Supporting information

Effects of Substrate, Protein Environment, and Proximal Ligand Mutation on Compound I and Compound 0 of Chloroperoxidase

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Part I. QM Energies and QM/MM Energies.

Table S1. Absolute energies (in hartree) obtained from B3LYP/CHARMM calculations.

	species	QM (B1)	QM/MM (B1)	QM (B2)	QM/MM (B2)
Prot3/QM1 AcO^-	S–HOOH	-2117.292087	-2190.449338	-3258.105746	-3331.262983
	S–Cpd 0	-2117.301955	-2190.462693	-3258.113614	-3331.274318
	S–Cpd I	-2117.290175	-2190.449301	-3258.117638	-3331.276745
Prot3/QM1 AcOH	S–HOOH	-2117.298311	-2190.617544	-3258.110584	-3331.429799
	S–Cpd 0	-2117.301755	-2190.624032	-3258.111949	-3331.434252
	S–Cpd I	-2117.313321	-2190.631837	-3258.136692	-3331.455154
Prot3/QM1 no Acetate	S–HOOH	-2117.296479	-2190.713638	-3258.108884	-3331.526025
	S–Cpd 0	-2117.300638	-2190.721119	-3258.110930	-3331.531424
	S–Cpd I	-2117.306795	-2190.728037	-3258.132267	-3331.553425
Prot1/QM2 AcO^-	S–HOOH	-2728.496830	-2805.459034	-3869.518481	-3946.480689
	S–Cpd 0	-2728.505494	-2805.470627	-3869.523553	-3946.488714
	S–Cpd I	-2728.498163	-2805.459273	-3869.532129	-3946.493269
Prot1/QM2 AcOH	S–HOOH	-2728.504268	-2805.473412	-3869.524356	-3946.493430
	S–Cpd 0	-2728.506579	-2805.477911	-3869.523322	-3946.494653
	S–Cpd I	-2728.521152	-2805.487702	-3869.551146	-3946.517697
Prot1/QM2 no Acetate	S–HOOH	-2728.503300	-2805.341348	-3869.521750	-3946.359729
	S–Cpd 0	-2728.505122	-2805.346130	-3869.522055	-3946.363045
	S–Cpd I	-2728.515243	-2805.355518	-3869.546683	-3946.386933
Prot3/QM2 no Acetate	S–HOOH	-2728.519307	-2801.971395	-3869.537871	-3942.989975
	S–Cpd 0	-2728.525013	-2801.980754	-3869.542337	-3942.998081
	S–Cpd I	-2728.528977	-2801.983131	-3869.558490	-3943.012682
Prot2/QM2 no Acetate	S–HOOH	-2728.521995	-2805.411425	-3869.541313	-3946.430744
	S–Cpd 0	-2728.526780	-2805.419795	-3869.544080	-3946.436629
	S–Cpd I	-2728.530542	-2805.421530	-3869.559611	-3946.450605

Table S2. Relative energies (in kcal/mol) obtained from B3LYP/CHARMM calculations.

	species	QM (B1)	QM/MM (B1)	QM (B2)	QM/MM (B2)
Prot3/QM1 AcO^-	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-6.2	-8.4	-4.9	-7.1
	S–Cpd I	1.2	0.02	-7.5	-8.6
Prot3/QM1 AcOH	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-2.2	-4.1	-0.9	-2.8
	S–Cpd I	-9.4	-9.0	-16.4	-15.9
Prot3/QM1 no Acetate	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-2.6	-4.7	-1.3	-3.4
	S–Cpd I	-6.5	-9.0	-14.7	-17.2
Prot1/QM2 AcO^-	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-5.4	-7.3	-3.2	-5.0
	S–Cpd I	-0.8	-0.2	-8. 6	-7.9
Prot1/QM2 AcOH	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-1.5	-2.8	0.6	-0.8
	S–Cpd I	-10.6	-9.0	-16.8	-15.2
Prot1/QM2 no Acetate	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-1.1	-3.0	-0.2	-2.1
	S–Cpd I	-7.5	-8.9	-15.6	-17.1
Prot3/QM2 no acetate	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-3.6	-5.9	-2.8	-5.1
	S–Cpd I	-6.1	-7.4	-12.9	-14.2
Prot2/QM2 no Acetate	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-3.0	-5.3	-1.7	-3.7
	S–Cpd I	-5.4	-6.3	-11.5	-12.5

