

Supporting Information

DFT Study of the Mechanism for Methane Hydroxylation by Soluble Methane Monooxygenase (sMMO) : Effects of Oxidation State, Spin State, and Coordination Number

Shu-Ping Huang, Yoshihito Shiota, and Kazunari Yoshizawa*

Institute for Materials Chemistry and Engineering, and International Research Center for Molecular Systems, Kyushu University, Fukuoka 819-0395, Japan

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* E-mail: kazunari@ms.ifoc.kyushu-u.ac.jp

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Cartesian coordinates

Table S1. Mulliken spin density during the reaction of Model1 with methane.

Spin density		Methane complex	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	3.48	3.48	3.43 (3.44)	4.26 (4.25)	4.23
	HS-AF	3.49	3.39	3.39	4.21	4.15
	IS-AF	1.75	1.92	1.67		
Fe2	HS-FM	3.30	4.16	4.26 (4.26)	3.57 (3.16)	4.21
	HS-AF	-3.32	-4.12	-4.21	-3.50	-4.14
	IS-AF	-1.80	-1.96	-2.16		
O3	HS-FM	0.15	0.31	0.39 (0.39)	0.48 (0.43)	0.71
	HS-AF	-0.15	0.05	0.00	-0.27	-0.06
	IS-AF	-0.30	-0.09	0.27		
O4	HS-FM	0.47	-0.12	0.24 (0.21)	0.05 (0.20)	0.05
	HS-AF	-0.19	0.24	-0.07	0.15	-0.05
	IS-AF	0.32	-0.03	0.00		
C	HS-FM	0.00	-0.53	1.11 (-1.10)	0.94 (-0.88)	0.00
	HS-AF	0.00	0.56	1.11	-1.01	0.00
	IS-AF	0.00	0.08	0.00		

¹¹**IM** (¹¹**TS2**) is energetically slightly more stable than ⁹**IM** (⁹**TS2**). Values in parenthesis represent the data at nonet.

Table S2. Mulliken spin density during the reaction of Model1H with methane.

Spin density		Methane complex	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	4.25	4.25	4.26	4.26	4.28
	HS-AF	4.21	4.24	4.26	4.26	4.27
	IS-AF	2.85	2.89	2.89		
Fe2	HS-FM	3.29	4.17	4.25	4.16	3.79
	HS-AF	-3.32	-4.16	-4.25	-4.14	-3.76
	IS-AF	-1.66	-1.76	-2.24		
O3	HS-FM	0.19	0.24	0.30	0.26	0.20
	HS-AF	-0.01	-0.03	-0.13	-0.02	0.05
	IS-AF	0.05	0.00	-0.07		
O4	HS-FM	0.46	-0.13	0.26	0.25	0.06
	HS-AF	-0.21	0.32	-0.26	-0.08	0.06
	IS-AF	-0.41	-0.36	0.03		
C	HS-FM	0.00	-0.49	-1.11	-0.85	0.00
	HS-AF	0.00	0.55	1.12	0.85	0.00
	IS-AF	0.00	0.08	0.30		

Table S3. Mulliken spin density during the reaction of Model2 with methane.

Spin density		Methane complex	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	3.50	4.21	3.39 (3.39)	3.70 (3.37)	4.25
	HS-AF	3.47	4.15	3.36	3.57	4.15
Fe2	HS-FM	3.44	3.32	4.29 (4.28)	4.28 (4.23)	4.20
	HS-AF	-3.42	-3.30	-4.25	-4.22	-4.17
O3	HS-FM	0.12	0.40	0.39 (0.39)	0.37 (0.35)	0.70
	HS-AF	-0.06	-0.30	0.11	-0.01	-0.02
O4	HS-FM	0.31	-0.26	0.23 (0.20)	0.11 (0.26)	0.08
	HS-AF	-0.05	-0.40	0.10	-0.19	-0.06
C	HS-FM	0.00	-0.47	1.11 (-1.10)	0.96 (-0.92)	0.00
	HS-AF	0.00	-0.55	1.10	1.04	0.00

¹¹**IM** (¹¹**TS2**) is energetically slightly more stable than ⁹**IM** (⁹**TS2**). Values in parenthesis represent the data at nonet.

Table S4. Mulliken spin density during the reaction of Model2H with methane.

Spin density		Methane complex	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	4.24	4.23	4.25	4.24	4.26
	HS-AF	4.19	4.21	4.24	4.24	4.25
Fe2	HS-FM	3.37	4.26	4.29	4.17	3.78
	HS-AF	-3.39	-4.22	-4.28	-4.14	-3.75
O3	HS-FM	0.14	0.19	0.26	0.22	0.19
	HS-AF	0.07	0.02	-0.07	0.03	0.07
O4	HS-FM	0.42	-0.20	0.26	0.24	0.05
	HS-AF	-0.16	0.40	-0.02	-0.08	0.04
C	HS-FM	0.00	-0.48	-1.11	-0.82	0.00
	HS-AF	0.00	0.54	1.11	0.82	0.00

Table S5. Mulliken spin density during the reaction of Model3H with methane.

Spin density		Q	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	4.27	4.26	4.27	4.27	4.24
	HS-AF	4.25	4.25	4.25	4.25	4.25
Fe2	HS-FM	3.13	4.06	4.21	4.14	3.83
	HS-AF	-3.12	-4.05	-4.19	-4.12	-3.77
O3	HS-FM	0.22	0.26	0.28	0.27	0.26
	HS-AF	0.09	0.08	0.07	0.10	0.17
O4	HS-FM	0.64	0.06	0.38	0.38	0.02
	HS-AF	-0.63	-0.04	-0.37	-0.37	-0.02
C	HS-FM	0.00	-0.55	-1.13	-0.99	0.00
	HS-AF	0.00	0.55	1.13	0.99	0.00

Table S6. Mulliken spin density during the reaction of Model4H with methane.

Spin density		Q	TS1	IM
Fe1	HS-FM	4.22	4.21	4.21
	HS-AF	4.21	4.21	4.20
Fe2	HS-FM	3.19	4.13	4.22
	HS-AF	-3.18	-4.11	-4.20
O3	HS-FM	0.16	0.24	0.27
	HS-AF	-0.03	-0.11	-0.14
O4	HS-FM	0.54	-0.59	0.27
	HS-AF	-0.52	0.11	-0.27
C	HS-FM	0.00	-0.59	-1.13
	HS-AF	0.00	0.58	1.13

Table S7. Mulliken spin density during the reaction of Model5 with methane.

Spin density		Q	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	4.23	4.25 (4.22)	4.24 (4.26)	2.22 (3.21)	4.22
	HS-AF	4.17	-4.23 (4.23)	-4.23 (4.26)	3.58	4.13
Fe2	HS-FM	3.14	3.97 (3.43)	3.17 (3.74)	4.12 (4.05)	4.12
	HS-AF	-3.12	3.97 (-3.55)	3.21 (-3.86)	-4.12	-4.13
O3	HS-FM	-0.08	-0.11 (-0.08)	0.59 (-0.21)	0.56 (0.49)	0.76
	HS-AF	-0.65	1.06 (-1.03)	0.42 (-1.03)	-0.11	-0.02
O4	HS-FM	0.37	-0.03 (0.19)	0.32 (0.16)	0.02 (0.15)	0.03
	HS-AF	-0.07	-0.21 (0.03)	0.12 (-0.02)	-0.23	-0.04
C	HS-FM		-0.50 (-0.12)	-1.06 (-0.37)	0.88 (-0.42)	0.00
	HS-AF		-0.45 (0.20)	1.09 (0.58)	0.98	0.00

The value in parenthesis is the spin density for the species via nonradical mechanism.

Table S8. Mulliken spin density during the reaction of Model5H with methane.

Spin density		Q	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	3.43	4.23	4.24 (4.25)	4.25	4.26
	HS-AF	-3.46	4.20	4.22 (4.24)	4.23	4.25
Fe2	HS-FM	4.13	4.03	4.14 (3.81)	4.08	3.80
	HS-AF	4.09	-4.02	-4.14 (-3.79)	-4.06	-3.76
O3	HS-FM	0.24	0.30	0.38 (0.29)	0.32	0.24
	HS-AF	0.29	-0.15	-0.26 (-0.15)	-0.15	0.09
O4	HS-FM	0.51	-0.07	0.27 (0.20)	0.30	0.04
	HS-AF	0.19	0.16	-0.14 (-0.09)	-0.20	-0.04
C	HS-FM		-0.44	-1.05 (-0.45)	-0.91	0.00
	HS-AF		0.47	1.06 (0.46)	0.91	0.00

The values in parenthesis are the spin densities for the nonradical **IM**.

Table S9. Mulliken spin density during the reaction of Model5H* with methane.

Spin density		Q	TS1	IM	TS2	Methanol complex
Fe1	HS-FM	4.26	4.27 (4.26)	4.27 (4.25)	4.27 (4.25)	4.26
	HS-AF	4.24	4.25 (4.25)	4.24 (4.25)	4.24 (4.25)	4.25
Fe2	HS-FM	3.18	4.01 (3.28)	4.16 (3.81)	4.10 (3.93)	3.80
	HS-AF	-3.14	-3.98 (-3.28)	-4.13 (-3.81)	-4.06 (-3.91)	-3.76
O3	HS-FM	0.19	0.29 (0.26)	0.29 (0.27)	0.28 (0.29)	0.24
	HS-AF	-0.01	-0.05 (-0.06)	-0.06 (0.03)	-0.01 (0.03)	0.09
O4	HS-FM	0.57	-0.07 (0.36)	0.36 (0.25)	0.34 (0.06)	0.04
	HS-AF	-0.56	0.08 (-0.33)	-0.35 (-0.24)	-0.34 (-0.05)	-0.04
C	HS-FM		-0.38 (0.08)	-1.05 (-0.41)	-0.94 (-0.28)	0.00
	HS-AF		0.37 (-0.05)	1.06 (0.45)	0.94 (0.29)	0.00

The values in parenthesis are the spin densities for the nonradical **TS1**, **IM** and **TS2**.

