Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supporting Information

Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes

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Full Gaussian Reference:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, N.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al–Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, revision C.02; Gaussian, Inc.,

Table S1: Absolute energies, zero point energies (ZPE), free energies in the gas-phase (G) and solvent energies (Esolv) with values in au for optimized geometries, of structures A_X and B_X, X = OTf or Cl.

	E (land12dz)	ZPE (land12dz)	G (land12dz)	E (LACVP+*)	Esolv (LACVP+*)
AOTf					
singlet	-2536.19	0.82	-2535.46	-3313.37	-3313.39
triplet	-2536.22	0.82	-2535.49	-3313.40	-3313.43
quintet	-2536.23	0.82	-2535.51	-3313.42	-3313.44
septet	-2536.23	0.82	-2535.51	-3313.42	-3313.45
BOTf					
singlet	-2536.17	0.82	-2535.44	-3313.35	-3313.39
triplet	-2536.20	0.82	-2535.48	-3313.37	-3313.40
quintet	-2536.20	0.81	-2535.49	-3313.38	-3313.41
septet	-2536.22	0.81	-2535.51	-3313.40	-3313.43
ACl					
singlet	-1977.97	0.80	-1977.25	-2812.03	-2812.06
triplet	-1977.99	0.80	-1977.28	-2812.05	-2812.08
quintet	-1978.01	0.79	-1977.30	-2812.07	-2812.11
septet	-1978.01	0.79	-1977.30	-2812.08	-2812.11
BCl					
singlet	-1977.96	0.80	-1977.25	-2812.03	-2812.06
triplet	-1977.99	0.80	-1977.28	-2812.06	-2812.08
quintet	-1978.00	0.79	-1977.26	-2812.02	-2812.09
septet	-1978.02	0.79	-1977.32	-2812.10	-2812.12

Table S2: Group spin densities and charges of optimized geometries

Table S2a: A_{Cl}/B_{Cl} UB3LYP/BS1 results.

Spin densities							Charges					
	Fe	O1	O2	Cl	SPh	BIP	Fe	O1	O2	Cl	SPh	BIP
A_{Cl}												
Singlet	0.00	0.00	0.00	0.00	0.00	0.00	-0.08	-0.17	-0.18	-0.34	-0.01	0.78
Triplet	0.98	0.31	0.60	-0.02	0.17	-0.04	-0.11	-0.23	-0.18	-0.34	-0.03	0.89
Quintet	3.46	0.21	0.40	0.03	-0.22	0.12	0.14	-0.20	-0.14	-0.37	-0.04	0.60
Septet	3.76	0.80	0.90	0.12	0.31	0.11	0.10	-0.09	-0.06	-0.38	-0.19	0.61
B_{Cl}												
Singlet	0.00	0.00	0.00	0.00	0.00	0.00	-0.16	-0.14	-0.22	-0.32	-0.11	0.94
Triplet	1.02	0.47	0.61	0.02	0.00	-0.12	-0.15	-0.17	-0.18	-0.27	-0.11	0.88
Quintet	2.02	0.58	0.65	-0.03	0.89	-0.11	0.22	-0.21	-0.20	-0.35	0.02	0.52
Septet	3.69	0.97	0.96	0.14	0.20	0.04	0.12	0.00	-0.03	-0.34	-0.25	0.50

Table S2b: A_{Cl}/B_{Cl} UB3LYP/BS2 results.

Spin densities							Charges					
	Fe	O1	O2	Cl	SPh	BIP	Fe	O1	O2	Cl	SPh	BIP
A_{Cl}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	-1.59	0.80	0.26	-0.54	-0.33	1.40
triplet	0.91	0.33	0.59	-0.02	0.20	-0.01	-1.45	0.45	0.20	-0.85	0.19	1.46
quintet	3.07	0.19	0.37	0.02	0.02	0.33	1.79	0.49	0.37	-0.78	-1.06	-0.82
septet	3.35	0.79	0.89	0.12	0.34	0.50	2.66	0.00	0.19	-0.70	-1.64	-0.51
B_{Cl}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	-2.73	1.24	-0.07	-1.65	-0.04	3.25
triplet	1.10	0.45	0.57	0.00	0.02	-0.14	-2.57	0.75	-0.08	-1.73	-0.02	3.65
quintet	3.47	0.53	0.55	0.15	-1.05	0.34	2.13	0.26	-0.10	-2.12	-0.02	-0.14
septet	3.52	0.99	0.97	0.14	0.16	0.21	0.95	-0.03	0.16	-1.64	-0.27	0.84

Table S2c: A_{OTf}/B_{OTf} UB3LYP/BS1 results.

Spin densities							Charges					
	Fe	O1	O2	Otf	SPh	BIP	Fe	O1	O2	Otf	SPh	BIP
A_{OTf}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	0.16	-0.15	-0.17	-0.73	0.04	0.85
triplet	0.87	0.35	0.58	-0.01	0.23	-0.02	0.07	-0.17	-0.21	-0.72	0.03	0.99
quintet	3.57	0.20	0.30	0.04	-0.25	0.13	0.38	-0.16	-0.11	-0.75	-0.01	0.65
septet	3.74	0.82	0.93	0.05	0.33	0.13	0.37	-0.07	-0.04	-0.76	-0.16	0.65
B_{OTf}												
	Fe	O1	O2	Otf	SPh	BIP	Fe	O1	O2	Otf	SPh	BIP
singlet	0.00	0.00	0.00	0.00	0.00	0.00	0.14	-0.14	-0.14	-0.70	-0.10	0.94
triplet	-0.07	0.45	0.61	0.00	1.00	0.01	0.43	-0.19	-0.22	-0.72	0.01	0.70
quintet	2.06	0.55	0.64	0.01	1.00	-0.24	0.51	-0.21	-0.21	-0.71	0.01	0.60
septet	3.69	0.53	0.61	0.08	1.00	0.09	0.72	-0.26	-0.22	-0.73	0.01	0.48

Table S2d: A_{OTf}/B_{OTf} UB3LYP/BS2 results.

Spin densities							Charges					
	Fe	O1	O2	Otf	SPh	BIP	Fe	O1	O2	Otf	SPh	BIP
A_{OTf}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	-2.17	1.03	0.21	0.07	-0.96	1.81
triplet	0.87	0.35	0.57	-0.01	0.28	-0.06	-2.67	1.06	-0.01	0.40	-1.22	2.43
quintet	3.30	0.15	0.20	0.03	0.01	0.30	1.45	0.49	0.36	0.04	-1.66	-0.68
septet	3.46	0.83	0.95	0.04	0.32	0.40	1.24	0.03	0.28	-0.11	-1.30	-0.14
B_{OTf}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	-3.58	0.88	0.15	0.37	-0.49	2.67
triplet	0.00	0.48	0.54	-0.01	1.00	-0.01	0.00	0.00	0.00	0.00	0.00	2.70
quintet	2.31	0.55	0.57	-0.04	1.00	-0.39	-0.40	0.05	-0.08	0.07	-0.04	0.40
septet	3.72	0.54	0.54	0.08	1.01	0.12	-0.12	0.14	-0.10	-0.02	-0.09	0.19

Table S3: Absolute energies, zero point energies (ZPE), free energies in the gas-phase (G) and solvent energies (Esolv) with values in au for optimized geometries, of structures A_{SPh} and $C_{Cl,Cl}$.

	E (land12dz)	ZPE (6-311g)	G (6-311g)	E (6-311+g*)	Esolv (6-311+g*)
$C_{Cl,Cl}$					
singlet	-1751.25	0.70	-1750.63	-2642.34	-2642.38
triplet	-1751.24	0.70	-1750.62	-2642.36	-2642.43
quintet	-1751.27	0.70	-1750.65	-2642.42	-2642.45
A_{SPh}					
singlet	-2204.70	0.89	-2203.90	-2981.68	-2981.71
triplet	-2204.73	0.89	-2203.93	-2981.71	-2981.74
quintet	-2204.74	0.89	-2203.95	-2981.73	-2981.76

Table S4: Group spin densities and charges of optimized geometries.

	Spin densities						Charge					
	Fe	O1	O2	Cl1	Cl2	CDO	Fe	O1	O2	Cl1	Cl2	CDO
$C_{Cl,Cl}$												
singlet	1.74	-0.71	-0.89	0.00	-0.03	-0.11	0.00	-0.10	-0.04	-0.36	-0.28	0.78
triplet	2.07	-0.05	-0.06	0.10	0.03	-0.09	0.08	-0.03	-0.04	-0.37	-0.32	0.68
quintet	3.80	0.01	-0.40	0.16	0.24	0.18	0.26	-0.18	-0.08	-0.37	-0.27	0.64
A_{SPh}												
singlet	0.00	0.00	0.00	0.00	0.00	0.00	-0.13	-0.16	-0.23	-0.24	-0.08	0.83
triplet	0.79	0.45	0.60	0.02	0.23	-0.09	-0.20	-0.18	-0.20	-0.17	-0.09	0.84
quintet	3.22	0.33	0.55	-0.08	-0.15	0.12	0.07	-0.22	-0.22	-0.19	-0.05	0.61

Table S5. Absolute and relative energies, zero point energies and free energies of UB3LYP/BS1 optimized geometries of $^{7}[Fe^{III}O_2(LN_3S)]$. M7 = septet spin state. Absolute energies in au and relative energies in kcal mol^{-1}.