Table S3. Absolute energies (in hartree) obtained from B3LYP/CHARMM calculations.[a]

	species	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
snapshot 0	S–HOOH	-2728.503300	-2805.340649	-3869.521750	-3946.359729
	S–Cpd 0	-2728.505122	-2805.346130	-3869.522055	-3946.363045
	S–Cpd I	-2728.515243	-2805.355518	-3869.546683	-3946.386933
	Se–HOOH	-4729.238732	-4806.076013	-5870.277223	-5947.114417
	Se–Cpd 0	-4729.240253	-4806.079790	-5870.276064	-5947.115537
	Se–Cpd I	-4729.251220	-4806.090061	-5870.302156	-5947.140909
snapshot 80	S–HOOH	-2728.510956	-2813.334798	-3869.528935	-3954.353785
	S–Cpd 0	-2728.510956	-2813.334798	-3869.527667	-3954.351530
	S–Cpd I	-2728.525303	-2813.347702	-3869.553672	-3954.376105
	Se–HOOH	-4729.247458	-4814.071661	-5870.286292	-5955.110477
	Se–Cpd 0	-4729.246842	-4814.069821	-5870.282920	-5955.105892
	Se–Cpd I	-4729.262355	-4814.083752	-5870.310958	-5955.132311
snapshot 150	S–HOOH	-2728.513222	-2813.195542	-3869.531402	-3954.213762
	S–Cpd 0	-2728.512836	-2813.192822	-3869.529630	-3954.209612
	S–Cpd I	-2728.529444	-2813.208864	-3869.558861	-3954.238292
	Se–HOOH	-4729.249613	-4813.931430	-5870.288513	-5954.970258
	Se–Cpd 0	-4729.248439	-4813.927767	-5870.284503	-5954.963805
	Se–Cpd I	-4729.266298	-4813.945105	-5870.315431	-5954.994311
snapshot 220	S–HOOH	-2728.513654	-2813.336331	-3869.531550	-3954.354199
	S–Cpd 0	-2728.513753	-2813.334391	-3869.530169	-3954.350826
	S–Cpd I	-2728.528746	-2813.349240	-3869.557733	-3954.378253
	Se–HOOH	-4729.250102	-4814.072139	-5870.288666	-5955.110700
	Se–Cpd 0	-4729.249382	-4814.069382	-5870.285022	-5955.105040
	Se–Cpd I	-4729.265711	-4814.085267	-5870.314534	-5955.134023
snapshot 290	S–HOOH	-2728.550397	-2813.423084	-3869.566026	-3954.438546
	S–Cpd 0	-2728.538660	-2813.411386	-3869.550896	-3954.423675
	S–Cpd I	-2728.582150	-2813.438232	-3869.605571	-3954.461683
	Se–HOOH	-4729.286973	-4814.159273	-5870.322576	-5955.194887
	Se–Cpd 0	-4729.275008	-4814.146398	-5870.306424	-5955.177766
	Se–Cpd I	-4729.318910	-4814.173911	-5870.362189	-5955.217207
		QM(B1a)	QM/MM(B1a)	QM(B2)	QM/MM(B2)
snapshot 0	S–Cpd 0[b]	-2728.564569	-2805.405229	-3869.524790	-3946.365416
	S–**TS**$_{OO}$[b]	-2728.544170	-2805.386869	-3869.506617	-3946.349332
	Se–Cpd 0[b]	-4729.300261	-4806.139661	-5870.278738	-5947.118180
	Se–**TS**$_{OO}$[b]	-4729.280292	-4806.121530	-5870.261075	-5947.102313

[a] Geometry was optimized with B1 basis set unless specified. [b] Geometry was optimized with B1a basis set.