Table S10. The calculated free energies (Hartree) of the species along the reaction pathway of the different diiron models with methane at the B3LYP level.

G(hartree)	Q	TS1	IM	TS2	Methanol complex
Model1					
HS-FM	-4199.6791288	-4240.1542552	-4240.1716309	-4240.1652037	-4240.2825488
HS-AF	-4199.6868326	-4240.1579868	-4240.1743716	-4240.1687268	-4240.2919309
Model2					
HS-FM	-4199.6821623	-4240.1596728	-4240.1772057	-4240.1678966	-4240.2735076
HS-AF	-4199.6889084	-4240.1627377	-4240.1772273	-4240.173781	-4240.2863704
Model1H					
HS-FM	-4200.3405441	-4240.8215524	-4240.8387713	-4240.8234817	-4240.8992213
HS-AF	-4200.3411858	-4240.8185387	-4240.8370802	-4240.8263954	-4240.8188521
Model2H					
HS-FM	-4200.3454796	-4240.8226497	-4240.8450376	-4240.8252422	-4240.8997947
HS-AF	-4200.3473705	-4240.8206255	-4240.8429331	-4240.8218354	-4240.9003831
Model3H					
HS-FM	-4200.3398187	-4240.8155668	-4240.836652	-4240.826657	-4240.9098379
HS-AF	-4200.3394609	-4240.8161438	-4240.8361878	-4240.826934	-4240.9088249
Model4H					
HS-FM	-4276.2640178	-4316.7425009	-4316.7601525		
HS-AF	-4276.2638232	-4316.7419969	-4316.7600436		

Table S11. Calculated relative free energies (kcal/mol) during the reaction of Model1 with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	4.8	27.5	16.6	20.6	-53.0
	HS-AF	0.0	25.2	14.9	18.4	-58.9
B3LYP+PCM	HS-FM	4.9	27.6	16.6	20.7	-52.3
	HS-AF	0.0	25.2	14.8	18.4	-58.1
B3LYP*	HS-FM	5.5	32.0	24.2	28.1	-40.7
	HS-AF	0.0	29.0	21.6	25.3	-48.0
OPBE	HS-FM	8.9	42.4	41.7	47.1	-16.3
	HS-AF	0.0	37.4	35.8	41.8	-26.8

Table S12. Calculated relative free energies (kcal/mol) during the reaction of Model1H with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	0.4	19.4	8.6	18.2	-29.4
	HS-AF	0.0	21.3	9.6	21.1	-26.2
B3LYP+PCM	HS-FM	0.2	20.3	9.3	19.5	-29.4
	HS-AF	0.0	22.3	10.3	22.6	-26.5
B3LYP*	HS-FM	0.9	23.6	15.8	23.4	-21.5
	HS-AF	0.0	25.4	16.7	26.3	-18.7
OPBE	HS-FM	2.7	32.6	30.0	38.8	-2.2
	HS-AF	0.0	33.7	30.0	42.3	1.9

Table S13. Calculated relative free energies (kcal/mol) during the reaction of Model2 with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	4.2	25.4	14.6	20.2	-46.0
	HS-AF	0.0	23.5	14.4	16.6	-54.1
B3LYP+PCM	HS-FM	4.4	25.8	14.7	21.3	-45.5
	HS-AF	0.0	23.5	14.6	17.6	-52.3
B3LYP*	HS-FM	5.1	30.2	21.8	27.6	-34.2
	HS-AF	0.0	27.6	21.1	23.2	-43.3
OPBE	HS-FM	9.0	43.5	40.0	46.8	-9.5
	HS-AF	0.0	39.4	37.5	39.1	-22.1

Table S14. Calculated relative free energies (kcal/mol) during the reaction of Model2H with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	1.2	22.6	8.5	21.0	-25.8
	HS-AF	0.0	23.8	9.8	23.1	-26.2
B3LYP+PCM	HS-FM	1.0	23.0	8.9	21.7	-25.3
	HS-AF	0.0	24.3	10.4	24.0	-25.8
B3LYP*	HS-FM	1.8	27.3	15.7	25.9	-18.0
	HS-AF	0.0	28.2	16.8	28.1	-18.5
OPBE	HS-FM	4.0	39.5	18.0	42.5	1.8
	HS-AF	0.0	38.9	31.9	45.0	3.7

Table S15. Calculated relative free energies (kcal/mol) during the reaction of Model3H with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	0.0	22.3	9.1	15.3	-36.9
	HS-AF	0.2	21.9	9.3	13.6	-36.2
B3LYP+PCM	HS-FM	0.0	23.6	10.4	17.0	-34.4
	HS-AF	0.1	23.1	10.6	16.7	-33.8
B3LYP*	HS-FM	0.0	25.1	14.9	20.1	-30.4
	HS-AF	0.0	25.1	14.9	19.6	-29.3
OPBE	HS-FM	0.6	30.9	29.7	34.7	-14.5
	HS-AF	0.0	29.8	27.0	33.6	-9.1

Table S16. Calculated relative free energies (kcal/mol) during the reaction of Model4H with methane.

Method	Spin state	Q+CH ₄	TS1	IM
B3LYP	HS-FM	0.0	20.6	9.5
	HS-AF	0.1	20.9	9.6
B3LYP+PCM	HS-FM	0.0	21.3	10.3
	HS-AF	0.2	21.6	10.4
OPBE	HS-FM	0.3	29.5	26.4
	HS-AF	0.0	29.3	25.6

Table S17. Calculated relative free energies (kcal/mol) during the reaction of Model5 with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	0.0	18.0	-1.3(8.4)	12.0(11.9)	-72.6
	HS-AF	2.9	17.4	0.7(6.2)	2.1	-79.0
B3LYP+PCM	HS-FM	0.0	18.4	1.0(5.7)	12.2(12.7)	-67.8
	HS-AF	2.9	18.9	2.8(7.7)	4.0	-73.8
OPBE	HS-FM	0.0	31.8	11.1(4.4)	28.5(26.3)	-44.2
	HS-AF	5.2	39.1	5.2(2.3)	14.6	-55.6

The values in parenthesis are for the nonradical **IM** and **TS2**.

Table S18. Calculated relative free energies (kcal/mol) during the reaction of Model5H with methane.

Method	Spin state	Q+CH ₄	TS1	IM	TS2	Methanol complex
B3LYP	HS-FM	2.7	14.3	4.4(2.4)	10.8	-55.9
	HS-AF	0.0	15.3	5.7(3.2)	11.6	-56.8
B3LYP+PCM	HS-FM	2.5	15.2	4.9(3.5)	10.7	-52.2
	HS-AF	0.0	16.1	6.2(4.3)	11.6	-53.0
OPBE	HS-FM	5.7	28.3	27.4(21.1)	32.6	-25.0
	HS-AF	0.0	28.5	27.5(20.2)	32.3	-25.0

The values in parenthesis are for the nonradical **IM**.

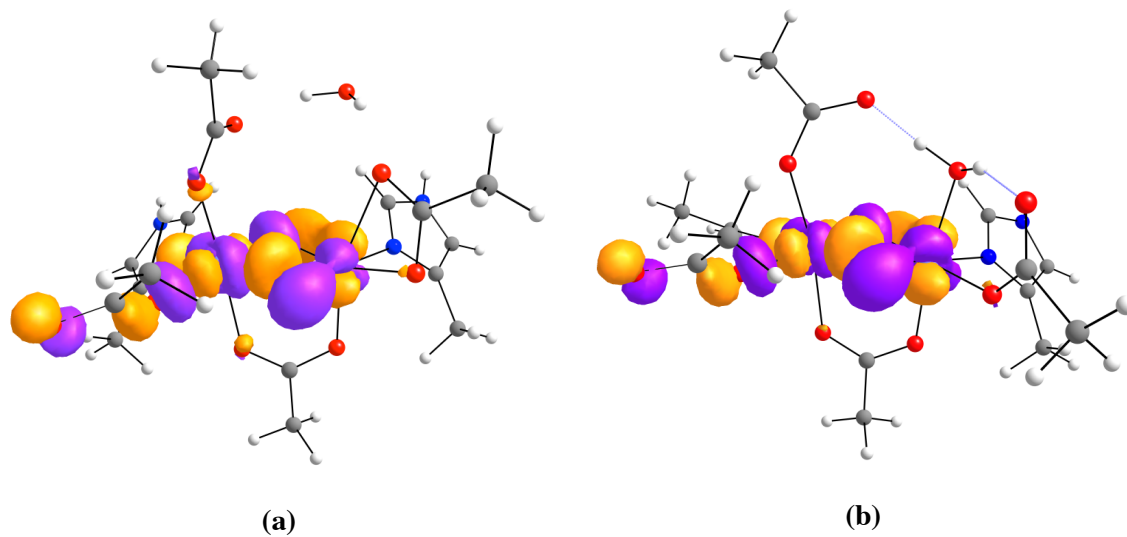


Fig. S1 (a) The LUMO of Model1 in the HS-AF state; (b) The LUMO of Model2 in the HS-AF state.