(a)

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPC^a$	ΔG^a
M7	-1646.868998	-1646.517425	-1646.577093	-0.91	-1.76	-4.62

[a] with respect to ^{1}A.

(b)

B1 -> LACVP (Solv = Chlorobenzene)			
Multip	E_{sol}	$\Delta(E+Esol)^a$	$\Delta(E+ZPC+Esol)^a$
M7	-39.09	-0.94	-1.79

[a] with respect to ^{1}A.

(c)

	B2 –> LACV3P+*					
Multip	E	E+ZPE	ΔE^a	$\Delta(E+Esol)^a$	$\Delta E+ZPC^a$	$\Delta(E+ZPC+Esol)^a$
M7	-1647.470770	-1647.119197	-6.07	-6.11	-6.92	-6.95

[a] with respect to ^{1}A.

Table S6. Group spin densities and group charges of UB3LYP/BS1 optimized geometries of $^{7}[Fe^{III}O_2(LN_3S)]$. M7 = septet spin state.

	Spin densities					Charges				
	Fe	O1	O2	S	Rest	Fe	O1	O2	S	Rest
M7	3.63	0.96	0.82	0.36	0.23	0.72	0.01	-0.15	0.10	0.32

Table S7. Group spin densities and group charges of UB3LYP/BS2//UB3LYP/BS1 calculations of $^{7}[Fe^{III}O_2(LN_3S)]$. M7 = septet spin state.

	Spin densities					Charges				
	Fe	O1	O2	S	Rest	Fe	O1	O2	S	Rest
M7	3.66	0.97	0.72	0.33	0.31	0.02	0.34	0.35	-0.48	0.77

Table S8. Group spin densities and group charges of UB3LYP/BS1 single point in solvent chlorobenzene calculations of $^{7}[Fe^{III}O_2(LN_3S)]$. M7 = septet spin state.

	Spin densities					Charges				
	Fe	O1	O2	S	Rest	Fe	O1	O2	S	Rest
M7	3.68	0.95	0.82	0.31	0.24	0.77	-0.01	-0.14	-0.01	0.39

Table S9. Important bond distances and angles of UB3LYP/BS1 optimized geometries of $^{7}[Fe^{III}O_2(LN_3S)]$. M7 = septet spin state.

	Fe-N_{av}	Fe-S	Fe-O2	O1-O2	O1-S	Ang(FeO2O1)
M7	2.166	2.336	2.075	1.278	4.364	179.9

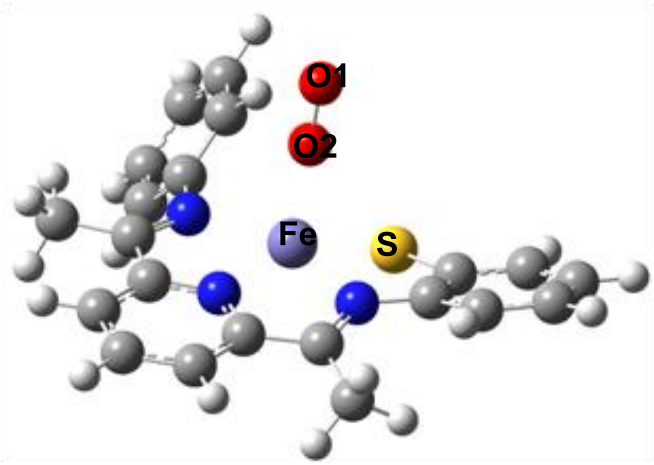

Figure S1. Optimized geometry of $^{7}[Fe^{III}O_2(LN_3S)]$ at UB3LYP/BS1 level of theory.

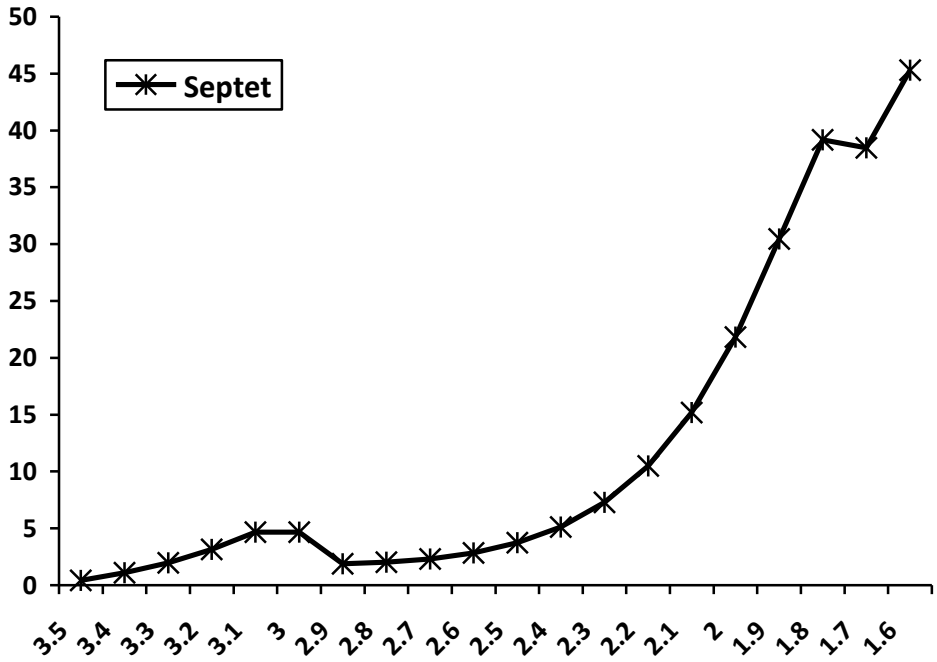

Figure S2. Geometry scan for the S–O bond formation step starting from $^{7}[Fe^{III}O_2(LN_3S)]$ at the left-hand-side. Each point represents a full geometry optimization with fixed S–O distance at UB3LYP/BS1.

Table S10. Absolute (in au) and relative (in kcal mol^{-1}) energies of optimized UB3LYP-D/BS1 and subsequent single point UB3LYP-D/BS2 calculations.

	E(B1, au)	E(B2, au)	ΔE(B1)	ΔE+ZPE(B1)	ΔE(B2)	ΔE+ZPE(B2)
A$_{OTF}$						
triplet	-2534.65186	-3311.73613	16.33	18.50	29.10	31.27
quintet	-2534.67789	-3311.78251	0.00	0.00	0.00	0.00
septet	-2534.67638	-3311.77972	0.95	0.65	1.75	1.46
B$_{OTF}$						
triplet	-2534.58061	-3311.66188	61.04	61.03	75.70	75.68
quintet	-2534.60754	-3311.71911	44.14	43.55	39.79	39.19
septet	-2534.63194	-3311.72624	28.83	27.42	35.31	33.90
A$_{Cl}$						
triplet	-1976.63141	-2810.60531	25.48	27.16	37.50	39.19
quintet	-1976.67201	-2810.66507	0.00	0.00	0.00	0.00
septet	-1976.67173	-2810.66429	0.18	-0.11	0.49	0.21
B$_{Cl}$						
triplet	-1976.63585	-2810.61118	22.69	24.58	33.82	35.71
quintet	-1976.63689	-2810.64399	22.04	20.96	13.23	12.15
septet	-1976.68242	-2810.67811	-6.53	-7.55	-8.18	-9.21

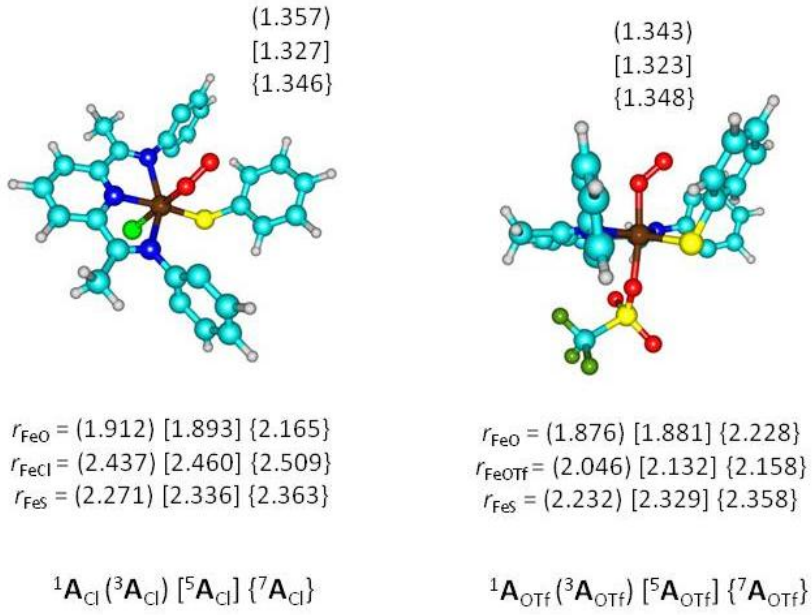

Figure S3. B3LYP-D/B1 optimized geometries of ^{3,5,7}**A**$_{Cl}$ (left-hand-side) and ^{3,5,7}**A**$_{OTf}$ (right-hand-side) with bond lengths in angstroms. H-atoms and isopropyl groups have been hidden.