Table S4. Relative energies (in kcal/mol) obtained from B3LYP/CHARMM calculations.

	species	QM(B1)	QM/MM(B1)	QM(B2)	QM/MM(B2)
snapshot 0	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-1.1	-3.4	-0.2	-2.1
	S–Cpd I	-7.5	-9.3	-15.6	-17.1
	Se–HOOH	0.0	0.0	0.0	0.0
	Se–Cpd 0	-1.0	-2.4	0.8	-0.7
	Se–Cpd I	-7.8	-8.8	-15.6	-16.6
snapshot 80	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	0.1	0.7	0.8	1.4
	S–Cpd I	-8.9	-7.4	-15.5	-14.0
	Se–HOOH	0.0	0.0	0.0	0.0
	Se–Cpd 0	0.4	1.2	2.1	2.9
	Se–Cpd I	-9.3	-7.6	-15.5	-13.7
snapshot 150	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	0.2	1.7	1.1	2.6
	S–Cpd I	-10.2	-8.4	-17.2	-15.4
	Se–HOOH	0.0	0.0	0.0	0.0
	Se–Cpd 0	0.7	2.3	2.5	4.0
	Se–Cpd I	-10.5	-8.6	-16.9	-15.1
snapshot 220	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	-0.1	1.2	0.9	2.1
	S–Cpd I	-9.5	-8.1	-16.4	-15.1
	Se–HOOH	0.0	0.0	0.0	0.0
	Se–Cpd 0	0.5	1.7	2.3	3.6
	Se–Cpd I	-9.8	-8.2	-16.2	-14.6
snapshot 290	S–HOOH	0.0	0.0	0.0	0.0
	S–Cpd 0	7.4	7.3	9.5	9.3
	S–Cpd I	-19.9	-9.5	-24.8	-14.5
	Se–HOOH	0.0	0.0	0.0	0.0
	Se–Cpd 0	7.5	8.1	10.1	10.7
	Se–Cpd I	-20.0	-9.2	-24.9	-14.0
		QM(B1a)	QM/MM(B1a)	QM(B2)	QM/MM(B2)
snapshot 0	S–Cpd 0	0.0	0.0	0.0	0.0
	S–**TS**$_{OO}$	12.8	11.5	11.4	10.1
	Se–Cpd 0	0.0	0.0	0.0	0.0
	Se–**TS**$_{OO}$	12.5	11.4	11.1	10.0

Part II. Spin and Charge Distributions.

Table S5. Spin distribution calculated at the QM/MM B2 level.

species		Fe	HOOH	S	Porp
S–HOOH	Prot3/QM1/AcO^-	1.15	0.00	-0.08	-0.07
	Prot3/QM1/AcOH	1.16	0.00	-0.09	-0.07
	Prot3/QM1/no Acetate	1.16	0.00	-0.08	-0.07
	Prot1/QM2/AcO^-	1.15	0.00	-0.06	-0.10
	Prot1/QM2/AcOH	1.15	0.00	-0.06	-0.10
	Prot1/QM2/no Acetate	1.15	0.00	-0.06	-0.10
	Prot3/QM2/no Acetate	1.12	0.00	-0.04	-0.09
	Prot2/QM2/no Acetate	1.15	0.00	-0.06	-0.09
		Fe	OOH	S	Porp
S–Cpd 0	Prot3/QM1/AcO^-	1.02	0.07	-0.02	-0.07
	Prot3/QM1/AcOH	1.03	0.06	-0.02	-0.07
	Prot3/QM1/no Acetate	1.03	0.06	-0.02	-0.07
	Prot1/QM2/AcO^-	1.02	0.07	-0.01	-0.08
	Prot1/QM2/AcOH	1.03	0.06	-0.01	-0.08
	Prot1/QM2/no Acetate	1.02	0.06	-0.01	-0.08
	Prot3/QM2/no Acetate	1.03	0.07	-0.01	-0.08
	Prot2/QM2/no Acetate	1.03	0.07	-0.01	-0.08
		Fe	O	S	Porp
S–Cpd I	Prot3/QM1/AcO^-	1.22	0.89	-0.13	-0.96
	Prot3/QM1/AcOH	1.24	0.87	-0.15	-0.97
	Prot3/QM1/no Acetate	1.24	0.88	-0.16	-0.96
	Prot1/QM2/AcO^-	1.40	0.84	-0.16	-1.07
	Prot1/QM2/AcOH	1.44	0.81	-0.19	-1.05
	Prot1/QM2/no Acetate	1.45	0.82	-0.22	-1.03
	Prot3/QM2/no Acetate	1.42	0.83	-0.18	-1.06
	Prot2/QM2/no Acetate	1.43	0.83	-0.20	-1.05