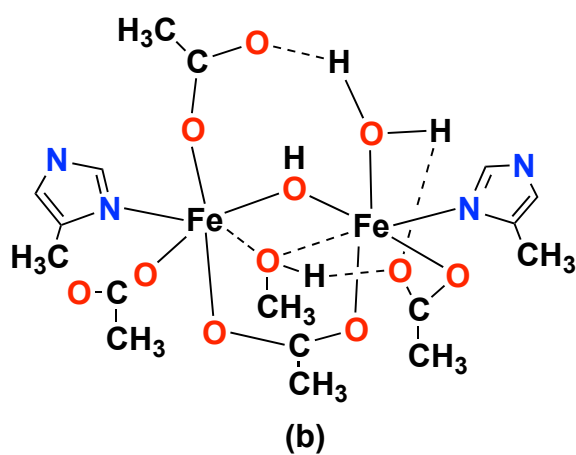
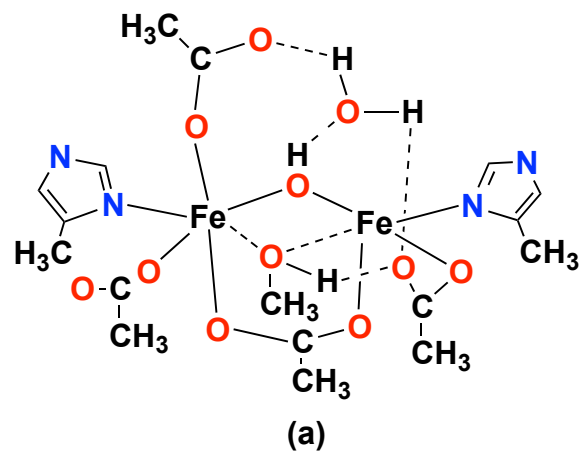


Fig. S2 Methanol complexes for (a) Model1H and (b) Model2H.

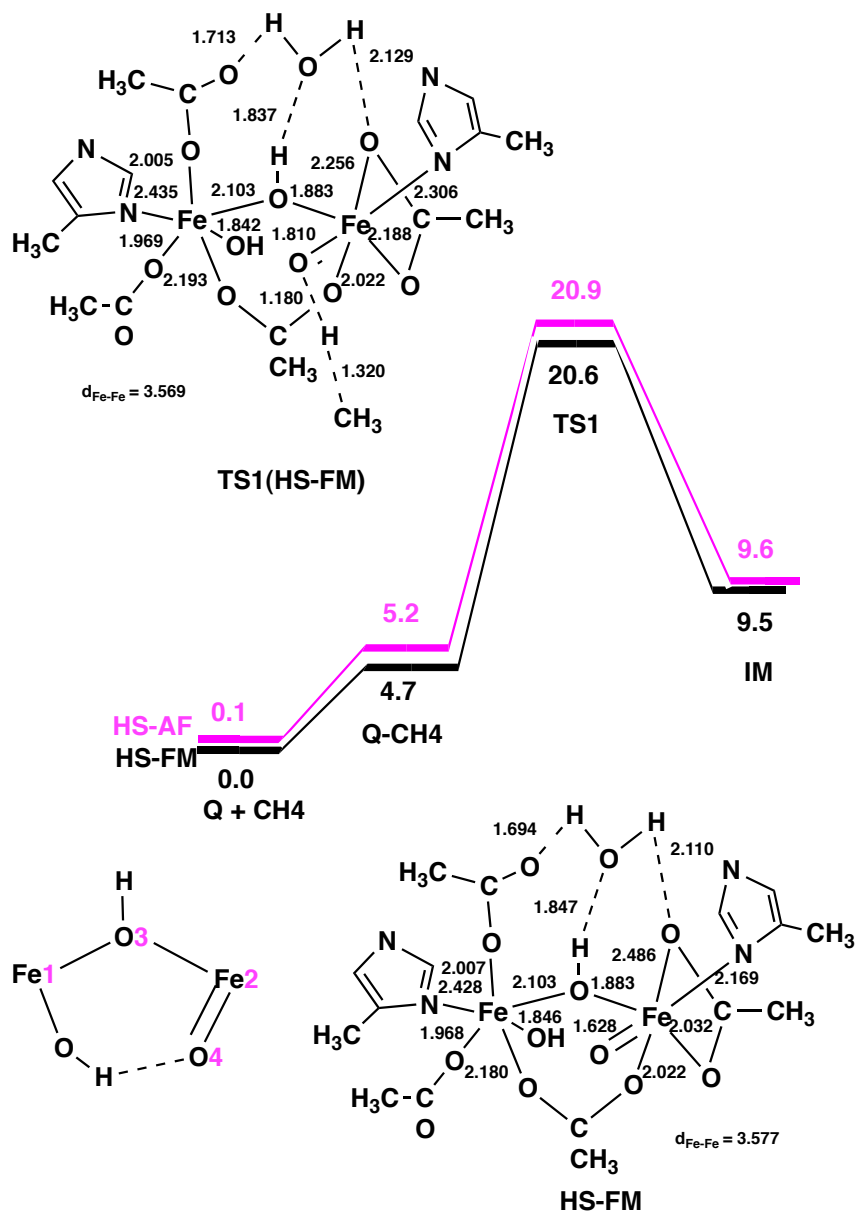


Fig. S3 Calculated free energy profiles of the reactions of Model4H with methane in the HS-FM and HS-AF states at the B3LYP level, and the structures of Model4H and **TS1** in the HS-FM state. The relative free energy is in kcal/mol. Distances are in angstroms.

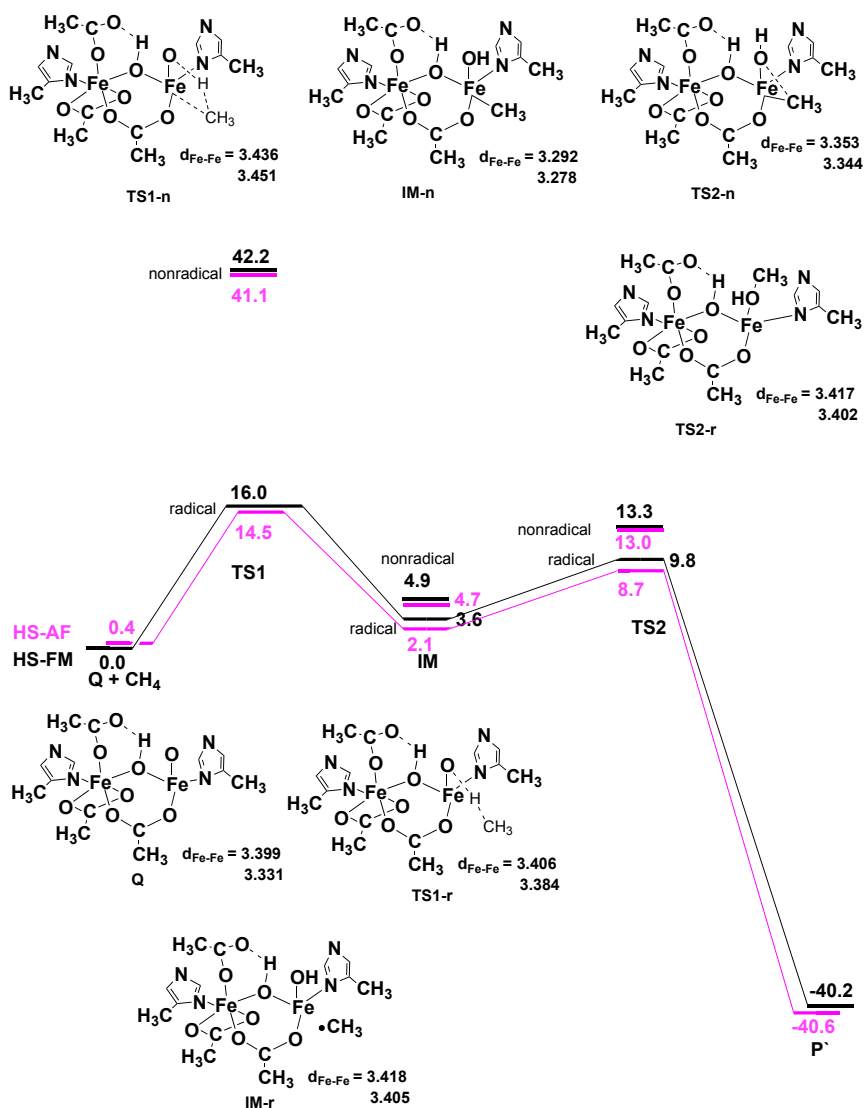


Fig. S4 Calculated free energy profiles of the reactions of Model5H* with methane in the HS-FM and HS-AF states at the B3LYP level. Distances are in angstroms. The above distance is for the HS-FM state, and the other one is for the HS-AF state.