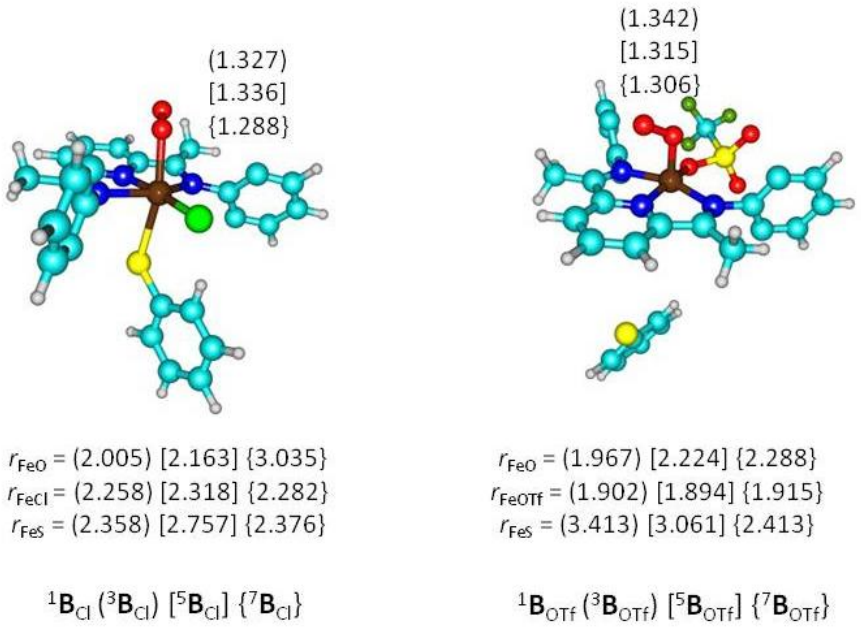

Figure S4. B3LYP-D/B1 optimized geometries of $^{3,5,7}\mathbf{B}_{Cl}$ (left-hand-side) and $^{3,5,7}\mathbf{B}_{OTf}$ (right-hand-side) with bond lengths in angstroms. H-atoms and isopropyl groups have been hidden.

Cartesian Coordinates:

$A_{Cl,\ 5}$

Fe	-0.044338000	-0.513358000	0.236930000
C	-2.439307000	-2.057915000	-0.924660000
C	-1.207044000	-2.843571000	-1.244090000
C	-1.233620000	-4.128224000	-1.822748000
H	-2.174850000	-4.603062000	-2.072629000
C	-0.017945000	-4.791241000	-2.059439000
H	-0.013713000	-5.785387000	-2.496647000
C	1.191101000	-4.163919000	-1.719614000
H	2.135061000	-4.667628000	-1.888467000
C	1.154809000	-2.874451000	-1.148709000
C	2.381779000	-2.117862000	-0.752171000
C	-3.778766000	-2.640010000	-1.322961000
H	-4.593189000	-1.969632000	-1.046019000
H	-3.936813000	-3.602368000	-0.818760000
H	-3.824018000	-2.817832000	-2.404701000
C	3.719282000	-2.801795000	-0.944736000
H	3.871355000	-3.091556000	-1.991263000
H	3.757414000	-3.715413000	-0.337044000
H	4.540102000	-2.151710000	-0.641164000
C	-3.367167000	-0.021781000	-0.016055000
C	-3.813410000	0.881157000	-1.024023000
C	-4.865450000	1.763240000	-0.696415000
H	-5.221187000	2.461952000	-1.449272000
C	-5.457579000	1.758427000	0.574604000
H	-6.267261000	2.447497000	0.802893000
C	-5.000294000	0.859093000	1.548818000
H	-5.460297000	0.854187000	2.533304000
C	-3.950923000	-0.044136000	1.281086000
C	-3.224431000	0.932783000	-2.440837000
H	-2.343797000	0.285544000	-2.481204000
C	-4.251400000	0.431891000	-3.493415000
H	-4.599564000	-0.586343000	-3.277347000
H	-3.800067000	0.434009000	-4.494898000
H	-5.134888000	1.083287000	-3.523312000
C	-2.735302000	2.357022000	-2.810065000
H	-3.568375000	3.071710000	-2.852946000
H	-2.255580000	2.343461000	-3.797755000
H	-2.001016000	2.721062000	-2.085783000
C	-3.518813000	-1.038357000	2.362797000
H	-2.592445000	-1.526625000	2.048586000
C	-3.205830000	-0.341763000	3.710144000
H	-2.434128000	0.424036000	3.577793000
H	-2.826875000	-1.081358000	4.426702000
H	-4.097344000	0.127811000	4.148953000
C	-4.596499000	-2.140691000	2.558296000
H	-5.543183000	-1.712121000	2.915315000
H	-4.253080000	-2.872619000	3.300918000
H	-4.805384000	-2.677963000	1.622917000
C	3.340809000	-0.066968000	0.079310000
C	3.831372000	-0.039061000	1.415311000
C	4.912730000	0.819184000	1.705703000
H	5.298592000	0.853176000	2.720735000
C	5.494851000	1.623463000	0.716305000
H	6.327479000	2.278192000	0.962123000
C	4.997529000	1.577533000	-0.593960000
H	5.451215000	2.202281000	-1.358383000
C	3.916498000	0.741278000	-0.945839000
C	3.273788000	-0.939455000	2.521358000
H	2.330369000	-1.375887000	2.184202000
C	2.955215000	-0.158222000	3.819756000
H	3.860492000	0.251067000	4.289597000
H	2.475840000	-0.830229000	4.542650000
H	2.261078000	0.663846000	3.616551000
C	4.254144000	-2.106661000	2.825501000
H	5.208888000	-1.729952000	3.217971000
H	4.473164000	-2.702110000	1.929321000
H	3.816507000	-2.775754000	3.577591000
C	3.448101000	0.723518000	-2.408944000
H	2.471020000	0.232187000	-2.457609000
C	4.441439000	-0.069766000	-3.304684000
H	5.426171000	0.416352000	-3.314220000
H	4.073826000	-0.105287000	-4.339234000
H	4.585087000	-1.099439000	-2.958139000
C	3.265386000	2.149164000	-2.989944000
H	4.226293000	2.671325000	-3.090883000
H	2.601877000	2.748080000	-2.361247000
H	2.816768000	2.087025000	-3.990138000
N	2.206028000	-0.928236000	-0.249071000
N	-0.028134000	-2.251166000	-0.933620000
N	-2.262260000	-0.925660000	-0.309751000
S	-0.078799000	1.246288000	1.815368000
C	-0.006299000	2.883967000	1.025593000
C	-1.189505000	3.643219000	0.850042000
H	-2.145525000	3.212597000	1.135258000
C	-1.123192000	4.940151000	0.315384000
H	-2.036107000	5.517625000	0.187074000
C	0.121865000	5.494475000	-0.053942000
H	0.169937000	6.500517000	-0.465377000
C	1.299875000	4.740827000	0.111808000
H	2.261631000	5.160652000	-0.174247000
C	1.238789000	3.440048000	0.644330000
H	2.143786000	2.853672000	0.771293000
O	-0.240781000	0.709008000	-1.356059000
O	0.543488000	1.738030000	-1.683714000
Cl	-0.094841000	-2.123802000	2.066046000