Table S6. NBO charge distribution calculated at the QM/MM B2 level.

species		Fe	HOOH	S	Porp
S–HOOH	Prot3/QM1/AcO^-	1.01	0.05	-0.64	-0.71
	Prot3/QM1/AcOH	0.99	0.02	-0.61	-0.70
	Prot3/QM1/no Acetate	0.99	0.02	-0.61	-0.70
	Prot1/QM2/AcO^-	0.96	0.05	-0.25	-0.73
	Prot1/QM2/AcOH	0.95	0.02	-0.22	-0.73
	Prot1/QM2/no Acetate	0.95	0.02	-0.22	-0.73
	Prot3/QM2/no Acetate	0.96	0.01	-0.25	-0.73
	Prot2/QM2/no Acetate	0.96	0.01	-0.25	-0.72
		Fe	OOH	S	Porp
S–Cpd 0	Prot3/QM1/AcO^-	0.98	-0.47	-0.75	-0.81
	Prot3/QM1/AcOH	0.96	-0.51	-0.71	-0.79
	Prot3/QM1/no Acetate	0.96	-0.50	-0.71	-0.80
	Prot1/QM2/AcO^-	0.96	-0.48	-0.25	-0.82
	Prot1/QM2/AcOH	0.95	-0.52	-0.22	-0.81
	Prot1/QM2/no Acetate	0.95	-0.51	-0.22	-0.81
	Prot3/QM2/no Acetate	0.96	-0.51	-0.25	-0.80
	Prot2/QM2/no Acetate	0.96	-0.51	-0.25	-0.81
		Fe	O	S	Porp
S–Cpd I	Prot3/QM1/AcO^-	1.15	-0.49	-0.78	0.00
	Prot3/QM1/AcOH	0.95	-0.49	-0.75	0.11
	Prot3/QM1/no Acetate	0.96	-0.48	-0.75	0.10
	Prot1/QM2/AcO^-	0.94	-0.46	-0.38	0.06
	Prot1/QM2/AcOH	0.95	-0.50	-0.35	0.05
	Prot1/QM2/no Acetate	0.95	-0.49	-0.35	0.03
	Prot3/QM2/no Acetate	0.95	-0.48	-0.38	0.06
	Prot2/QM2/no Acetate	0.95	-0.48	-0.37	0.04

Table S7. Spin distribution calculated at the QM/MM B2 level.

species		Fe	HOOH	S	Porp
S–HOOH	snapshot 0	1.15	0.00	-0.06	-0.10
	snapshot 80	1.16	0.00	-0.07	-0.10
	snapshot 150	1.17	0.00	-0.07	-0.10
	snapshot 220	1.17	0.00	-0.07	-0.10
	snapshot 290	1.15	0.00	-0.06	-0.10
		Fe	OOH	S	Porp
S–Cpd 0	snapshot 0	1.02	0.06	-0.01	-0.08
	snapshot 80	1.04	0.06	-0.01	-0.08
	snapshot 150	1.03	0.06	-0.01	-0.08
	snapshot 220	1.04	0.06	-0.01	-0.08
	snapshot 290	1.05	0.04	-0.01	-0.08
		Fe	O	S	Porp
S–Cpd I	snapshot 0	1.45	0.82	-0.22	-1.03
	snapshot 80	1.43	0.83	-0.25	-1.00
	snapshot 150	1.45	0.82	-0.30	-0.96
	snapshot 220	1.44	0.81	-0.26	-0.99
	snapshot 290	1.51	0.75	-0.19	-1.03
		Fe	HOOH	Se	Porp
Se–HOOH	snapshot 0	1.18	0.00	-0.10	-0.10
	snapshot 80	1.19	0.00	-0.10	-0.09
	snapshot 150	1.20	0.00	-0.11	-0.10
	snapshot 220	1.20	0.00	-0.11	-0.09
	snapshot 290	1.21	0.00	-0.11	-0.10
		Fe	OOH	Se	Porp
Se–Cpd 0	snapshot 0	1.03	0.07	-0.03	-0.07
	snapshot 80	1.04	0.06	-0.03	-0.07
	snapshot 150	1.04	0.06	-0.03	-0.07
	snapshot 220	1.04	0.06	-0.03	-0.07
	snapshot 290	1.06	0.04	-0.03	-0.07
		Fe	O	Se	Porp
Se–Cpd I	snapshot 0	1.42	0.81	-0.28	-0.95
	snapshot 80	1.41	0.82	-0.29	-0.92
	snapshot 150	1.42	0.81	-0.34	-0.89
	snapshot 220	1.42	0.81	-0.30	-0.92
	snapshot 290	1.49	0.74	-0.28	-0.95