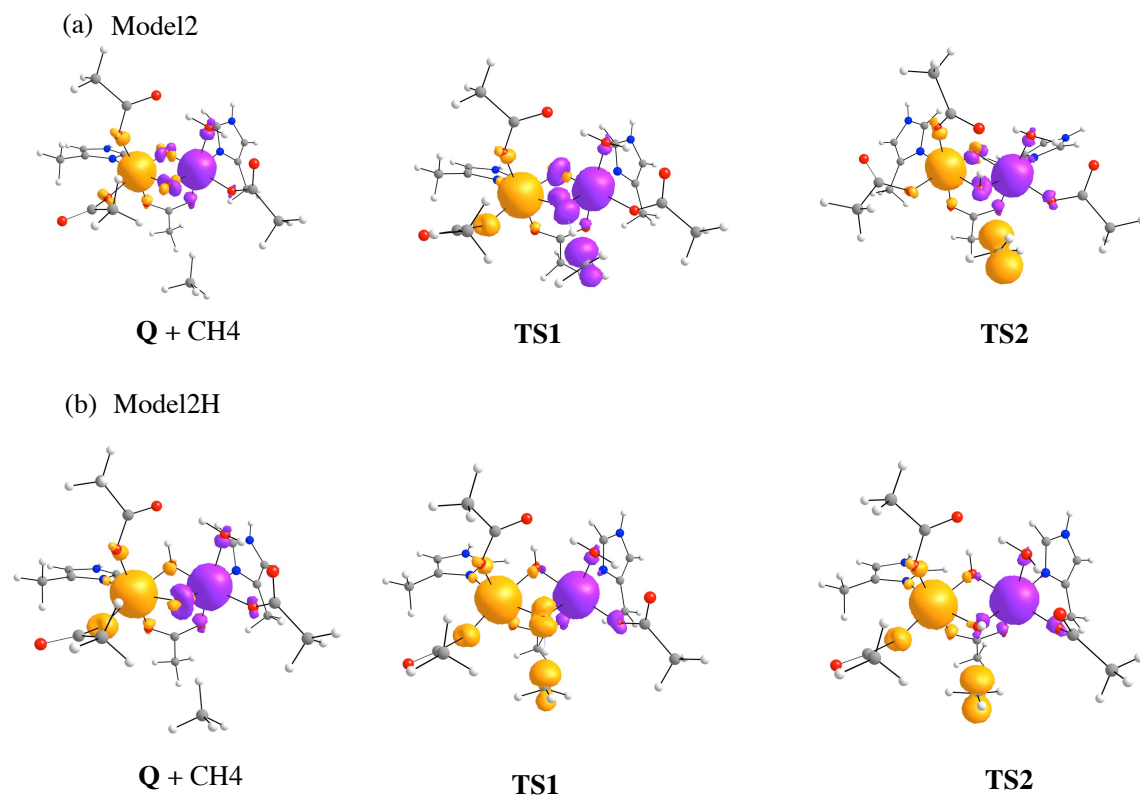


Fig. S5 The spin density distribution of (a) Model2 and (b) Model2H in the HS-AF state.

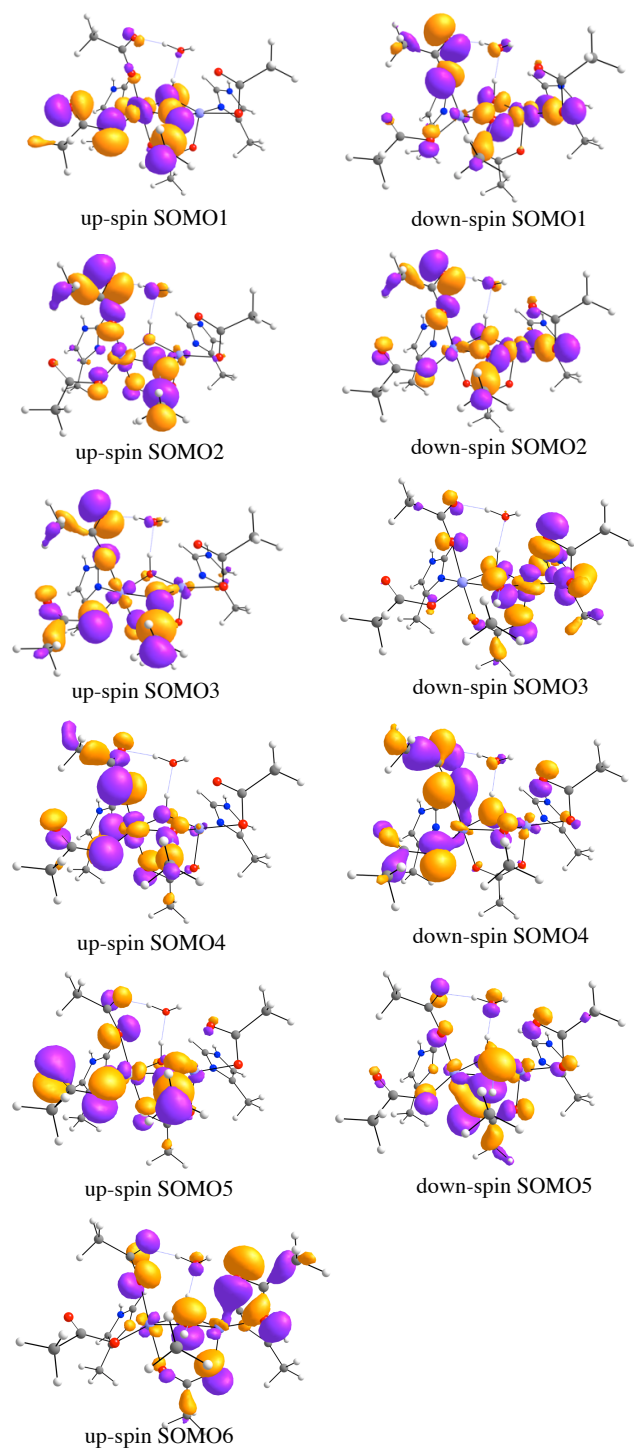


Fig. S6 The SOMO orbitals of Model1H.

Cartesian coordinates

Modell-RC-nonet (HS-FM)

C	-3.11066100	1.87902600	0.35684700	C	2.30744800	-2.07550100	1.55391400
O	-2.90659200	1.43591900	-0.84557300	N	2.53394600	-1.47190500	0.39225900
O	-2.43663500	1.42110300	1.31038900	H	4.83377600	-3.83604500	0.51938200
C	0.08342600	-0.93643800	-2.71787700	H	1.54931600	-1.77092600	2.26854500
O	1.13935000	-0.69757000	-2.06375600	Fe	1.29382200	0.16029300	-0.14975100
O	-1.10705600	-0.69382100	-2.32282500	Fe	-1.41575700	0.20373900	-0.52003000
C	-3.86190400	-1.78580500	-0.77336200	O	-0.12905400	-0.77205700	0.37122100
C	-4.54119200	-2.66665800	0.03807500	O	-2.11895900	-0.25330400	3.77097100
N	-3.89687100	-2.63735000	1.26807400	H	-2.34517900	0.46975400	3.15869900
H	-4.16272400	-3.13633400	2.10878100	H	-1.13995200	-0.23748700	3.80045800
C	-2.86816100	-1.76502300	1.19059100	O	-0.21289000	1.36934400	-0.78455300
N	-2.81669000	-1.23915600	-0.03158000	C	-0.46997400	4.85663800	-2.11061700
H	-5.40240400	-3.29049500	-0.15547200	H	-0.48693300	5.56983700	-1.27809300
H	-2.24852000	-1.49013100	2.03929800	H	-0.39417900	3.83549300	-1.72199500
C	3.74448800	1.71068900	-0.33423000	H	-1.39023700	4.95799700	-2.69753600
O	2.64261400	1.17545300	-0.87230700	H	0.39323300	5.06910500	-2.75182100
O	4.45498700	1.15362700	0.48650700	C	4.03391000	3.09331000	-0.90204000
C	0.93300100	0.98519500	2.68686600	H	5.00229500	3.44879900	-0.53947300
O	1.48465600	1.11869000	1.51051700	H	4.02250300	3.06237700	-1.99775000
O	0.65025300	-0.09953000	3.21980800	H	3.23948800	3.78074600	-0.58592500
C	3.61444300	-2.10381200	-0.21192400	C	-4.15188200	2.95936200	0.53712500
C	4.02931100	-3.12094900	0.61883300	H	-4.41522400	3.06202900	1.59322300
N	3.19453400	-3.08150700	1.72880800	H	-3.73564000	3.90846000	0.17560700
H	3.24120600	-3.68163200	2.54305600	H	-5.04035100	2.73625400	-0.06316500

C	-4.15477100	-1.41727500	-2.19572400	C	0.22761500	-1.59399000	-4.08124600
H	-4.29499600	-0.33395600	-2.28943200	H	0.02710400	-2.66836600	-3.97660100
H	-3.32343200	-1.69417200	-2.85187700	H	-0.50752000	-1.17810000	-4.77748800
H	-5.06569400	-1.92365000	-2.53358100	H	1.24122600	-1.45901800	-4.46749800
C	0.64445800	2.30934500	3.38038900	C	4.20798300	-1.68128400	-1.51964100
H	1.49002100	2.99426600	3.25896700	H	3.42566700	-1.52244200	-2.26746400
H	-0.22865800	2.76503900	2.89552700	H	4.75451100	-0.73948900	-1.39542300
H	0.42913600	2.14772700	4.44028100	H	4.90741000	-2.44487300	-1.87892100

Model1-TS1-nonet (HS-FM)

