

Supporting Information for

Computational Toxicological Investigation on the Mechanism and Pathways of Xenobiotics

Metabolized by Cytochrome P450: A Case of BDE-47

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Table S1. Comparison of the barriers obtained with B3LYP versus B3LYP-D

Reaction Pathways	C1	C2	C3	C4	C5	C6
$\Delta E_{\text{B3LYP,sol}}^{\ddagger}$ (kcal/mol)	22.6	24.1	20.2	23.2	19.2	19.8
$\Delta E_{\text{B3LYP-D,sol}}^{\ddagger}$ (kcal/mol)	14.5	16.7	8.3	16.1	14.1	11.6
$\Delta E_{\text{B3LYP,sol}}^{\ddagger} - \Delta E_{\text{B3LYP-D,sol}}^{\ddagger}$ (kcal/mol)	8.1	7.4	11.9	7.1	5.1	8.2

As the attack of Cpd I on the π -system was found to be the rate limiting step, we only considered the effects of dispersion on the addition of Cpd I to the different aromatic C atoms of BDE-47. The single-point energies were calculated using the empirical dispersion-corrected B3LYP method (B3LYP-D) [refs. 40 and 41] on top of the B3LYP-optimized geometries in solvation environment ($\epsilon = 5.7$). The results indicate that the inclusion of the empirical dispersion correction can differentially lower the barriers among the reaction paths by 5.1 ~ 11.9 kcal/mol. The inclusion of the empirical dispersion correction cannot change the conclusion of the study, i.e., the approach of Cpd I to the non-substituted C atoms (C3, C5 and C6) is the most favorable; and the addition of Cpd I to C1, C2 and C4 atoms has higher $\Delta E^{\ddagger}$ values.

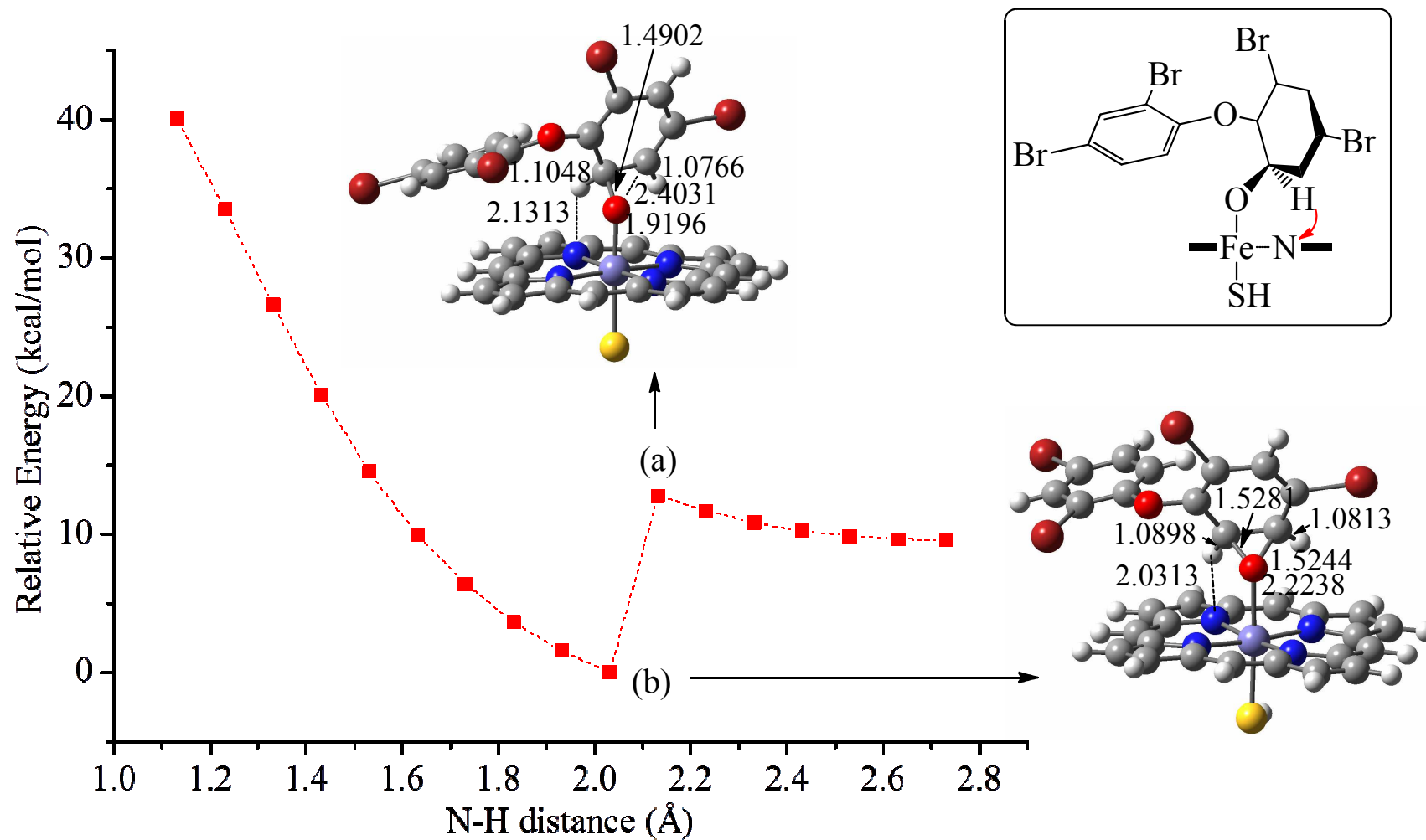
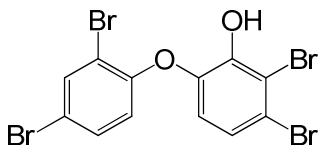
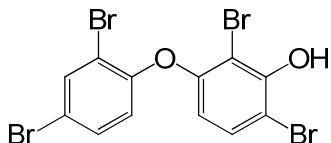
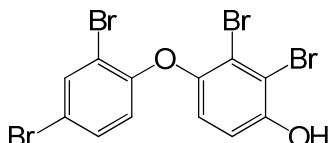
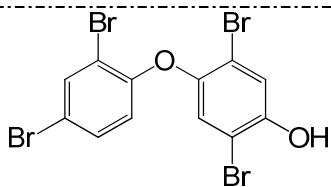
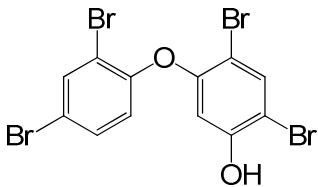
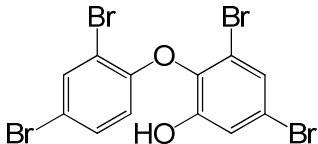
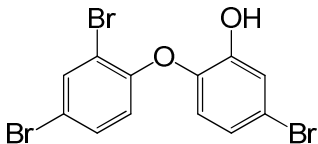
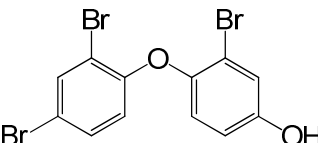
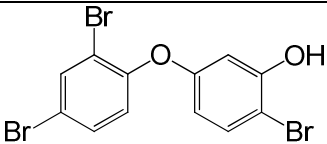
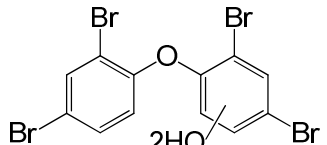
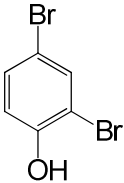


Figure S1. Geometry Scans for H Atom Transfer From C6 in IM_{C6} to One N Atom on the Porphyrin Ring (Similar results were obtained in the geometry scans of IM_{C5})

Table S2. Comparison of the Metabolites Predicted in the Current Study With Those Identified in the *in vivo* and *in vitro* Tests*

Compounds	Structures	Prediction	Experimental detection
2'-HO-BDE-66		It can be predicted by the current computation. To save computational resources, however, it was not calculated.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from faeces of BDE-47 exposed rats. ²
3-HO-BDE-47		It can be predicted by the current computation. To save computational resources, however, it was not calculated.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in hepatic microsomes from phenobarbital-treated rats. ³ (3) Detected from faeces of BDE-47 exposed rats. ²
4-HO-BDE-42		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in hepatic microsomes from phenobarbital-treated rats. ³ (3) Detected from faeces of BDE-47 exposed rats. ²
4'-HO-BDE-49		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in hepatic

			microsomes from phenobarbital-treated rats. ³ (3) Detected from faeces of BDE-47 exposed rats. ²
5-HO-BDE-47		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in hepatic microsomes from phenobarbital-treated rats. ³ (3) Detected from faeces of BDE-47 exposed rats. ²
6-HO-BDE-47		It can be predicted by the current computation. To save computational resources, however, it was not calculated.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in hepatic microsomes from phenobarbital-treated rats. ³ (3) Detected from faeces of BDE-47 exposed rats. ²
2'-HO-BDE-28		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from faeces of BDE-47 exposed rats. ²
4'-HO-BDE-17		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from faeces of BDE-47 exposed rats. ²

3'-HO-BDE-28		It cannot be predicted by the current computation. According to Marsh et al., ² it might be a natural product.	Detected from faeces of BDE-47 exposed rats. ²
Dihydroxy BDE 47		It cannot be predicted by the current computation. The formation of this compound needs the catalysis of epoxide hydrolase. ⁴	Detected from incubation of BDE-47 in human liver microsomes <i>in vitro</i> . ⁵
2,4-dibromophenol		It has been predicted by the current computation.	(1) Detected in mouse plasma after exposure to DE-71 mixture (BDE-47, 85, 99, 100, 153, 154). ¹ (2) Detected from incubation of BDE-47 in human liver microsomes <i>in vitro</i> . ⁵

*(1) Qiu, X. H.; Mercado-Feliciano, M.; Bigsby, R. M.; Hites, R. A. Measurement of polybrominated diphenyl ethers and metabolites in mouse plasma after exposure to a commercial pentabromodiphenyl ether mixture. *Environ. Health Persp.* **2007**, 115 (7), 1052-1058.
 (2) Marsh, G.; Athanasiadou, M.; Athanassiadis, I.; Sandholm, A. Identification of hydroxylated metabolites in 2,2',4,4'-tetrabromodiphenyl ether exposed rats. *Chemosphere* **2006**, 70 (4), 690-697.
 (3) Erratico, C. A.; Moffatt, S. C.; Bandiera, S. M. Comparative oxidative metabolism of BDE-47 and BDE-99 by rat hepatic microsomes. *Toxicol. Sci.* **2011**, 123 (1), 37-47.
 (4) Rietjens, I. M. C. M.; Soffers, A. E. M. F.; Veeger, C.; Vervoort, J. Regioselectivity of cytochrome P-450 catalyzed hydroxylation of fluorobenzenes predicted by calculated frontier orbital substrate characteristics. *Biochemistry-US* **1993**, 32 (18), 4801-4812.
 (5) Lupton, S. J.; McGarrgle, B. P.; Olson, J. R.; Wood, T. D.; Aga, D. S. Human liver microsome-mediated metabolism of brominated diphenyl ethers 47, 99, and 153 and identification of their major metabolites. *Chem. Res. Toxicol.* **2009**, 22 (11), 1802-1809.

Table S3. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C1) by Cpd I.

C1	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C1}	-12407.018228	0.0	1.23	0.87	-0.58	-0.52	0.00	0.52	-0.37	-0.04	-0.11	0.00
TS _{C1}	-12406.973730	27.9	1.73	0.37	-0.36	-0.42	-0.32	0.53	-0.45	-0.02	-0.19	0.11
IM _{C1}	-12406.992186	16.3	1.04	0.01	0.01	0.39	-0.54	0.39	-0.51	0.00	-0.16	0.27
TS(1,2)	-12407.020327	-1.3	1.11	0.00	-0.02	-0.12	0.02	0.33	-0.44	0.10	-0.39	0.39
IM(1,2)	-12407.000611	11.1	1.22	0.00	-0.11	-0.12	0.01	0.40	-0.37	0.03	-0.49	0.44
TS(1,6)	-12407.018930	-0.4	1.09	0.00	-0.01	-0.10	0.02	0.29	-0.43	0.10	-0.42	0.46
IM(1,6)	-12407.031851	-8.5	1.16	0.00	-0.06	-0.11	0.01	0.32	-0.42	0.12	-0.49	0.47

Table S4. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C2) by Cpd I.

C2	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C2}	-12407.018249	0.0	1.23	0.87	-0.58	-0.52	0.00	0.52	-0.37	-0.04	-0.11	0.00
TS _{C2}	-12406.972761	28.5	1.82	0.30	-0.41	-0.38	-0.33	0.54	-0.43	-0.02	-0.20	0.12
PC _{C2}	-12407.050747	-20.4	1.11	0.37	0.00	-0.65	0.17	0.37	-0.50	0.03	-0.09	0.18

Table S5. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C3) by Cpd I.

C3	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C3}	-12407.014901	0.0	1.22	0.88	-0.57	-0.53	0.00	0.51	-0.37	-0.05	-0.09	-0.01
TS _{C3}	-12406.977888	23.2	1.84	0.29	-0.37	-0.38	-0.39	0.56	-0.47	-0.01	-0.20	0.14
IM _{C3}	-12406.984934	18.8	1.01	0.06	0.02	-0.04	-0.06	0.42	-0.52	-0.06	-0.17	0.32
TS(3,2)	-12406.975669	24.6	1.08	0.00	-0.04	-0.17	0.12	0.41	-0.47	-0.01	-0.30	0.37
IM(3,2)	-12407.000540	9.0	1.23	0.00	-0.13	-0.13	0.00	0.38	-0.37	0.03	-0.49	0.44
TS(3,4)	-12406.978994	22.5	1.17	-0.05	-0.11	-0.34	0.34	0.39	-0.45	-0.01	-0.32	0.39
IM(3,4)	-12407.001653	8.3	1.21	0.00	-0.10	-0.11	0.01	0.41	-0.38	0.03	-0.50	0.45

Table S6. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C4) by Cpd I.

C4	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C4}	-12407.052014	0.0	1.29	0.83	-0.55	-0.58	0.00	0.43	-0.38	0.02	-0.09	0.02
TS _{C4}	-12407.011455	25.4	1.81	0.20	-0.30	-0.38	-0.34	0.47	-0.44	0.05	-0.22	0.13
PC _{C4}	-12407.085995	-21.3	1.14	0.00	-0.04	-0.10	0.00	0.23	-0.42	0.10	-0.49	0.58

Table S7. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C5) by Cpd I.

C5	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C5}	-12407.017960	0.0	1.23	0.87	-0.59	-0.52	0.00	0.52	-0.37	-0.04	-0.11	0.00
TS _{C5}	-12406.980546	23.5	1.86	0.02	-0.21	-0.29	-0.38	0.40	-0.41	0.06	-0.22	0.18
IM _{C5}	-12406.985723	20.2	1.08	0.07	0.01	-0.12	-0.03	0.29	-0.47	0.04	-0.32	0.45
TS(5,4)	-12407.014399	2.23	1.14	-0.03	-0.07	-0.22	0.18	0.34	-0.45	0.07	-0.38	0.42
IM(5,4)	-12407.032285	-9.0	1.15	0.00	-0.05	-0.10	0.01	0.34	-0.40	0.10	-0.51	0.46
TS(5,6)	-12407.019364	-0.9	1.06	0.06	0.06	0.03	-0.20	0.29	-0.44	0.06	-0.35	0.44
IM(5,6)	-12407.035854	-11.2	1.13	0.00	-0.02	-0.10	0.01	0.29	-0.40	0.10-	-0.50	0.50

Table S8. Relative Energies, Spin and Charge Densities at the UB3LYP/B-I//B-I Level for the Species in the Metabolism of BDE-47 (C6) by Cpd I.

C6	E (a.u.)	E_{rel} (Kcal/mol)	Spin Density					Charge				
			Fe	O	SH	Por	sub	Fe	O	SH	Por	sub
RC _{C6}	-12407.018069	0.0	1.23	0.87	-0.58	-0.52	0.00	0.50	-0.37	-0.04	-0.09	0.00
TS _{C6}	-12406.978806	24.6	1.83	0.15	-0.31	-0.30	-0.37	0.50	-0.43	-0.01	-0.23	0.17
IM _{C6}	-12406.986439	19.8	1.11	0.05	-0.17	-0.54	0.54	0.39	-0.51	-0.04	-0.21	0.37
TS(6,5)	-12407.016174	1.2	1.11	0.05	-0.02	-0.16	0.01	0.29	-0.43	0.07	-0.39	0.47
IM(6,5)	-12407.035854	-11.2	1.13	0.00	-0.02	-0.10	0.01	0.29	-0.40	0.10	-0.50	0.50
TS(6,1)	-12407.017268	0.5	1.13	-0.01	-0.06	-0.17	0.11	0.32	-0.47	0.06	-0.43	0.51
IM(6,1)	-12407.031851	-8.6	1.16	0.00	-0.06	-0.11	0.01	0.32	-0.42	0.12	-0.49	0.47

Table S9. Self-Consistent Field (SCF) Energies at Various Computational Levels for the Metabolism of BDE-47 (C1) by Cpd I.

BDE-47 (C1)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C1}	-12407.018228	0.0	-12406.581725	0.0	-12418.962364	0.0	-12418.525861	0.0	-12418.962364	0.0	-12418.525861	0.0
TS _{C1}	-12406.973730	27.9	-12406.539533	26.5	-12418.924077	24.0	-12418.489880	22.6	-12418.924077	24.0	-12418.48988	22.6
IM _{C1}	-12406.992186	16.3	-12406.557318	15.3	-12418.935679	16.7	-12418.500811	15.7	-12418.950699	7.3	-12418.515831	6.3
TS(1,2)	-12407.020327	-1.3	-12406.584517	-1.8	-12418.934847	17.3	-12418.499037	16.8	-12418.950988	7.1	-12418.515178	6.7
IM(1,2)	-12407.000611	11.1	-12406.564207	11.0	-12418.956346	3.8	-12418.519942	3.7	-12418.971327	-5.6	-12418.534923	-5.7
TS(1,6)	-12407.018930	-0.4	-12406.583154	-0.9	-12418.933620	18.0	-12418.497845	17.6	-12418.950174	7.6	-12418.514399	7.2
IM(1,6)	-12407.031851	-8.5	-12406.594619	-8.1	-12418.955760	4.1	-12418.518528	4.6	-12418.971336	-5.6	-12418.534104	-5.2

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S10. SCF Energies at Various Computational Levels for the Metabolism of BDE-47 (C2) by Cpd I.

BDE-47 (C2)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C2}	-12407.018249	0.0	-12406.581656	0.0	-12418.962470	0.0	-12418.525876	0.0	-12418.962469	0.0	-12418.525875	0.0
TS _{C2}	-12406.972761	28.5	-12406.538671	27.0	-12418.921552	25.7	-12418.487462	24.1	-12418.921552	25.7	-12418.487462	24.1
PC _{C2}	-12407.050747	-20.4	-12406.613661	-20.1	-12418.990252	-17.4	-12418.553166	-17.1	-12419.009320	-29.4	-12418.572234	-29.1

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S11. SCF Energies at Various Computational Levels for the Metabolism of BDE-47 (C3) by Cpd I.

BDE-47 (C3)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C3}	-12407.014901	0.0	-12406.578372	0.0	-12418.962429	0.0	-12418.525900	0.0	-12418.962429	0.0	-12418.525900	0.0
TS _{C3}	-12406.977888	23.2	-12406.543338	22.0	-12418.928193	21.5	-12418.493642	20.2	-12418.928193	21.4	-12418.493642	20.2
IM _{C3}	-12406.984934	18.8	-12406.548356	18.8	-12418.927509	21.9	-12418.490931	21.9	-12418.946776	9.8	-12418.510198	9.8
TS(3,2)	-12406.975669	24.6	-12406.540157	24.0	-12418.919870	26.7	-12418.484358	26.1	-12418.936924	16.0	-12418.501412	15.3
IM(3,2)	-12407.000540	9.0	-12406.563643	9.2	-12418.953896	5.4	-12418.517000	5.6	-12418.969318	-4.3	-12418.532422	-4.1
TS(3,4)	-12406.978994	22.5	-12406.543586	21.8	-12418.922845	24.8	-12418.487437	24.1	-12418.940556	13.7	-12418.505148	13.0
IM(3,4)	-12407.001653	8.3	-12406.564741	8.6	-12418.954484	5.0	-12418.517572	5.2	-12418.969770	-4.6	-12418.532858	-4.4

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S12. SCF Energies at Various Computational Levels for the Metabolism of BDE-47 (C4) by Cpd I.

BDE-47 (C4)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C4}	-12407.052014	0.0	-12406.615445	0.0	-12418.962760	0.0	-12418.526191	0.0	-12418.962760	0.0	-12418.526191	0.0
TS _{C4}	-12407.011455	25.4	-12406.576865	24.2	-12418.923864	24.4	-12418.489275	23.1	-12418.923864	24.4	-12418.489275	23.2
PC _{C4}	-12407.085995	-21.3	-12406.648086	-20.5	-12419.001847	-24.5	-12418.563939	-23.7	-12419.018299	-34.9	-12418.580391	-34.0

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S13. SCF Energies at Various Computational Levels for the Metabolism of BDE-47 (C5) by Cpd I.