Table S8. NBO charge distribution calculated at the QM/MM B2 level.

species		Fe	HOOH	S	Porp
S–HOOH	snapshot 0	0.95	0.02	-0.22	-0.73
	snapshot 80	0.96	0.03	-0.22	-0.73
	snapshot 150	0.95	0.02	-0.20	-0.73
	snapshot 220	0.96	0.03	-0.21	-0.73
	snapshot 290	0.94	0.00	-0.19	-0.73
		Fe	OOH	S	Porp
S–Cpd 0	snapshot 0	0.95	-0.51	-0.22	-0.81
	snapshot 80	0.96	-0.51	-0.22	-0.81
	snapshot 150	0.95	-0.52	-0.20	-0.81
	snapshot 220	0.96	-0.51	-0.21	-0.81
	snapshot 290	0.94	-0.55	-0.19	-0.79
		Fe	O	S	Porp
S–Cpd I	snapshot 0	0.95	-0.49	-0.35	0.03
	snapshot 80	0.97	-0.48	-0.34	0.00
	snapshot 150	0.98	-0.49	-0.31	-0.03
	snapshot 220	0.97	-0.49	-0.34	0.00
	snapshot 290	0.98	-0.53	-0.33	0.03
		Fe	HOOH	Se	Porp
Se–HOOH	snapshot 0	0.91	0.02	-0.12	-0.73
	snapshot 80	0.91	0.03	-0.12	-0.73
	snapshot 150	0.91	0.02	-0.10	-0.73
	snapshot 220	0.91	0.02	-0.11	-0.73
	snapshot 290	0.90	0.00	-0.09	-0.73
		Fe	OOH	Se	Porp
Se–Cpd 0	snapshot 0	0.90	-0.51	-0.24	-0.81
	snapshot 80	0.91	-0.51	-0.24	-0.81
	snapshot 150	0.90	-0.52	-0.22	-0.82
	snapshot 220	0.91	-0.52	-0.23	-0.81
	snapshot 290	0.89	-0.56	-0.19	-0.80
		Fe	O	Se	Porp
Se–Cpd I	snapshot 0	0.93	-0.49	-0.25	0.00
	snapshot 80	0.95	-0.48	-0.25	-0.03
	snapshot 150	0.96	-0.49	-0.22	-0.07
	snapshot 220	0.96	-0.49	-0.24	-0.03
	snapshot 290	0.96	-0.53	-0.23	0.00

Part III. Geometrical Parameters.