C	-3.09237500	1.98380800	-0.93654900	C	1.33336600	2.34449200	1.77723200
O	-2.98826300	1.01213300	-1.76592000	O	1.69193500	1.78966000	0.65660100
O	-2.38175200	1.96301900	0.11661700	O	0.85516600	1.75318200	2.75996900
C	-0.12251000	-2.19566000	-1.76271900	C	3.37182600	-2.09565500	0.97316500
O	0.96751200	-1.73173000	-1.34416400	C	3.70075400	-2.56168200	2.22686700
O	-1.28133600	-1.66327800	-1.59093900	N	2.91232300	-1.85236300	3.12434200
C	-4.13474000	-1.71456000	0.26405200	H	2.91631600	-1.93713100	4.13321700
C	-4.84801600	-1.99504300	1.40826900	C	2.13333800	-1.00083500	2.41851200
N	-4.22422500	-1.29273300	2.43172700	N	2.38734900	-1.12562900	1.12057600
H	-4.50736200	-1.25472900	3.40358000	H	4.41726500	-3.30697000	2.54250400
C	-3.17578500	-0.61621200	1.90733200	H	1.43120000	-0.29001100	2.84162700
N	-3.09190900	-0.85505000	0.59970600	Fe	1.27620400	0.09793400	-0.20850800
H	-5.72045300	-2.61218600	1.57134100	Fe	-1.55253400	0.04963600	-0.59931500
H	-2.55172100	0.07449800	2.47469400	O	-0.16806400	-0.24626500	0.70659200
C	3.90800000	0.89513100	-1.17891000	O	-1.96208400	1.95117600	3.06838300
O	2.69404800	0.39675300	-1.39388200	H	-2.14059400	2.23632200	2.15425900
O	4.51344400	0.86305400	-0.11716100	H	-0.98503200	1.90368000	3.11703800

O	-0.05547200	0.85543600	-1.46185700	H	-4.52097800	-1.32747500	-1.80914100
C	0.58179700	2.04842500	-3.57541900	H	-3.55088500	-2.77032300	-1.51502800
H	0.76170800	3.07736900	-3.25648000	H	-5.30226900	-2.79606300	-1.16696300
H	0.25684200	1.43143500	-2.49557200	C	1.56836600	3.85214600	1.80341800
H	-0.29121300	1.92250100	-4.22025400	H	2.61129500	4.06528500	1.54222700
H	1.47516600	1.51881000	-3.90992600	H	0.93394700	4.33013400	1.04656200
C	4.50374000	1.50576600	-2.44608700	H	1.33497700	4.25613200	2.79221100
H	5.55145200	1.76666400	-2.27334200	C	-0.10956400	-3.50649800	-2.53479900
H	4.42012200	0.80424100	-3.28458200	H	-0.61625100	-4.27693000	-1.93995400
H	3.94001700	2.40934700	-2.71064600	H	-0.66958000	-3.38812900	-3.46930100
C	-4.06664300	3.10598000	-1.20389300	H	0.91509200	-3.82269000	-2.74504000
H	-3.77358900	4.00631400	-0.65649700	C	3.96272900	-2.50267700	-0.34102000
H	-4.12786300	3.30692600	-2.27800600	H	3.17843800	-2.63579400	-1.09137600
H	-5.06251400	2.79605800	-0.86002200	H	4.65138300	-1.72883700	-0.69890400
C	-4.39406300	-2.18386400	-1.13548400	H	4.52248400	-3.43833300	-0.22700200

Modell-**IM**-undecet (HS-FM)

C	3.31513300	-0.71385600	2.20202300	O	4.52791800	0.51397400	-0.68865300
C	3.63219400	-0.14254200	3.41441000	C	-3.03833600	0.70595500	-2.19435900
N	2.84776700	0.99893900	3.52406200	O	-2.96194400	-0.56182500	-2.03317900
H	2.84688100	1.66300500	4.28833300	O	-2.36836000	1.45452400	-1.41136900
C	2.08179400	1.09180600	2.41344800	C	-0.17772000	-2.73399100	0.37338000
N	2.34032400	0.07317300	1.59979900	O	0.91888200	-2.12853800	0.31682400
H	4.33886600	-0.43988100	4.17637300	O	-1.32263100	-2.23546000	0.04821300
H	1.38834000	1.89591200	2.19016700	C	-4.18825000	-0.92868200	1.37633000
C	3.88467200	-0.17487300	-1.46719600	C	-4.92137300	-0.28516600	2.34820600
O	2.68169800	-0.69183000	-1.22377500	N	-4.30868200	0.94691300	2.53869700

H	-4.60713800	1.68325000	3.16712900	H	-4.69600000	0.61290300	-3.56200500
C	-3.24732400	1.02976800	1.70309500	H	-4.25833900	2.27396200	-3.01629900
N	-3.14421700	-0.09160700	0.99071700	C	-0.20350900	-4.17026700	0.87307000
H	-5.80117300	-0.59058800	2.89712000	H	-0.62186300	-4.18159000	1.88802500
H	-2.62428800	1.91859000	1.59270100	H	-0.85597400	-4.77918100	0.23801400
C	1.40103400	2.99162200	-0.43197200	H	0.80583800	-4.58882600	0.89841700
O	1.74216200	1.79179500	-0.80176200	C	-4.42907000	-2.27660600	0.76677400
O	0.88369300	3.29417300	0.65701400	H	-4.52613000	-2.19350600	-0.32262000
Fe	1.26533000	0.00449500	-0.21182000	H	-3.59108000	-2.95324400	0.96473000
Fe	-1.58630200	-0.33560500	-0.47664700	H	-5.34846200	-2.71501900	1.17067700
O	-0.18453500	0.44634200	0.62760500	C	3.91065600	-1.94065500	1.58430700
O	-1.94629400	3.58386500	0.63531200	H	3.12920900	-2.57370600	1.15521800
H	-2.09421000	3.12070000	-0.20855600	H	4.60273800	-1.65828300	0.78296000
H	-0.97214600	3.59324000	0.73674900	H	4.46689500	-2.50755100	2.33997800
O	0.00371600	-0.36790600	-1.69964000	C	4.40589800	-0.56252500	-2.84824300
H	0.24649800	-1.14444500	-2.23919000	H	4.30219300	-1.64173600	-3.01157200
C	1.02705400	-3.09152900	-3.35439600	H	3.80310200	-0.05267400	-3.61074700
H	1.77224500	-2.82098700	-2.61108600	H	5.45275300	-0.26297300	-2.94821400
H	1.12653800	-2.73925000	-4.37759000	C	1.71479000	4.05560800	-1.47888600
H	0.22239900	-3.77689700	-3.10116900	H	2.78358200	4.02333200	-1.72121800
C	-3.87623000	1.28979900	-3.30410900	H	1.16207300	3.83403200	-2.40006800
H	-3.23942800	1.41522700	-4.18983100	H	1.44209400	5.04699600	-1.10721500
Modell-TS2-undecet (HS-FM)							
C	3.10046700	-1.93658900	1.16844700	C	0.28891400	-0.33841000	-2.77071700
O	3.05412400	-1.90412300	-0.11028400	O	-0.82540100	-0.23264100	-2.18299800
O	2.33097600	-1.16876700	1.82743900	O	1.41766600	-0.49616700	-2.19430900

C	4.33136900	1.06639200	-0.98452900	H	1.85334800	0.43691400	3.07333700
C	5.07447500	2.12664200	-0.51490500	H	0.63706300	1.37415600	3.20144700
N	4.39373700	2.61552200	0.59377300	O	0.18259900	-1.74730300	0.00582400
H	4.67917300	3.38226400	1.19103900	C	-0.64633700	-4.02706900	-0.69038000
C	3.27837600	1.87146600	0.77451300	H	-0.68296100	-4.50685900	0.28442300
N	3.21481700	0.92960500	-0.16474700	H	0.13394700	-1.98203700	0.95266900
H	5.99833400	2.56087000	-0.87051200	H	-1.51543600	-3.50068500	-1.06843700
H	2.57515700	1.98647900	1.60160400	H	0.24874400	-4.11864200	-1.29602800
C	-4.02973100	-1.52053900	-0.13810900	C	-4.69187200	-2.87195000	-0.39361000
O	-2.83046300	-1.41488900	-0.68083100	H	-5.71530100	-2.86982900	-0.00877300
O	-4.58914400	-0.62951200	0.49913500	H	-4.69298300	-3.09398400	-1.46777300
C	-1.85028700	0.14637100	2.83614400	H	-4.11494200	-3.66273800	0.10324100
O	-1.60635600	-0.52382000	1.73982600	C	4.07734400	-2.85314000	1.86646500
O	-1.23304100	1.16443300	3.18552000	H	4.32330800	-3.70937100	1.23164800
C	-3.18032500	2.18249800	-1.19039700	H	3.66617500	-3.18468400	2.82490800
C	-3.37081800	3.50739400	-0.86742300	H	5.00035200	-2.29320200	2.06820900
N	-2.53077800	3.76757500	0.20889300	C	4.60844700	0.17448200	-2.15603100
H	-2.43821900	4.64407000	0.70744000	H	4.68643900	-0.87009000	-1.83348400
C	-1.86130400	2.62952000	0.50354200	H	3.79183600	0.22550300	-2.88444400
N	-2.23067900	1.65512300	-0.32191300	H	5.54423700	0.47070500	-2.64287100
H	-4.01999500	4.25897700	-1.29412700	C	-2.97814500	-0.42810900	3.67947300
H	-1.15383600	2.52284800	1.31547600	H	-3.89689200	-0.42335700	3.08065900
Fe	-1.35472300	-0.28917500	-0.16640400	H	-2.75631000	-1.47303100	3.93025800
Fe	1.61722900	-0.42686000	-0.17643300	H	-3.10918800	0.15644100	4.59404200
O	0.47322000	0.78329000	0.12746700	C	0.29498200	-0.25209100	-4.28844700
O	1.61488400	1.35792700	3.27861000	H	0.30503000	0.80768700	-4.57638200