BDE-47 (C5)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C5}	-12407.017960	0.0	-12406.581554	0.0	-12418.963235	0.0	-12418.526829	0.0	-12418.963235	0.0	-12418.526829	0.0
TS _{C5}	-12406.980546	23.5	-12406.545282	22.8	-12418.931831	19.7	-12418.496279	19.2	-12418.931831	19.7	-12418.496279	19.2
IM _{C5}	-12406.985723	20.2	-12406.549406	20.2	-12418.927754	22.3	-12418.491347	22.3	-12418.946116	10.7	-12418.509709	10.7
TS(5,4)	-12407.014399	2.23	-12406.578593	1.9	-12418.925626	23.6	-12418.48982	23.2	-12418.942590	13.0	-12418.506784	12.6
IM(5,4)	-12407.032285	-9.0	-12406.595198	-8.6	-12418.953431	6.2	-12418.516343	6.6	-12418.968842	-3.5	-12418.531754	-3.1
TS(5,6)	-12407.019364	-0.9	-12406.583406	-1.2	-12418.928476	21.8	-12418.492518	21.5	-12418.946232	10.7	-12418.510274	10.4
IM(5,6)	-12407.035854	-11.2	-12406.597679	-10.1	-12418.955794	4.7	-12418.517619	5.8	-12418.971221	-5.0	-12418.533046	-3.9

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S14. SCF Energies at Various Computational Levels for the Metabolism of BDE-47 (C6) by Cpd I.

BDE-47 (C6)	UB3LYP/BS-I		UB3LYP/BS-I +ZPE		UB3LYP/BS-II		UB3LYP/BS-II +ZPE		UB3LYP/BS-II + solvent		UB3LYP/BS-II + solvent + ZPE	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>
RC _{C6}	-12407.018069	0.0	-12406.581556	0.0	-12418.963027	0.0	-12418.526514	0.0	-12418.963027	0.0	-12418.526514	0.0
TS _{C6}	-12406.978806	24.6	-12406.543812	23.7	-12418.929948	20.8	-12418.494953	19.8	-12418.929948	20.8	-12418.494953	19.8
IM _{C6}	-12406.986439	19.8	-12406.550815	19.3	-12418.926614	22.8	-12418.49099	22.3	-12418.944264	11.8	-12418.508640	11.2
TS(6,5)	-12407.016174	1.2	-12406.579599	1.2	-12418.923654	24.7	-12418.487079	24.7	-12418.941405	13.6	-12418.504830	13.6
IM(6,5)	-12407.035854	-11.2	-12406.597679	-10.1	-12418.955794	4.5	-12418.517619	5.6	-12418.971221	-5.1	-12418.533046	-4.1
TS(6,1)	-12407.017268	0.5	-12406.580889	0.4	-12418.928977	21.4	-12418.492598	21.3	-12418.946652	10.3	-12418.510273	10.2
IM(6,1)	-12407.031851	-8.6	-12406.594619	-8.2	-12418.955760	4.5	-12418.518528	5.0	-12418.971336	-5.2	-12418.534104	-4.8

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol.

Table S15. Sum of Electronic and Thermal Enthalpies and Reaction Enthalpies at Various Levels for Hydroxylation of BDE-47 by Cpd I.

		UB3LYP/BS-I//BS-I		UB3LYP/ BS-II//BS-I		UB3LYP/BS-II//BS-I +Bulk Polarity	
C1	RC _{C1}	-12406.541478	0.00	-12418.485614	0.00	-12418.485614	0.00
	IM _{C1}	-12406.517812	14.8	-12418.461305	15.3	-12418.476325	5.8
	IM(1,2)	-12406.524768	10.5	-12418.480503	3.2	-12418.495484	-6.2
	IM(1,6)	-12406.555383	-8.7	-12418.479292	4.0	-12418.494868	-5.8
C2	RC _{C2}	-12406.541473	0.00	-12418.485693	0.00	-12418.485692	0.00
	IM _{C2}	-12406.573943	-20.4	-12418.513448	-17.4	-12418.532516	-29.4
C3	RC _{C3}	-12406.538108	0.00	-12418.485636	0.00	-12418.485636	0.00
	IM _{C3}	-12406.509480	18.0	-12418.452054	21.0	-12418.471321	9.0
	IM(3,2)	-12406.524127	8.8	-12418.477484	5.1	-12418.492906	-4.6
	IM(3,4)	-12406.525307	8.0	-12418.478138	4.7	-12418.493424	-4.9
C4	RC _{C4}	-12406.575320	0.00	-12418.486066	0.00	-12418.486066	0.00
	IM _{C4}	-12406.608616	-20.9	-12418.524468	-24.1	-12418.540920	-34.4
C5	RC _{C5}	-12406.541211	0.00	-12418.486486	0.00	-12418.486486	0.00
	IM _{C5}	-12406.510141	19.5	-12418.452159	21.5	-12418.470521	10.0
	IM(5,4)	-12406.556021	-9.3	-12418.477167	5.8	-12418.492578	-3.8
	IM(5,6)	-12406.558634	-10.9	-12418.478574	5.0	-12418.494001	-4.7
C6	RC _{C6}	-12406.541321	0.00	-12418.486279	0.00	-12418.486279	0.00
	IM _{C6}	-12406.511409	18.8	-12418.451584	21.8	-12418.469234	10.7
	IM(6,5)	-12406.558634	-10.9	-12418.478574	4.8	-12418.494001	-4.8
	IM(6,1)	-12406.555383	-8.8	-12418.480503	3.6	-12418.495484	-5.8

Absolute SCF energies E are in Hartree and relative SCF energies dE are in kcal/mol.

Table S16. SCF Energies at Various Computational Levels, Sum of Electronic and Thermal Enthalpies and Reaction Enthalpies at Various Levels for Proton Catalyzed Rearrangement of Three Representative Hydroxyl-Cyclohexadienyl Cations.

	B3LYP/6-311G(d)		UB3LYP/6-311G(d) + ZPE		UB3LYP/6-311+G(d,p) + solvent		UB3LYP/6-311+G(d,p) + solvent + ZPE		UB3LYP/6-311+G(d,p) + solvent	
	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>E</i>	d <i>E</i>	<i>H</i>	d <i>H</i>
#1	-10908.332855	0.0	-10908.173892	0.0	-10908.432191	0.0	-10908.273228	0.0	-10908.254559	0.0
TS _{#1-#4}	-10908.324890	5.0	-10908.166189	4.8	-10908.425891	4.0	-10908.267190	3.8	n.a.	n.a.
#4	-10908.337920	-3.2	-10908.177924	-2.5	-10908.438776	-4.1	-10908.278779	-3.5	-10908.26036	-3.6
TS _{#1-#5}	-10908.328456	2.8	-10908.169680	2.6	-10908.428644	2.2	-10908.269869	2.1	n.a.	n.a.
#5	-10908.344199	-7.1	-10908.184549	-6.7	-10908.443619	-7.2	-10908.283969	-6.7	-10908.265558	-6.9
#2	-10908.316751	0.0	-10908.158505	0.0	-10908.417456	0.0	-10908.259210	0.0	-10908.240497	0.0
TS _{#2-#6}	-10908.300600	10.1	-10908.145643	8.1	-10908.403059	9.0	-10908.248102	7.0	n.a.	n.a.
#6	-10908.356695	-25.1	-10908.196611	-24.0	-10908.455012	-23.6	-10908.294928	-22.4	-10908.276534	-22.6
TS _{#2-#7}	-10908.302788	8.8	-10908.147578	6.9	-10908.404682	8.0	-10908.249471	6.1	n.a.	n.a.
#7	-10908.357831	-25.8	-10908.198499	-25.1	-10908.455142	-23.6	-10908.295810	-23.0	-10908.277272	-23.1
#3	-10908.312781	0.0	n.a.	n.a.	-10908.410631	0.0	-10908.252429	0.0	-10908.233881	0.0
TS _{#3}	-10908.306671	3.8	n.a.	n.a.	-10908.404478	3.9	-10908.247777	2.9	n.a.	n.a.
PC _{#3}	-10908.329546	-10.5	n.a.	n.a.	-10908.426827	-10.2	-10908.269282	-10.1	-10908.250034	-10.1
#8+#9	-10908.303913	5.6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
#10+#11	-10908.308652	2.6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Absolute SCF energies *E* are in Hartree and relative SCF energies d*E* are in kcal/mol; n.a. = not applicable.

Table S17. Vertical and Adiabatic Electron Affinities (VEA and AEA) (eV) of Phenoxide Radical and Cyclohexadienone.

	UB3LYP/6-311+G(d,p)		UB3LYP/6-311+G(d,p) + solvent ($\epsilon = 5.6$)		UB3LYP/6-311+G(d,p) + solvent ($\epsilon = 78.4$)	
	E	d E	E	d E	E	d E
phenoxide	-8333.875747	0.00	-8333.884822	0.00	-8333.888067	0.00
phenoxide anion (neutral geometry)	-8333.969430	-2.55	-8334.035141	-4.09	-8334.051395	-4.44
phenoxide anion (anion geometry)	-8333.989629	-3.10	-8334.046789	-4.41	-8334.060622	-4.70
cyclohexadienone	-10908.037002	0.00	-10908.037002	0.00	-10908.039741	0.00
cyclohexadienone anion (neutral geometry)	-10908.094331	-1.56	-10908.154917	-3.21	-10908.169157	-3.52
cyclohexadienone anion (anion geometry)	-10908.142273	-2.86	-10908.206874	-4.62	-10908.222326	-4.97

Absolute SCF energies E are in Hartree and relative SCF energies d E are in eV.

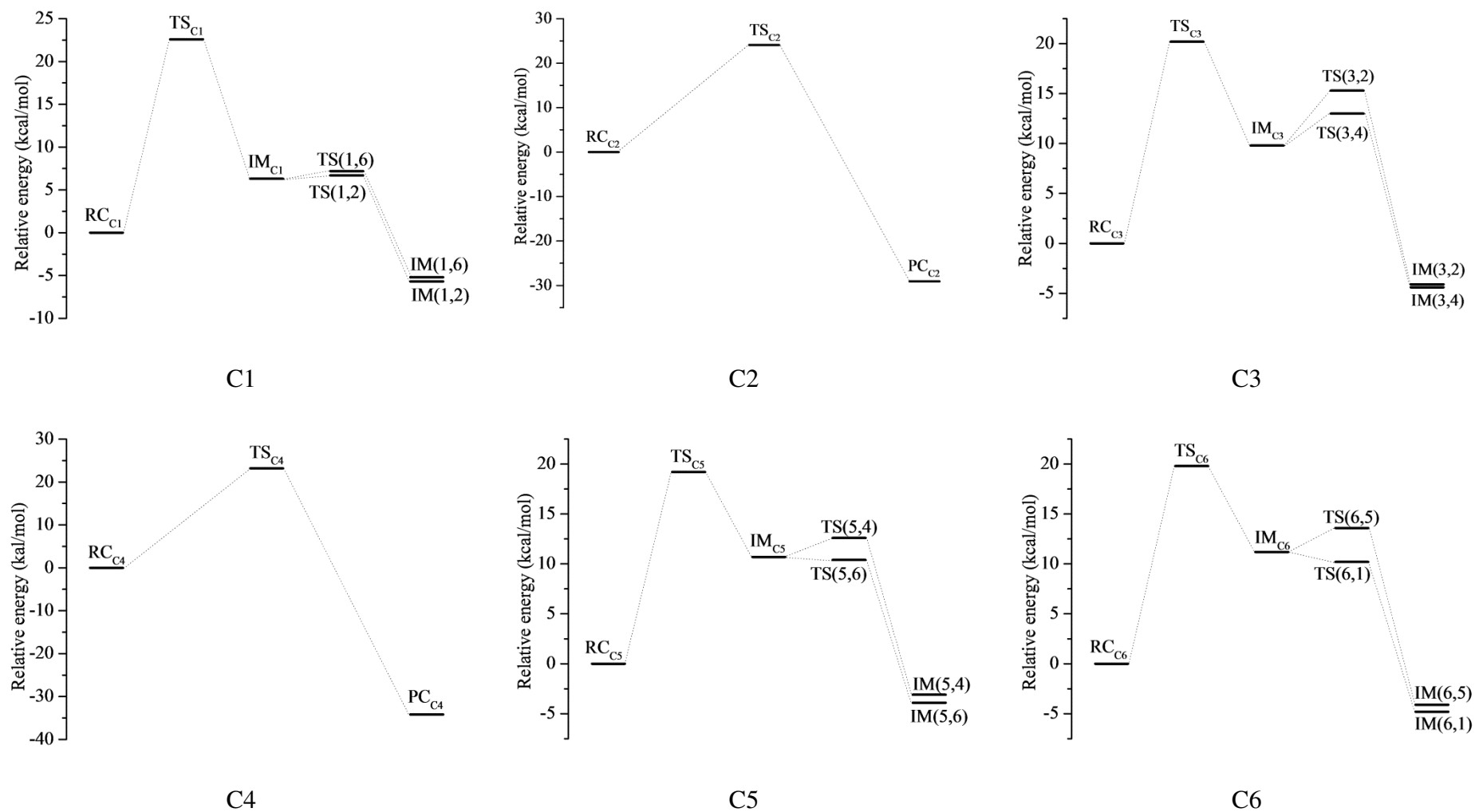


Figure S2. Profiles of the Potential Energy Surface (PES) for the Addition of Cpd I to BDE-47 at UB3LYP/BS-II + Solvent + ZPE Level.

Table S18. Cartesian Coordinates of the Reaction Species.

RC_{C1}

Fe	-0.11789500	1.47651100	0.33386400
N	-1.56659900	2.86870000	0.51829700
C	-2.14434200	3.31477100	1.69905000
C	-3.22610000	4.22966500	1.40483900
C	-3.30707900	4.32921200	0.04619300
C	-2.27213000	3.48052900	-0.50470500
H	-3.83244500	4.72180500	2.15100400
H	-3.99224800	4.92027000	-0.54349000
C	-2.02515600	3.31983700	-1.86022400
H	-2.66642200	3.85663600	-2.55104600
N	-0.10998500	1.78132400	-1.66851500
C	-1.01732400	2.54161700	-2.40103500
C	-0.76493100	2.38019300	-3.81581200
C	0.27852300	1.50971400	-3.94522700
C	0.68211500	1.12616400	-2.61050500
H	-1.32667600	2.87192700	-4.59636900
H	0.73869600	1.13848800	-4.84877200
C	1.68951500	0.22409200	-2.31705000
H	2.20191900	-0.23886000	-3.15274800
N	1.51396300	0.30511400	0.14136000
C	2.07977200	-0.15200000	-1.03700900
C	3.15071300	-1.07987800	-0.74686400
C	3.23208400	-1.18280200	0.61259800
C	2.20773000	-0.32350300	1.16423500
H	3.74755500	-1.57854700	-1.49604000

H	3.91236100	-1.78146800	1.20030000
C	1.95872500	-0.15972900	2.51795200
H	2.58662100	-0.71023500	3.21050600
N	0.07311400	1.41415300	2.33318600
C	0.96826400	0.64685400	3.05904700
C	0.72748100	0.81170000	4.47597500
C	-0.31659300	1.68270900	4.60367900
C	-0.72082700	2.05557700	3.26554100
H	1.29226100	0.32187900	5.25549500
H	-0.77799400	2.04951700	5.50873200
C	-1.75120700	2.93964700	2.97207600
H	-2.29145500	3.36998700	3.80861600
O	-1.17240600	0.20759800	0.24772800
S	1.37289500	3.58063000	0.13230700
H	2.39996700	3.03200600	-0.61307500
C	-0.86865700	-4.36710700	0.38804500
C	-1.02548200	-3.01965700	0.06856000
C	-0.68947500	-2.58712200	-1.21727300
C	-0.20387700	-3.49562400	-2.16067100
C	-0.05382500	-4.84431500	-1.82303100
C	-0.38554400	-5.28829300	-0.54187000
O	0.22739700	-3.02868600	-3.41691800
C	-0.68059800	-2.83392100	-4.45788100
C	-2.04463500	-3.12908800	-4.35666500
C	-2.89556100	-2.90991400	-5.44330900
C	-2.37475600	-2.39614100	-6.62843400
C	-1.01738000	-2.09817800	-6.74716000

C	-0.17749200	-2.31838300	-5.65808900	H	-1.29104600	4.26255000	-4.19910400
Br	0.63264900	-6.11683400	-3.12124000	H	1.24555800	3.53769000	-4.80495600
Br	1.71603200	-1.90231700	-5.82819300	C	2.43470400	1.95696900	-2.73852300
Br	-3.55603600	-2.08411100	-8.15326000	H	3.10337500	2.12454300	-3.57579100
H	-0.78926400	-1.53761500	-1.46442300	N	2.21463800	0.92021700	-0.51487600
H	-0.26494900	-6.33058400	-0.27970400	C	2.92259100	1.22786400	-1.66642600
H	-2.44155200	-3.52765200	-3.43137900	C	4.26572400	0.69621200	-1.57300300
H	-3.95025600	-3.13997400	-5.36076800	C	4.36529200	0.06901100	-0.36492800
H	-0.61508700	-1.70197900	-7.66964400	C	3.08186700	0.20449700	0.29116200
H	-1.38343000	-2.29636900	0.78937400	H	5.01925700	0.79876300	-2.34004000
Br	-1.32228000	-4.99317100	2.18356400	H	5.21652900	-0.44570300	0.05593800
TS_{C1}				C	2.77382100	-0.32390700	1.53525500
Fe	0.26057200	1.28870600	-0.14976700	H	3.56052300	-0.85527100	2.05985500
N	-1.61945600	1.83814100	0.30732800	N	0.41270700	0.38207500	1.63925800
C	-2.34941500	1.47981300	1.42877000	C	1.53951700	-0.23795400	2.15790800
C	-3.67654000	2.05041000	1.35636100	C	1.23347500	-0.80862300	3.45184900
C	-3.74298700	2.76348700	0.19317800	C	-0.07824500	-0.53310900	3.71266400
C	-2.45945800	2.63204300	-0.46101400	C	-0.58646800	0.21542100	2.58368300
H	-4.43964500	1.92356200	2.11030600	H	1.94164500	-1.34438000	4.06687600
H	-4.57233700	3.33583000	-0.19620800	H	-0.65974600	-0.79667800	4.58388500
C	-2.13593200	3.21105700	-1.67764400	C	-1.87821700	0.70788000	2.47989300
H	-2.90260800	3.80170300	-2.16780400	H	-2.56311400	0.49467200	3.29290700
N	0.17969400	2.38885700	-1.84659700	O	-0.16890800	-0.13156300	-1.04308300
C	-0.91533400	3.09021500	-2.32308500	S	1.00275200	3.35112400	0.96915100
C	-0.60635500	3.66518400	-3.61505200	H	1.92328900	3.75670100	0.02233000
C	0.67285300	3.29925900	-3.92071900	C	-2.68251800	-2.34608700	0.70616700
C	1.16260000	2.50235800	-2.81638600	C	-3.20595400	-1.53208200	-0.31052500

C	-2.41632400	-1.21790800	-1.40121400	C	-2.52358100	2.36628300	-0.43135100
C	-1.04131900	-1.63736800	-1.47380800	H	-4.41046200	1.80177600	2.24442500
C	-0.59122100	-2.55760300	-0.46284500	H	-4.65804900	3.00382500	-0.16569800
C	-1.38408600	-2.86425600	0.63170500	C	-2.25642300	2.81752600	-1.71492000
O	-0.45738200	-1.70683100	-2.77237100	H	-3.05531700	3.33391100	-2.23713900
C	-0.84568700	-2.70197800	-3.66966400	N	0.07597000	2.04111100	-1.88329300
C	-1.70285700	-3.76509400	-3.35717800	C	-1.05969200	2.64053600	-2.40042300
C	-2.02564300	-4.72138000	-4.32535200	C	-0.82592400	3.04229600	-3.77139400
C	-1.48811100	-4.61010700	-5.60406200	C	0.45370300	2.67913400	-4.08107700
C	-0.63235700	-3.55926400	-5.93385600	C	1.01934200	2.06744500	-2.89837000
C	-0.31612300	-2.60992200	-4.96513400	H	-1.55500700	3.53055700	-4.40136100
Br	1.17741400	-3.32103100	-0.60668800	H	0.98001300	2.80971700	-5.01497000
Br	0.87033200	-1.14717900	-5.43315100	C	2.33370600	1.63901800	-2.78429300
Br	-1.93364400	-5.94155200	-6.96476700	H	2.95884800	1.71378000	-3.66745100
H	-2.78866500	-0.60353400	-2.21119500	N	2.27056000	0.99145900	-0.41592200
H	-1.00555100	-3.51119400	1.41150300	C	2.91979500	1.14752000	-1.62595600
H	-2.11732000	-3.85612800	-2.36199300	C	4.30432200	0.73686400	-1.50270300
H	-2.68678800	-5.54176100	-4.07599400	C	4.48263700	0.32544200	-0.21337200
H	-0.21628600	-3.47425100	-6.92854600	C	3.20492400	0.47236200	0.45734700
H	-4.22175400	-1.16379900	-0.24531100	H	5.02716400	0.76198600	-2.30491100
Br	-3.80573400	-2.82279400	2.22701500	H	5.38033100	-0.05591600	0.25097600
IM_{C1}				C	2.95151800	0.09012300	1.76886100
Fe	0.30661900	1.31388600	-0.02286500	H	3.78818300	-0.29783400	2.34094200
N	-1.62838900	1.66744300	0.37583900	N	0.53401100	0.57272000	1.83865800
C	-2.31651900	1.39059200	1.55176300	C	1.71751500	0.12717400	2.40241000
C	-3.67041900	1.89143700	1.46249000	C	1.47697200	-0.32774300	3.75677400
C	-3.79472900	2.50102400	0.24558300	C	0.14421800	-0.16126300	4.00393000