$A_{Cl,\ 7}$

Fe	-0.031617000	-0.617272000	0.346964000
C	-2.425304000	-2.018341000	-0.939860000
C	-1.211600000	-2.796406000	-1.327658000
C	-1.248133000	-4.028242000	-2.011936000
H	-2.191980000	-4.477949000	-2.296717000
C	-0.035274000	-4.670932000	-2.314267000
H	-0.038260000	-5.623065000	-2.836715000
C	1.181301000	-4.078992000	-1.933348000
H	2.121756000	-4.568663000	-2.156869000
C	1.152139000	-2.844648000	-1.253179000
C	2.369404000	-2.111102000	-0.797205000
C	-3.778742000	-2.592910000	-1.297835000
H	-4.585318000	-1.944197000	-0.955289000
H	-3.899723000	-3.576539000	-0.825472000
H	-3.876647000	-2.729874000	-2.381852000
C	3.717302000	-2.748291000	-1.055598000
H	3.876246000	-2.921666000	-2.126880000
H	3.766317000	-3.721610000	-0.549768000
H	4.528142000	-2.123319000	-0.680618000
C	-3.329217000	-0.004349000	0.039094000
C	-3.851652000	0.866447000	-0.962127000
C	-4.892869000	1.745028000	-0.592592000
H	-5.303246000	2.420538000	-1.338858000
C	-5.406496000	1.767398000	0.711248000
H	-6.208071000	2.454532000	0.971251000
C	-4.879980000	0.898009000	1.676985000
H	-5.278518000	0.914316000	2.687515000
C	-3.837009000	0.000836000	1.368578000
C	-3.356769000	0.900577000	-2.415564000
H	-2.479737000	0.252042000	-2.508893000
C	-4.444944000	0.378934000	-3.395507000
H	-4.774743000	-0.636546000	-3.145496000
H	-4.057435000	0.370877000	-4.423205000
H	-5.330824000	1.027050000	-3.377163000
C	-2.915347000	2.325569000	-2.840905000
H	-3.766160000	3.019804000	-2.852538000
H	-2.491040000	2.301030000	-3.853292000
H	-2.154295000	2.726776000	-2.165487000
C	-3.336276000	-0.965666000	2.443503000
H	-2.405529000	-1.426910000	2.104376000
C	-3.010413000	-0.254056000	3.779096000
H	-2.296001000	0.560711000	3.618030000
H	-2.555346000	-0.971816000	4.473157000
H	-3.908901000	0.155708000	4.261259000
C	-4.362277000	-2.110466000	2.670925000
H	-5.315634000	-1.719742000	3.053244000
H	-3.966602000	-2.825561000	3.403376000
H	-4.572961000	-2.659149000	1.742579000
C	3.293324000	-0.113266000	0.193840000
C	3.727707000	-0.096111000	1.549104000
C	4.788346000	0.766510000	1.894603000
H	5.131619000	0.791776000	2.924995000
C	5.403652000	1.588298000	0.939652000
H	6.218859000	2.247539000	1.227934000
C	4.962085000	1.553866000	-0.390197000
H	5.441289000	2.192644000	-1.127572000
C	3.905566000	0.710700000	-0.796666000
C	3.133384000	-1.019264000	2.614324000
H	2.204225000	-1.451343000	2.234897000
C	2.767530000	-0.269694000	3.918302000
H	3.653781000	0.128306000	4.431958000
H	2.263835000	-0.960354000	4.606253000
H	2.080969000	0.557758000	3.708100000
C	4.099706000	-2.198479000	2.915597000
H	5.046754000	-1.837836000	3.340884000
H	4.336147000	-2.773158000	2.009565000
H	3.637920000	-2.883211000	3.638267000
C	3.491232000	0.728339000	-2.275534000
H	2.585664000	0.125489000	-2.398267000
C	4.599794000	0.119906000	-3.179970000
H	5.518258000	0.718783000	-3.126431000
H	4.269582000	0.106589000	-4.227433000
H	4.857203000	-0.905122000	-2.888526000
C	3.154224000	2.160928000	-2.765855000
H	4.046963000	2.800499000	-2.772140000

H	2.397768000	2.633503000	-2.133266000
H	2.764358000	2.123848000	-3.791638000
N	2.174902000	-0.973859000	-0.184006000
N	-0.027994000	-2.244274000	-0.974909000
N	-2.224883000	-0.900580000	-0.294836000
S	-0.064254000	1.308461000	1.697024000
C	0.086363000	2.906963000	0.805162000
C	-1.073694000	3.628469000	0.444921000
H	-2.052424000	3.202110000	0.646829000
C	-0.960955000	4.894519000	-0.159640000
H	-1.861984000	5.441555000	-0.430045000
C	0.307505000	5.455766000	-0.407825000
H	0.392363000	6.436894000	-0.869852000
C	1.464640000	4.737610000	-0.046658000
H	2.449796000	5.162650000	-0.228175000
C	1.357888000	3.470469000	0.557258000
H	2.251877000	2.924449000	0.845256000
O	0.013708000	0.296635000	-1.970958000
O	0.097283000	1.581184000	-2.166413000
Cl	-0.101380000	-2.445790000	2.001687000

$B_{Cl,\ 5}$

Fe	0.352933000	-0.300568000	-0.317098000
C	2.801541000	0.780970000	1.033850000
C	2.530113000	-0.542343000	1.662510000
C	3.376077000	-1.158918000	2.614177000
H	4.295316000	-0.678785000	2.927745000
C	3.017743000	-2.410161000	3.130531000
H	3.647115000	-2.895650000	3.871005000
C	1.857793000	-3.058753000	2.656243000
H	1.601272000	-4.051289000	3.007106000
C	1.061337000	-2.400846000	1.703298000
C	-0.079844000	-3.041685000	0.987568000
C	4.147220000	1.418289000	1.299768000
H	4.249585000	2.364510000	0.766957000
H	4.936150000	0.737245000	0.958409000
H	4.301815000	1.603868000	2.370100000
C	-0.471073000	-4.450667000	1.383535000
H	-0.755829000	-4.491726000	2.442685000
H	0.375634000	-5.134631000	1.241072000
H	-1.306009000	-4.811748000	0.782211000
C	1.946846000	2.649913000	-0.231628000
C	1.671836000	3.747314000	0.640219000
C	1.777435000	5.056142000	0.123723000
H	1.574712000	5.900706000	0.777496000
C	2.130335000	5.289169000	-1.211953000
H	2.209915000	6.306104000	-1.588795000
C	2.371742000	4.199397000	-2.059839000
H	2.634620000	4.378482000	-3.098274000
C	2.282861000	2.869061000	-1.599524000
C	1.252790000	3.584616000	2.108703000
H	1.076210000	2.521616000	2.309190000
C	2.355077000	4.081452000	3.084748000
H	3.309760000	3.569255000	2.923615000
H	2.046997000	3.915286000	4.126146000
H	2.531353000	5.157389000	2.954519000
C	-0.071359000	4.335608000	2.408717000
H	0.065625000	5.423245000	2.352202000
H	-0.421923000	4.097402000	3.421976000
H	-0.857455000	4.059020000	1.699252000
C	2.611578000	1.724318000	-2.561574000
H	2.202696000	0.799197000	-2.152688000
C	1.976828000	1.909884000	-3.960762000
H	0.893224000	2.049000000	-3.880990000
H	2.156774000	1.009961000	-4.563149000
H	2.406453000	2.762001000	-4.505506000
C	4.148655000	1.535111000	-2.679818000
H	4.626093000	2.437188000	-3.088478000
H	4.372840000	0.691970000	-3.345204000
H	4.602594000	1.314335000	-1.706480000
C	-1.640496000	-2.934693000	-0.843942000
C	-1.246267000	-3.513209000	-2.081880000
C	-2.244990000	-4.090825000	-2.892256000
H	-1.960470000	-4.541519000	-3.839810000
C	-3.592626000	-4.088288000	-2.504108000
H	-4.347358000	-4.541835000	-3.142115000
C	-3.962828000	-3.481728000	-1.295548000
H	-5.010942000	-3.459635000	-1.007374000
C	-3.004039000	-2.888225000	-0.447689000
C	0.210102000	-3.534341000	-2.554950000
H	0.823163000	-2.965327000	-1.851773000
C	0.367464000	-2.836796000	-3.930373000
H	-0.166443000	-3.376813000	-4.724526000
H	1.429433000	-2.792668000	-4.204101000
H	-0.017893000	-1.812053000	-3.887543000
C	0.768860000	-4.981720000	-2.599304000
H	0.224475000	-5.598390000	-3.327420000
H	0.691131000	-5.475366000	-1.620411000
H	1.827146000	-4.968038000	-2.891026000
C	-3.478829000	-2.199892000	0.836656000
H	-2.619239000	-1.704296000	1.304413000
C	-4.056531000	-3.211686000	1.862612000
H	-4.934863000	-3.727858000	1.453032000
H	-4.368722000	-2.690863000	2.777816000
H	-3.320919000	-3.977003000	2.139846000
C	-4.522990000	-1.098057000	0.520438000
H	-5.447580000	-1.528864000	0.114497000
H	-4.130041000	-0.387488000	-0.214467000
H	-4.783894000	-0.545250000	1.432593000
N	-0.603266000	-2.358345000	0.003711000
N	1.370741000	-1.142980000	1.292143000
N	1.847278000	1.292617000	0.292140000
O	2.144472000	-1.214123000	-1.263931000
O	3.391194000	-1.156512000	-0.732464000
S	-1.304550000	0.666446000	1.952439000
C	-2.623859000	1.836732000	1.668132000
C	-3.409734000	2.290264000	2.769267000
H	-3.192092000	1.912059000	3.764371000
H	-5.039788000	3.556017000	3.405683000
C	-4.443236000	3.212768000	2.564286000
C	-4.707466000	3.699830000	1.262599000
H	-5.509018000	4.418100000	1.105891000
H	-4.140376000	3.627105000	-0.832664000
C	-3.934792000	3.255120000	0.167420000
C	-2.899988000	2.327643000	0.358762000
H	-2.310435000	1.970336000	-0.481941000
Cl	-1.000152000	0.462867000	-2.057062000