H	1.18556900	-0.73485700	-4.70025300	H	-3.12699700	0.80645100	-2.83494400
H	-0.61391100	-0.70513300	-4.69558800	H	-4.55691700	0.66726400	-1.79683700
C	-3.85936600	1.37741600	-2.25465700	H	-4.41932600	2.03684400	-2.92770100
Modell- P -undecet (HS-FM)							
C	3.75497700	-1.15356200	1.20622500	N	-3.02135000	3.67446300	0.06548400
O	3.69089600	-1.36396600	-0.04613100	H	-3.04399400	4.56282300	0.55103400
O	2.74747400	-0.63226200	1.79868400	C	-2.38305400	2.56279200	0.50265800
C	0.04903300	-0.58769400	-2.53705800	N	-2.57543000	1.56129300	-0.35072500
O	-1.06012900	-0.42475000	-1.96192300	H	-4.25159200	4.08425600	-1.67749100
O	1.18838000	-0.72269900	-1.96735200	H	-1.84001700	2.47500000	1.43938400
C	3.43346200	1.85716000	-1.34085600	Fe	-1.69754500	-0.34600700	0.09310100
C	3.74977400	3.16730900	-1.05496600	Fe	1.64720600	-0.53598500	-0.00603100
N	3.05677800	3.48358200	0.10724000	O	0.03834900	0.01549600	0.62818700
H	3.08694000	4.36123600	0.61162400	O	1.22976300	1.64665800	3.24268800
C	2.35281200	2.39199500	0.49388100	H	1.64352200	0.79293500	3.02525200
N	2.55666900	1.39563800	-0.36471900	H	0.26618600	1.47545500	3.20532700
H	4.39175300	3.87395600	-1.56220100	O	1.14254300	-2.64567400	0.20416900
H	1.76338700	2.32822100	1.41071000	C	1.63410900	-3.66923500	-0.67510700
C	-2.74312400	-2.58271300	-0.44227900	H	1.41155200	-4.65871300	-0.25336100
O	-1.55222000	-2.50716700	0.03240700	H	0.15920000	-2.71224400	0.24042300
O	-3.37185200	-1.51255100	-0.67493300	H	2.71459300	-3.53410000	-0.75294200
C	-2.24519800	0.13728100	3.00359300	H	1.18478400	-3.58122100	-1.67324000
O	-2.53547100	-0.41969900	1.86613400	C	-3.37197700	-3.93616600	-0.67795000
O	-1.60867600	1.19870500	3.14031400	H	-4.25911200	-3.84290200	-1.31005500
C	-3.37788000	2.03914300	-1.38094700	H	-2.64570200	-4.61879400	-1.13274700
C	-3.66132900	3.36382700	-1.12872200	H	-3.66671400	-4.35922100	0.29118100

C	4.98726000	-1.51501100	2.00337500	H	-2.23364000	-1.57310900	4.30479700
H	4.73262400	-2.31363300	2.71136700	H	-2.61434800	-0.03241600	5.13182300
H	5.79281900	-1.85039200	1.34479600	C	0.05757500	-0.60520500	-4.06118100
H	5.31230600	-0.64885200	2.59145100	H	0.18415900	0.42495300	-4.42110000
C	3.92829800	1.00112200	-2.46707900	H	0.89357300	-1.20260300	-4.43708100
H	4.42810700	0.10827200	-2.07329400	H	-0.89350000	-0.98609100	-4.44500600
H	3.09705100	0.65585900	-3.09165400	C	-3.83739400	1.18712300	-2.52450000
H	4.63535700	1.56218800	-3.08860600	H	-2.98024100	0.80909500	-3.09203100
C	-2.76813600	-0.61794800	4.22133800	H	-4.38479500	0.31318500	-2.15394600
H	-3.83163900	-0.84973400	4.09029200	H	-4.48817100	1.76550900	-3.19000200

Model1-RC(HS-AF)

C	-2.99559900	1.94472400	-0.29811200	C	3.75112200	1.45546000	-0.87779800
O	-2.80558300	1.15000400	-1.30461300	O	2.61180700	0.84281900	-1.21533300
O	-2.36619700	1.74818400	0.77036000	O	4.46467700	1.13536600	0.05935500
C	0.01224600	-1.75719100	-2.36024000	C	1.03034300	1.66566500	2.36946300
O	1.08628500	-1.40168900	-1.81319600	O	1.53518900	1.45549300	1.19072500
O	-1.16503800	-1.36060700	-2.02528000	O	0.67408400	0.77272300	3.16118200
C	-3.95811800	-1.82586100	-0.25356800	C	3.55768900	-2.10711900	0.31098400
C	-4.69085300	-2.38330600	0.77003200	C	3.96867200	-2.86620300	1.38356500
N	-4.04836500	-2.02574000	1.94827300	N	3.16297500	-2.49984800	2.45447800
H	-4.34578000	-2.23542600	2.89386900	H	3.21606500	-2.85368500	3.40176700
C	-2.96808100	-1.27761700	1.63657700	C	2.29439400	-1.55704000	2.02757800
N	-2.88245600	-1.14467900	0.31389600	N	2.50601000	-1.30340600	0.73903100
H	-5.58739600	-2.98684400	0.75357900	H	4.75488500	-3.60280600	1.47033500
H	-2.33692400	-0.79409100	2.37818400	H	1.55865400	-1.04785300	2.64395600

Fe	1.27753400	0.09057600	-0.19218300	H	-3.45106800	3.88046900	-1.05801700
Fe	-1.39664600	-0.00203500	-0.54843300	H	-4.83581000	2.77607400	-1.04578200
O	-0.16771700	-0.66984600	0.57085300	C	-4.22689300	-1.88422400	-1.72620000
O	-2.09863600	0.87862500	3.63185200	H	-4.30431400	-0.87282500	-2.14183300
H	-2.28197900	1.40453100	2.83287400	H	-3.41098200	-2.38768800	-2.25419200
H	-1.11966400	0.86228100	3.68294700	H	-5.16453900	-2.41907100	-1.91355200
O	-0.10580000	0.99146200	-1.10530100	C	0.89092100	3.13895300	2.73157000
C	-0.38160400	4.43986300	-2.57497900	H	1.81044400	3.67690200	2.47687800
H	-0.55440600	5.15606400	-1.76306600	H	0.07783000	3.56922600	2.13269100
H	-0.22494800	3.43917700	-2.15842700	H	0.66168200	3.25425900	3.79456700
H	-1.24895300	4.42610300	-3.24523700	C	0.06807100	-2.73182300	-3.52721100
H	0.50609400	4.74377700	-3.14142200	H	-0.60695100	-3.57489900	-3.34008600
C	4.08031900	2.59423200	-1.83438200	H	-0.28197500	-2.22161900	-4.43303300
H	5.07197200	2.99514200	-1.60765000	H	1.08832600	-3.09195600	-3.68080100
H	4.03701900	2.24130200	-2.87135000	C	4.13417000	-2.08359900	-1.07000900
H	3.32411500	3.38142400	-1.72445400	H	3.34058400	-2.10887100	-1.82150900
C	-3.95581300	3.09678600	-0.47844300	H	4.71602200	-1.16655700	-1.21563700
H	-4.24847500	3.50379100	0.49320100	H	4.79971400	-2.94315400	-1.21031400
Modell-TS1(HS-AF)							
C	-3.11225800	1.79612200	-1.28432600	C	-4.82139500	-1.70266000	1.75677600
O	-3.01192900	0.69317100	-1.92616500	N	-4.19718300	-0.82657400	2.63552400
O	-2.38714200	1.96503900	-0.25254700	H	-4.47718900	-0.61638500	3.58606000
C	-0.15461000	-2.44536100	-1.39796100	C	-3.15652200	-0.24715100	1.99240600
O	0.94155200	-1.93933000	-1.05644200	N	-3.07698000	-0.71372800	0.74736500
O	-1.30490700	-1.86886400	-1.32280400	H	-5.68871100	-2.28630900	2.03207400
C	-4.11609000	-1.62510600	0.57629600	H	-2.53741500	0.53952800	2.42458800