C	-0.43774300	0.40613400	2.80545500	H	-3.18930100	-4.61602200	-4.37289800
H	2.23678000	-0.72132900	4.41610500	H	0.20645800	-3.45880500	-6.74543500
H	-0.40427900	-0.38691200	4.90676100	H	-4.09273400	-0.99708400	-0.30700600
C	-1.77142600	0.77179700	2.66622900	Br	-4.11729800	-3.43593100	1.42434200
H	-2.42661100	0.60363100	3.51459700				
O	0.15544700	-0.51159800	-0.68424200	TS(1,2)			
S	0.80001300	3.44456200	0.77501500	Fe	0.37231600	1.32398600	-0.04100100
H	1.93904500	3.67638300	0.02879800	N	-1.60912500	1.58668700	0.12547800
C	-2.78541700	-2.62268200	0.27517000	C	-2.41760000	1.27970800	1.21278900
C	-3.10759400	-1.43305500	-0.41550800	C	-3.77010700	1.72770400	0.96681900
C	-2.16129400	-0.83799700	-1.21033200	C	-3.77731100	2.32865700	-0.26095400
C	-0.75251900	-1.33992100	-1.31645600	C	-2.43134900	2.24929600	-0.78373400
C	-0.57862100	-2.69318700	-0.67303300	H	-4.59074000	1.61068100	1.66012100
C	-1.53321700	-3.25281000	0.14382100	H	-4.60612200	2.79703900	-0.77219300
O	-0.34604000	-1.34552200	-2.77713800	C	-2.03417100	2.74543600	-2.01472700
C	-0.77665900	-2.29381000	-3.68698600	H	-2.78730000	3.23765100	-2.62117100
C	-1.92566800	-3.08771600	-3.53117600	N	0.33580000	2.07379800	-1.90679700
C	-2.30165900	-4.01132900	-4.51109500	C	-0.75315200	2.65308600	-2.53984400
C	-1.53247600	-4.13910800	-5.66296800	C	-0.36681400	3.13669000	-3.84891300
C	-0.39234800	-3.35886700	-5.85034100	C	0.95664800	2.84472800	-4.00938300
C	-0.02240700	-2.44777600	-4.86429200	C	1.39678400	2.18873900	-2.79708500
Br	1.13527000	-3.53947700	-0.85776600	H	-1.03493600	3.62608600	-4.54259000
Br	1.58264100	-1.38644000	-5.14527400	H	1.59169600	3.05166800	-4.85847500
Br	-2.04893100	-5.42629100	-7.04313200	C	2.69780600	1.78509500	-2.54842800
H	-2.37872100	0.05796400	-1.77483300	H	3.42849000	1.93263900	-3.33652000
H	-1.32977200	-4.17159200	0.67784500	N	2.34878300	0.98910400	-0.24614300
H	-2.54300900	-2.97849000	-2.65055300	C	3.14165200	1.23384500	-1.35557700
				C	4.51266100	0.85978800	-1.07862100

C	4.54620600	0.38996900	0.20258200
C	3.19410700	0.46503500	0.71763600
H	5.32768100	0.95264700	-1.78166100
H	5.39453800	0.01866400	0.75918300
C	2.81017200	0.03591700	1.97995400
H	3.58759400	-0.34994800	2.63129200
N	0.39203700	0.48614900	1.78689900
C	1.51408400	0.03974500	2.47115800
C	1.13112400	-0.44929600	3.77935400
C	-0.22188400	-0.29646400	3.88489700
C	-0.67732800	0.29482700	2.64474700
H	1.81953700	-0.84965600	4.50960200
H	-0.86288800	-0.54544000	4.71803200
C	-1.99218000	0.64838300	2.37159800
H	-2.73292000	0.45657400	3.14061500
O	0.23576200	-0.55163300	-0.90595600
S	0.76410000	3.39799600	0.87024700
H	1.75421200	3.80934800	-0.00098500
C	-2.08305900	-2.50328300	0.70745800
C	-2.79641500	-1.63280800	-0.18011900
C	-2.17206500	-1.10575300	-1.26581100
C	-0.73465600	-1.38488700	-1.54906900
C	-0.11304000	-2.41704200	-0.66391900
C	-0.77626900	-2.88147700	0.49427100
O	-0.45212500	-1.42009000	-2.96362400
C	-1.09174800	-2.33417500	-3.79971700
C	-1.73404200	-3.49522700	-3.34727600

C	-2.32344600	-4.38007300	-4.25551400
C	-2.26271700	-4.10290800	-5.61801800
C	-1.62412600	-2.95588800	-6.08858900
C	-1.04470100	-2.07535900	-5.17736700
Br	1.54135900	-3.24507300	-1.17151500
Br	-0.17192900	-0.47432600	-5.83614100
Br	-3.08105200	-5.33366500	-6.89534800
H	-2.69231800	-0.45847800	-1.96086200
H	-0.26464400	-3.54982900	1.17258600
H	-1.77137600	-3.72582000	-2.29053700
H	-2.81725700	-5.27465800	-3.89783500
H	-1.57806300	-2.74277800	-7.14790100
H	-3.83153300	-1.39942700	0.03066700
Br	-3.03689400	-3.22098700	2.23813900
IM(1,2)			
Fe	0.39706600	1.44615400	0.05172400
N	-1.58089000	1.75374300	0.24615900
C	-2.38479100	1.44700300	1.33586300
C	-3.72931700	1.93162000	1.11260600
C	-3.73513000	2.54834000	-0.10657900
C	-2.39662500	2.43986900	-0.64540300
H	-4.54522000	1.82113300	1.81238900
H	-4.55820800	3.03993500	-0.60512200
C	-2.00577600	2.92848400	-1.88198500
H	-2.75289300	3.44613500	-2.47437900
N	0.33619800	2.15440500	-1.82495200
C	-0.74212600	2.78451800	-2.43256900

C	-0.36911100	3.23801800	-3.75526300	H	1.87943900	3.86198700	0.05703800
C	0.93265700	2.87606500	-3.95226700	C	-2.05533100	-2.43150000	0.74781700
C	1.37370600	2.20667800	-2.74860300	C	-2.92449200	-1.75910400	-0.19618700
H	-1.03110500	3.75582200	-4.43414900	C	-2.46030900	-1.33065800	-1.39540200
H	1.55130000	3.04187300	-4.82223900	C	-1.03831600	-1.47175700	-1.73250400
C	2.65598100	1.72632100	-2.53966800	C	-0.13857500	-2.15658700	-0.71591500
H	3.37084800	1.83064500	-3.34872200	C	-0.74043900	-2.66135900	0.52193200
N	2.32089600	0.94477800	-0.22731800	O	-0.69752000	-1.44226800	-3.09598500
C	3.09868000	1.14980500	-1.36001100	C	-1.16957800	-2.43795300	-3.96125900
C	4.45444800	0.70846700	-1.11708500	C	-1.64750300	-3.67805000	-3.52352500
C	4.50056500	0.24482100	0.16640700	C	-2.07551600	-4.63277200	-4.45059100
C	3.17072100	0.38747000	0.71915900	C	-2.01628900	-4.33942700	-5.81069300
H	5.25365400	0.75631600	-1.84240900	C	-1.53685900	-3.10972800	-6.26119200
H	5.34509500	-0.16542200	0.70097600	C	-1.11686500	-2.15928100	-5.33204500
C	2.80373500	-0.01685400	1.99283800	Br	1.47485500	-3.11621700	-1.30467600
H	3.57872400	-0.43405900	2.62715800	Br	-0.46011800	-0.44593700	-5.95468200
N	0.40368200	0.53540600	1.84325800	Br	-2.61136000	-5.66636600	-7.11355000
C	1.51926700	0.04348100	2.50976400	H	-3.11391400	-0.88712600	-2.13686900
C	1.14078200	-0.43016400	3.82368100	H	-0.12639200	-3.22745100	1.20843800
C	-0.20250500	-0.22075500	3.95561700	H	-1.67694500	-3.91158300	-2.46691300
C	-0.65879900	0.39155200	2.72757700	H	-2.44345200	-5.59235300	-4.11064600
H	1.82514600	-0.86191500	4.53970300	H	-1.49114800	-2.88654500	-7.31842200
H	-0.83701900	-0.44700200	4.79999900	H	-3.96779900	-1.63574900	0.06478100
C	-1.96091900	0.79901600	2.48609800	Br	-2.88832500	-3.10060100	2.38156100
H	-2.69434500	0.62584200	3.26614700				
O	-0.06310600	-0.69061200	-0.94297200	TS(1,6)			
S	0.91499900	3.48486400	0.97292000	Fe	0.24735400	1.33341400	0.01894100
				N	-1.65733300	1.73868400	0.55472300

C	-2.24546800	1.52911200	1.79324600	C	1.83236200	0.24332700	2.37144000
C	-3.60497900	2.02442300	1.78587000	C	1.70055000	-0.12172900	3.76777300
C	-3.83141500	2.55693100	0.54720300	C	0.39751100	0.08648900	4.11501000
C	-2.61682200	2.37991200	-0.22038400	C	-0.27815300	0.59447700	2.93818500
H	-4.27846100	1.98112900	2.62972400	H	2.50784500	-0.49232100	4.38275900
H	-4.72768100	3.03363300	0.17662800	H	-0.07575400	-0.07405700	5.07286300
C	-2.45827600	2.75053200	-1.54832100	C	-1.61124800	0.97269700	2.89535500
H	-3.29329400	3.24753400	-2.03128000	H	-2.19235800	0.86374600	3.80517700
N	-0.16185800	1.89664200	-1.87085600	O	-0.26593300	-0.70110000	-0.26436600
C	-1.32424600	2.51775700	-2.31635900	S	0.88681000	3.46153100	0.58845800
C	-1.19651100	2.85452000	-3.71754200	H	1.68527900	3.72330000	-0.50854000
C	0.04263300	2.44090600	-4.11912500	C	-3.10166800	-2.59499100	0.09968700
C	0.69053400	1.85782300	-2.96580500	C	-3.15074200	-1.34325600	-0.48249800
H	-1.96177400	3.34395200	-4.30269800	C	-2.03084800	-0.88967600	-1.19576600
H	0.49307200	2.52694200	-5.09730600	C	-0.74494100	-1.63357500	-1.21693500
C	1.99645000	1.39013000	-2.94593200	C	-0.83061000	-3.00643600	-0.61426100
H	2.55014300	1.41094600	-3.87799400	C	-1.94658900	-3.43620200	0.03465900
N	2.10618600	0.84371200	-0.54777400	O	0.02969400	-1.59102400	-2.44171100
C	2.65795400	0.93347300	-1.81761500	C	-0.36338000	-2.33900600	-3.55304200
C	4.04492200	0.52026500	-1.78444200	C	-1.68940200	-2.72369400	-3.79902900
C	4.33297000	0.19054700	-0.49186600	C	-2.02354900	-3.43787000	-4.95323800
C	3.12197500	0.38859800	0.27846100	C	-1.02585400	-3.76241100	-5.86751900
H	4.69756300	0.49639200	-2.64492900	C	0.29914800	-3.39156000	-5.64279000
H	5.26869500	-0.16094100	-0.08183500	C	0.62545800	-2.68679800	-4.48528300
C	3.00071300	0.12572900	1.63467600	Br	0.75745000	-4.08495500	-0.64173200
H	3.88452600	-0.22980000	2.15398800	Br	2.48124000	-2.21575600	-4.17763900
N	0.61337500	0.68203800	1.88081200	Br	-1.48020700	-4.75627400	-7.48633200

H	-2.02887400	0.05718100	-1.71596600	N	2.70728800	0.27169800	-0.63683700
H	-1.96716300	-4.40280900	0.51977500	C	2.84194800	0.04157100	-2.00171800
H	-2.47348000	-2.46237900	-3.09952900	C	4.02452300	-0.75118300	-2.25628200
H	-3.05051500	-3.73008300	-5.13272400	C	4.60916100	-0.99698700	-1.04655600
H	1.07398400	-3.65162400	-6.35121000	C	3.78850100	-0.36097100	-0.03855500
H	-4.02518800	-0.71347500	-0.38815300	H	4.35265400	-1.06609400	-3.23643200
Br	-4.63607200	-3.26370500	1.07112000	H	5.50995100	-1.55622500	-0.83868100
IM(1,6)				C	4.04584600	-0.40493200	1.32281400
Fe	1.31589600	1.37628400	0.30672300	H	4.93189900	-0.94165100	1.64481800
N	-0.17125300	2.33713700	1.25819000	N	2.08884900	0.88584900	2.09314000
C	-0.32520300	2.53444900	2.62455200	C	3.25798900	0.16936100	2.30675400
C	-1.48487400	3.36049100	2.87908200	C	3.53881200	0.09130500	3.72506900
C	-2.02809900	3.67207000	1.66574900	C	2.54218900	0.76436400	4.36959400
C	-1.20759200	3.03680000	0.65600000	C	1.64285100	1.26457000	3.35241500
H	-1.82135200	3.65798600	3.86167600	H	4.39123500	-0.41626100	4.15284600
H	-2.89868000	4.27672000	1.45581300	H	2.41311400	0.91875100	5.43097300
C	-1.44752300	3.11049800	-0.70741800	C	0.51468800	2.02867000	3.60379200
H	-2.30184200	3.69488600	-1.03219700	H	0.28116800	2.25889100	4.63758600
N	0.43352000	1.70419800	-1.47053600	O	0.14428800	-0.53023300	0.41218800
C	-0.68875300	2.49413900	-1.69066700	S	2.57375000	3.28315200	0.18664500
C	-0.97348000	2.56419100	-3.10663200	H	2.99252900	3.14794400	-1.12337100
C	-0.02066500	1.82274600	-3.74741600	C	-2.80248900	-0.46833300	-0.65533800
C	0.86078100	1.29454800	-2.73056800	C	-1.72320500	-0.98519500	-1.28835600
H	-1.79779500	3.11305000	-3.53839700	C	-0.60787300	-1.49733500	-0.49328700
H	0.09348900	1.65032100	-4.80805300	C	-0.74441000	-1.51951000	1.02184400
C	1.97889600	0.51292800	-2.97925500	C	-2.00540600	-1.00316800	1.58576200
H	2.20434700	0.26884200	-4.01210800	C	-2.95605500	-0.46718300	0.78434200

O	-0.02585800	-2.46133800	1.77606300	H	-3.18991500	3.43122900	-2.08580100
C	-0.35443400	-3.82051100	1.71060600	N	-0.15583600	1.90039200	-1.85703500
C	-1.46768800	-4.31813600	1.02435100	C	-1.27614000	2.56246700	-2.33609000
C	-1.72421600	-5.69306700	1.00554600	C	-1.12164500	2.83937200	-3.74736200
C	-0.86560900	-6.55797300	1.67805700	C	0.09061900	2.33499800	-4.12412900
C	0.24381300	-6.07408900	2.37193400	C	0.69057200	1.75302400	-2.94334700
C	0.49671900	-4.70408500	2.38605300	H	-1.85420500	3.34888600	-4.35602300
Br	-2.26573100	-1.12167100	3.49878900	H	0.55071800	2.33956700	-5.10094100
Br	2.03779300	-4.03291200	3.34896700	C	1.94331800	1.15054700	-2.91310800
Br	-1.21440600	-8.47858500	1.65874100	H	2.48394100	1.08326800	-3.85025000
Br	-4.30005700	0.24218800	-1.68423800	N	1.96921400	0.56765100	-0.51736500
H	0.08273500	-2.19550700	-0.95086900	C	2.54191800	0.61307300	-1.78767500
H	-3.86425600	-0.06022900	1.20834200	C	3.84463600	-0.01351700	-1.76227800
H	-2.14525900	-3.64610200	0.51259100	C	4.05560500	-0.45463800	-0.48800300
H	-2.58718800	-6.07605400	0.47579000	C	2.88502400	-0.10638500	0.28620400
H	0.90708200	-6.74942000	2.89513500	H	4.49487700	-0.10395900	-2.61974700
H	-1.66993300	-1.04926100	-2.36716000	H	4.91596500	-0.97515500	-0.09385600
RC_{C2}				C	2.69705500	-0.41771700	1.62088600
Fe	0.08741100	1.12358700	-0.01082100	H	3.49283200	-0.95569800	2.12471700
N	-1.64840800	1.95408800	0.56765700	N	0.46426400	0.58811800	1.89699400
C	-2.22005800	1.89571100	1.82487400	C	1.57819100	-0.08518500	2.37080700
C	-3.51596800	2.53905900	1.81223700	C	1.41378600	-0.38604900	3.77693700
C	-3.72523400	2.98763100	0.53947600	C	0.19826200	0.10756800	4.15311500
C	-2.55892900	2.62069900	-0.23399500	C	-0.39566900	0.71090700	2.97976900
H	-4.16444500	2.62999100	2.67119700	H	2.14457400	-0.90229400	4.38186300
H	-4.57961800	3.51915900	0.14691000	H	-0.26637900	0.07594700	5.12765700
C	-2.38706200	2.90436900	-1.58097300	C	-1.63920700	1.31817400	2.94661400

H	-2.20580900	1.34654100	3.87127700
O	-0.57842500	-0.33277900	-0.41800500
S	1.45797000	3.20536300	0.67726200
H	1.91558000	3.56875200	-0.57562900
C	0.91874300	-4.53489900	-1.62173600
C	0.40869300	-3.24275400	-1.51044600
C	0.48966500	-2.38721400	-2.61278100
C	1.07579900	-2.82625500	-3.80208900
C	1.58416600	-4.12571400	-3.89556100
C	1.50851000	-4.98951300	-2.80178700
O	1.23967600	-1.92121600	-4.86803100
C	0.22631300	-1.73334700	-5.80829000
C	-0.99579200	-2.41362300	-5.77098000
C	-1.96524200	-2.17470400	-6.74865800
C	-1.70500300	-1.25411600	-7.76089000
C	-0.49204700	-0.56755300	-7.81313100
C	0.46717300	-0.81088400	-6.83300900
Br	2.41800300	-4.74403200	-5.53901100
Br	2.15851900	0.14906700	-6.90844900
Br	-3.05374400	-0.91170800	-9.13210300
H	0.11127300	-1.37637700	-2.52559800
H	1.90563000	-5.99293400	-2.87284100
H	-1.19008800	-3.12730700	-4.98006800
H	-2.90935700	-2.70348200	-6.71636800
H	-0.29148500	0.14485100	-8.60177200
H	-0.03532400	-2.87777900	-0.59368300
Br	0.82001900	-5.74840600	-0.09252200

TS_{C2}

Fe	0.77358100	1.04752200	-0.32475100
N	-1.17956400	1.30444400	0.10690000
C	-1.90559200	0.67944700	1.10706300
C	-3.29178500	1.08780600	1.03826500
C	-3.39856300	1.96671500	-0.00096200
C	-2.08001000	2.10143300	-0.58207900
H	-4.06506300	0.74373500	1.70940900
H	-4.27788500	2.48617100	-0.35288400
C	-1.78201200	2.90705000	-1.66913500
H	-2.59596000	3.47453000	-2.10721500
N	0.62357400	2.40103300	-1.82104800
C	-0.52895700	3.04209100	-2.24332000
C	-0.23531500	3.87442000	-3.39111000
C	1.09413100	3.72457200	-3.66613300
C	1.62982200	2.80510000	-2.68488800
H	-0.96215600	4.48685800	-3.90449100
H	1.67459700	4.18975400	-4.44942100
C	2.95775700	2.42078800	-2.60527100
H	3.63884200	2.81083900	-3.35372000
N	2.77386600	1.01163800	-0.59013400
C	3.48806400	1.59640800	-1.62469500
C	4.88721700	1.24690700	-1.51412900
C	5.01615500	0.44903900	-0.41355800
C	3.69595600	0.29503300	0.15629700
H	5.65613400	1.57866100	-2.19644600
H	5.91163100	-0.00508700	-0.01518800

C	3.40339100	-0.47924700	1.26692400	Br	2.39030900	-2.27080600	-2.31461500
H	4.22970600	-0.98181600	1.75794100	Br	-0.41254700	1.13833900	-5.81550700
N	0.96256200	-0.11892900	1.30027900	Br	-1.98582200	-2.69991100	-9.82613800
C	2.13687800	-0.66714700	1.79721300	H	-2.44347700	-2.17186900	-3.72742500
C	1.84822200	-1.46807500	2.96607700	H	0.68839300	-2.83432400	0.08559200
C	0.50131200	-1.39359000	3.18252700	H	-0.41786400	-3.86976700	-5.15586500
C	-0.04909600	-0.54353500	2.15141700	H	-1.24475400	-4.38434700	-7.44828300
H	2.59066900	-2.00391100	3.53920800	H	-1.33573400	-0.17387800	-8.33981300
H	-0.07918100	-1.85943700	3.96494100	H	-3.26830300	-3.13971300	-1.59126700
C	-1.38446500	-0.18808800	2.05369100	Br	-1.97651600	-3.91437800	0.99646700
H	-2.06863800	-0.60652500	2.78307400				
O	0.50554700	-0.22319500	-1.47865000	PC_{C2}			
S	1.13440100	3.03173100	1.14901600	Fe	0.71592100	1.14649500	-0.18027900
H	2.20211500	3.57682400	0.46170900	N	-1.15748600	1.87324800	-0.04518400
C	-1.33080800	-3.04076700	-0.63421200	C	-2.11818600	1.57552900	0.90858700
C	-2.23049800	-2.85009600	-1.69306600	C	-3.32724400	2.32216900	0.63934400
C	-1.76379100	-2.30278600	-2.89398500	C	-3.08629800	3.07996000	-0.47264400
C	-0.42636800	-1.94567700	-3.03097200	C	-1.73418100	2.78777700	-0.89853500
C	0.46407600	-2.01237500	-1.90854900	H	-4.22788100	2.27073200	1.23336200
C	-0.00448100	-2.66926200	-0.72637800	H	-3.75337700	3.76684700	-0.97246600
O	0.10428400	-1.42656300	-4.20614000	C	-1.13283300	3.32305600	-2.03796200
C	-0.43770900	-1.74043700	-5.45703200	H	-1.71649800	4.03487500	-2.61263900
C	-0.63477300	-3.06893700	-5.85282600	N	1.00047900	2.09152600	-1.93741600
C	-1.09440200	-3.35794600	-7.13907100	C	0.11475700	2.98854300	-2.52876200
C	-1.34394400	-2.30838600	-8.02343300	C	0.66905200	3.46419400	-3.77922500
C	-1.14258800	-0.98169900	-7.64709800	C	1.86983700	2.83598300	-3.94972300
C	-0.69091700	-0.70024000	-6.35640500	C	2.06696100	1.98599400	-2.79610700
				H	0.18277500	4.16958500	-4.43699400