Table S9. Key Bond Length (in Å) of Ferric-Hydrogen Peroxide, Cpd 0, and Cpd I.

species		Fe–O	Fe–S	O–O	Fe–N_{por}
S–HOOH	Prot3/QM1/AcO^-	2.093	2.409	1.518	2.026
	Prot3/QM1/AcOH	2.133	2.393	1.518	2.025
	Prot3/QM1/no Acetate	2.132	2.390	1.518	2.025
	Prot1/QM2/AcO^-	2.119	2.370	1.521	2.026
	Prot1/QM2/AcOH	2.167	2.350	1.521	2.026
	Prot1/QM2/no Acetate	2.148	2.357	1.519	2.025
	Prot3/QM2/no Acetate	2.119	2.376	1.523	2.026
	Prot2/QM2/no Acetate	2.126	2.369	1.519	2.026
S–Cpd 0	Prot3/QM1/AcO^-	1.873	2.476	1.528	2.029
	Prot3/QM1/AcOH	1.890	2.453	1.544	2.023
	Prot3/QM1/no Acetate	1.888	2.455	1.543	2.028
	Prot1/QM2/AcO^-	1.878	2.444	1.529	2.028
	Prot1/QM2/AcOH	1.896	2.423	1.544	2.029
	Prot1/QM2/no Acetate	1.895	2.422	1.544	2.028
	Prot3/QM2/no Acetate	1.888	2.436	1.542	2.028
	Prot2/QM2/no Acetate	1.892	2.427	1.542	2.028
S–Cpd I	Prot3/QM1/AcO^-	1.648	2.543	2.711	2.030
	Prot3/QM1/AcOH	1.651	2.545	2.746	2.028
	Prot3/QM1/no Acetate	1.653	2.563	2.880	2.027
	Prot1/QM2/AcO^-	1.648	2.542	2.729	2.028
	Prot1/QM2/AcOH	1.652	2.544	2.751	2.026
	Prot1/QM2/no Acetate	1.653	2.563	2.832	2.025
	Prot3/QM2/no Acetate	1.652	2.570	2.866	2.026
	Prot2/QM2/no Acetate	1.652	2.565	2.844	2.026

Table S10. Key Bond Length (in Å) of Ferric-Hydrogen Peroxide, Cpd 0, and Cpd I.

	species	Fe–O	Fe–S(Se)	O–O	Fe–N_{por}
snapshot 0	S–HOOH	2.148	2.357	1.519	2.025
	S–Cpd 0	1.895	2.422	1.544	2.028
	S–Cpd I	1.653	2.563	2.832	2.025
	Se–HOOH	2.150	2.434	1.519	2.025
	Se–Cpd 0	1.898	2.503	1.544	2.027
	Se–Cpd I	1.653	2.654	2.844	2.024
snapshot 80	S–HOOH	2.149	2.376	1.520	2.028
	S–Cpd 0	1.907	2.439	1.545	2.032
	S–Cpd I	1.654	2.628	2.896	2.029
	Se–HOOH	2.152	2.454	1.520	2.028
	Se–Cpd 0	1.910	2.518	1.546	2.032
	Se–Cpd I	1.654	2.711	2.885	2.028
snapshot 150	S–HOOH	2.163	2.372	1.521	2.029
	S–Cpd 0	1.911	2.438	1.548	2.033
	S–Cpd I	1.653	2.639	2.896	2.030
	Se–HOOH	2.163	2.453	1.521	2.028
	Se–Cpd 0	1.914	2.513	1.549	2.033
	Se–Cpd I	1.653	2.726	2.888	2.029
snapshot 220	S–HOOH	2.165	2.378	1.521	2.028
	S–Cpd 0	1.911	2.442	1.548	2.032
	S–Cpd I	1.654	2.633	2.866	2.028
	Se–HOOH	2.166	2.457	1.521	2.027
	Se–Cpd 0	1.913	2.523	1.548	2.031
	Se–Cpd I	1.654	2.718	2.860	2.027
snapshot 290	S–HOOH	2.185	2.363	1.519	2.030
	S–Cpd 0	1.934	2.414	1.561	2.034
	S–Cpd I	1.656	2.585	2.636	2.033
	Se–HOOH	2.177	2.450	1.519	2.029
	Se–Cpd 0	1.938	2.495	1.560	2.033
	Se–Cpd I	1.656	2.678	2.630	2.031

Part IV. Cartesian Coordinates of the QM Region.