$B_{Cl,\ 7}$

Fe	0.030196000	-0.039303000	0.080241000
C	2.713549000	0.870195000	1.192176000
C	2.441636000	-0.470809000	1.770767000
C	3.214488000	-1.087435000	2.773936000
H	4.064569000	-0.574931000	3.209426000
C	2.866610000	-2.380971000	3.201525000
H	3.442231000	-2.871928000	3.980455000
C	1.777017000	-3.041512000	2.604326000
H	1.508620000	-4.046124000	2.910592000
C	1.040753000	-2.375558000	1.606137000
C	-0.086538000	-2.968164000	0.842515000
C	3.957690000	1.606846000	1.633706000
H	4.113555000	2.508086000	1.039398000
H	4.838867000	0.961701000	1.531973000
H	3.878985000	1.900230000	2.688499000
C	-0.440918000	-4.418062000	1.087686000
H	-0.821501000	-4.550796000	2.108870000
H	0.445158000	-5.055714000	0.977882000
H	-1.205572000	-4.760968000	0.389819000
C	2.000059000	2.581040000	-0.357973000
C	1.675340000	3.788517000	0.321333000
C	1.838228000	5.001627000	-0.382371000
H	1.590270000	5.936385000	0.113889000
C	2.299123000	5.025539000	-1.704942000
H	2.416068000	5.972933000	-2.225610000
C	2.597004000	3.820491000	-2.359655000
H	2.941074000	3.844481000	-3.389579000
C	2.448255000	2.580150000	-1.709581000
C	1.127619000	3.841444000	1.753589000
H	0.991044000	2.820440000	2.125600000
C	2.091541000	4.590575000	2.713321000
H	3.094522000	4.146632000	2.726332000
H	1.694725000	4.569880000	3.737025000
H	2.200560000	5.642995000	2.419681000
C	-0.270651000	4.512434000	1.787100000
H	-0.210980000	5.574874000	1.514308000
H	-0.698336000	4.443638000	2.795248000
H	-0.963477000	4.019639000	1.099210000
C	2.828873000	1.284521000	-2.432924000
H	2.320161000	0.455471000	-1.928063000
C	2.368779000	1.259393000	-3.909460000
H	1.295942000	1.464892000	-3.982755000
H	2.556509000	0.266591000	-4.339482000
H	2.913306000	1.989654000	-4.522617000
C	4.361050000	1.040245000	-2.337626000
H	4.912739000	1.859307000	-2.818156000
H	4.633799000	0.104537000	-2.843348000
H	4.699931000	0.973849000	-1.295385000
C	-1.711646000	-2.665193000	-0.912986000
C	-1.336107000	-3.048974000	-2.230460000
C	-2.337530000	-3.553052000	-3.083658000
H	-2.073599000	-3.857778000	-4.092808000
C	-3.670318000	-3.658415000	-2.657306000
H	-4.429481000	-4.049489000	-3.330446000
C	-4.021783000	-3.241613000	-1.366217000
H	-5.059725000	-3.302681000	-1.049248000
C	-3.058942000	-2.732622000	-0.467994000
C	0.112863000	-2.962418000	-2.721958000
H	0.670141000	-2.324758000	-2.027886000
C	0.220829000	-2.305862000	-4.119790000
H	-0.244798000	-2.923137000	-4.899295000
H	1.277493000	-2.175964000	-4.391008000

H	-0.258634000	-1.321415000	-4.118538000
C	0.785366000	-4.362937000	-2.721062000
H	0.268923000	-5.044137000	-3.410639000
H	0.767431000	-4.821785000	-1.723381000
H	1.833116000	-4.284727000	-3.040428000
C	-3.511835000	-2.259350000	0.918429000
H	-2.666942000	-1.780758000	1.425554000
C	-4.002970000	-3.440231000	1.798713000
H	-4.883707000	-3.923573000	1.354910000
H	-4.286449000	-3.074280000	2.794260000
H	-3.231092000	-4.209690000	1.925397000
C	-4.626243000	-1.186412000	0.804122000
H	-5.551224000	-1.608902000	0.388637000
H	-4.310762000	-0.355497000	0.165583000
H	-4.856514000	-0.776049000	1.795065000
N	-0.661477000	-2.176901000	-0.027696000
N	1.367667000	-1.108220000	1.235771000
N	1.848879000	1.294003000	0.304718000
O	3.162639000	-2.142356000	-1.240271000
O	4.125474000	-1.901156000	-0.442027000
S	-1.027544000	0.513805000	2.206295000
C	-2.511642000	1.588415000	2.039391000
C	-3.235103000	1.893055000	3.217144000
H	-2.897895000	1.489409000	4.168813000
H	-4.923703000	2.932180000	4.078877000
C	-4.380150000	2.709579000	3.162482000
C	-4.821290000	3.235984000	1.931763000
H	-5.706422000	3.866674000	1.888119000
H	-4.428618000	3.331930000	-0.199897000
C	-4.101397000	2.934544000	0.758821000
C	-2.955433000	2.118188000	0.806961000
H	-2.416575000	1.895600000	-0.109614000
Cl	-0.832997000	0.714486000	-1.944668000

$A_{OTF,\ 5}$

Fe	-0.037877000	0.030847000	0.090797000
C	2.531969000	-0.197423000	1.771851000
C	1.533839000	-1.140279000	2.373248000
C	1.823428000	-2.013735000	3.437983000
H	2.815897000	-2.052660000	3.870425000
C	0.800561000	-2.848011000	3.924170000
H	1.001252000	-3.535709000	4.740410000
C	-0.473618000	-2.801272000	3.340688000
H	-1.260788000	-3.457535000	3.689729000
C	-0.700187000	-1.908896000	2.272040000
C	-2.013937000	-1.771715000	1.570313000
C	3.927536000	-0.172960000	2.353328000
H	4.553271000	0.556914000	1.838302000
H	4.389614000	-1.163296000	2.249305000
H	3.906296000	0.075162000	3.421699000
C	-3.120709000	-2.718919000	1.970232000
H	-3.337777000	-2.660440000	3.043200000
H	-2.795764000	-3.743172000	1.745356000
H	-4.037833000	-2.515002000	1.416997000
C	2.926625000	1.582177000	0.178647000
C	2.980530000	2.861985000	0.805230000
C	3.734141000	3.873080000	0.171455000
H	3.788620000	4.856640000	0.630752000
C	4.407450000	3.638762000	-1.035749000
H	4.980482000	4.434500000	-1.505553000
C	4.340433000	2.371031000	-1.631194000
H	4.865833000	2.188549000	-2.564504000
C	3.604782000	1.321272000	-1.044128000
C	2.277796000	3.195390000	2.129140000
H	1.625206000	2.361095000	2.403761000
C	3.308729000	3.408529000	3.272351000
H	3.955548000	2.533929000	3.413753000
H	2.790150000	3.608520000	4.219734000
H	3.957899000	4.267533000	3.057849000
C	1.368527000	4.445729000	2.003750000
H	1.957058000	5.353593000	1.815317000
H	0.812232000	4.598193000	2.938184000
H	0.640845000	4.330237000	1.195211000
C	3.621331000	-0.063398000	-1.697680000
H	2.851337000	-0.680463000	-1.226765000
C	3.283558000	-0.014097000	-3.208191000
H	2.315434000	0.470442000	-3.372906000
H	3.224270000	-1.034753000	-3.606905000
H	4.048972000	0.524135000	-3.783877000
C	5.001445000	-0.742657000	-1.471750000
H	5.806777000	-0.153036000	-1.930364000
H	5.011264000	-1.741459000	-1.923729000
H	5.232398000	-0.850641000	-0.403439000
C	-3.367262000	-0.518331000	0.012369000
C	-3.662463000	-1.015608000	-1.288599000
C	-4.887706000	-0.646394000	-1.880445000
H	-5.126779000	-1.021142000	-2.871180000
C	-5.797193000	0.189016000	-1.216213000
H	-6.738294000	0.459420000	-1.688868000
C	-5.484447000	0.675444000	0.060781000
H	-6.187985000	1.329529000	0.568691000
C	-4.272121000	0.343050000	0.703047000
C	-2.732593000	-1.983812000	-2.021951000
H	-1.738867000	-1.890788000	-1.575882000
C	-2.571463000	-1.665200000	-3.526954000
H	-3.501462000	-1.838667000	-4.085507000
H	-1.799985000	-2.320368000	-3.948209000
H	-2.257297000	-0.626781000	-3.678611000
C	-3.211204000	-3.450933000	-1.837253000
H	-4.206367000	-3.589871000	-2.281945000
H	-3.267805000	-3.734299000	-0.779514000
H	-2.508232000	-4.132604000	-2.328724000
C	-4.007289000	0.922576000	2.101721000
H	-2.957389000	0.749058000	2.361686000
C	-4.895702000	0.235294000	3.176687000
H	-5.959103000	0.416480000	2.972204000
H	-4.671040000	0.642621000	4.171752000
H	-4.747026000	-0.849469000	3.209541000
C	-4.239088000	2.455672000	2.153293000
H	-5.301553000	2.706062000	2.033837000
H	-3.668617000	2.967875000	1.374233000
H	-3.914462000	2.848631000	3.125947000
N	-2.092807000	-0.858069000	0.641233000
N	0.291435000	-1.102127000	1.834380000
N	2.114267000	0.531952000	0.778894000
C	2.477720000	-3.844113000	-0.741011000
F	2.515787000	-5.184542000	-0.405488000
F	3.236394000	-3.645700000	-1.878947000
F	3.051784000	-3.119022000	0.307046000
S	0.567384000	-3.255112000	-1.027535000
O	0.757046000	-1.598776000	-0.971036000
O	0.182023000	-3.827772000	-2.488251000
O	-0.206260000	-3.868662000	0.268097000
S	-0.316200000	1.084875000	-2.026407000
C	-0.967497000	2.769013000	-1.876314000
C	-0.085938000	3.879784000	-1.917455000
H	0.984785000	3.706127000	-1.980369000
C	-0.595660000	5.186497000	-1.879178000
H	0.087163000	6.032509000	-1.912129000
C	-1.989310000	5.405395000	-1.800530000
H	-2.380272000	6.420221000	-1.775211000
C	-2.869410000	4.307119000	-1.755682000
H	-3.942932000	4.468891000	-1.693289000
C	-2.364741000	2.994834000	-1.787955000
H	-3.039535000	2.144701000	-1.754620000
O	-0.456184000	1.713752000	1.171430000
O	-1.346731000	2.673948000	0.981905000