H	2.55973400	2.91526800	-4.77619700	C	-0.51431100	-1.99861100	-2.92699900
C	3.20563200	1.19775100	-2.57318000	C	0.10220000	-1.56462000	-1.68548100
H	4.01872900	1.28492700	-3.28005700	C	0.86494500	-2.53147000	-0.94648200
N	2.57939600	0.39354500	-0.32760200	O	-1.26645300	-1.04792000	-3.56994800
C	3.46383200	0.51567500	-1.37427100	C	-1.63281200	-1.18505500	-4.92458700
C	4.72136800	-0.11485400	-1.04664900	C	-0.65192700	-1.14016600	-5.91977600
C	4.60047500	-0.61109800	0.22112300	C	-1.03234400	-1.18160200	-7.26333700
C	3.26044200	-0.30500400	0.67096000	C	-2.38728500	-1.25777700	-7.58762200
H	5.56722500	-0.17575100	-1.71441700	C	-3.37149000	-1.29439600	-6.60049900
H	5.33420200	-1.15162300	0.80086800	C	-2.98627400	-1.25944000	-5.25909900
C	2.71556500	-0.70782400	1.87703000	Br	2.78524700	-0.99362300	-4.33950800
H	3.36229900	-1.25519500	2.55498200	Br	-4.34579900	-1.31100500	-3.87433800
N	0.43012500	0.16548900	1.55876400	Br	-2.92780800	-1.30890200	-9.46298200
C	1.39435400	-0.51271700	2.28149800	H	-0.82168200	-3.62148300	-4.30783300
C	0.82287100	-1.03264000	3.50262000	H	1.32663400	-2.21270400	-0.02400800
C	-0.49616500	-0.66751100	3.51425500	H	0.39376200	-1.05702600	-5.63333000
C	-0.73351800	0.09303600	2.30956700	H	-0.28088500	-1.14463400	-8.04160500
H	1.36587300	-1.60277300	4.24211600	H	-4.41893900	-1.35086400	-6.86340900
H	-1.24115800	-0.87475100	4.26841300	H	0.49904500	-5.23944600	-2.97505900
C	-1.92855400	0.72708500	1.98994100	Br	2.01421500	-5.13208100	-0.41148700
H	-2.76446100	0.58614800	2.66721400				
O	-0.05729500	-0.34584800	-1.28866100	RC_{C3}			
S	1.48826900	2.97605400	0.98205700	Fe	1.29044800	1.16887400	0.40022100
H	2.57660800	3.27425500	0.18406400	N	0.28596800	2.86702200	0.81950000
C	0.98686500	-3.81343100	-1.41804400	C	0.33745800	3.60070000	1.99157200
C	0.38216700	-4.21981600	-2.63054300	C	-0.63162200	4.67396400	1.94895900
C	-0.36324500	-3.31015400	-3.37791100	C	-1.27375900	4.58410800	0.74689700
				C	-0.70312600	3.45470500	0.04629800

H	-0.78736100	5.39163500	2.74103400	H	4.50849400	0.48749900	4.50885900
H	-2.06061800	5.21346500	0.35778200	H	3.05125600	2.67955000	5.12791900
C	-1.09215200	3.03016800	-1.21452500	C	1.19847700	3.35760000	3.05519700
H	-1.87873100	3.59089500	-1.70837300	H	1.12664400	4.01656200	3.91396400
N	0.44358400	1.11697500	-1.42254400	O	0.16020700	0.19495400	1.10666200
C	-0.55795800	1.94671000	-1.89620800	S	3.29386900	2.56454800	-0.43632700
C	-0.96229800	1.52965200	-3.22133100	H	3.07015900	3.70460600	0.31335200
C	-0.19829800	0.44589900	-3.54774600	C	-3.20524700	-1.98608000	1.80056300
C	0.67601200	0.19228400	-2.42305300	C	-4.09523600	-3.04429800	1.98751300
H	-1.72708200	2.01378900	-3.81059400	C	-3.61773100	-4.35367600	1.89820100
H	-0.21228900	-0.13598400	-4.45752500	C	-2.26747300	-4.58900600	1.62592300
C	1.61349700	-0.83134000	-2.36989800	C	-1.39348200	-3.51347700	1.43763800
H	1.68621400	-1.48528500	-3.23230700	C	-1.85458400	-2.19773200	1.52365400
N	2.49943400	-0.36042700	-0.12232600	O	-1.83321900	-5.91472300	1.45438500
C	2.45409000	-1.09096400	-1.30145800	C	-1.35025300	-6.65500300	2.53546100
C	3.40817700	-2.17764700	-1.24688300	C	-1.23416000	-6.13991700	3.83086300
C	4.02161300	-2.10980800	-0.02964600	C	-0.74312000	-6.94148800	4.86536600
C	3.45470100	-0.97569200	0.66899600	C	-0.37214700	-8.25594000	4.59390000
H	3.57139300	-2.89019200	-2.04190800	C	-0.48312200	-8.78442800	3.30792000
H	4.79143500	-2.75303600	0.37055700	C	-0.97386800	-7.97939000	2.28195300
C	3.83360100	-0.56413900	1.93814200	Br	0.47741500	-3.84161500	1.03358500
H	4.59260900	-1.14933900	2.44608900	Br	-1.13392000	-8.71370700	0.49243000
N	2.35555500	1.40000000	2.10647300	Br	0.31717300	-9.38497700	6.03347700
C	3.33516000	0.54393700	2.59952200	Br	-3.87673700	-0.15527800	1.92445300
C	3.75167200	0.97813400	3.91466500	H	-4.28253000	-5.20018400	2.02411600
C	3.01676200	2.08503900	4.22677300	H	-1.17272700	-1.36446200	1.37602600
C	2.13596400	2.34214300	3.10900600	H	-1.52181100	-5.11525500	4.03159300

H	-0.65152000	-6.53999900	5.86664000	C	3.08268000	-1.34928400	0.85741400
H	-0.19464100	-9.80606400	3.10108800	H	2.54441400	-3.81303800	-1.30180400
H	-5.14068100	-2.85370500	2.19425500	H	4.34598900	-3.18489200	0.61452700
TS _{C3}				C	3.75233300	-0.70320800	1.88139700
Fe	0.91722100	0.78143800	0.65022400	H	4.63380700	-1.18972400	2.28441100
N	0.04482300	2.59166900	0.91756300	N	2.30236300	1.27985500	2.04319400
C	0.34349200	3.52835100	1.89540400	C	3.38337300	0.51262300	2.43758200
C	-0.58138000	4.63772700	1.80873500	C	4.07358800	1.16096600	3.53180500
C	-1.43603000	4.36793600	0.77812700	C	3.40058000	2.31847200	3.80056900
C	-1.04615400	3.08812700	0.22727800	C	2.29456100	2.39304900	2.87028200
H	-0.56348500	5.50188800	2.45673100	H	4.95304500	0.76749600	4.02008600
H	-2.25865300	4.96606300	0.41430800	H	3.62006200	3.06313400	4.55174200
C	-1.68715500	2.45599900	-0.82792800	C	1.38298000	3.43489000	2.80772000
H	-2.52588000	2.97177600	-1.28274300	H	1.49975300	4.24622100	3.51813400
N	-0.32201600	0.39956200	-0.88469100	O	-0.08625300	0.10714900	1.90695600
C	-1.34575900	1.21859500	-1.34471700	S	2.38603600	1.90505100	-0.98520700
C	-2.02107000	0.58051600	-2.45260200	H	2.66813300	3.03213200	-0.23761400
C	-1.40277400	-0.61902100	-2.66419800	C	-2.30575300	-1.14145600	1.70255000
C	-0.33921600	-0.72618400	-1.69038400	C	-2.49492600	-2.15002300	0.77808900
H	-2.85283700	1.01061900	-2.99115300	C	-1.62113100	-3.24924900	0.76717600
H	-1.62376300	-1.36458800	-3.41415700	C	-0.59826500	-3.34253600	1.72973400
C	0.54473200	-1.79135500	-1.60097100	C	-0.40070400	-2.33011700	2.64964400
H	0.41798300	-2.61150900	-2.29900600	C	-1.16095400	-1.10333800	2.58048800
N	1.92703500	-0.90084400	0.23123800	O	0.24862000	-4.46666600	1.71241500
C	1.61085000	-1.85902100	-0.71851000	C	-0.18128500	-5.67971900	2.25582200
C	2.57782500	-2.93401800	-0.67600800	C	-1.34914100	-5.80771600	3.01653700
C	3.48564700	-2.61789900	0.29171800	C	-1.71287200	-7.04834500	3.54704100

C	-0.90137700	-8.15590700	3.31358800
C	0.26648600	-8.04508700	2.55943000
C	0.62085000	-6.80501800	2.03156500
Br	0.92915900	-2.49065300	4.03920600
Br	2.24502300	-6.65898100	0.97698500
Br	-1.39819100	-9.89520300	4.05241500
Br	-3.58237800	0.31591700	1.82783000
H	-1.74063600	-4.04930400	0.04696300
H	-1.26846800	-0.55073800	3.50639200
H	-1.97003300	-4.93944700	3.19901600
H	-2.61552300	-7.14292700	4.13731900
H	0.89461900	-8.90715100	2.38066800
H	-3.31856300	-2.10386000	0.07685900
IM_{C3}			
Fe	0.91865500	0.77100500	0.69123900
N	0.01435400	2.56776900	0.95350000
C	0.33250000	3.55206700	1.87688400
C	-0.60424700	4.65200000	1.76884500
C	-1.48631100	4.32553300	0.77861400
C	-1.09473800	3.02148600	0.28004800
H	-0.57567800	5.54659000	2.37383800
H	-2.32528200	4.89848400	0.41124100
C	-1.76086000	2.33228000	-0.73444100
H	-2.60359000	2.83591000	-1.19732700
N	-0.41704600	0.25959600	-0.72864100
C	-1.44013800	1.07816500	-1.21360300
C	-2.11976000	0.41489500	-2.30536100

C	-1.49783900	-0.78672300	-2.49524500
C	-0.43099500	-0.86876900	-1.52014400
H	-2.94990500	0.83356300	-2.85564100
H	-1.71571900	-1.54439900	-3.23420500
C	0.46030200	-1.93403100	-1.40393900
H	0.35172700	-2.75734100	-2.10209800
N	1.85529400	-0.97871300	0.37944000
C	1.55701700	-1.95855700	-0.55097700
C	2.56008200	-3.00137500	-0.51963800
C	3.47799700	-2.64220300	0.42314900
C	3.04602900	-1.37766100	0.97910300
H	2.54251400	-3.89019500	-1.13167200
H	4.36586200	-3.17515900	0.72956200
C	3.72359600	-0.68347000	1.96528200
H	4.62215000	-1.14576700	2.36142300
N	2.29624100	1.31596300	2.07628300
C	3.37118500	0.55858900	2.48671100
C	4.08906900	1.24186000	3.54500500
C	3.43195400	2.41697800	3.77433600
C	2.31232200	2.45882200	2.85546700
H	4.97208200	0.85999300	4.03636000
H	3.67031100	3.19038800	4.48997100
C	1.39819000	3.49936300	2.76123600
H	1.53163000	4.34232900	3.43179800
O	-0.08855200	0.21039800	2.19535700
S	2.26350000	1.72647400	-0.99904300
H	2.63357700	2.88004100	-0.33568400

C	-2.12149300	-1.02775800	1.56998400
C	-2.34120600	-2.04743800	0.67982700
C	-1.45428700	-3.14268400	0.65132000
C	-0.42766400	-3.26495300	1.61848400
C	-0.17296300	-2.24680700	2.49920700
C	-0.92607600	-0.94505600	2.47245000
O	0.36556300	-4.42831200	1.59898000
C	-0.13603200	-5.62218700	2.12862800
C	-1.30191700	-5.68820000	2.89979700
C	-1.73918900	-6.91229400	3.41329700
C	-1.00222900	-8.06504700	3.15322100
C	0.16431800	-8.01491800	2.39024700
C	0.59250900	-6.79122200	1.87892700
Br	1.14683700	-2.43764700	3.87822800
Br	2.21331000	-6.72978500	0.81317000
Br	-1.60412200	-9.78043400	3.86544600
Br	-3.41834600	0.38754700	1.74938400
H	-1.60966800	-3.95788000	-0.04507800
H	-1.28209700	-0.74956400	3.49649700
H	-1.86396500	-4.78593900	3.10677800
H	-2.64013800	-6.95954900	4.01165400
H	0.73518600	-8.91176400	2.19150700
H	-3.17836900	-2.01508800	-0.00580500
TS(3,2)			
Fe	1.04860400	0.76736000	0.62418200
N	-0.04500900	2.41297000	0.98455000
C	0.16372000	3.32458400	2.01333400

C	-0.77974400	4.41704700	1.90127800
C	-1.53537300	4.18218500	0.78865800
C	-1.07122500	2.93674600	0.21688000
H	-0.83185300	5.25386700	2.58263800
H	-2.33199400	4.78609000	0.37904000
C	-1.58073100	2.35887200	-0.93864900
H	-2.37370000	2.88815300	-1.45610300
N	-0.16595600	0.34802700	-0.92749600
C	-1.16133400	1.15046000	-1.47018600
C	-1.71686300	0.52038100	-2.64785000
C	-1.05556300	-0.66362700	-2.81675200
C	-0.07740300	-0.75918200	-1.75229600
H	-2.50455700	0.94123100	-3.25581800
H	-1.18952600	-1.39970500	-3.59659000
C	0.82342600	-1.80704700	-1.60249500
H	0.75914300	-2.62011700	-2.31881300
N	2.12128800	-0.91208100	0.29012000
C	1.86007100	-1.86287300	-0.67662800
C	2.83802600	-2.92976800	-0.60018600
C	3.69194800	-2.61477900	0.41744600
C	3.23549200	-1.36026800	0.97812000
H	2.85260700	-3.79842600	-1.24185300
H	4.54342100	-3.17425200	0.77581100
C	3.81186700	-0.71714600	2.06378700
H	4.68104800	-1.18272100	2.51681600
N	2.26056700	1.19189200	2.18012300
C	3.34967400	0.46135700	2.63062800

C	3.92642500	1.09877600	3.79691600	H	-1.36312400	-3.87551600	-0.08671400
C	3.17526900	2.20829300	4.05636900	H	-1.66442500	-0.23176600	3.22065900
C	2.13544700	2.26177900	3.04736600	H	-2.29228400	-4.76045100	2.91368400
H	4.78654900	0.72910800	4.33605300	H	-3.12768400	-6.98796200	3.61382300
H	3.29831400	2.93101200	4.84994800	H	0.69437000	-8.71341500	2.64722600
C	1.15998900	3.24671000	2.97244200	H	-2.94034700	-1.97609400	-0.45041800
H	1.19395600	4.03596800	3.71644800				
O	0.08000100	-0.28099100	2.01965600	IM(3,2)			
S	2.40806700	1.94532300	-0.85134600	Fe	1.30128000	0.73584200	0.44781600
H	3.62155300	1.70324100	-0.23654700	N	0.11974800	2.27564600	0.96657400
C	-2.25325100	-0.89847600	1.25820600	C	0.16799800	3.03529800	2.13279300
C	-2.26299300	-1.95425800	0.39349700	C	-0.78845900	4.11613400	2.05879700
C	-1.39154200	-3.05440200	0.61975000	C	-1.40059200	4.02806100	0.83989100
C	-0.62386600	-3.13739400	1.78068100	C	-0.83532300	2.88500200	0.15891800
C	-0.63017700	-2.09259800	2.70276700	H	-0.95130600	4.84520200	2.83938400
C	-1.26188600	-0.77745500	2.36648700	H	-2.16754700	4.66791500	0.42793500
O	0.20903900	-4.25179700	1.98721200	C	-1.22338300	2.44881000	-1.09828300
C	-0.33398500	-5.48016500	2.37888100	H	-1.98547700	3.02417000	-1.61274400
C	-1.64313500	-5.62504800	2.85048600	N	0.22498100	0.45746200	-1.22581300
C	-2.11488200	-6.87954900	3.24691100	C	-0.74115100	1.31574500	-1.73292500
C	-1.26869600	-7.98318400	3.17002800	C	-1.21432300	0.82870100	-3.01120500
C	0.03998400	-7.85426300	2.70528700	C	-0.53646200	-0.32619800	-3.27660200
C	0.50261100	-6.60051700	2.30953500	C	0.36752900	-0.55128200	-2.16943600
Br	0.21494100	-2.27854700	4.40857900	H	-1.97069700	1.31524400	-3.60978300
Br	2.32158200	-6.42498400	1.65794400	H	-0.62174000	-0.97095300	-4.13930400
Br	-1.91774900	-9.74154800	3.71873500	C	1.27331900	-1.59651900	-2.09215400
Br	-3.61270800	0.47013500	1.15093800	H	1.28601500	-2.31349900	-2.90609000
				N	2.32201400	-0.94282900	0.03921700

C	2.19564600	-1.76508000	-1.07231100
C	3.20210600	-2.80413800	-1.03758500
C	3.94724600	-2.60142300	0.09000000
C	3.39677400	-1.44302900	0.76092500
H	3.31964300	-3.56894000	-1.79170100
H	4.79333400	-3.17064800	0.44707000
C	3.86413500	-0.93852000	1.96358700
H	4.71057300	-1.43979700	2.42084000
N	2.23464500	0.89698900	2.21594100
C	3.31579900	0.13697600	2.64353900
C	3.77303100	0.60870400	3.93234600
C	2.96625500	1.65133000	4.28899600
C	2.01301400	1.83516200	3.21768100
H	4.59989800	0.18261500	4.48185500
H	3.00318200	2.25151500	5.18661400
C	1.03985900	2.82108200	3.18872700
H	0.97559100	3.49142600	4.03916900
O	-0.40489700	-0.80790800	1.39384700
S	2.83383600	2.06560100	-0.63589800
H	2.95216600	3.04184300	0.33636000
C	-2.90074500	-1.09322400	0.99196400
C	-3.00622100	-2.42369000	0.76510000
C	-2.14141400	-3.37363500	1.43170800
C	-1.20186100	-2.97242400	2.32604400
C	-0.94890600	-1.53758900	2.54899300
C	-1.84394700	-0.55280100	1.83880400
O	-0.39916600	-3.81458800	3.08498000

C	-0.59909900	-5.20623900	3.07079600
C	-1.58497200	-5.76875300	3.88563400
C	-1.73293000	-7.15648400	3.94747100
C	-0.88211100	-7.96233500	3.19011300
C	0.10888200	-7.41271300	2.37756500
C	0.24698000	-6.02445800	2.31682300
Br	-0.20363800	-1.04394400	4.30488200
Br	1.61614600	-5.23473400	1.19685600
Br	-1.07470500	-9.90261200	3.27012700
Br	-4.19641300	0.16611400	0.27017000
H	-2.28650500	-4.42802800	1.23060400
H	-1.95425200	0.43809500	2.25878500
H	-2.21853900	-5.11605600	4.47459500
H	-2.49117600	-7.60016300	4.57976000
H	0.76607600	-8.04813800	1.79958300
H	-3.77925100	-2.80988100	0.11157500
TS(3,4)			
Fe	1.12114900	0.91788900	0.32881200
N	-0.11128300	2.35989000	1.00211200
C	-0.13061900	2.95410700	2.25441800
C	-1.13985900	3.99020000	2.29674200
C	-1.71712500	4.03419100	1.05953300
C	-1.07525000	3.01624100	0.25470800
H	-1.35423200	4.60428000	3.15935400
H	-2.50235200	4.68863900	0.70948200
C	-1.41664800	2.72418300	-1.05838200
H	-2.20778400	3.31612700	-1.50725900

N	0.17435800	0.88480200	-1.44810600	O	-0.07816100	-0.62343800	0.80615700
C	-0.84914600	1.72850500	-1.84168000	S	2.60603200	2.54812300	-0.45424000
C	-1.27740900	1.39222500	-3.18463400	H	2.85492100	2.00010100	-1.69823100
C	-0.51742700	0.33324300	-3.59299800	C	-1.95477700	-1.19804500	1.41936100
C	0.38965100	0.02123000	-2.50801800	C	-2.34121700	-2.42076800	0.85172200
H	-2.05978300	1.90403500	-3.72614600	C	-1.61401900	-3.56079700	1.14355700
H	-0.55083800	-0.19198500	-4.53654500	C	-0.51360200	-3.52104000	2.05923700
C	1.35576800	-0.97555400	-2.54018100	C	-0.09195800	-2.34161800	2.59465700
H	1.41773900	-1.58504800	-3.43581900	C	-0.64456300	-1.03922000	2.10812200
N	2.34428500	-0.53591900	-0.32953900	O	0.15717600	-4.71758500	2.35747700
C	2.27143600	-1.22697000	-1.53065300	C	-0.50997200	-5.76509000	2.99985800
C	3.32752800	-2.21603600	-1.59596600	C	-1.65857200	-5.57223200	3.77542800
C	4.04478400	-2.11245500	-0.43943800	C	-2.25808500	-6.65455700	4.42548600
C	3.42683500	-1.06826700	0.35295900	C	-1.69597600	-7.92303500	4.29859800
H	3.48892100	-2.88731600	-2.42689000	C	-0.54717200	-8.12904300	3.53465800
H	4.90690600	-2.68594400	-0.13149200	C	0.04225800	-7.04605900	2.88459700
C	3.84947700	-0.68124400	1.61548100	Br	1.26886600	-2.30288900	3.94802300
H	4.73530500	-1.16575800	2.01248800	Br	1.63652500	-7.32947400	1.81673600
N	2.05759000	0.93922400	2.11057500	Br	-2.52201100	-9.44258200	5.20501400
C	3.22027000	0.25322200	2.42561400	Br	-3.14854800	0.30082800	1.29755400
C	3.66428500	0.61471700	3.75482600	H	-1.88347100	-4.51525700	0.70573300
C	2.76701800	1.51865600	4.24710400	H	-0.58959300	-0.24912300	2.85622900
C	1.77438400	1.73343900	3.21713100	H	-2.07582400	-4.57801600	3.88115900
H	4.54749200	0.21851900	4.23461000	H	-3.14541600	-6.50449800	5.02736000
H	2.77280600	2.01497100	5.20667900	H	-0.11425000	-9.11569500	3.44045500
C	0.73490600	2.64693100	3.29613000	H	-3.20952900	-2.46787300	0.20700200
H	0.62238900	3.20116800	4.22203600				