S-$\mathbf{TS}_{OO}$

C	4.739000	-1.954000	0.314000	H	-3.384000	-0.484000	1.589000
O	4.251000	-0.888000	-0.143000	N	1.812000	-1.429000	3.343000
N	4.048000	-2.826000	1.078000	C	1.484000	-0.213000	2.536000
H	4.538000	-3.597000	1.509000	H	0.475000	-0.299000	2.119000
C	2.610000	-2.727000	1.367000	H	2.193000	-0.094000	1.716000
H	2.224000	-1.890000	0.793000	C	1.617000	-1.182000	4.806000
C	1.914000	-4.020000	0.925000	H	2.560000	-1.372000	5.326000
H	2.309000	-4.851000	1.514000	C	1.134000	0.290000	4.891000
H	2.097000	-4.197000	-0.134000	H	1.560000	0.793000	5.761000
C	2.430000	-2.550000	2.876000	H	0.043000	0.377000	4.968000
O	2.807000	-3.480000	3.649000	C	1.596000	0.919000	3.563000
S	0.048000	-3.956000	1.221000	H	1.006000	1.793000	3.284000
O	-2.029000	-2.949000	-2.209000	H	2.635000	1.235000	3.648000
H	-1.115000	-2.250000	-4.203000	C	3.497000	1.360000	-9.517000
O	-1.493000	-3.192000	-3.892000	H	3.142000	0.424000	-9.955000
H	-0.706000	-3.743000	-3.709000	H	3.492000	2.116000	-10.305000
FE	-1.030000	-3.452000	-0.905000	C	1.826000	0.906000	-7.591000
N	0.669000	-3.403000	-1.948000	H	1.670000	-0.160000	-7.644000
N	-1.208000	-5.447000	-1.308000	C	2.608000	1.720000	-8.374000
N	-2.755000	-3.513000	0.198000	N	1.221000	1.700000	-6.631000
N	-0.874000	-1.485000	-0.458000	H	0.555000	1.363000	-5.796000
C	1.419000	-2.265000	-2.233000	N	2.447000	3.018000	-7.860000
C	2.500000	-2.608000	-3.143000	H	2.912000	3.866000	-8.207000
C	2.401000	-3.944000	-3.412000	C	1.604000	2.969000	-6.799000
C	1.268000	-4.449000	-2.650000	H	1.297000	3.789000	-6.167000
C	-0.302000	-6.256000	-1.973000	C	-2.404000	0.096000	-3.942000
C	-0.762000	-7.646000	-1.957000	H	-3.020000	-0.310000	-4.755000
C	-1.960000	-7.673000	-1.296000	H	-2.476000	-0.627000	-3.122000
C	-2.247000	-6.274000	-0.920000	C	-0.993000	0.092000	-4.503000
C	-3.654000	-4.558000	0.214000	O	-0.384000	1.207000	-4.774000
C	-4.842000	-4.198000	0.991000	O	-0.479000	-1.042000	-4.773000
C	-4.599000	-2.976000	1.553000	h	5.763381	-2.251517	0.089962
C	-3.319000	-2.516000	0.977000	h	3.220286	-1.874538	-3.505339
C	-1.773000	-0.719000	0.255000	h	2.990991	-4.531756	-4.115221
C	-1.472000	0.699000	0.074000	h	-0.192726	-8.470594	-2.385997
C	-0.358000	0.775000	-0.710000	h	-2.631874	-8.485662	-1.019898
C	0.027000	-0.601000	-1.025000	h	-5.755042	-4.790364	0.931615
C	1.120000	-0.980000	-1.789000	h	-5.143763	-2.399053	2.300283
H	1.783000	-0.185000	-2.106000	h	-2.132463	1.484557	0.441090
C	0.833000	-5.773000	-2.614000	h	0.140259	1.653373	-1.120201
H	1.431000	-6.480000	-3.177000	h	0.889537	-1.863502	5.246930
C	-3.408000	-5.822000	-0.297000	h	4.527757	1.158376	-9.225530
H	-4.201000	-6.544000	-0.137000	h	-2.818582	1.050536	-3.617885
C	-2.829000	-1.218000	1.011000				