$A_{OTF,\ 7}$

Fe	0.001393000	-0.029616000	-0.020778000
C	2.528558000	0.109522000	1.708257000
C	1.615716000	-0.877610000	2.365288000
C	1.960917000	-1.646557000	3.492633000
H	2.942361000	-1.564379000	3.944216000
C	1.007547000	-2.537776000	4.017927000
H	1.251662000	-3.147118000	4.883099000
C	-0.252400000	-2.650500000	3.411174000
H	-0.983819000	-3.352856000	3.791078000
C	-0.535289000	-1.855624000	2.281468000
C	-1.836813000	-1.878732000	1.548196000
C	3.925829000	0.262427000	2.264443000
H	4.497172000	0.999377000	1.699113000
H	4.448836000	-0.701171000	2.211119000
H	3.900939000	0.571015000	3.316748000
C	-2.850580000	-2.920646000	1.955589000
H	-3.117899000	-2.837865000	3.015621000
H	-2.404726000	-3.910568000	1.792548000
H	-3.760166000	-2.844390000	1.359421000
C	2.789850000	1.830207000	0.031832000
C	2.783558000	3.133197000	0.609759000
C	3.480426000	4.157234000	-0.066350000
H	3.487448000	5.158890000	0.355513000
C	4.156742000	3.912547000	-1.269546000
H	4.685202000	4.718241000	-1.773269000
C	4.147928000	2.622575000	-1.818225000
H	4.673385000	2.432873000	-2.750097000
C	3.469686000	1.559763000	-1.187374000
C	2.067444000	3.483561000	1.922002000
H	1.468652000	2.623817000	2.240216000
C	3.083478000	3.805523000	3.052996000
H	3.778963000	2.976855000	3.232280000
H	2.553862000	4.017688000	3.991547000
H	3.682465000	4.689699000	2.799113000
C	1.089255000	4.674498000	1.745699000
H	1.627865000	5.605032000	1.523423000
H	0.519999000	4.833225000	2.671083000
H	0.376450000	4.492176000	0.935776000
C	3.545891000	0.158771000	-1.799490000
H	2.831319000	-0.490780000	-1.286505000
C	3.157330000	0.147111000	-3.299135000
H	2.167621000	0.591678000	-3.448324000
H	3.125854000	-0.886879000	-3.665023000
H	3.883219000	0.696589000	-3.914050000
C	4.968552000	-0.434828000	-1.600233000

H	5.724791000	0.186656000	-2.098411000
H	5.022004000	-1.443407000	-2.026344000
H	5.236182000	-0.500129000	-0.536793000
C	-3.274755000	-0.820188000	-0.074867000
C	-3.478804000	-1.332965000	-1.387323000
C	-4.719820000	-1.092854000	-2.011255000
H	-4.888634000	-1.477349000	-3.012693000
C	-5.735477000	-0.373701000	-1.365892000
H	-6.685626000	-0.200208000	-1.865005000
C	-5.518221000	0.119985000	-0.072547000
H	-6.308133000	0.677791000	0.423518000
C	-4.294790000	-0.084400000	0.601849000
C	-2.438521000	-2.200452000	-2.096722000
H	-1.472789000	-2.034273000	-1.613046000
C	-2.248018000	-1.839146000	-3.588733000
H	-3.141468000	-2.068424000	-4.185284000
H	-1.416177000	-2.426543000	-3.995451000
H	-2.007856000	-0.776788000	-3.707594000
C	-2.797930000	-3.705742000	-1.946522000
H	-3.754945000	-3.925043000	-2.439570000
H	-2.882403000	-4.002498000	-0.893413000
H	-2.015118000	-4.320142000	-2.404812000
C	-4.149636000	0.497991000	2.016656000
H	-3.112358000	0.378260000	2.348163000
C	-5.066645000	-0.242493000	3.030503000
H	-6.123795000	-0.108268000	2.767324000
H	-4.919617000	0.161850000	4.041158000
H	-4.869319000	-1.319732000	3.059322000
C	-4.468941000	2.016420000	2.054263000
H	-5.529837000	2.204979000	1.844761000
H	-3.871633000	2.570820000	1.325046000
H	-4.251659000	2.420460000	3.051995000
N	-1.981833000	-1.011802000	0.579437000
N	0.388925000	-0.992765000	1.805743000
N	2.045039000	0.757709000	0.684927000
C	2.834836000	-3.726803000	-0.506682000
F	3.000463000	-5.022247000	-0.053350000
F	3.599336000	-3.547511000	-1.643544000
F	3.303928000	-2.858434000	0.483998000
S	0.880433000	-3.360684000	-0.881908000
O	0.885628000	-1.691257000	-0.941267000
O	0.596841000	-4.068509000	-2.305852000
O	0.126551000	-3.952161000	0.435370000
S	-0.398656000	1.226672000	-1.978856000
C	-1.304688000	2.798744000	-1.740061000
C	-0.612962000	4.025916000	-1.873172000
H	0.457311000	4.016263000	-2.059961000
C	-1.307763000	5.244744000	-1.774998000
H	-0.764570000	6.181765000	-1.878936000
C	-2.700407000	5.255895000	-1.552411000
H	-3.236705000	6.199724000	-1.484158000
C	-3.391703000	4.035434000	-1.426802000
H	-4.467447000	4.031340000	-1.264180000
C	-2.700954000	2.812296000	-1.518867000
H	-3.239635000	1.873473000	-1.436841000
O	-0.761494000	1.628133000	1.680873000
O	-1.438885000	2.691815000	1.387671000

$B_{OTF,\ 5}$

Fe	-0.758290000	0.082845000	0.829155000
C	0.222041000	2.480246000	2.022313000
C	0.570988000	1.377562000	2.928333000
C	1.136821000	1.465831000	4.207884000
H	1.401904000	2.429021000	4.629463000
C	1.346909000	0.277052000	4.940640000
H	1.783049000	0.322615000	5.933802000
C	0.982908000	-0.962666000	4.388760000
H	1.122459000	-1.878686000	4.951905000
C	0.421209000	-0.999490000	3.098356000
C	0.024292000	-2.180145000	2.321298000
C	0.498160000	3.902807000	2.439021000
H	0.304525000	4.604592000	1.627304000
H	1.541255000	4.010831000	2.760007000
H	-0.138906000	4.175890000	3.290275000
C	0.161765000	-3.558843000	2.911821000
H	-0.627078000	-3.724947000	3.657207000
H	1.128473000	-3.672096000	3.416727000
H	0.072988000	-4.329735000	2.144422000
C	-0.762233000	3.101440000	-0.088611000
C	-2.018375000	3.746377000	0.073832000
C	-2.374374000	4.721969000	-0.879819000
H	-3.335654000	5.221063000	-0.791518000
C	-1.526372000	5.039420000	-1.949417000
H	-1.828168000	5.787493000	-2.678437000
C	-0.298136000	4.375670000	-2.094925000
H	0.339216000	4.610986000	-2.941623000
C	0.111196000	3.392036000	-1.173486000
C	-2.991810000	3.420309000	1.215302000
H	-2.593873000	2.585820000	1.802861000
C	-3.174194000	4.634093000	2.167573000
H	-2.220376000	4.985147000	2.581747000
H	-3.830816000	4.360675000	3.004120000
H	-3.636738000	5.479519000	1.641264000
C	-4.372770000	2.958669000	0.678507000
H	-4.893696000	3.776607000	0.162162000
H	-5.002624000	2.628831000	1.514846000
H	-4.263115000	2.133296000	-0.029854000
C	1.477276000	2.707633000	-1.316029000
H	1.421671000	1.737360000	-0.804033000
C	1.870816000	2.428699000	-2.786131000
H	1.072021000	1.889370000	-3.302878000
H	2.783236000	1.815723000	-2.812841000
H	2.088849000	3.356064000	-3.332834000
C	2.590695000	3.542929000	-0.622596000
H	2.685514000	4.526803000	-1.101628000
H	3.557650000	3.029026000	-0.698886000
H	2.386075000	3.704558000	0.441702000
C	-0.726509000	-2.950025000	0.143587000
C	0.186177000	-3.171871000	-0.925089000
C	-0.108842000	-4.193973000	-1.846982000
H	0.574949000	-4.386249000	-2.668583000
C	-1.284897000	-4.952232000	-1.733812000
H	-1.503289000	-5.729829000	-2.461838000
C	-2.186848000	-4.692400000	-0.692489000
H	-3.106561000	-5.267432000	-0.625388000
C	-1.931096000	-3.693262000	0.270667000
C	1.483801000	-2.366521000	-1.047202000
H	1.363847000	-1.446055000	-0.463095000
C	1.799047000	-1.941599000	-2.501123000
H	2.002172000	-2.805588000	-3.147598000
H	2.695924000	-1.306927000	-2.515432000
H	0.970937000	-1.371604000	-2.936668000
C	2.674269000	-3.152253000	-0.430753000
H	2.853088000	-4.085059000	-0.982378000
H	2.482969000	-3.415454000	0.618411000
H	3.592611000	-2.551496000	-0.468303000
C	-2.972465000	-3.415988000	1.360915000
H	-2.551964000	-2.726597000	2.098228000
C	-3.395756000	-4.703151000	2.114939000
H	-3.924562000	-5.405498000	1.457489000
H	-4.076957000	-4.444516000	2.935964000
H	-2.532168000	-5.232157000	2.540453000
C	-4.214477000	-2.703518000	0.761586000
H	-4.705457000	-3.329613000	0.004542000
H	-3.932977000	-1.756575000	0.291223000
H	-4.939801000	-2.486988000	1.556585000
N	-0.386875000	-1.906356000	1.093812000
N	0.248965000	0.161539000	2.399598000
N	-0.339644000	2.100053000	0.887291000
O	-2.393444000	0.122764000	2.245133000
O	-2.373870000	-0.766659000	3.270686000
C	7.769260000	-0.609285000	-2.234511000
H	8.421912000	-0.847685000	-3.070908000
C	6.479974000	-0.083952000	-2.474357000
H	6.140304000	0.081648000	-3.493277000
C	5.635325000	0.224851000	-1.398572000
H	4.644147000	0.632352000	-1.575831000
C	6.068561000	0.011153000	-0.057000000
S	4.999051000	0.400118000	1.322470000
C	7.372578000	-0.519562000	0.170040000
H	7.702571000	-0.682122000	1.192177000
C	8.212310000	-0.825450000	-0.910355000
H	9.204771000	-1.229200000	-0.727881000
O	-1.535199000	-0.340794000	-0.885950000
S	-2.071137000	0.468383000	-2.265376000
O	-3.287421000	1.503661000	-2.019432000
O	-0.853255000	0.879092000	-3.251545000
C	-2.910056000	-1.106183000	-3.174880000
F	-3.522647000	-0.669550000	-4.338919000
F	-1.948382000	-2.041814000	-3.504548000
F	-3.864528000	-1.694479000	-2.366997000