IM(3,4)

Fe	1.17630400	0.81427700	0.53791600	H	5.20170300	-0.13660800	2.31609900
N	-0.13429100	2.32338700	0.73164700	N	2.36052000	1.70220900	1.89547500
C	-0.02081900	3.45025200	1.53794700	C	3.61261100	1.26286300	2.30394000
C	-1.14508800	4.33241600	1.31641800	C	4.18711700	2.20854500	3.23688400
C	-1.93353100	3.74658300	0.36758600	C	3.27997600	3.21710000	3.39765300
C	-1.30675000	2.49330000	0.00652800	C	2.14599400	2.90591500	2.55530200
H	-1.29450600	5.27409100	1.82449100	H	5.15532400	2.09755000	3.70335700
H	-2.85869100	4.11239800	-0.05393000	H	3.35929200	4.09765900	4.01861600
C	-1.83208500	1.58487200	-0.89961500	C	1.03115400	3.71468500	2.40029800
H	-2.75903600	1.85324300	-1.39558800	H	0.99325600	4.63538200	2.97274300
N	-0.10638200	-0.16376800	-0.66176400	O	0.09852200	-0.09068500	2.41854100
C	-1.28176100	0.34829300	-1.19883600	S	2.25006000	1.79301500	-1.23982200
C	-1.87654600	-0.61979400	-2.09492400	H	2.32183600	3.07561300	-0.72875100
C	-1.06189000	-1.71706000	-2.10019600	C	-1.19577100	-0.62347200	2.85587500
C	0.04601300	-1.42689800	-1.21649500	C	-1.95081800	-1.46872600	1.92339900
H	-2.79363400	-0.46360500	-2.64471000	C	-1.47041500	-2.69173400	1.59625100
H	-1.17648500	-2.63510100	-2.65853000	C	-0.27037600	-3.23815600	2.20716700
C	1.11222300	-2.28244200	-0.98167300	C	0.43659300	-2.54414500	3.13576500
H	1.09861300	-3.25253000	-1.46571300	C	0.04584900	-1.18724200	3.49340600
N	2.38866200	-0.78610800	0.50198900	O	0.17771600	-4.49623100	1.79609400
C	2.21191300	-1.97276700	-0.19782200	C	-0.68653400	-5.59690200	1.77807900
C	3.36564600	-2.82829300	-0.02367000	C	-1.72933200	-5.74360100	2.69993400
C	4.25123100	-2.14956400	0.76231400	C	-2.53190300	-6.88675600	2.67761600
C	3.64186600	-0.87862800	1.09265800	C	-2.27505500	-7.88214100	1.73630600
H	3.46338200	-3.81611900	-0.44858300	C	-1.23188800	-7.75469000	0.81930100
H	5.22423500	-2.46943700	1.10581900	C	-0.44050100	-6.60674000	0.84190100
C	4.21522800	0.07551700	1.91765700	Br	1.93262600	-3.31853200	4.08133700

Br	1.00692200	-6.43304300	-0.43910100	C	0.60129300	-1.57167900	-1.86650400
Br	-3.38618000	-9.48486900	1.69736500	H	0.46675900	-2.37142000	-2.58741500
Br	-2.29664000	0.67384300	3.87607700	N	1.95673600	-0.76695000	0.02870200
H	-1.98225000	-3.30380500	0.86324200	C	1.63543200	-1.69853400	-0.94957500
H	0.37183800	-0.79870700	4.44877700	C	2.61339900	-2.76629800	-0.95314000
H	-1.90419000	-4.97194100	3.44041800	C	3.54663500	-2.45725300	-0.00191000
H	-3.33816700	-7.00034900	3.39095700	C	3.13777100	-1.21024900	0.60852600
H	-1.03496300	-8.53203600	0.09350600	H	2.59918100	-3.60845500	-1.63064300
H	-2.86790100	-1.08344100	1.49788800	H	4.43709500	-3.00764800	0.26639300
TS(3,2) _{NIH}				C	3.81830400	-0.57708100	1.63830500
				H	4.73046800	-1.04510800	1.99410800
Fe	1.06398100	1.00080400	0.39413200	N	2.27370200	1.31727100	1.95990200
N	0.12897600	2.72323700	0.79896500	C	3.40101500	0.58016500	2.28196400
C	0.30552300	3.54452200	1.90019600	C	4.03892500	1.14584000	3.45387800
C	-0.57589400	4.69063500	1.80607300	C	3.28206700	2.21329300	3.84763100
C	-1.26488200	4.56921500	0.63319100	C	2.18938300	2.32892900	2.90429800
C	-0.83064600	3.33464600	0.00960500	H	4.94105900	0.76101000	3.90789400
H	-0.63393000	5.48216800	2.53943200	H	3.44553800	2.87933800	4.68273200
H	-2.00522300	5.23830500	0.21840800	C	1.24675700	3.34712400	2.90107600
C	-1.34259100	2.82742300	-1.17649700	H	1.28970500	4.07678500	3.70302100
H	-2.07259300	3.43350900	-1.70346300	O	-0.37498100	0.12522500	1.77926200
N	-0.15146400	0.66875300	-1.17247800	S	2.55077600	2.05523000	-1.02370600
C	-1.03305200	1.58816000	-1.71771000	H	2.84107000	3.13688300	-0.21418600
C	-1.65257000	1.03225700	-2.90330100	C	-2.25896200	-1.38248700	1.31810800
C	-1.15229200	-0.22815500	-3.06535700	C	-2.73684900	-2.67304700	1.33166100
C	-0.20180100	-0.44701800	-1.99480000	C	-2.06385800	-3.69941700	2.02442400
H	-2.37621900	1.54965700	-3.51695500	C	-0.91238100	-3.42799800	2.75076300
H	-1.37735600	-0.94439900	-3.84263900				

C	-0.35449400	-2.13538100	2.75615000	H	-2.02268900	5.21770400	0.21215900
C	-0.99079600	-0.99974800	2.00056300	C	-1.35704500	2.80433800	-1.17715800
O	-0.26284600	-4.38312900	3.53513200	H	-2.09072700	3.40624800	-1.70386100
C	-0.45063600	-5.75820200	3.29485500	N	-0.15625700	0.65069400	-1.17108600
C	-1.23542400	-6.48747600	4.19034700	C	-1.04310300	1.56521600	-1.71644200
C	-1.37305900	-7.86965300	4.03541900	C	-1.66286500	1.00431600	-2.89938400
C	-0.71889200	-8.50057800	2.97725200	C	-1.15680500	-0.25403800	-3.06063800
C	0.07480100	-7.78339600	2.08130600	C	-0.20267000	-0.46655300	-1.99230600
C	0.21141500	-6.40418400	2.24428000	H	-2.38960700	1.51761800	-3.51289100
Br	1.23082800	-1.77320400	3.73232200	H	-1.37964100	-0.97228700	-3.83673200
Br	1.34029100	-5.39155700	1.03628500	C	0.60723400	-1.58635600	-1.86557000
Br	-0.90495400	-10.42756000	2.74412200	H	0.47472300	-2.38785000	-2.58490500
Br	-3.25326900	0.00320100	0.45466100	N	1.96440500	-0.77170300	0.02374000
H	-2.47480000	-4.70165100	2.02407700	C	1.64470200	-1.70642400	-0.95150000
H	-1.52342500	-1.04399100	3.13030000	C	2.62529800	-2.77194300	-0.95319500
H	-1.71821900	-5.96697300	5.00894800	C	3.55724700	-2.45918100	-0.00195900
H	-1.97652300	-8.44205300	4.72806200	C	3.14561300	-1.21159900	0.60539800
H	0.58751100	-8.28673300	1.27274100	H	2.61356200	-3.61515500	-1.62946500
H	-3.65691900	-2.90566600	0.80956100	H	4.44819000	-3.00762700	0.26857400
TS(3,4)_{NIH}				C	3.82593000	-0.57407600	1.63258100
Fe	1.06543400	0.99293300	0.38905900	H	4.73776900	-1.04099100	1.99058400
N	0.12316200	2.71228800	0.79261600	N	2.28246400	1.32215800	1.94675700
C	0.30354600	3.53988300	1.88874600	C	3.40959600	0.58627500	2.27093200
C	-0.58272300	4.68211300	1.79443300	C	4.04968700	1.15764100	3.43905700
C	-1.27804700	4.55281200	0.62604400	C	3.29341100	2.22668600	3.82892700
C	-0.84265800	3.31727400	0.00540600	C	2.19850900	2.33690700	2.88723900
H	-0.63912400	5.47708200	2.52420500	H	4.95212000	0.77441700	3.89376800

H	3.45752700	2.89627500	4.66104400
C	1.25205400	3.35147700	2.88443800
H	1.29637800	4.08480000	3.68294900
O	-0.33202300	0.10664700	1.80516100
S	2.53975600	2.04918700	-1.04068500
H	2.83284500	3.13306600	-0.23514300
C	-2.25193500	-1.38361800	1.36114900
C	-2.75677700	-2.68688900	1.41335700
C	-2.07663200	-3.68886400	2.09120300
C	-0.88867700	-3.40649800	2.79599000
C	-0.34074100	-2.13503100	2.79042200
C	-0.96533200	-1.00707500	2.03548900
O	-0.24718100	-4.37798500	3.56900200
C	-0.43055000	-5.74920900	3.30788500
C	-1.18327300	-6.49861800	4.21476300
C	-1.31744600	-7.87892900	4.04240100
C	-0.69219600	-8.48906200	2.95493100
C	0.07037400	-7.75281700	2.04770300
C	0.20432400	-6.37551100	2.22873400
Br	1.23448500	-1.75755700	3.77424300
Br	1.29712200	-5.33943200	1.00701500
Br	-0.87477200	-10.41339300	2.69643100
Br	-3.23585900	-0.01779300	0.45270400
H	-2.48182700	-4.69326200	2.11582800
H	-1.88441600	-0.87250600	2.86977000
H	-1.64393100	-5.99361700	5.05553600
H	-1.89644100	-8.46582400	4.74378100

H	0.56230500	-8.24010200	1.21667700
H	-3.69121100	-2.90742200	0.91284000
RC_{C4}			
Fe	0.73743300	0.59773900	-0.04478600
N	-1.09682500	0.79902200	0.75156600
C	-1.48054100	0.50934900	2.04805300
C	-2.90673000	0.69785300	2.19976000
C	-3.38723500	1.09935400	0.98596600
C	-2.25592400	1.16515500	0.08700600
H	-3.45247900	0.53771700	3.11797900
H	-4.40356500	1.33028600	0.70403400
C	-2.33126300	1.55308800	-1.24353600
H	-3.31398700	1.78496000	-1.63828000
N	0.06543500	1.36459600	-1.78382400
C	-1.25318800	1.64694100	-2.11042800
C	-1.34493800	2.05667100	-3.49385600
C	-0.07906400	2.02086800	-4.00534900
C	0.79560700	1.58509000	-2.93918700
H	-2.26394100	2.32817300	-3.99170000
H	0.24688200	2.26013500	-5.00690500
C	2.16975400	1.41611200	-3.06521300
H	2.60939400	1.62495300	-4.03476600
N	2.62682200	0.67118000	-0.76135900
C	3.01962200	0.99297600	-2.05917700
C	4.44390000	0.79218600	-2.20641800
C	4.91130200	0.32807500	-1.01112400
C	3.78145700	0.24389300	-0.11263000

H	4.99724800	0.97941500	-3.11496600	C	-6.78848300	-1.65447600	-0.15136100
H	5.92390900	0.06189200	-0.74584700	C	-5.92700600	-1.22099200	-1.15643800
C	3.84317200	-0.19942600	1.19668300	Br	-4.82342800	-3.21476500	-5.11135900
H	4.81210400	-0.50915800	1.57341600	Br	-6.22295300	0.52284400	-1.96716600
N	1.46371900	0.08674200	1.76615500	Br	-7.78108000	-3.51224100	1.84530300
C	2.77004900	-0.25719900	2.07383600	H	-1.58838600	-1.52274900	-1.58473600
C	2.86107500	-0.67066500	3.45759700	H	-2.09687100	-4.30464600	-5.66662500
C	1.60752900	-0.57352500	3.98820100	H	-3.84058800	-3.89880000	-1.30864600
C	0.73514700	-0.10863400	2.93182000	H	-5.36417100	-4.68400600	0.48303500
H	3.77304800	-0.98422000	3.94393200	H	-7.60998800	-1.02656800	0.16590100
H	1.28629000	-0.79380200	4.99563000	H	0.36190700	-2.67929200	-2.50731500
C	-0.62786600	0.09515500	3.06394400	Br	0.79374700	-4.49499300	-4.90317000
H	-1.06870900	-0.09469000	4.03686400				
O	0.50536100	-0.97319900	-0.52072700	TS_{c4}			
S	1.44562100	2.92544200	0.72727200	Fe	0.91640800	0.52035500	-0.31695100
H	1.68378900	3.48467300	-0.51378400	N	-0.81382500	0.46572400	0.69798900
C	-0.75245700	-3.57069100	-4.14366500	C	-1.01530200	-0.00271300	1.99020900
C	-0.59635900	-2.79539000	-2.99622300	C	-2.40856900	0.13677200	2.35052300
C	-1.71110500	-2.13846700	-2.46725900	C	-3.04654700	0.69945900	1.28119300
C	-2.95776800	-2.26162500	-3.08468200	C	-2.04958400	0.91081500	0.25557400
C	-3.09645600	-3.04395700	-4.23562200	H	-2.82440200	-0.14852600	3.30606000
C	-1.99023700	-3.70354200	-4.77390400	H	-4.08933700	0.96271000	1.18022900
O	-4.04827200	-1.51676700	-2.59563400	C	-2.30872400	1.48002800	-0.98148400
C	-4.86263400	-2.02363600	-1.58304000	H	-3.33588900	1.74340000	-1.20542500
C	-4.66383100	-3.27351100	-0.98626600	N	-0.00081600	1.45172200	-1.84527300
C	-5.52140100	-3.71606300	0.02443400	C	-1.35440200	1.73358100	-1.95368300
C	-6.57599800	-2.90312600	0.43261400	C	-1.63226300	2.32847200	-3.24144300
				C	-0.44596900	2.40123700	-3.91384700

C	0.57068100	1.84811900	-3.04733400	C	-1.22806200	-2.64301300	-0.46073800
H	-2.61321100	2.63359700	-3.57403900	C	-2.52357100	-2.26873500	-0.77612400
H	-0.26083800	2.78152500	-4.90775300	C	-2.85674700	-1.89416000	-2.09016300
C	1.91092900	1.73077600	-3.38206400	C	-1.87339900	-1.91130500	-3.09567000
H	2.21364100	2.08222100	-4.36250400	C	-0.57533600	-2.28555700	-2.80438500
N	2.68701700	0.71520100	-1.27858400	O	-4.13580800	-1.44596700	-2.42961000
C	2.89176700	1.20137600	-2.55975200	C	-5.28519600	-2.04604600	-1.91035800
C	4.29277800	1.09192900	-2.90870200	C	-5.39602300	-3.43366700	-1.75843800
C	4.93060100	0.54057300	-1.83583500	C	-6.59076400	-3.99873400	-1.30836600
C	3.92763800	0.30567400	-0.81823400	C	-7.67330900	-3.16768700	-1.02108000
H	4.71406200	1.40340300	-3.85338600	C	-7.58135400	-1.78505300	-1.17485900
H	5.97974200	0.30868500	-1.72480200	C	-6.38122800	-1.22851100	-1.61708400
C	4.18380500	-0.24116400	0.42741000	Br	-2.34723700	-1.44255200	-4.92076500
H	5.21008000	-0.50884700	0.65436900	Br	-6.25527800	0.69889800	-1.82569500
N	1.87702100	-0.20648200	1.30212200	Br	-9.34941800	-3.94639200	-0.39515700
C	3.23313200	-0.47364800	1.40817800	H	-3.28522000	-2.24731100	-0.00636000
C	3.51975300	-1.04667000	2.70517300	H	0.17888400	-2.32010900	-3.57723800
C	2.33586600	-1.12597000	3.38042600	H	-4.55063900	-4.06635400	-2.00152600
C	1.31171300	-0.60252000	2.50320100	H	-6.67678300	-5.07176000	-1.19416500
H	4.50360800	-1.34288000	3.03839100	H	-8.42490000	-1.14585900	-0.95245900
H	2.15552000	-1.49858300	4.37820100	H	-0.96302500	-2.93324600	0.54676100
C	-0.03344200	-0.50925200	2.82600200	Br	1.31374400	-3.83948400	-1.22649900
H	-0.33709100	-0.84397700	3.81206100				
O	0.80158400	-1.05340400	-1.04182000	PC _{C4}			
S	1.39799800	2.69322900	0.67266900	Fe	1.10031200	0.93854300	-0.27639100
H	1.24880900	3.44719300	-0.47491700	N	-0.64852300	1.03110400	0.72459500
C	-0.21164200	-2.58959400	-1.45807500	C	-0.87417400	0.56809500	2.01760800
				C	-2.21561000	0.91283700	2.43407600

C	-2.80065900	1.58667700	1.39747200	C	2.18567200	-1.38272600	3.14395500
C	-1.81918700	1.67537400	0.34000800	C	1.29182900	-0.55166100	2.36544800
H	-2.64002800	0.66792800	3.39713600	H	4.18562600	-2.16143000	2.63700000
H	-3.79545100	2.00551900	1.34782200	H	1.96688400	-1.75673100	4.13369200
C	-2.00703700	2.34096800	-0.86374100	C	0.02775800	-0.15947700	2.77962200
H	-2.97543300	2.79703600	-1.04015600	H	-0.29074500	-0.46784000	3.76981500
N	0.26575400	2.01700600	-1.75877800	O	0.39172900	-0.78035700	-1.45441400
C	-1.02745500	2.51733700	-1.82941300	S	1.84361500	2.84180300	0.75403400
C	-1.19317600	3.28962300	-3.04281500	H	3.11196500	2.39663300	1.07383500
C	0.00554500	3.26963200	-3.69585800	C	-0.64167700	-1.44317200	-1.72632800
C	0.91397800	2.47332300	-2.89666200	C	-1.63023400	-1.84873100	-0.65931100
H	-2.10816100	3.78443900	-3.33486900	C	-2.95500700	-2.27749700	-1.12971000
H	0.26680000	3.74192800	-4.63189400	C	-3.18219100	-2.53672300	-2.43892300
C	2.22321000	2.18432700	-3.24987300	C	-2.12816300	-2.35866700	-3.43145100
H	2.59477600	2.60966700	-4.17632900	C	-0.91835700	-1.84878700	-3.09579000
N	2.79198800	0.73910000	-1.33246600	O	-4.39623200	-2.96996500	-2.96366700
C	3.08497400	1.36752800	-2.53318900	C	-5.47413700	-3.27866200	-2.11561800
C	4.41820300	1.00345000	-2.96741200	C	-5.53245400	-4.53684900	-1.50965700
C	4.92392800	0.14393600	-2.03491700	C	-6.63985300	-4.89059200	-0.73558600
C	3.91088100	-0.01617600	-1.01336700	C	-7.68077500	-3.97389900	-0.58278500
H	4.88638000	1.36138000	-3.87302100	C	-7.63690700	-2.71756100	-1.18641100
H	5.88988800	-0.33985800	-2.02196000	C	-6.52374100	-2.37033600	-1.95430900
C	4.05610000	-0.78401100	0.13227000	Br	-2.50229300	-2.84131800	-5.26331600
H	4.98734400	-1.32499200	0.26199600	Br	-6.45697300	-0.62739500	-2.80219700
N	1.87275200	-0.24929800	1.14166200	Br	-9.23469500	-4.45403900	0.49165900
C	3.11304800	-0.87370000	1.14488300	H	-3.73586100	-2.40902500	-0.39169000
C	3.30362700	-1.58929700	2.38800600	H	-0.14418600	-1.67475100	-3.83099100

