52355700
C	4.02580700	-0.88126500	0.73353000
C	4.17431700	0.46177800	0.54295100
C	2.86421800	0.98344600	0.24553000
C	2.56300800	2.33169600	0.12362800
C	1.28350100	2.85976600	0.03722300
C	0.98119900	4.26832700	0.07879700
C	-0.37737900	4.37986500	0.07004000
C	-0.90148000	3.04040800	-0.00775400
C	-2.24249400	2.72210300	-0.15553100
C	-2.73054700	1.44876300	-0.41275300
C	-4.09815900	1.15290100	-0.76228300
C	-4.15302100	-0.17705200	-1.04424000
C	-2.82861900	-0.70567700	-0.83123600
C	-2.50647200	-2.04716800	-0.88757400
C	-1.28216800	-2.59018200	-0.50747900
C	-1.00992000	-3.99796800	-0.37941400
C	0.26228800	-4.10908500	0.10242200
H	4.78056200	-1.61048100	0.98802200
H	1.71887700	5.05559100	0.12432400
H	-0.97765400	5.27681100	0.09767700
H	-5.00791100	-0.76245400	-1.34785800
H	0.81533200	-5.00716200	0.33388900
H	-4.89599900	1.87961800	-0.79690100
H	-1.70987900	-4.78686300	-0.61043000
H	5.07384500	1.05430500	0.61866300
O	-0.13412600	0.13861800	1.82188200
N	-0.99635900	-0.51463400	2.60154000
O	-2.00422600	-1.07721900	2.09619000
O	-0.74024400	-0.51812200	3.82891000
H	2.74089400	-3.27148700	0.83039800
H	-3.28946700	-2.73631300	-1.18502600
H	-2.95749200	3.53724900	-0.13792400
H	3.38855500	3.03403400	0.16552200
C	2.69443800	-0.42535500	-2.96011200
H	2.92736000	0.37987300	-3.65183400
H	3.44283200	-0.63788800	-2.20210700
C	1.53808400	-1.09441900	-3.02662700
H	1.30166100	-1.90507800	-2.34880200
H	0.80715000	-0.88927500	-3.80054800

Estimated minimum energy point for Comp-F

Fe	0.08119700	0.03535400	-0.37726500
O	0.19165700	0.01059600	1.78775000
N	0.63483100	-1.95368600	-0.17559300
N	-1.91136100	-0.54355500	-0.23919400
N	-0.50558500	2.00925500	-0.18849400

N	2.04801300	0.59772300	-0.11965500
C	-0.20531200	-3.04577400	-0.23562800
C	-1.59699700	-2.98837200	-0.29906700
C	-2.38552700	-1.83752600	-0.31326900
C	-3.82762900	-1.80638300	-0.41168800
C	-4.20643700	-0.49201700	-0.40982000
C	-3.00175900	0.30173000	-0.31067900
C	-2.94570900	1.69533200	-0.28834300
C	-1.79755000	2.48437900	-0.22643100
C	-1.76902600	3.93124300	-0.18949000
C	-0.45639500	4.30756100	-0.12977600
C	0.33678700	3.09665600	-0.13059000
C	1.72890000	3.03874300	-0.07594100
C	2.51851600	1.89094200	-0.06534200
C	3.96366200	1.86180300	0.01532000
C	4.34265300	0.54890300	0.01295200
C	3.13500500	-0.24535300	-0.06851600
C	3.07723700	-1.63784000	-0.08216600
C	1.92919200	-2.42641800	-0.13386400
C	1.90238200	-3.87301300	-0.15859400
C	0.59107600	-4.25377100	-0.22231800
H	-4.46107500	-2.67875000	-0.48364000
H	-2.64177900	4.56785300	-0.21093800
H	-0.05444000	5.30975500	-0.09316800
H	5.34439700	0.14722800	0.06153500
H	0.19277700	-5.25732800	-0.26203300
H	4.59729000	2.73541000	0.06594700
H	2.77684900	-4.50722600	-0.13757600
H	-5.20707400	-0.09044900	-0.48040900
F	0.11486100	0.03108200	-2.21642100
H	4.02607900	-2.16383700	-0.04869200
H	2.25263700	3.98852000	-0.03377000
H	-2.12100800	-3.93716100	-0.35657600
H	-3.89461400	2.22024800	-0.33717300
C	-0.48717000	-0.88105700	2.65284900
H	0.14300600	-1.22251400	3.47658200
H	-0.92460700	-1.73704300	2.13639300
C	-1.38113500	0.20359100	2.94180700
H	-2.22824600	0.39499500	2.29223000
H	-1.12817600	0.93828300	3.69810300