$B_{OTF,\ 7}$

Fe	-0.682658000	0.147738000	0.716844000
C	0.891766000	2.468030000	1.843460000
C	1.231440000	1.290344000	2.689056000
C	1.960196000	1.334222000	3.891768000
H	2.384609000	2.263449000	4.253765000
C	2.116831000	0.141450000	4.625674000
H	2.672234000	0.148700000	5.558965000
C	1.542065000	-1.052438000	4.160004000
H	1.632230000	-1.967147000	4.734449000
C	0.833799000	-1.031609000	2.940790000
C	0.198440000	-2.210590000	2.285986000
C	1.500464000	3.807282000	2.188877000
H	1.153842000	4.587178000	1.509862000
H	2.595313000	3.752098000	2.134649000
H	1.234098000	4.096381000	3.213457000
C	0.288247000	-3.556081000	2.962071000
H	-0.306643000	-3.549612000	3.884750000
H	1.325486000	-3.788457000	3.233919000
H	-0.090481000	-4.348367000	2.314372000

C	-0.380752000	3.309357000	-0.027611000
C	-1.620526000	3.950079000	0.247009000
C	-2.030551000	4.978962000	-0.624639000
H	-2.976839000	5.480646000	-0.444153000
C	-1.253268000	5.348442000	-1.732561000
H	-1.594625000	6.137639000	-2.397745000
C	-0.049051000	4.680632000	-1.996284000
H	0.531741000	4.953232000	-2.873751000
C	0.412839000	3.646410000	-1.156871000
C	-2.483351000	3.576585000	1.459054000
H	-2.164282000	2.597039000	1.832806000
C	-2.288486000	4.600985000	2.612036000
H	-1.237816000	4.678284000	2.921680000
H	-2.879652000	4.300404000	3.486946000
H	-2.620329000	5.601699000	2.303302000
C	-3.985985000	3.448726000	1.105119000
H	-4.429124000	4.421405000	0.850394000
H	-4.533028000	3.051771000	1.970182000
H	-4.131533000	2.769361000	0.259211000
C	1.726794000	2.930747000	-1.495959000
H	1.873462000	2.108604000	-0.784757000
C	1.684911000	2.306479000	-2.915672000
H	0.821688000	1.645188000	-3.037835000
H	2.608338000	1.738755000	-3.101773000
H	1.614372000	3.081742000	-3.689581000
C	2.943443000	3.886986000	-1.364121000
H	2.868777000	4.714415000	-2.081606000
H	3.878609000	3.348161000	-1.567260000
H	3.014700000	4.322052000	-0.359488000
C	-0.934838000	-3.015046000	0.289028000
C	-0.229168000	-3.342241000	-0.904185000
C	-0.772402000	-4.330621000	-1.746002000
H	-0.253919000	-4.600446000	-2.661149000
C	-1.986835000	-4.961725000	-1.430507000
H	-2.396047000	-5.717717000	-2.096341000
C	-2.681551000	-4.599002000	-0.268954000
H	-3.635131000	-5.071108000	-0.047981000
C	-2.178919000	-3.620370000	0.615718000
C	1.110710000	-2.675980000	-1.233514000
H	1.116548000	-1.687493000	-0.755181000
C	1.328285000	-2.446464000	-2.746635000
H	1.453861000	-3.391106000	-3.291950000
H	2.241622000	-1.857119000	-2.903376000
H	0.487551000	-1.901590000	-3.189060000
C	2.289865000	-3.489397000	-0.630639000
H	2.328482000	-4.495523000	-1.069331000
H	2.189616000	-3.602025000	0.456810000
H	3.246306000	-2.989827000	-0.833837000
C	-3.020252000	-3.198088000	1.825387000
H	-2.423759000	-2.554172000	2.477789000
C	-3.494491000	-4.406721000	2.672532000
H	-4.194212000	-5.044965000	2.117695000
H	-4.016638000	-4.048247000	3.568998000
H	-2.653363000	-5.035288000	2.995563000
C	-4.232432000	-2.344961000	1.362621000
H	-4.888312000	-2.917880000	0.693508000
H	-3.901578000	-1.446854000	0.830155000
H	-4.818211000	-2.021791000	2.232615000
N	-0.355596000	-1.980890000	1.122402000
N	0.727779000	0.119598000	2.235296000
N	0.056622000	2.240921000	0.862122000
O	-2.015138000	0.235348000	2.312168000
O	-1.886353000	-0.528972000	3.434812000
C	6.782188000	-1.687374000	-2.560356000
H	7.243087000	-2.169137000	-3.419282000
C	5.632132000	-0.885620000	-2.735295000
H	5.208768000	-0.749771000	-3.726894000
C	5.035358000	-0.262606000	-1.630100000
H	4.152314000	0.356889000	-1.755478000
C	5.581179000	-0.433600000	-0.323854000
S	4.825796000	0.355441000	1.091278000
C	6.742244000	-1.245905000	-0.162070000
H	7.158742000	-1.375224000	0.832852000
C	7.334649000	-1.864890000	-1.271901000
H	8.219626000	-2.481842000	-1.139998000
O	-1.351033000	0.044186000	-1.119961000
S	-2.382005000	0.752943000	-2.239974000
O	-3.641289000	1.500702000	-1.554779000
O	-1.579135000	1.465673000	-3.448791000
C	-3.130723000	-0.930070000	-3.039674000
F	-4.098430000	-0.606742000	-3.975301000
F	-2.125808000	-1.645709000	-3.669338000
F	-3.703004000	-1.715648000	-2.057570000