H	-4.71431400	-5.23182300	-1.65775300	C	3.08075500	1.32109600	-1.66625700
H	-6.69197900	-5.86454400	-0.26630400	C	3.38867100	1.01189700	-0.37281800
H	-8.45208500	-2.01724700	-1.06559600	C	2.14452000	0.99205200	0.36559700
H	-1.63757800	-1.13720600	0.16217400	H	3.74905700	1.42786900	-2.50763700
Br	-0.73759700	-3.51790900	0.28025400	H	4.35957700	0.81395500	0.05663700
RC_{C5}				C	2.03147600	0.70728300	1.71535800
Fe	-0.87641600	1.27794200	-0.01343700	H	2.94512900	0.48765600	2.25769600
N	-2.81086600	1.54231900	0.49738900	N	-0.41270400	0.93650600	1.91153700
C	-3.37197000	1.33164500	1.74789300	C	0.84191300	0.68137000	2.43255800
C	-4.80738000	1.49833100	1.68016300	C	0.74413600	0.39506100	3.84722300
C	-5.11412200	1.80017000	0.38362500	C	-0.57766600	0.47974000	4.18014300
C	-3.86783700	1.82694400	-0.35029400	C	-1.29568300	0.81820500	2.97068600
H	-5.47791500	1.39150800	2.51986100	H	1.58362000	0.16534400	4.48672100
H	-6.08478500	1.98720600	-0.05065100	H	-1.03760800	0.33346700	5.14638900
C	-3.75861500	2.10634700	-1.70807600	C	-2.66884400	1.00292100	2.89605600
H	-4.67528300	2.29042600	-2.25780400	H	-3.23875100	0.87473800	3.81024900
N	-1.30642900	1.92019900	-1.88636400	O	-1.08384300	-0.31532900	-0.39684300
C	-2.57266000	2.15719600	-2.41864300	S	-0.49303000	3.82415900	0.20213500
C	-2.46763600	2.44204000	-3.83238700	H	-1.79354800	4.24260900	-0.00785700
C	-1.14539600	2.36616500	-4.16091400	C	-1.40124700	-3.58359800	-3.64671800
C	-0.42109600	2.03017600	-2.95503400	C	-1.53237900	-2.55440300	-2.71585600
H	-3.30976800	2.65086100	-4.47488600	C	-2.67440300	-1.75033200	-2.75403900
H	-0.68702900	2.51246800	-5.12791700	C	-3.66607400	-1.98212100	-3.71053900
C	0.94520100	1.82708400	-2.88278200	C	-3.52014900	-3.02095700	-4.63469200
H	1.51599200	1.94209000	-3.79732000	C	-2.38067100	-3.82771700	-4.60959900
N	1.08674500	1.29688100	-0.47973300	O	-4.76598700	-1.10954900	-3.80438000
C	1.64552300	1.49833200	-1.73098800	C	-5.84563200	-1.21690600	-2.92995000

C	-5.97008700	-2.23341000	-1.97621900
C	-7.08665800	-2.27963700	-1.13703800
C	-8.07645100	-1.30734200	-1.25879200
C	-7.97091700	-0.28947600	-2.20670500
C	-6.85207100	-0.24891200	-3.03676900
Br	-4.88904400	-3.35008300	-5.97352400
Br	-6.70419200	1.17300000	-4.35583600
Br	-9.64070300	-1.36147000	-0.08916300
H	-2.77237900	-0.94073500	-2.04225800
H	-2.26567700	-4.62772600	-5.32824600
H	-5.19649200	-2.98582200	-1.88823000
H	-7.17808400	-3.06751000	-0.40017900
H	-8.74450200	0.45948200	-2.30441300
H	-0.77331300	-2.35342500	-1.97141900
Br	0.19245100	-4.71454500	-3.61829800
RS_{C5}			
Fe	7.25863900	-13.79667200	21.84685000
N	5.55862900	-14.23415900	22.84150400
C	5.45908400	-14.83960800	24.08404600
C	4.06598900	-15.06395500	24.40746900
C	3.32923300	-14.58468600	23.36332700
C	4.26238700	-14.07486600	22.38079600
H	3.71696200	-15.52350600	25.32054000
H	2.25533200	-14.57655000	23.24781300
C	3.90294300	-13.54678200	21.15197800
H	2.84438300	-13.47698100	20.92702200
N	6.17537000	-13.16397100	20.27057500

C	4.79290300	-13.14025400	20.17190100
C	4.40559200	-12.66959500	18.85896300
C	5.55428700	-12.42386200	18.16455700
C	6.65859400	-12.72958600	19.04868100
H	3.38367700	-12.55625600	18.52800900
H	5.66298600	-12.06435600	17.15181200
C	7.99644000	-12.57107700	18.72489600
H	8.23381400	-12.20756600	17.73125300
N	8.94235400	-13.26879900	20.89726900
C	9.05173300	-12.79328200	19.59466000
C	10.43332000	-12.49478500	19.29836000
C	11.15615400	-12.75737500	20.42811600
C	10.22946300	-13.23494200	21.42726500
H	10.78631700	-12.11602000	18.35032800
H	12.21822300	-12.63960800	20.58635900
C	10.58211800	-13.62037200	22.71004800
H	11.62856500	-13.55067900	22.98609700
N	8.32916000	-14.26130600	23.48189600
C	9.69868400	-14.11460100	23.65788500
C	10.08130800	-14.62068100	24.95641300
C	8.94567500	-15.08657200	25.55842100
C	7.85108800	-14.85359000	24.64479900
H	11.09144700	-14.62291300	25.33918900
H	8.84356800	-15.55040400	26.52838000
C	6.52295000	-15.14297200	24.91749500
H	6.29904500	-15.61577100	25.86720200
O	7.18548600	-15.45131500	21.26054100

S	7.01475400	-11.55146500	22.67376800	N	-2.27678300	-0.06909800	1.25609900
H	7.00505700	-11.86324100	24.01901000	C	-2.24225200	-0.75302700	2.46373900
C	7.89766600	-17.35264600	19.69656500	C	-3.58395100	-0.91901400	2.97866500
C	8.59057300	-16.55827900	20.66125800	C	-4.43076200	-0.32469600	2.08587900
C	8.96077500	-17.20851900	21.88241700	C	-3.61794500	0.21098400	1.01563500
C	8.49072400	-18.47536100	22.17979200	H	-3.82977600	-1.42127800	3.90294800
C	7.70641300	-19.17979000	21.24845200	H	-5.50701000	-0.24711700	2.13353600
C	7.42108100	-18.61596300	19.99626000	C	-4.11750100	0.89305900	-0.08229400
O	8.73721600	-19.01888400	23.45260600	H	-5.19460800	1.00991400	-0.14184300
C	9.91165200	-19.72601600	23.71646800	N	-1.98426100	1.40310400	-1.20104200
C	10.85745300	-20.04286800	22.73571800	C	-3.36285000	1.43534800	-1.11386200
C	12.00973300	-20.75823200	23.07409400	C	-3.91822300	2.11444000	-2.26901000
C	12.20690100	-21.15114000	24.39554500	C	-2.86705300	2.48600800	-3.05551600
C	11.27293900	-20.84299900	25.38484400	C	-1.66088800	2.04063200	-2.38602900
C	10.12728900	-20.12928700	25.03969000	H	-4.97322000	2.27315000	-2.43893700
Br	7.02515800	-20.94008600	21.66997600	H	-2.88720000	3.01225900	-3.99879800
Br	8.82746700	-19.69589900	26.41551200	C	-0.37186700	2.24677100	-2.85569200
Br	13.81487700	-22.14903600	24.88094100	H	-0.26006200	2.77328100	-3.79782700
Br	7.55788100	-16.59928100	17.94250700	N	0.82850000	1.15842400	-1.00256300
H	9.55587500	-16.67693800	22.61299800	C	0.78499900	1.84115600	-2.20812100
H	6.84347000	-19.17579600	19.27312900	C	2.13056700	2.08640400	-2.68655800
H	10.69511100	-19.73444400	21.71030400	C	2.98449300	1.55026100	-1.76710500
H	12.73920700	-21.00472300	22.31288200	C	2.16788900	0.96513900	-0.72178600
H	11.42990800	-21.14978800	26.41005800	H	2.37064600	2.60358300	-3.60421700
H	9.17040700	-15.70819800	20.32426900	H	4.06473800	1.53801700	-1.78111800
				C	2.66784900	0.28587300	0.38095200
IM_{C5}				H	3.74697200	0.22602800	0.47885500
Fe	-0.72964800	0.52649400	0.12098900				

N	0.51835300	-0.36588300	1.41232000	Br	-5.98793500	-5.64626900	4.71586600
C	1.91005800	-0.32714900	1.36608300	Br	1.83788000	-2.59552200	-2.42797500
C	2.46000000	-1.01281600	2.51462200	H	-2.25000100	-2.49537900	0.61119400
C	1.40765400	-1.44827200	3.26907100	H	-0.29970200	-4.30138100	-3.60730800
C	0.19933300	-1.03044300	2.59459800	H	-2.52180000	-5.43767900	1.03434600
H	3.51628200	-1.12704300	2.71082700	H	-3.38584000	-6.08797800	3.27048300
H	1.43250100	-1.98620000	4.20570400	H	-7.11094200	-4.12101700	2.38778100
C	-1.08684700	-1.21949200	3.07791700	H	0.22485400	-2.34790200	0.12402900
H	-1.19659700	-1.74208200	4.02240100				
O	-0.81996800	-0.96270600	-1.08037100	TS(5,4)			
S	-0.65758300	2.51264300	1.34800300	Fe	-0.41656100	0.78725900	0.16110500
H	-0.51237900	3.39168200	0.29350100	N	-1.84408400	0.39479600	1.52176900
C	0.04036100	-3.04432700	-1.90987600	C	-1.68649800	-0.05948300	2.82773600
C	-0.49806400	-2.37763600	-0.70034300	C	-2.97271300	-0.13487200	3.48400300
C	-1.82645000	-2.89473900	-0.29923000	C	-3.90826600	0.29388500	2.58379700
C	-2.56754200	-3.73569300	-1.10385700	C	-3.20661000	0.63546100	1.36663300
C	-2.01478700	-4.23293300	-2.29686800	H	-3.12397200	-0.45989400	4.50327900
C	-0.70193700	-3.88690000	-2.69279500	H	-4.97630900	0.38216000	2.71968100
O	-3.90355700	-4.06071700	-0.82859900	C	-3.81291300	1.13372800	0.22471000
C	-4.31936100	-4.39829000	0.46327700	H	-4.89020800	1.25953900	0.25082800
C	-3.51934800	-5.14296300	1.33773400	N	-1.79788300	1.38957900	-1.17191600
C	-4.00457900	-5.51151700	2.59454700	C	-3.16246200	1.47387400	-0.95202300
C	-5.29658800	-5.13831900	2.96178800	C	-3.83003700	1.94892900	-2.14818200
C	-6.10886400	-4.40589100	2.09731100	C	-2.86627500	2.14347200	-3.09377400
C	-5.61401200	-4.03407000	0.84737500	C	-1.59930400	1.79386000	-2.48456500
Br	-3.03977500	-5.40061300	-3.42428400	H	-4.89611900	2.10079800	-2.23491200
Br	-6.73883200	-3.00481700	-0.35042600	H	-2.98322100	2.48930200	-4.11056100
				C	-0.36966600	1.86525700	-3.11879100

H	-0.35441600	2.20360600	-4.14952900	C	-1.15243300	-3.51760900	-1.96827800
N	1.00605600	1.10010000	-1.22712000	O	-4.39207700	-3.40044800	-0.13033000
C	0.84491100	1.54453100	-2.52955500	C	-4.88772900	-4.59449900	0.40495500
C	2.13269600	1.64295800	-3.18460100	C	-4.07111300	-5.65481300	0.80891600
C	3.07316700	1.25768100	-2.27356200	C	-4.63885700	-6.81408600	1.34607100
C	2.36808100	0.91635200	-1.05455600	C	-6.02251500	-6.89948300	1.47771400
H	2.27923600	1.96799900	-4.20444300	C	-6.84900400	-5.84705100	1.08319700
H	4.14500300	1.20283200	-2.39799000	C	-6.27649000	-4.69554600	0.54705500
C	2.97969500	0.45980000	0.10349500	Br	-3.67603200	-4.44326100	-2.96506300
H	4.06191700	0.37958100	0.09374300	Br	-7.42228600	-3.22965400	-0.00188500
N	0.95699300	0.12504100	1.47711400	Br	-6.82664300	-8.51451000	2.22590700
C	2.33001700	0.10591100	1.27718400	Br	1.60463600	-3.05482300	-1.28404900
C	3.00001600	-0.33956000	2.48020200	H	-2.63248400	-2.33147600	1.48477900
C	2.03315800	-0.57901200	3.41470800	H	-0.76220300	-3.86806900	-2.91383700
C	0.76166900	-0.28199700	2.79284000	H	-2.99526200	-5.57734000	0.71020700
H	4.07059900	-0.44286800	2.58277000	H	-4.00571100	-7.63539200	1.65672200
H	2.15424900	-0.91602900	4.43401400	H	-7.92318100	-5.91664700	1.18820300
C	-0.47235100	-0.37688600	3.41957000	H	-0.15815800	-2.21069000	1.04440600
H	-0.48771400	-0.70580600	4.45336800				
O	-0.71981200	-1.02972100	-0.65443800	IM(5,4)			
S	-0.20031000	2.95122000	0.97035100	Fe	-0.52364400	0.69444500	0.18540200
H	-0.18248500	3.60902300	-0.24401400	N	-1.93863900	0.06238000	1.47126000
C	-0.29434600	-2.92732300	-1.02279500	C	-1.76552700	-0.49837100	2.73156700
C	-0.82518300	-2.26379400	0.18628600	C	-3.05176200	-0.72426400	3.35371500
C	-2.22746400	-2.62163800	0.52342600	C	-4.00281500	-0.28249700	2.47759100
C	-3.02231300	-3.23509700	-0.39064000	C	-3.30956700	0.20953100	1.30681300
C	-2.49104500	-3.65636300	-1.66391300	H	-3.19134700	-1.14974400	4.33718100
				H	-5.07644800	-0.28179700	2.59783500

C	-3.93704500	0.72421500	0.18303700	C	-0.54057100	-0.77299100	3.32203400
H	-5.02069800	0.76818900	0.19514200	H	-0.54555900	-1.19827300	4.32014800
N	-1.92279600	1.17432000	-1.16950600	O	-0.73961200	-1.36362000	-0.70051600
C	-3.29527200	1.15651200	-0.96681100	S	-0.52401600	2.79173200	1.10067200
C	-3.97634800	1.61887200	-2.15813700	H	-0.48895000	3.51135800	-0.07868600
C	-3.01569700	1.90755400	-3.08420400	C	-0.11641300	-2.58743200	-1.24915200
C	-1.73617100	1.63483300	-2.46590300	C	-0.79259900	-2.69757800	0.08117700
H	-5.04920400	1.69885700	-2.25770100	C	-2.08066200	-3.37612000	0.14930600
H	-3.14384400	2.27412900	-4.09238800	C	-2.66960100	-3.82727200	-0.98807800
C	-0.50542900	1.83343000	-3.07252400	C	-2.00412400	-3.73131600	-2.28393700
H	-0.49910700	2.20511400	-4.09162700	C	-0.77673900	-3.18390800	-2.41907600
N	0.89050800	1.15680600	-1.15658800	O	-3.90763200	-4.46064200	-1.03669100
C	0.71757000	1.62586200	-2.45425400	C	-4.60516400	-4.78756300	0.13701000
C	2.00274700	1.91680800	-3.05063900	C	-4.19935900	-5.88434000	0.90363600
C	2.95246100	1.64308800	-2.10843200	C	-4.94184500	-6.27299200	2.02055100
C	2.26009100	1.16825500	-0.92974700	C	-6.09251900	-5.55668900	2.35155200
H	2.14182300	2.29005400	-4.05496700	C	-6.51314000	-4.46685400	1.59063100
H	4.02527500	1.74282800	-2.18937900	C	-5.76112200	-4.08111500	0.47897000
C	2.88867700	0.75348300	0.23376400	Br	-2.89558600	-4.48168900	-3.83506700
H	3.97067000	0.82498900	0.26882500	Br	-6.34620400	-2.57520800	-0.59045500
N	0.87713600	0.05726800	1.48216000	Br	-7.14201200	-6.09118200	3.90587300
C	2.24837500	0.23179000	1.34657000	Br	1.85628000	-2.58597400	-1.35706300
C	2.92674700	-0.23621400	2.53560200	H	-2.54586800	-3.51049600	1.11716300
C	1.96758100	-0.69026800	3.39523200	H	-0.26157200	-3.17791800	-3.36981700
C	0.68992200	-0.49354500	2.74669000	H	-3.31115200	-6.43262200	0.61217900
H	3.99744700	-0.21274400	2.67862100	H	-4.63356500	-7.12303200	2.61541500
H	2.09570300	-1.10732200	4.38371000	H	-7.41084000	-3.92342300	1.85230500

H	-0.19119200	-2.62268200	0.97748300
TS(5,6)			
Fe	-0.70375800	0.54270700	0.18154900
N	-2.13668600	-0.02956200	1.47167700
C	-1.98061800	-0.58571100	2.73465600
C	-3.27245000	-0.77405600	3.35681700
C	-4.21155200	-0.31722900	2.47523000
C	-3.50609600	0.15319600	1.30314800
H	-3.42496300	-1.19244000	4.34113700
H	-5.28481900	-0.29104800	2.59489600
C	-4.11820800	0.68826400	0.18053500
H	-5.20160900	0.74325100	0.18715000
N	-2.09665600	1.16531500	-1.14473800
C	-3.46679400	1.14590100	-0.95622000
C	-4.13649500	1.66013700	-2.13457400
C	-3.16442700	1.98399500	-3.03604800
C	-1.89243800	1.67497100	-2.41476500
H	-5.20782100	1.74863200	-2.24118700
H	-3.27913200	2.39432100	-4.02880200
C	-0.65275400	1.88407600	-3.00293100
H	-0.63731300	2.29580600	-4.00664600
N	0.73163400	1.10039300	-1.12363400
C	0.56627900	1.62010300	-2.39998800
C	1.86007500	1.87303800	-3.00085400
C	2.80413200	1.51042400	-2.08479000
C	2.09716100	1.02356300	-0.91656100
H	2.00708400	2.27795400	-3.99162700

H	3.87973800	1.55570700	-2.17574600
C	2.70935200	0.52960400	0.22657700
H	3.79385600	0.54904000	0.25679900
N	0.67770800	-0.12292800	1.47284400
C	2.05593400	0.00215400	1.32988500
C	2.72142400	-0.50352200	2.51026300
C	1.75048700	-0.92099800	3.37571500
C	0.47718600	-0.66987300	2.73925300
H	3.79291400	-0.52279200	2.64738300
H	1.86972900	-1.34597400	4.36183300
C	-0.76042300	-0.90014600	3.31932000
H	-0.77638200	-1.32403500	4.31795000
O	-0.71956100	-1.10430600	-0.86474000
S	-0.69685100	2.64251100	1.15743300
H	-0.55835800	3.39364100	0.00713500
C	0.36599700	-3.22799100	-1.41209300
C	-0.32010200	-2.45696500	-0.34749600
C	-1.72836300	-2.85421200	-0.14553400
C	-2.39841700	-3.66686900	-1.05534300
C	-1.69850300	-4.26032100	-2.10493000
C	-0.30026400	-4.04694200	-2.27347600
O	-3.79017800	-3.83035800	-1.00114400
C	-4.42112000	-4.25709800	0.17149300
C	-3.79398900	-5.08353400	1.11055000
C	-4.49123700	-5.52142600	2.23927800
C	-5.81829700	-5.13373600	2.41387400
C	-6.45934200	-4.31854600	1.48151400

C	-5.75510500	-3.87969000	0.36106900	H	-5.24655100	1.88402500	-2.07300500	
Br	-2.60590700	-5.39617600	-3.36232200	H	-3.34714400	2.40310300	-3.93032400	
Br	-6.64273000	-2.73912900	-0.93228300	C	-0.72118900	1.78054900	-2.98216100	
Br	-6.80234500	-5.73773000	3.98826700	H	-0.71679000	2.18240500	-3.98969100	
Br	2.26657800	-2.96136300	-1.59918200	N	0.68051800	0.97015200	-1.12539300	
H	-2.25519600	-2.39392500	0.67848500	C	0.50218100	1.48537400	-2.40203500	
H	0.21358800	-4.55215100	-3.08017500	C	1.78684000	1.70782300	-3.03049700	
H	-2.76619700	-5.39008900	0.95656100	C	2.74265300	1.34109600	-2.12794300	
H	-4.00589600	-6.16184500	2.96471300	C	2.05290800	0.88067200	-0.94063900	
H	-7.49021000	-4.02249400	1.62077500	H	1.92114500	2.10033300	-4.02799000	
H	0.27809400	-2.33869900	0.55749400	H	3.81687300	1.36925700	-2.23968600	
IM(5,6)				C	2.68415500	0.39620500	0.19439800	
	Fe	-0.73342400	0.55913000	0.24003800	H	3.76896600	0.39180800	0.19881500
	N	-2.15233000	-0.02038100	1.54321400	N	0.66192600	-0.18801200	1.48839200
	C	-1.98137900	-0.60469400	2.79697500	C	2.04105200	-0.10080300	1.31794300
	C	-3.26189300	-0.75471200	3.45008400	C	2.71502000	-0.63460500	2.47986400
	C	-4.20689600	-0.24601000	2.60347400	C	1.74924800	-1.03896600	3.35904000
	C	-3.51811700	0.21518300	1.41914100	C	0.47147200	-0.74910100	2.75011600
	H	-3.40344600	-1.18547700	4.43080500	H	3.78810000	-0.68501900	2.59538700
	H	-5.27480500	-0.18204400	2.75328500	H	1.87650500	-1.48139900	4.33655700
	C	-4.14179100	0.78406200	0.31896200	C	-0.76052000	-0.96188400	3.35133900
	H	-5.22029400	0.88878600	0.35774900	H	-0.76761700	-1.40282000	4.34258600
	N	-2.13572100	1.14115800	-1.07049200	O	-0.91443000	-1.35598300	-0.84629100
	C	-3.50157500	1.20218400	-0.83681000	S	-0.60159800	2.65475300	1.13966700
	C	-4.17865800	1.73866500	-1.99961400	H	-0.60026600	2.29386900	2.47409100
	C	-3.22145900	1.99835800	-2.93664300	C	0.37278400	-3.34733700	-1.68901800
	C	-1.94764500	1.63177900	-2.35430700	C	-0.11431600	-2.61283600	-0.52136800