C	3.92647700	0.65090400	-1.29187000	H	1.55106800	0.36937200	-4.04370500
O	2.70290800	0.14468000	-1.42177900	C	4.51847400	1.06193900	-2.63839500
O	4.54312500	0.75914800	-0.24202600	H	5.55207600	1.39141800	-2.50243900
C	1.37815000	2.63287700	1.36411300	H	4.48091400	0.22109200	-3.34172100
O	1.75090100	1.89541800	0.36258300	H	3.92257200	1.87837600	-3.06473100
O	0.85780700	2.21735600	2.41592900	C	-4.09389500	2.85186400	-1.73226100
C	3.30576000	-1.91813900	1.33060600	H	-3.80595400	3.83298500	-1.34438600
C	3.61517400	-2.17317600	2.64825400	H	-4.15735300	2.86955200	-2.82479700
N	2.84044400	-1.30406600	3.40584700	H	-5.08746700	2.59712600	-1.33988300
H	2.83745700	-1.21693800	4.41455000	C	-4.38191900	-2.33790200	-0.71509600
C	2.08645400	-0.56551100	2.56024200	H	-4.49974900	-1.61685700	-1.53303500
N	2.34423400	-0.91437800	1.30400100	H	-3.54613600	-2.99286200	-0.98219300
H	4.31129200	-2.87126100	3.09149000	H	-5.29692400	-2.93549800	-0.63494100
H	1.40338200	0.22695800	2.84955100	C	1.65345400	4.11979100	1.16038800
Fe	1.28069600	0.08207900	-0.21271600	H	2.72015400	4.26700500	0.95392100
Fe	-1.54988300	-0.02138200	-0.60984300	H	1.09690500	4.47726100	0.28529200
O	-0.17337800	-0.06783200	0.69895300	H	1.35983000	4.68759300	2.04742800
O	-1.95034800	2.49107400	2.65681900	C	-0.17137900	-3.86632600	-1.94226300
H	-2.12796100	2.60729300	1.70619000	H	-0.66380600	-4.52190400	-1.21263200
H	-0.97289400	2.45488400	2.71541600	H	-0.75728200	-3.90223100	-2.86752300
O	-0.04639400	0.64584800	-1.56931600	H	0.84566900	-4.22353900	-2.12221300
C	0.71151300	1.05543100	-3.92770500	C	3.89659800	-2.55547500	0.11149100
H	0.98202500	2.11306800	-3.92739400	H	3.11610600	-2.78620100	-0.61860300
H	0.32063800	0.83025300	-2.69455600	H	4.61543600	-1.87342600	-0.35675500
H	-0.17588200	0.81075800	-4.51592000	H	4.42296900	-3.47639200	0.38840700

Model1-**IM**(HS-AF)

C	3.06390200	0.40775000	2.16355600	H	-4.49009900	0.07249500	-4.08510800
O	3.02805000	-0.81305500	1.78850700	H	-1.57159900	2.17957900	-1.81575200
O	2.32863000	1.25050600	1.54926200	Fe	-1.29938000	-0.08109400	0.22452700
C	0.22195100	-2.65091900	-0.81756900	Fe	1.55335200	-0.34568700	0.34133800
O	-0.89187400	-2.09942300	-0.65869800	O	0.10568900	0.53606100	-0.54411900
O	1.35655200	-2.16156600	-0.44309700	O	1.74573400	3.69954700	-0.06267500
C	4.09542000	-0.51438600	-1.68614700	H	1.94248400	3.10319500	0.68167600
C	4.76244600	0.31817500	-2.55696700	H	0.76862200	3.68372900	-0.13389600
N	4.10488000	1.54044400	-2.49966500	O	0.02374300	-0.63627900	1.59882200
H	4.35183900	2.38727100	-2.99772800	C	0.69388600	-3.26008800	3.43265800
C	3.08195800	1.43372800	-1.61999900	H	1.60989100	-2.82432900	3.04258000
N	3.04565900	0.20102200	-1.11545900	H	-0.18717700	-1.50226000	1.99789800
H	5.62461100	0.14846600	-3.18661900	H	0.28295100	-4.16099600	2.98465000
H	2.43931900	2.26494800	-1.32550900	H	0.24202100	-2.85662000	4.33497400
C	-3.85725700	-0.60807800	1.51352100	C	-4.28729200	-1.25716300	2.82558300
O	-2.63837500	-0.99662600	1.14534000	H	-5.34185300	-1.04257100	3.01934900
O	-4.57555800	0.15438100	0.88341900	H	-4.11818700	-2.33980600	2.79005100
C	-1.56121700	2.81911100	0.94588500	H	-3.67243700	-0.85287600	3.63980900
O	-1.84319500	1.56351000	1.12620800	C	3.92877200	0.83783500	3.32235700
O	-1.06603600	3.30971900	-0.08501800	H	3.31931400	0.82130000	4.23568000
C	-3.39130800	-0.47791700	-2.21186700	H	4.76747800	0.14782200	3.45223000
C	-3.77096700	0.27168400	-3.30312900	H	4.28566700	1.86146500	3.17203300
N	-3.03668400	1.44953600	-3.24208900	C	4.40748600	-1.93803800	-1.33644400
H	-3.08907500	2.23064000	-3.88417700	H	4.56998700	-2.04118200	-0.25658800
C	-2.23789100	1.39210700	-2.15283400	H	3.57604600	-2.59972300	-1.60092800
N	-2.42849200	0.24234900	-1.51341100	H	5.31082200	-2.26653300	-1.86250400

C	-1.91507100	3.69640300	2.14259900	H	1.00578300	-4.65391300	-1.00986300
H	-2.98074600	3.58208100	2.37381600	H	-0.70169800	-4.46671000	-1.54471900
H	-1.35091400	3.35998000	3.02104500	C	-3.91649500	-1.81528400	-1.79227400
H	-1.68606100	4.74382900	1.92851800	H	-3.09616200	-2.48100200	-1.51018600
C	0.28669500	-4.00085200	-1.51550700	H	-4.57870200	-1.70044900	-0.92705900
H	0.63898100	-3.84811800	-2.54421000	H	-4.48890500	-2.26548900	-2.61171100

Model1-TS2(HS-AF)

C	3.09885400	-1.99091500	1.05384500	O	-1.23843300	1.01586600	3.22201400
O	3.05090000	-1.87670600	-0.22188400	C	-3.16335200	2.24615100	-1.09566500
O	2.33183600	-1.26246300	1.75683600	C	-3.36710400	3.55109700	-0.70577200
C	0.30305800	-0.19896500	-2.78713900	N	-2.53681400	3.76203900	0.38855400
O	-0.81263200	-0.12345300	-2.20204100	H	-2.45778600	4.61111400	0.93457500
O	1.43054700	-0.38681100	-2.21205000	C	-1.86018000	2.61503700	0.62841300
C	4.30524400	1.14691600	-0.90924100	N	-2.21509800	1.68192900	-0.24914200
C	5.03516300	2.18629700	-0.37679700	H	-4.02033500	4.31825900	-1.09710300
N	4.34701800	2.60299000	0.75623500	H	-1.16150900	2.47043500	1.44222500
H	4.62341700	3.33606800	1.39843100	Fe	-1.33297400	-0.26992500	-0.18149300
C	3.23971500	1.83807500	0.89129800	Fe	1.61709400	-0.42231400	-0.20324300
N	3.18828900	0.95134600	-0.10127800	O	0.45879100	0.73715000	0.15366200
H	5.95471000	2.65048400	-0.70457900	O	1.59056200	1.18367200	3.35474400
H	2.53591400	1.89428800	1.72446600	H	1.83162300	0.27079900	3.11949200
C	-4.01069400	-1.50543200	-0.22960300	H	0.61201300	1.20192100	3.27700200
O	-2.80894800	-1.36570900	-0.75618700	O	0.17711400	-1.74921900	-0.08808800
O	-4.59359300	-0.63835200	0.42067700	C	-0.65897200	-4.18202400	-0.77167300
C	-1.85870100	0.01419900	2.82912000	H	-0.70647300	-4.70938300	0.17806100
O	-1.62152700	-0.60881300	1.70600000	H	0.12311600	-2.05120200	0.83866700

H	-1.49946100	-3.58370100	-1.10572300	H	5.53500200	0.66118900	-2.58952700
H	0.23734500	-4.25153000	-1.37904500	C	-2.98603100	-0.59236300	3.65085100
C	-4.64622000	-2.86268200	-0.51980900	H	-3.90670200	-0.55830800	3.05586100
H	-5.67666800	-2.88380700	-0.15452700	H	-2.76755100	-1.64805000	3.85494100
H	-4.62265000	-3.06758100	-1.59705300	H	-3.11261300	-0.04779900	4.59040700
H	-4.06580500	-3.65186200	-0.02439100	C	0.32310900	-0.03635900	-4.29811200
C	4.07167500	-2.95760100	1.68463300	H	0.36084000	1.03590000	-4.53265000
H	4.16316000	-3.85858100	1.06975900	H	1.20559500	-0.51885400	-4.72743400
H	3.75365800	-3.21103400	2.69981300	H	-0.59269400	-0.44762400	-4.73276400
H	5.05957500	-2.48064900	1.73498100	C	-3.83147700	1.49174900	-2.20306800
C	4.59756600	0.32892800	-2.13001600	H	-3.09349400	0.95022200	-2.80386500
H	4.68107100	-0.73262000	-1.87076100	H	-4.52999800	0.75886100	-1.78423800
H	3.78711200	0.41771000	-2.86159500	H	-4.38814300	2.18150400	-2.84795000

Model1-P(HS-AF)

C	3.72293600	-1.12181800	1.25577300	H	4.37343700	3.83348200	-1.61484200
O	3.68515800	-1.35683000	0.00825900	H	1.73144700	2.34590900	1.37465600
O	2.69839900	-0.59858200	1.81892000	C	-2.74763500	-2.57292900	-0.44190200
C	0.05654600	-0.62270400	-2.54168200	O	-1.55208500	-2.49290100	0.02844100
O	-1.05409100	-0.43467100	-1.97758500	O	-3.37886200	-1.50923800	-0.68085000
O	1.18957200	-0.77531400	-1.96182600	C	-2.25694500	0.15105600	2.98321100
C	3.40458800	1.82521200	-1.36605300	O	-2.54144900	-0.41312800	1.84960300
C	3.72551600	3.13825900	-1.09947400	O	-1.57665800	1.18606100	3.12029700
N	3.02939200	3.47616500	0.05452600	C	-3.32995900	2.05193700	-1.38249400
H	3.06304200	4.36099100	0.54602200	C	-3.60974700	3.37753900	-1.13044900
C	2.31905700	2.39406500	0.45563500	N	-2.95952100	3.69004500	0.05749100
N	2.52102600	1.38325000	-0.38653000	H	-2.97841100	4.57896800	0.54214700