Se-**TS**$_{OO}$

C	4.773000 -1.940000 0.316000	H	-3.399000 -0.484000 1.575000
O	4.276000 -0.886000 -0.159000	N	1.828000 -1.423000 3.356000
N	4.095000 -2.792000 1.113000	C	1.493000 -0.211000 2.547000
H	4.592000 -3.558000 1.547000	H	0.484000 -0.307000 2.128000
C	2.655000 -2.713000 1.386000	H	2.200000 -0.086000 1.727000
H	2.263000 -1.882000 0.808000	C	1.618000 -1.179000 4.816000
C	1.988000 -4.016000 0.937000	H	2.557000 -1.365000 5.344000
H	2.397000 -4.844000 1.518000	C	1.130000 0.292000 4.900000
H	2.157000 -4.183000 -0.125000	H	1.554000 0.796000 5.770000
C	2.452000 -2.542000 2.893000	H	0.039000 0.376000 4.975000
O	2.819000 -3.473000 3.669000	C	1.592000 0.923000 3.572000
SE	0.014000 -3.982000 1.263000	H	0.997000 1.792000 3.290000
O	-2.048000 -2.934000 -2.252000	H	2.628000 1.247000 3.661000
H	-1.121000 -2.235000 -4.239000	C	3.497000 1.360000 -9.518000
O	-1.499000 -3.177000 -3.929000	H	3.141000 0.423000 -9.954000
H	-0.713000 -3.725000 -3.732000	H	3.493000 2.115000 -10.306000
FE	-1.060000 -3.448000 -0.936000	C	1.825000 0.910000 -7.591000
N	0.652000 -3.402000 -1.961000	H	1.667000 -0.155000 -7.643000
N	-1.237000 -5.442000 -1.338000	C	2.608000 1.723000 -8.375000
N	-2.781000 -3.509000 0.169000	N	1.221000 1.706000 -6.632000
N	-0.897000 -1.483000 -0.481000	H	0.553000 1.372000 -5.796000
C	1.405000 -2.265000 -2.242000	N	2.449000 3.021000 -7.863000
C	2.492000 -2.609000 -3.145000	H	2.915000 3.868000 -8.210000
C	2.393000 -3.946000 -3.414000	C	1.606000 2.975000 -6.802000
C	1.255000 -4.449000 -2.658000	H	1.301000 3.795000 -6.171000
C	-0.325000 -6.253000 -1.993000	C	-2.403000 0.101000 -3.950000
C	-0.779000 -7.644000 -1.968000	H	-3.019000 -0.305000 -4.763000
C	-1.979000 -7.671000 -1.309000	H	-2.470000 -0.626000 -3.134000
C	-2.272000 -6.271000 -0.945000	C	-0.996000 0.104000 -4.516000
C	-3.678000 -4.555000 0.192000	O	-0.384000 1.220000 -4.777000
C	-4.858000 -4.198000 0.981000	O	-0.486000 -1.027000 -4.806000
C	-4.613000 -2.977000 1.543000	h	5.792213 -2.247782 0.082460
C	-3.340000 -2.514000 0.957000	h	3.213590 -1.875700 -3.505063
C	-1.792000 -0.717000 0.236000	h	2.985391 -4.534665 -4.114437
C	-1.484000 0.701000 0.066000	h	-0.204882 -8.469573 -2.388575
C	-0.368000 0.776000 -0.717000	h	-2.646373 -8.485462 -1.027342
C	0.011000 -0.600000 -1.039000	h	-5.770152 -4.792494 0.929789
C	1.107000 -0.980000 -1.798000	h	-5.152428 -2.401453 2.295216
H	1.774000 -0.186000 -2.109000	h	-2.140710 1.487412 0.437962
C	0.816000 -5.772000 -2.626000	h	0.133207 1.654397 -1.123543
H	1.418000 -6.481000 -3.182000	h	0.890567 -1.862672 5.253608
C	-3.433000 -5.819000 -0.320000	h	4.527578 1.158411 -9.225873
H	-4.222000 -6.544000 -0.153000	h	-2.819344 1.053459 -3.622058
C	-2.848000 -1.216000 0.991000		