C	-1.59970500	-2.60195000	-0.29505100
C	-2.44805600	-3.32688700	-1.24930900
C	-1.90603300	-3.89257200	-2.35594700
C	-0.47465000	-3.90588700	-2.58281900
O	-3.82928500	-3.32301200	-1.04753600
C	-4.39049600	-3.91844400	0.08886200
C	-3.71261400	-4.87248300	0.85459600
C	-4.33446700	-5.45652300	1.96183500
C	-5.63744600	-5.08543700	2.28531200
C	-6.32983200	-4.14585200	1.52092800
C	-5.70201500	-3.56271700	0.42182500
Br	-3.01605700	-4.78285900	-3.66853300
Br	-6.66823500	-2.26588200	-0.64710000
Br	-6.51899200	-5.89368400	3.82807200
Br	2.29716300	-3.50812100	-1.89306300
H	-1.98857800	-2.42931600	0.70073900
H	-0.10404300	-4.41751300	-3.46113400
H	-2.70936200	-5.17414900	0.57586100
H	-3.80983300	-6.19547600	2.55398800
H	-7.34427300	-3.86757000	1.77245500
H	0.55379500	-2.44961200	0.31349900
RC_{C6}			
Fe	1.31984300	1.11685400	-0.00869400
N	0.54008200	2.76438200	0.87211400
C	0.64853700	3.12453200	2.21209600
C	-0.17019700	4.28694000	2.47683000
C	-0.78760200	4.62221800	1.30677300

C	-0.35744800	3.66891900	0.30800200
H	-0.25297800	4.76941900	3.43957300
H	-1.47675300	5.43304000	1.12166500
C	-0.78624700	3.64983000	-1.00698900
H	-1.49625400	4.41134300	-1.31151800
N	0.51590500	1.69991300	-1.76555100
C	-0.37706900	2.73709000	-1.97234500
C	-0.81210400	2.75062000	-3.35190000
C	-0.17841600	1.71658500	-3.98024100
C	0.64469500	1.05984300	-2.98872400
H	-1.50829000	3.46338700	-3.76883900
H	-0.25251000	1.41396400	-5.01442900
C	1.43913300	-0.04959400	-3.23232600
H	1.44799900	-0.44386700	-4.24304400
N	2.33054700	-0.34140300	-0.95523100
C	2.21702200	-0.70210700	-2.28697500
C	3.03201100	-1.86703700	-2.55598500
C	3.63739100	-2.21013600	-1.37993500
C	3.19835200	-1.25392400	-0.38623100
H	3.12196600	-2.34345500	-3.52126000
H	4.31768100	-3.02578600	-1.18469800
C	3.60714300	-1.25728600	0.94182400
H	4.28241600	-2.04713900	1.25179200
N	2.33469400	0.71449900	1.68779200
C	3.20869300	-0.34308500	1.90127600
C	3.63708300	-0.35862800	3.28346300
C	3.01533500	0.68410600	3.90642500

C	2.20245600	1.35031700	2.91105400	H	-0.91512500	-3.79662500	0.00588000
H	4.32280300	-1.07953900	3.70350800	H	1.46268400	-4.42162300	-0.31770900
H	3.09008700	0.98926800	4.93972500	H	1.85612000	-5.06895800	3.92219900
C	1.41108700	2.46263700	3.15759500	H	-2.68976700	0.17957300	0.09070800
H	1.39623300	2.84930300	4.17087200				
O	0.03956800	0.15525500	0.39433700	TS _{c6}			
S	3.23063400	2.81889200	-0.33262800	Fe	1.03175900	1.16700100	0.32835400
H	2.55425100	3.73882400	-1.11224000	N	0.12635800	2.78790900	1.12393500
C	-4.48157800	-1.03559600	0.18866100	C	0.23340900	3.23859200	2.42900200
C	-3.14326800	-0.73936000	0.43741500	C	-0.64385000	4.37291600	2.62759000
C	-2.36470800	-1.65116600	1.15449400	C	-1.28490900	4.59810500	1.44369800
C	-2.92436400	-2.85319400	1.59923300	C	-0.80028100	3.61033900	0.50296900
C	-4.26876400	-3.13681900	1.33664600	H	-0.74623000	4.91067900	3.55869800
C	-5.05722200	-2.22512900	0.63361800	H	-2.01506700	5.35898600	1.20982300
O	-2.20708800	-3.76897400	2.38129700	C	-1.17942700	3.53272200	-0.82691800
C	-0.86540100	-4.05936400	2.14266100	H	-1.91152600	4.24905600	-1.18306600
C	-0.30710900	-4.07202900	0.85858500	N	0.26304000	1.63441000	-1.47303500
C	1.03108500	-4.42726200	0.67473600	C	-0.66855500	2.62961200	-1.74639800
C	1.79741700	-4.78106400	1.78303200	C	-1.00765600	2.60708700	-3.15044000
C	1.25627900	-4.78930300	3.06689600	C	-0.27448900	1.60782500	-3.72816900
C	-0.07812900	-4.42305900	3.24176800	C	0.51398800	0.99779800	-2.68197900
Br	-5.06060700	-4.80227200	1.94685500	H	-1.71238400	3.27755400	-3.61997100
Br	-0.83358500	-4.42264300	5.02888100	H	-0.26099000	1.30003800	-4.76354600
Br	3.67965200	-5.27257000	1.54232000	C	1.35752700	-0.08856600	-2.86011400
Br	-5.58564200	0.23640300	-0.80798700	H	1.46354600	-0.48164300	-3.86534400
H	-1.32591000	-1.40667900	1.34276200	N	2.04679800	-0.35545500	-0.50524400
H	-6.09694600	-2.44812700	0.43641400	C	2.06704100	-0.71490700	-1.84872900
				C	2.93584300	-1.85425700	-2.03620300

C	3.44851200	-2.17672300	-0.81128400
C	2.90918800	-1.23212800	0.14022300
H	3.12402200	-2.33022100	-2.98747800
H	4.13990900	-2.96815600	-0.56183900
C	3.25698800	-1.18129300	1.48098900
H	3.93731000	-1.93962300	1.85145700
N	1.97153800	0.83159500	2.07822900
C	2.83276000	-0.21075600	2.37317000
C	3.25177600	-0.12459700	3.75643900
C	2.64278600	0.97220200	4.29163400
C	1.83786900	1.56655900	3.24451300
H	3.92218700	-0.82227400	4.23554400
H	2.71393600	1.35531300	5.29894800
C	1.03793500	2.68433300	3.41057800
H	1.02622100	3.15019100	4.38974400
O	-0.33917000	0.21781600	0.85395700
S	2.92182600	2.65348000	-0.14822100
H	2.21920500	3.60395900	-0.86435000
C	-3.41636200	-0.49969000	-0.27787900
C	-2.12074200	-0.65409600	-0.72547500
C	-1.14391800	-1.26669900	0.13450000
C	-1.62955800	-1.93057700	1.31623400
C	-2.93687700	-1.74075900	1.73744400
C	-3.84156400	-1.00735400	0.95828400
O	-0.75516000	-2.66097400	2.11977100
C	-0.14642600	-3.83091900	1.66091700
C	-0.52383400	-4.47930800	0.47930400

C	0.11080100	-5.66207700	0.09008300
C	1.11574600	-6.19367400	0.89434400
C	1.48998300	-5.56946000	2.08417000
C	0.85533000	-4.38856800	2.46482000
Br	-3.55680600	-2.51948800	3.40486400
Br	1.35882500	-3.53805100	4.13254000
Br	2.01342500	-7.84489000	0.35995100
Br	-4.72004500	0.44099900	-1.39329700
H	-0.22919800	-1.64189700	-0.31175100
H	-4.85830400	-0.86488200	1.29667900
H	-1.32124700	-4.06950400	-0.12878200
H	-0.18398000	-6.16129400	-0.82418400
H	2.26112000	-5.99380100	2.71279000
H	-1.80700900	-0.26256400	-1.68240900
IM_{C6}			
Fe	0.99471500	0.93012400	0.19192200
N	0.19696800	2.35484600	1.37610100
C	0.38003600	2.52747900	2.73462700
C	-0.43431000	3.62983800	3.21059600
C	-1.10645900	4.12096000	2.13044300
C	-0.70544200	3.32402900	0.98494200
H	-0.47088300	3.96934900	4.23537300
H	-1.80404000	4.94483000	2.09162300
C	-1.14444000	3.53620900	-0.31443900
H	-1.83164800	4.36074300	-0.47491300
N	0.07623800	1.70386200	-1.42914300
C	-0.76065500	2.81076000	-1.43387600

C	-1.16641400	3.11650300	-2.78903100	H	2.98607600	2.16735500	-1.57189500
C	-0.56733500	2.20120700	-3.60715900	C	-3.25889700	-0.57116600	-1.11833700
C	0.20485400	1.31888500	-2.76083700	C	-1.91090700	-0.74316600	-1.15782800
H	-1.82221000	3.92970700	-3.06333600	C	-1.14634000	-1.23097200	0.03962100
H	-0.63819000	2.11621600	-4.68164700	C	-2.05269200	-1.81378800	1.09886100
C	0.93311300	0.22134800	-3.19691200	C	-3.41744600	-1.56106700	1.09570800
H	0.93750500	0.01371000	-4.26202800	C	-4.03248500	-0.93560300	0.01150500
N	1.81719300	-0.47339900	-1.00180700	O	-1.55869500	-2.46107200	2.19859200
C	1.67414400	-0.62320100	-2.37706700	C	-0.36596800	-3.18524900	2.25047600
C	2.46788300	-1.73899400	-2.84021400	C	0.03766600	-4.03393500	1.21457200
C	3.11510400	-2.24937200	-1.74936600	C	1.19952300	-4.79688200	1.34880500
C	2.72451500	-1.44992600	-0.60905500	C	1.93231000	-4.71466900	2.53159600
H	2.52846100	-2.06526400	-3.86838400	C	1.51683800	-3.90471500	3.58735200
H	3.81072900	-3.07513100	-1.70991300	C	0.35913900	-3.14051000	3.44520200
C	3.24089200	-1.60212900	0.67142000	Br	-4.52386600	-2.10568900	2.60083000
H	3.96414400	-2.39742900	0.82008900	Br	-0.24078800	-2.03856400	4.91710900
N	2.02524800	0.22963100	1.78034200	Br	3.57272900	-5.75895200	2.72269400
C	2.93383000	-0.81353700	1.77079200	Br	-4.21763700	0.18518500	-2.65491400
C	3.51881100	-0.97386400	3.08819700	H	-0.37301800	-1.93870500	-0.28350100
C	2.95231400	-0.02788100	3.89220700	H	-5.09810100	-0.75224700	0.02758900
C	2.02016800	0.72014800	3.07197100	H	-0.56424800	-4.11771400	0.31803200
H	4.26224000	-1.71522600	3.34255200	H	1.51767900	-5.45120000	0.54743300
H	3.13628100	0.16055700	4.93965300	H	2.08107000	-3.86092500	4.50851000
C	1.24023500	1.77692500	3.52212200	H	-1.33584400	-0.48247900	-2.03223500
H	1.31484700	2.03975500	4.57211300				
O	-0.50583600	-0.12255600	0.75567700	TS(6,5)			
S	2.80473300	2.43632000	-0.22786500	Fe	0.97763300	1.03962100	0.09551000
				N	0.17547100	2.47339900	1.26011800

C	0.31409100	2.63383200	2.62743700	C	2.79305600	-0.77953400	1.73438500
C	-0.45650800	3.77843400	3.07287500	C	3.33731200	-0.94954500	3.06653800
C	-1.05286900	4.31077200	1.96784700	C	2.75861400	-0.00108300	3.85905300
C	-0.65325700	3.49550700	0.83598400	C	1.86184200	0.76477200	3.01861900
H	-0.51636800	4.11654500	4.09714000	H	4.06596200	-1.69934800	3.33855300
H	-1.70042300	5.17319900	1.90401100	H	2.91543100	0.18032800	4.91215700
C	-1.03847700	3.73001500	-0.47585800	C	1.10818100	1.84654500	3.44710300
H	-1.66756700	4.59472300	-0.66050200	H	1.15915100	2.10820000	4.49863800
N	0.07875000	1.80121100	-1.53726700	O	-0.65999000	0.05450700	0.67967700
C	-0.68354400	2.96101300	-1.57423100	S	2.81822700	2.40089700	-0.26700000
C	-1.07193700	3.25130200	-2.93793300	H	2.99931100	2.13525800	-1.61127000
C	-0.54474100	2.26897200	-3.72694500	C	-3.17697500	-0.57520900	-0.88548900
C	0.17377700	1.36613600	-2.85500400	C	-1.80356800	-0.75944200	-0.92304700
H	-1.67176800	4.09891400	-3.23597000	C	-1.07531000	-1.31668800	0.23845100
H	-0.62659700	2.15290700	-4.79791400	C	-1.95821100	-1.92815800	1.27950000
C	0.84743200	0.22372400	-3.26494400	C	-3.31672900	-1.72325400	1.25516300
H	0.83452600	-0.01579000	-4.32301900	C	-3.93272000	-1.03616800	0.18481800
N	1.72547300	-0.43410900	-1.05241500	O	-1.44354800	-2.58921500	2.36414800
C	1.57343000	-0.61279900	-2.42568700	C	-0.26448600	-3.34405400	2.37478100
C	2.34649700	-1.75164700	-2.86539000	C	0.10793100	-4.16114900	1.30314500
C	2.99531800	-2.24491200	-1.76772500	C	1.25732600	-4.94948500	1.39411400
C	2.62264700	-1.41813100	-0.64200400	C	2.00751800	-4.92335300	2.56862600
H	2.39599800	-2.10183300	-3.88641200	C	1.62257100	-4.14116200	3.65708600
H	3.68000600	-3.07917800	-1.71403600	C	0.47758600	-3.35136400	3.55962800
C	3.12147800	-1.57059200	0.64353000	Br	-4.44884500	-2.39059000	2.68389900
H	3.83604300	-2.37062900	0.80648700	Br	-0.08314200	-2.28949900	5.07506900
N	1.89269200	0.27382200	1.72239300	Br	3.62404000	-6.00890400	2.70306100

Br	-4.07128600	0.34495700	-2.35528400	C	1.20795100	-0.29993100	-2.83664100
H	-0.19574300	-1.91010000	-0.00822700	H	1.27409500	-0.69497300	-3.84515200
H	-5.00376800	-0.88297200	0.20765700	N	2.03303300	-0.50884000	-0.52339100
H	-0.50649700	-4.20075800	0.41149600	C	1.97200000	-0.91329300	-1.85360500
H	1.55248200	-5.57997900	0.56533400	C	2.86813000	-2.02641200	-2.07418500
H	2.20030400	-4.14095700	4.57112200	C	3.48939800	-2.28175900	-0.88397100
H	-1.20979300	-0.42861300	-1.76003200	C	2.97641800	-1.33086900	0.07854800
IM(6,5) = IM(5,6)				H	3.00650800	-2.52490900	-3.02290200
TS(6,1)				H	4.23116600	-3.03622800	-0.66481800
Fe	1.07275100	1.02485600	0.35973000	C	3.39296200	-1.25009300	1.40007500
N	0.05185600	2.50882300	1.25544600	H	4.15713900	-1.95070900	1.72088600
C	0.08043000	2.87601500	2.59122500	N	1.94156100	0.60489600	2.12417000
C	-0.80859600	3.99806700	2.81742300	C	2.92016300	-0.35139300	2.34291400
C	-1.36457800	4.31394300	1.61267700	C	3.36306900	-0.30052100	3.72285900
C	-0.82479400	3.38359800	0.63930400	C	2.64122500	0.67942800	4.33781200
H	-0.96643300	4.47204700	3.77534600	C	1.75719000	1.24388300	3.33745800
H	-2.07154600	5.09833700	1.38402700	H	4.12096100	-0.94273300	4.14734400
C	-1.15084800	3.38553800	-0.70920800	H	2.69114100	1.00606200	5.36639900
H	-1.84049400	4.14938100	-1.05278500	C	0.87346100	2.28877300	3.56358400
N	0.18977500	1.42853500	-1.40151300	H	0.81638500	2.69036200	4.56975700
C	-0.67481700	2.49147800	-1.65496500	O	-0.44651800	-0.20836300	0.93739500
C	-1.02376900	2.51680900	-3.05712000	S	2.81116200	2.48745600	-0.11513200
C	-0.36616900	1.47915500	-3.65858000	H	2.97272800	2.17883400	-1.45259000
C	0.39608000	0.80660600	-2.63097300	C	-3.36147400	0.00094200	-0.39974500
H	-1.68597900	3.24034500	-3.50971800	C	-2.16579700	-0.40368200	-0.88274800
H	-0.38014600	1.19209300	-4.70024000	C	-1.19321600	-1.09088900	0.02763600
				C	-1.80794800	-1.64487600	1.27792700

C	-3.03026100	-1.09684000	1.75113800
C	-3.78591800	-0.29178100	0.93984700
O	-1.25886100	-2.61914200	2.03640200
C	-0.27017700	-3.52977000	1.62107900
C	-0.32740900	-4.17567700	0.38336600
C	0.63970600	-5.12733300	0.05035500
C	1.63734300	-5.43314000	0.97435600
C	1.67646700	-4.82266500	2.22729600
C	0.71298400	-3.86837700	2.55436700
Br	-3.65300600	-1.53862700	3.53422300
Br	0.74504200	-3.04583200	4.30143800
Br	2.99945000	-6.75320600	0.51992200
Br	-4.62773800	0.98142700	-1.52538100
H	-0.52235900	-1.75694100	-0.51369700
H	-4.72670800	0.10519400	1.29740400
H	-1.13251600	-3.95887400	-0.30794400
H	0.60586600	-5.62613200	-0.90943200
H	2.44233100	-5.08180900	2.94535700
H	-1.87640400	-0.22696300	-1.90851300

IM(6,1) = IM(1,6)

#1

C	-3.47058900	0.87488100	0.56339300
C	-2.43028900	1.29170900	1.39162600
C	-1.21630300	0.61667400	1.34896800
C	-1.03023800	-0.46209900	0.48866200
C	-2.08786500	-0.87716000	-0.32698700

C	-3.30896500	-0.21016800	-0.29597300
O	0.16773600	-1.17254800	0.55726400
C	1.22715000	-0.96555600	-0.37387100
C	0.96116700	0.18322800	-1.32025400
C	1.76191000	1.26409400	-1.41347700
C	2.88126300	1.38397500	-0.53010400
C	3.22784700	0.39581800	0.40965900
C	2.47749600	-0.74764700	0.48155300
Br	-1.90667400	-2.37917300	-1.50132900
Br	2.92602000	-2.11009400	1.63950200
Br	3.93512000	2.90612400	-0.64790300
Br	-5.13983900	1.78369100	0.60808200
H	-0.40456200	0.90559300	2.00709500
H	-4.12394600	-0.53750100	-0.92782800
H	0.11274400	0.06345400	-1.98501300
H	1.57631200	2.04273900	-2.14253000
H	4.09314600	0.53233600	1.04521200
H	-2.56816800	2.12498400	2.06869900
O	1.48162200	-2.10613300	-1.12169000
H	0.65218000	-2.40779900	-1.53172900

#2

C	3.41822100	-0.87711000	-0.36406300
C	2.16046400	-1.66455800	-0.61084000
C	0.90642000	-0.87427500	-0.49534800
C	0.89814800	0.48720000	-0.45647300
C	2.15966200	1.17203600	-0.38553700
C	3.39343900	0.49101700	-0.34395000

O	-0.19146000	1.27415700	-0.43393700	C	1.22715000	-0.96555600	-0.37387100
C	-1.47304900	0.70621400	-0.46072100	C	0.96116700	0.18322800	-1.32025400
C	-2.18454800	0.75640700	-1.65298200	C	1.76191000	1.26409400	-1.41347700
C	-3.49055700	0.28218300	-1.70351000	C	2.88126300	1.38397500	-0.53010400
C	-4.07091100	-0.23947200	-0.54831200	C	3.22784700	0.39581800	0.40965900
C	-3.36648700	-0.28571000	0.65344200	C	2.47749600	-0.74764700	0.48155300
C	-2.05980500	0.19372500	0.69693000	Br	-1.90667400	-2.37917300	-1.50132900
Br	2.16905200	3.02215100	-0.30206700	Br	2.92602000	-2.11009400	1.63950200
Br	-1.10108800	0.15999100	2.34285800	Br	3.93512000	2.90612400	-0.64790300
Br	-5.85730600	-0.88968900	-0.60154800	Br	-5.13983900	1.78369100	0.60808200
Br	5.01946300	-1.81240800	-0.20525100	H	-0.40456200	0.90559300	2.00709500
H	-0.01268000	-1.44752200	-0.50878500	H	-4.12394600	-0.53750100	-0.92782800
H	4.30602500	1.06456100	-0.24332100	H	0.11274400	0.06345400	-1.98501300
H	-1.71679600	1.18615100	-2.53155500	H	1.57631200	2.04273900	-2.14253000
H	-4.05047100	0.32501400	-2.62883900	H	4.09314600	0.53233600	1.04521200
H	-3.82821400	-0.68033200	1.54873000	H	-2.56816800	2.12498400	2.06869900
H	2.22234800	-1.84298400	-1.71324800	O	1.48162200	-2.10613300	-1.12169000
O	2.02593300	-2.86737900	0.08400300	H	0.65218000	-2.40779900	-1.53172900
H	2.60375500	-3.54664200	-0.28505000				
#3				#4			
C	-3.47058900	0.87488100	0.56339300	C	2.99911500	-0.33402900	1.99901500
C	-2.43028900	1.29170900	1.39162600	C	1.69384300	-0.69730900	2.28609300
C	-1.21630300	0.61667400	1.34896800	C	0.72119600	-0.55197600	1.30649500
C	-1.03023800	-0.46209900	0.48866200	C	0.97021000	-0.03987900	0.00369900
C	-2.08786500	-0.87716000	-0.32698700	C	2.25677600	0.31442100	-0.32842000
C	-3.30896500	-0.21016800	-0.29597300	C	3.37999300	0.06745300	0.61186600
O	0.16773600	-1.17254800	0.55726400	O	-0.00006700	0.13803300	-0.91590900
				C	-1.33962300	-0.14490400	-0.63334100