$A_{SPh,\,5}$

Fe	0.000638000	-0.093498000	-0.300613000
S	0.132852000	-0.020496000	2.110701000
S	2.328287000	0.091204000	-0.565861000
N	-0.765272000	2.067312000	-0.547191000
N	-2.029902000	-0.294349000	-0.294358000
N	-0.388437000	-2.424202000	-0.436402000
C	-2.066483000	2.113539000	-0.589625000
C	-2.793956000	0.819808000	-0.419392000
C	-4.199323000	0.729538000	-0.406435000
C	-4.800029000	-0.530586000	-0.263861000
C	-3.991543000	-1.673657000	-0.179273000
C	-2.589684000	-1.527297000	-0.215896000
C	-1.656384000	-2.692511000	-0.299572000
C	-2.888101000	3.363801000	-0.825218000
C	-2.261412000	-4.081590000	-0.295459000
C	0.046616000	3.276032000	-0.674257000
C	0.528201000	3.658899000	-1.957809000
C	1.344473000	4.806591000	-2.044890000
C	1.666338000	5.565411000	-0.911241000
C	1.163881000	5.182303000	0.339631000
C	0.350867000	4.039669000	0.489389000
C	0.169611000	2.914795000	-3.247661000
C	1.431196000	2.376604000	-3.969393000
C	-0.663413000	3.816991000	-4.198684000
C	-0.191363000	3.701946000	1.882634000
C	-1.273288000	4.727312000	2.322423000
C	0.929552000	3.621433000	2.947989000
C	0.572852000	-3.463771000	-0.791263000
C	0.629468000	-3.916773000	-2.144112000
C	1.594989000	-4.892206000	-2.473327000
C	2.470957000	-5.415872000	-1.514557000
C	2.393591000	-4.961497000	-0.190915000
C	1.456404000	-3.982616000	0.195907000
C	-0.276047000	-3.401601000	-3.271763000
C	0.557492000	-2.712818000	-4.384370000
C	-1.141150000	-4.542452000	-3.873369000
C	1.374543000	-3.566110000	1.664880000
C	2.767332000	-3.355961000	2.306423000
C	0.569011000	-4.614925000	2.482380000
C	-1.509576000	-0.402753000	2.855516000
C	-2.431620000	0.625668000	3.164818000
C	-3.644952000	0.334312000	3.816183000
C	-3.961501000	-0.991230000	4.174717000
C	-3.045913000	-2.020763000	3.880772000
C	-1.833385000	-1.729676000	3.227097000
C	3.233441000	1.015225000	0.731803000
C	3.741356000	2.297648000	0.413670000
C	4.550460000	2.989744000	1.331920000
C	4.849708000	2.419986000	2.586245000
C	4.329620000	1.152723000	2.914654000
C	3.530231000	0.450732000	1.993331000
H	-4.808967000	1.619100000	-0.506442000
H	-5.881763000	-0.621925000	-0.235493000
H	-4.440217000	-2.655931000	-0.098756000
H	-2.244341000	4.235692000	-0.945513000
H	-3.573363000	3.550360000	0.011154000
H	-3.492782000	3.250427000	-1.734313000
H	-2.868243000	-4.227666000	0.607111000
H	-1.482273000	-4.844514000	-0.321241000
H	-2.913525000	-4.229636000	-1.165339000
H	1.722909000	5.109641000	-3.017870000
H	2.295441000	6.447642000	-1.002519000
H	1.408190000	5.773608000	1.218094000
H	-0.445448000	2.047983000	-3.002662000
H	1.995020000	1.704647000	-3.314262000
H	2.093526000	3.192986000	-4.290174000
H	1.135752000	1.808438000	-4.860802000
H	-1.579182000	4.182064000	-3.713278000
H	-0.089912000	4.693274000	-4.529234000
H	-0.954787000	3.248750000	-5.091753000
H	-0.645505000	2.708330000	1.841697000
H	-1.689908000	4.446768000	3.299745000
H	-0.842112000	5.732490000	2.420516000
H	-2.099197000	4.791556000	1.602505000
H	0.504155000	3.321685000	3.914953000
H	1.430208000	4.588829000	3.087206000
H	1.682918000	2.880229000	2.668480000
H	1.659869000	-5.239396000	-3.501177000
H	3.206597000	-6.165619000	-1.795375000
H	3.072499000	-5.367058000	0.553784000
H	-0.951634000	-2.637376000	-2.879991000
H	-0.109731000	-2.317587000	-5.161185000
H	1.123664000	-1.873773000	-3.969724000
H	1.255666000	-3.416797000	-4.857129000
H	-1.824014000	-4.135423000	-4.631000000
H	-1.740740000	-5.052602000	-3.107854000
H	-0.516966000	-5.301673000	-4.362452000
H	0.852584000	-2.605725000	1.720434000
H	2.654268000	-2.885638000	3.292117000
H	3.392850000	-2.708378000	1.682350000
H	3.300441000	-4.304625000	2.454691000
H	0.503533000	-4.314519000	3.537207000
H	1.058604000	-5.597260000	2.441318000
H	-0.452091000	-4.738345000	2.096889000
H	-2.186091000	1.654833000	2.920327000
H	-4.333413000	1.142305000	4.056223000
H	-4.893687000	-1.213980000	4.688913000
H	-3.265999000	-3.045748000	4.173257000
H	-1.121640000	-2.523919000	3.029568000
H	3.504222000	2.740097000	-0.549635000

H	4.940200000	3.970876000	1.069723000
H	5.475979000	2.955920000	3.296167000
H	4.547747000	0.707001000	3.882693000
H	3.135698000	-0.525272000	2.248842000
O	0.094637000	-0.300617000	-2.319905000
O	-1.071254000	-0.104524000	-3.005956000

$C_{Cl,Cl,\,5}$

Fe	-0.001018000	-0.462589000	0.075919000
C	-2.419160000	-2.051220000	-0.946209000
C	-1.207516000	-2.854860000	-1.304138000
C	-1.255578000	-4.145486000	-1.870229000
H	-2.203840000	-4.618269000	-2.096180000
C	-0.047313000	-4.816552000	-2.125567000
H	-0.059686000	-5.812774000	-2.558154000
C	1.176603000	-4.203090000	-1.807004000
H	2.111861000	-4.720693000	-1.983542000
C	1.160220000	-2.910985000	-1.242935000
C	2.387764000	-2.165515000	-0.819285000
C	-3.775873000	-2.649803000	-1.247195000
H	-4.577736000	-1.964429000	-0.971567000
H	-3.905428000	-3.579617000	-0.677146000
H	-3.873989000	-2.894528000	-2.311974000
C	3.729121000	-2.829567000	-1.040473000
H	3.866767000	-3.105051000	-2.093207000
H	3.790546000	-3.749244000	-0.442978000
H	4.546638000	-2.172730000	-0.742024000
C	-3.317207000	0.002864000	-0.052296000
C	-3.813733000	0.871125000	-1.067539000
C	-4.885503000	1.726325000	-0.735951000
H	-5.280388000	2.396003000	-1.495192000
C	-5.444104000	1.737796000	0.549614000
H	-6.268055000	2.408285000	0.781407000
C	-4.928173000	0.885399000	1.534747000
H	-5.355181000	0.898797000	2.534090000
C	-3.859293000	0.006550000	1.261853000
C	-3.253614000	0.918854000	-2.495672000
H	-2.329255000	0.333980000	-2.531721000
C	-4.252561000	0.307074000	-3.517193000
H	-4.506943000	-0.732435000	-3.276105000
H	-3.823166000	0.328497000	-4.527956000
H	-5.188704000	0.880262000	-3.537712000
C	-2.890964000	2.365908000	-2.920285000
H	-3.786219000	2.995424000	-3.008979000
H	-2.391337000	2.355725000	-3.897782000
H	-2.209490000	2.827456000	-2.199852000
C	-3.351199000	-0.912556000	2.374044000
H	-2.471595000	-1.453231000	2.017503000
C	-2.885830000	-0.104444000	3.611722000
H	-2.115996000	0.621993000	3.329922000
H	-2.451662000	-0.784658000	4.355233000
H	-3.717658000	0.434294000	4.086720000
C	-4.423972000	-1.962991000	2.768910000
H	-5.324468000	-1.485228000	3.178501000
H	-4.021703000	-2.638726000	3.534836000
H	-4.732655000	-2.571389000	1.906943000
C	3.330516000	-0.155731000	0.130185000
C	3.823896000	-0.211481000	1.462134000
C	4.906536000	0.626932000	1.801667000
H	5.294374000	0.597910000	2.816526000
C	5.486342000	1.490641000	0.863451000
H	6.319570000	2.128859000	1.147283000
C	4.981558000	1.530394000	-0.443728000
H	5.429343000	2.204793000	-1.168491000
C	3.897487000	0.720121000	-0.840533000
C	3.245181000	-1.137894000	2.533975000
H	2.409071000	-1.699954000	2.111407000
C	2.661702000	-0.323625000	3.717657000
H	3.439240000	0.258949000	4.231115000
H	2.203616000	-1.003496000	4.446925000
H	1.886070000	0.364747000	3.365855000
C	4.301451000	-2.160750000	3.030644000
H	5.149898000	-1.662294000	3.518648000
H	4.701124000	-2.765107000	2.203924000
H	3.846489000	-2.841879000	3.761559000
C	3.406714000	0.807691000	-2.291874000
H	2.454440000	0.275190000	-2.373610000
C	4.416326000	0.140677000	-3.267680000
H	5.384632000	0.657518000	-3.239783000
H	4.038187000	0.189200000	-4.297802000
H	4.596302000	-0.912694000	-3.019218000
C	3.145601000	2.272774000	-2.727090000
H	4.077351000	2.851836000	-2.774795000
H	2.459394000	2.771591000	-2.036361000
H	2.690100000	2.290973000	-3.725714000
N	2.203053000	-1.004565000	-0.257467000
N	-0.015766000	-2.279618000	-1.028003000
N	-2.211202000	-0.901651000	-0.368853000
O	0.056909000	0.382546000	-1.755580000
O	0.093330000	1.640091000	-2.158141000
Cl	-0.075542000	-2.092912000	1.913165000
Cl	0.012283000	1.529030000	1.192735000