C	-1.90363600	-1.27194300	-1.22030700
C	-3.25610400	-1.54513900	-1.04903500
C	-4.03574100	-0.67867800	-0.28445000
C	-3.48199400	0.45760900	0.30285800
C	-2.12769800	0.72520500	0.12233800
Br	2.64922400	1.08787700	-1.97293200
Br	-1.36843100	2.28967600	0.90677000
Br	-5.88741400	-1.03860800	-0.04117700
H	-0.29936500	-0.82660900	1.55027900
H	-1.27967100	-1.91764000	-1.82774400
H	-3.69791000	-2.41857600	-1.51113000
H	-4.09532300	1.13295900	0.88449800
H	1.41812400	-1.05057200	3.27383200
O	3.98875700	-0.30054600	2.85605000
H	3.74644900	-0.62546100	3.73767600
H	4.11334100	0.87176800	0.61889100
Br	4.40452900	-1.52953800	-0.06261300

#5

C	2.99911500	-0.33402900	1.99901500
C	1.69384300	-0.69730900	2.28609300
C	0.72119600	-0.55197600	1.30649500
C	0.97021000	-0.03987900	0.00369900
C	2.25677600	0.31442100	-0.32842000
C	3.37999300	0.06745300	0.61186600
O	-0.00006700	0.13803300	-0.91590900
C	-1.33962300	-0.14490400	-0.63334100
C	-1.90363600	-1.27194300	-1.22030700

C	-3.25610400	-1.54513900	-1.04903500
C	-4.03574100	-0.67867800	-0.28445000
C	-3.48199400	0.45760900	0.30285800
C	-2.12769800	0.72520500	0.12233800
Br	2.64922400	1.08787700	-1.97293200
Br	-1.36843100	2.28967600	0.90677000
Br	-5.88741400	-1.03860800	-0.04117700
H	-0.29936500	-0.82660900	1.55027900
H	-1.27967100	-1.91764000	-1.82774400
H	-3.69791000	-2.41857600	-1.51113000
H	-4.09532300	1.13295900	0.88449800
H	1.41812400	-1.05057200	3.27383200
O	3.98875700	-0.30054600	2.85605000
H	3.74644900	-0.62546100	3.73767600
H	4.11334100	0.87176800	0.61889100
Br	4.40452900	-1.52953800	-0.06261300

#6

C	3.39822900	-0.89194800	-1.06652600
C	2.05947500	-1.55857700	-1.11708100
C	0.90124600	-0.84508100	-0.93065000
C	0.96170400	0.52045200	-0.62074900
C	2.23785800	1.22571700	-0.51660300
C	3.38293700	0.55054100	-0.71680400
O	-0.09490100	1.25656300	-0.41334300
C	-1.40724600	0.72221600	-0.42275100
C	-2.18477000	0.94599100	-1.54937100
C	-3.50589200	0.51318800	-1.56340800

C	-4.02666900	-0.12706400	-0.43899500
C	-3.24741200	-0.33381000	0.69832100
C	-1.92300400	0.09782100	0.71162900
Br	2.23313500	3.06627400	-0.09823000
Br	-0.86603200	-0.14752200	2.27390500
Br	-5.83203100	-0.71761400	-0.44404300
Br	4.56945000	-1.88607400	0.21174300
H	-0.05179300	-1.35338600	-0.99604300
H	4.34242300	1.04865600	-0.65308800
H	-1.76140300	1.46723200	-2.40027400
H	-4.12309700	0.68054900	-2.43656200
H	-3.66413900	-0.81824200	1.57125400
O	1.96880200	-2.83737200	-1.39839300
H	2.82771700	-3.29152100	-1.38248500
H	3.90211100	-1.03074700	-2.02912700

#7

C	3.39822900	-0.89194800	-1.06652600
C	2.05947500	-1.55857700	-1.11708100
C	0.90124600	-0.84508100	-0.93065000
C	0.96170400	0.52045200	-0.62074900
C	2.23785800	1.22571700	-0.51660300
C	3.38293700	0.55054100	-0.71680400
O	-0.09490100	1.25656300	-0.41334300
C	-1.40724600	0.72221600	-0.42275100
C	-2.18477000	0.94599100	-1.54937100
C	-3.50589200	0.51318800	-1.56340800
C	-4.02666900	-0.12706400	-0.43899500

C	-3.24741200	-0.33381000	0.69832100
C	-1.92300400	0.09782100	0.71162900
Br	2.23313500	3.06627400	-0.09823000
Br	-0.86603200	-0.14752200	2.27390500
Br	-5.83203100	-0.71761400	-0.44404300
Br	4.56945000	-1.88607400	0.21174300
H	-0.05179300	-1.35338600	-0.99604300
H	4.34242300	1.04865600	-0.65308800
H	-1.76140300	1.46723200	-2.40027400
H	-4.12309700	0.68054900	-2.43656200
H	-3.66413900	-0.81824200	1.57125400
O	1.96880200	-2.83737200	-1.39839300
H	2.82771700	-3.29152100	-1.38248500
H	3.90211100	-1.03074700	-2.02912700

#8

O	-2.27067100	2.09660700	0.00154200
C	-1.19633900	1.55114100	0.00031600
C	-1.06941700	0.03298300	0.00021000
C	0.07471600	2.32060900	-0.00094000
C	0.16836900	-0.56072000	0.00030500
C	1.27034900	1.69832800	-0.00094200
H	-0.02283600	3.40058000	-0.00160900
C	1.31774400	0.25558900	-0.00018500
H	0.27245300	-1.63851400	0.00058300
H	2.20045000	2.25322400	-0.00148300
Br	2.97730100	-0.55314400	0.00018900
Br	-2.62522200	-0.94902000	-0.00025800

				Br	-3.02405800	-0.54535200	-0.00001500
#9				#11			
C	-0.21151000	-0.51519600	0.00004200	C	1.35851500	0.26277500	0.00003900
C	1.04954600	0.07024700	0.00008200	C	0.20958600	-0.55584500	0.00008800
C	1.19644900	1.46334400	0.00015600	C	-1.03223700	0.03296200	0.00000500
C	0.04425100	2.25385200	-0.00015000	C	-1.14685400	1.46979100	0.00018900
C	-1.22341400	1.68112300	-0.00017700	C	0.02718500	2.27396700	-0.00012700
C	-1.34162300	0.29667100	0.00001800	C	1.25872500	1.68444000	-0.00000400
H	-0.30413900	-1.59301400	0.00005200	H	0.30838400	-1.63364800	0.00003100
H	0.14082100	3.33669700	-0.00041200	H	-0.09549500	3.35052500	-0.00020000
H	-2.10439200	2.31061900	-0.00045700	H	2.15895600	2.28592100	0.00008900
Br	-3.07887500	-0.51240100	0.00003000	O	-2.29296100	2.09773300	-0.00000100
O	2.44816500	1.98746900	0.00002600	H	-3.05595700	1.48864800	-0.00000600
H	2.39924900	2.95037800	0.00122500	Br	-2.61171400	-0.99424300	-0.00002000
Br	2.59890200	-1.04201800	-0.00004200	Br	3.03966500	-0.52809500	-0.00001000
#10				TS _{#1-#4}			
C	-1.24314900	1.69816200	0.00007500	C	2.99911500	-0.33402900	1.99901500
C	-1.31910700	0.28920700	0.00000800	C	1.69384300	-0.69730900	2.28609300
C	-0.17075200	-0.51631300	-0.00002700	C	0.72119600	-0.55197600	1.30649500
C	1.06950100	0.08308300	0.00000500	C	0.97021000	-0.03987900	0.00369900
C	1.22918100	1.54269100	-0.00004300	C	2.25677600	0.31442100	-0.32842000
C	-0.01441900	2.30060000	0.00007500	C	3.37999300	0.06745300	0.61186600
H	-2.15314600	2.28585600	0.00013500	O	-0.00006700	0.13803300	-0.91590900
H	-0.26292300	-1.59459300	-0.00004600	C	-1.33962300	-0.14490400	-0.63334100
H	0.08793100	3.37997900	0.00014500	C	-1.90363600	-1.27194300	-1.22030700
O	2.33377000	2.10250700	-0.00011900	C	-3.25610400	-1.54513900	-1.04903500
Br	2.63407000	-0.97681600	0.00001900				

C	-4.03574100	-0.67867800	-0.28445000
C	-3.48199400	0.45760900	0.30285800
C	-2.12769800	0.72520500	0.12233800
Br	2.64922400	1.08787700	-1.97293200
Br	-1.36843100	2.28967600	0.90677000
Br	-5.88741400	-1.03860800	-0.04117700
H	-0.29936500	-0.82660900	1.55027900
H	-1.27967100	-1.91764000	-1.82774400
H	-3.69791000	-2.41857600	-1.51113000
H	-4.09532300	1.13295900	0.88449800
H	1.41812400	-1.05057200	3.27383200
O	3.98875700	-0.30054600	2.85605000
H	3.74644900	-0.62546100	3.73767600
H	4.11334100	0.87176800	0.61889100
Br	4.40452900	-1.52953800	-0.06261300

TS_{#1-#5}

C	-3.73367600	0.74629300	0.50829900
C	-2.44994800	1.47829900	0.73140600
C	-1.22616800	0.80994600	0.24430300
C	-1.25672100	-0.43231700	-0.29406400
C	-2.53657100	-1.11338400	-0.42160200
C	-3.73245200	-0.53458000	-0.02036800
O	-0.20032900	-1.13502400	-0.73613600
C	1.09107300	-0.60259600	-0.62167800
C	1.65804900	0.00350500	-1.73575000
C	2.96711800	0.46966400	-1.68218700
C	3.69561300	0.32009700	-0.50325300

C	3.13620700	-0.29403500	0.61595800
C	1.82523800	-0.75950100	0.55430100
Br	-2.56552300	-2.81459500	-1.15739100
Br	1.06642700	-1.63043900	2.07020600
Br	5.48834500	0.94989100	-0.41593800
H	-0.28883700	1.33513900	0.37567400
H	-4.67419200	-1.05432700	-0.14310200
H	1.07696900	0.08833600	-2.64710800
H	3.41561500	0.93553600	-2.55013900
H	3.71321100	-0.41928600	1.52248200
O	-4.87922500	1.27209700	0.85474000
H	-4.81065400	2.21407500	1.09017600
H	-2.35435300	1.68490100	1.80406600
Br	-2.61976100	3.31144800	-0.05839300

TS_{#2-#6}

C	3.39822900	-0.89194800	-1.06652600
C	2.05947500	-1.55857700	-1.11708100
C	0.90124600	-0.84508100	-0.93065000
C	0.96170400	0.52045200	-0.62074900
C	2.23785800	1.22571700	-0.51660300
C	3.38293700	0.55054100	-0.71680400
O	-0.09490100	1.25656300	-0.41334300
C	-1.40724600	0.72221600	-0.42275100
C	-2.18477000	0.94599100	-1.54937100
C	-3.50589200	0.51318800	-1.56340800
C	-4.02666900	-0.12706400	-0.43899500
C	-3.24741200	-0.33381000	0.69832100

C	-1.92300400	0.09782100	0.71162900	Br	2.25004600	3.02184700	-0.64482000
Br	2.23313500	3.06627400	-0.09823000	Br	-1.26821800	0.64919100	2.37724600
Br	-0.86603200	-0.14752200	2.27390500	Br	-5.80147100	-1.03763200	-0.61839000
Br	-5.83203100	-0.71761400	-0.44404300	Br	5.02949900	-1.92676700	-0.06247700
Br	4.56945000	-1.88607400	0.21174300	H	0.24016800	-1.45677200	-0.91757600
H	-0.05179300	-1.35338600	-0.99604300	H	4.28363100	0.92895800	-0.36735000
H	4.34242300	1.04865600	-0.65308800	H	-1.55002500	0.69512100	-2.64064900
H	-1.76140300	1.46723200	-2.40027400	H	-3.86655000	-0.21132500	-2.72082200
H	-4.12309700	0.68054900	-2.43656200	H	-3.92927100	-0.37328600	1.57862600
H	-3.66413900	-0.81824200	1.57125400	O	2.07638300	-3.00225200	0.01806500
O	1.96880200	-2.83737200	-1.39839300	H	2.94759400	-3.43570100	0.07705800
H	2.82771700	-3.29152100	-1.38248500	H	0.36977000	-1.17762500	0.79050900
H	3.90211100	-1.03074700	-2.02912700				
TS _{#2-#7}				TS _{#3}			
C	3.37427900	-0.99673500	-0.17004300	C	2.15226900	0.96022500	-0.43876800
C	2.19013900	-1.70202200	-0.11039500	C	2.48462200	-0.12830900	0.34281800
C	0.88504700	-0.98693000	-0.16399700	C	1.87584800	-0.29744100	1.69908500
C	0.94064400	0.49027700	-0.37259200	C	1.35524700	0.95881600	2.29100200
C	2.16369300	1.14636000	-0.41980000	C	1.09256800	2.03867400	1.53160700
C	3.33961300	0.39733100	-0.31894700	C	1.43238300	2.01144600	0.13323200
O	-0.15913400	1.19411400	-0.50713200	H	2.48588200	1.02054500	-1.46600900
C	-1.44462800	0.60840000	-0.50260300	H	1.13756700	0.95177100	3.35392100
C	-2.07163600	0.42781800	-1.72852700	H	0.66157500	2.93796200	1.95319300
C	-3.36973700	-0.06813500	-1.76994300	O	0.64995200	-1.24585300	1.35129800
C	-4.02679600	-0.36332800	-0.57567000	C	-0.60319700	-0.87422700	1.01327500
C	-3.40581900	-0.16003500	0.65601400	C	-1.10271900	-1.12063200	-0.28723800
C	-2.10451100	0.33422500	0.69453400	C	-1.49218700	-0.36996900	1.98250600
				C	-2.43859700	-0.88068800	-0.59469700

C	-2.81793900	-0.12706200	1.68566300
H	-1.13352600	-0.21312600	2.99302200
C	-3.28734900	-0.37834800	0.38750000
H	-2.81108000	-1.08955600	-1.58867700
H	-3.49298900	0.24055600	2.44795200
Br	0.97845700	3.48267500	-0.91510000
Br	-5.10080100	-0.03761000	-0.02947400
O	2.66342400	-1.05408200	2.50018300
H	2.20734600	-1.28580000	3.32097500
Br	0.01272600	-1.84867300	-1.63446900
Br	3.61054800	-1.45118600	-0.28673200

PC_{#3}

C	-1.39977800	-0.98306700	-0.84165600
C	-2.54972100	-0.68493200	-0.13256600
C	-2.73528400	-1.20666900	1.18171300
C	-1.77459900	-2.09001000	1.71173900
C	-0.62991800	-2.39026100	1.00648600
C	-0.42621400	-1.80709500	-0.26359400
H	-1.26643000	-0.59567500	-1.84301500
H	-1.94248100	-2.53144500	2.68932900
H	0.09307900	-3.09100100	1.40373600
O	-0.96323800	0.75309100	2.01192400
C	0.16837400	0.67219900	1.54957500
C	0.62116600	1.48285400	0.38125800
C	1.17942000	-0.22642800	2.12979100
C	1.89688400	1.36826500	-0.10983600
C	2.44346500	-0.31306000	1.63274200

H	0.87751000	-0.77803200	3.01144600
C	2.79845900	0.47173300	0.50238600
H	2.22510500	1.97027300	-0.94732400
H	3.18406200	-0.95998700	2.08609100
Br	1.12554800	-2.25041800	-1.24482400
Br	4.54971300	0.38723200	-0.13949200
O	-3.85054500	-0.87954900	1.81901700
H	-3.88899000	-1.25987000	2.70734000
Br	-0.57059900	2.72079500	-0.34207500
Br	-3.91395100	0.35656900	-0.90913400

Phenoxide

O	-2.43164000	1.69182100	2.39136400
C	-3.85098300	-0.51464900	-0.05355000
C	-2.67720100	-1.03954700	-0.64026500
C	-1.42121400	-0.62834900	-0.19399900
C	-1.31682800	0.30107200	0.82848300
C	-2.51446100	0.86968500	1.46766000
C	-3.79249400	0.40293500	0.95616500
O	-0.15188300	0.77522500	1.32778000
C	1.05350800	0.24624500	0.90645300
C	1.54353100	-0.90624200	1.51455700
C	2.79023600	-1.41344900	1.16666700
C	3.54353700	-0.75003100	0.20197300
C	3.07512800	0.40743400	-0.41065600
C	1.82244200	0.90443200	-0.05510000
Br	1.17719700	2.49364000	-0.88156200
Br	5.26149200	-1.43268600	-0.28857500

H	-0.53241400	-1.03690900	-0.65924700
H	-4.67819000	0.81795000	1.41990300
H	0.94105600	-1.39110700	2.27436900
H	3.17029200	-2.30711100	1.64493300
H	3.67029700	0.92104900	-1.15357600
H	-2.75256800	-1.76113600	-1.44388900
Br	-5.54387500	-1.12542000	-0.71460500

Phenoxide Anion

O	-1.13514500	-0.50050700	1.95581600
C	-4.10716900	-0.21373300	-0.10103900
C	-3.68449700	0.57594800	-1.16970300
C	-2.34619500	0.98689900	-1.14136600
C	-1.50400500	0.62165700	-0.11036600
C	-1.91129800	-0.18165000	1.02364000
C	-3.29902700	-0.59467900	0.94680900
O	-0.21123800	1.18318500	-0.11747100
C	0.88124300	0.40303200	-0.09271400
C	0.86570100	-0.99618000	-0.19905600
C	2.04387500	-1.72950000	-0.21900300
C	3.26531700	-1.07003600	-0.13096700
C	3.32449700	0.31275800	-0.02583400
C	2.13429200	1.03190300	-0.01014500
Br	2.22611100	2.94451300	0.11964500
Br	4.90871900	-2.08251900	-0.15155400
H	-1.95072600	1.61688700	-1.93389600
H	-3.67072100	-1.20150000	1.76380100
H	-0.08897000	-1.49923700	-0.25701700

H	2.00541900	-2.80984200	-0.29146800
H	4.27214000	0.83010700	0.04084800
H	-4.34975500	0.85862200	-1.97444100
Br	-5.97548000	-0.80870800	-0.10169400

Cyclohexadienone

O	-4.66645800	0.92900800	1.82726100
C	-3.72948800	0.66804200	1.10460600
C	-2.44050400	1.48560000	1.14355700
C	-1.22979300	0.81627800	0.63638900
C	-1.31050400	-0.31088400	-0.09411600
C	-2.61466300	-0.92761900	-0.38071500
C	-3.75449200	-0.45777600	0.15578700
O	-0.24887600	-0.98872500	-0.61962300
C	1.02137600	-0.45353000	-0.51965500
C	1.44242700	0.49322300	-1.44963900
C	2.74223000	0.98470500	-1.41825800
C	3.61857800	0.51469600	-0.44366300
C	3.21844200	-0.43404400	0.49137300
C	1.91109500	-0.91530600	0.45181900
Br	-2.65485800	-2.43842700	-1.53659900
Br	1.35709300	-2.22077400	1.72359100
Br	5.41216400	1.17545600	-0.38887000
H	-0.27176500	1.27886800	0.83696400
H	-4.71274900	-0.92853500	-0.02151300
H	0.74071100	0.83323000	-2.20280600
H	3.06748000	1.71813400	-2.14495700
H	3.90761500	-0.79815700	1.24126900

H	-2.31739500	1.92937000	2.12760900
Br	-2.80981200	3.13130300	-0.01419600

Cyclohexadienone Anion

O	-1.13514500	-0.50050700	1.95581600
C	-4.10716900	-0.21373300	-0.10103900
C	-3.68449700	0.57594800	-1.16970300
C	-2.34619500	0.98689900	-1.14136600
C	-1.50400500	0.62165700	-0.11036600
C	-1.91129800	-0.18165000	1.02364000
C	-3.29902700	-0.59467900	0.94680900
O	-0.21123800	1.18318500	-0.11747100
C	0.88124300	0.40303200	-0.09271400
C	0.86570100	-0.99618000	-0.19905600
C	2.04387500	-1.72950000	-0.21900300
C	3.26531700	-1.07003600	-0.13096700
C	3.32449700	0.31275800	-0.02583400
C	2.13429200	1.03190300	-0.01014500
Br	2.22611100	2.94451300	0.11964500
Br	4.90871900	-2.08251900	-0.15155400
H	-1.95072600	1.61688700	-1.93389600
H	-3.67072100	-1.20150000	1.76380100
H	-0.08897000	-1.49923700	-0.25701700
H	2.00541900	-2.80984200	-0.29146800
H	4.27214000	0.83010700	0.04084800
H	-4.34975500	0.85862200	-1.97444100
Br	-5.97548000	-0.80870800	-0.10169400