C	-2.31879400	2.57828200	0.49123200	H	-3.91177200	-0.75264300	4.04065700
N	-2.51906000	1.57515100	-0.35814900	H	-2.34918800	-1.52841300	4.32155400
H	-4.20411000	4.09729400	-1.67565400	H	-2.69730200	0.04321600	5.10238200
H	-1.77151600	2.49165200	1.42514000	C	4.94121200	-1.45624600	2.08589500
Fe	-1.66362800	-0.34314600	0.08892900	H	5.76723500	-1.78514200	1.44976900
Fe	1.62220900	-0.54604800	0.00068200	H	5.23885400	-0.58053600	2.67425800
O	0.03220500	-0.02041200	0.60595300	H	4.68203100	-2.25315700	2.79428000
O	1.23102400	1.68825000	3.21889400	C	3.90542600	0.94969300	-2.47449800
H	1.66150200	0.83736100	3.02217900	H	4.39561700	0.06011100	-2.06176900
H	0.27068400	1.49511200	3.20548500	H	3.07972100	0.60000800	-3.10373600
O	1.13515300	-2.65704500	0.24136700	H	4.62293600	1.49762500	-3.09577500
C	-3.80217000	1.19928900	-2.52036300	C	0.07783200	-0.65292400	-4.06528400
H	-2.95201300	0.82454800	-3.10035200	H	0.23588100	0.37019800	-4.43283000
H	-4.34099300	0.32311900	-2.14286800	H	0.90086200	-1.27593400	-4.42813900
H	-4.46403100	1.77648800	-3.17593400	H	-0.87972000	-1.01143300	-4.45437400
C	-3.36755700	-3.93342800	-0.66427900	C	1.65209800	-3.68932600	-0.61290200
H	-4.27988400	-3.84694400	-1.26033300	H	1.22507600	-3.61694300	-1.62196600
H	-2.65078700	-4.60113800	-1.15550700	H	1.42563200	-4.67441000	-0.18299100
H	-3.61564200	-4.37112600	0.31129000	H	2.73330100	-3.54894600	-0.66823000
C	-2.84505500	-0.55657100	4.20017500	H	0.15112500	-2.72839700	0.25720400
Model1-RC(IS-AF)							
C	1.76737700	2.42607400	1.63511000	O	1.37050900	-1.97164600	0.57053000
O	2.23759400	1.40230300	0.92058500	C	3.96636100	-1.21699900	-1.31940000
O	1.36269600	3.45721200	1.10451300	C	4.77946700	-0.70351600	-2.30455300
C	0.26565800	-2.62678500	0.65171000	N	4.30582300	0.57365300	-2.56997500
O	-0.88477900	-2.15849400	0.46400700	H	4.67693300	1.23580500	-3.24126600

C	3.25053800	0.81814100	-1.76365000	C	-3.99014600	0.48487100	3.20959700
N	3.01791000	-0.24911000	-0.99515900	C	1.82811000	2.23841400	3.13774900
H	5.63193600	-1.12994000	-2.81426600	C	-1.86515600	3.93616700	-0.10607800
H	2.68722300	1.75785000	-1.76555400	C	4.06809300	-2.56665500	-0.67535500
C	-3.70542600	0.20263700	1.73865900	C	-3.97370400	-2.53159400	-0.36996600
O	-2.56533100	-0.46696400	1.57372200	H	3.18907900	-3.18073300	-0.89955500
O	-4.47324100	0.52138900	0.84063200	H	4.95975900	-3.08395600	-1.04679800
C	-1.48929300	2.55843800	-0.63745100	H	4.14232800	-2.48448800	0.41495800
O	-1.78640800	1.60846400	0.20908400	H	-4.58224000	-3.33717100	-0.79743800
O	-0.95991700	2.41803400	-1.75050800	H	-3.17978200	-2.96343500	0.24460100
C	-3.40635300	-1.69154900	-1.47166100	H	-4.60802200	-1.91615400	0.27605400
C	-3.78390200	-1.69210200	-2.79534800	H	-5.00466600	0.87620500	3.32660200
N	-3.01431100	-0.72181800	-3.42359400	H	-3.85914500	-0.42506900	3.80684700
H	-3.05575800	-0.45104400	-4.39833100	H	-3.26375000	1.22291200	3.57340100
C	-2.19856000	-0.16737400	-2.50035200	H	-2.80556200	3.89201800	0.45191500
N	-2.41077700	-0.72979600	-1.31311600	H	-1.06996300	4.26030400	0.57709100
H	-4.52686500	-2.27734100	-3.31848300	H	-1.93843700	4.64559600	-0.93546600
H	-1.49841400	0.63992500	-2.67882700	H	1.06423000	1.50123000	3.41475700
Fe	-1.25849200	-0.19452900	0.29389900	H	2.80559700	1.83894300	3.43198900
Fe	1.42178900	-0.10604500	0.25982900	H	1.63190400	3.18591700	3.64628800
O	0.24309700	-0.06273900	-0.93124400	H	1.40107400	-4.45947100	0.84698000
O	1.70736700	3.45941700	-1.79121400	H	0.13891900	-4.20336000	2.08010000
H	1.67419900	3.58769400	-0.82032400	H	-0.33853800	-4.67797900	0.44016300
H	0.79123600	3.18986900	-2.00443800	C	4.18262200	-2.03317600	3.59923700
O	0.02147200	0.11043900	1.44447800	H	4.65441700	-3.02215100	3.58925300
C	0.38528600	-4.09351000	1.01632200	H	3.95232800	-1.75008400	4.63205500

H	4.86712800	-1.29599600	3.16472000	H	3.25628900	-2.05967200	3.01483200
Model1-TS1(IS-AF)							
C	-2.24779500	2.61461700	-0.42678100	C	1.60560100	-0.36557300	2.53315000
O	-2.04975800	1.55669000	-1.19035100	N	2.18436100	-0.68417500	1.38020700
O	-2.11861800	2.66740200	0.79223400	H	4.31252200	-1.75105400	3.66712200
C	-0.26332600	-2.75659700	-0.63258400	H	0.65700500	0.13904600	2.64267300
O	0.87571600	-2.24758900	-0.45685700	Fe	1.21366000	-0.29421900	-0.36988000
O	-1.35127000	-2.11134700	-0.82778500	Fe	-1.47070400	-0.16171200	-0.82606200
C	-4.27739700	-1.05234300	0.40377300	O	-0.30910600	-0.04680200	0.53294700
C	-4.85917600	-0.99817600	1.65022500	O	-0.77533900	2.01688900	3.21243900
N	-3.94266900	-0.36156800	2.47505100	H	-1.34356200	2.39485700	2.51556800
H	-4.05402300	-0.14070400	3.45761400	H	0.11529100	2.18069700	2.84224900
C	-2.85509900	-0.04508000	1.73965000	O	0.04006700	0.01544400	-1.86467900
N	-3.02631900	-0.44548500	0.48061800	H	-0.81646500	-0.43961100	-2.55686200
H	-5.81732500	-1.35324900	2.00278100	C	-2.16542600	-0.58429000	-3.00239100
H	-1.97962200	0.45508500	2.13619500	H	-2.04611100	-1.57435700	-3.45747100
C	3.44619300	0.17873100	-2.12986700	H	-2.08944200	0.23742900	-3.72418400
O	2.67987800	-0.65554500	-1.41273400	H	-3.15488100	-0.53060200	-2.54325400
O	4.59136200	0.44831100	-1.79584000	C	-4.85011100	-1.65927700	-0.84066300
C	1.85842100	2.43852400	0.47238700	H	-5.10082800	-0.89415100	-1.58678800
O	1.68601700	1.53379600	-0.45947300	H	-4.14235600	-2.36071000	-1.29604100
O	1.56707300	2.34509900	1.66715900	H	-5.77074500	-2.20174600	-0.59924900
C	3.39486100	-1.31409100	1.67330500	C	-2.67400600	3.82431900	-1.25215000
C	3.52393700	-1.35340500	3.04419100	H	-3.53344600	3.56973900	-1.88296700
N	2.38348500	-0.75627000	3.56433800	H	-2.92315400	4.65497300	-0.58677700
H	2.17499500	-0.58513900	4.54029300	H	-1.85165600	4.11426900	-1.91731800

C	2.50182700	3.70396800	-0.09340000	C	4.36333900	-1.86171300	0.67054100
H	1.98007600	4.02412700	-1.00198300	H	3.87576000	-2.59178800	0.01542400
H	2.48124000	4.49659700	0.65934700	H	4.76594100	-1.07110500	0.02934600
H	3.53962700	3.47964900	-0.36940100	H	5.18712300	-2.35367200	1.20194600
C	2.81154500	0.67618300	-3.41578900	C	-0.37693200	-4.26836300	-0.58314500
H	2.60674800	-0.18015700	-4.07127200	H	-1.17263400	-4.61319000	-1.24996500
H	1.85273900	1.15273600	-3.18712100	H	0.57964500	-4.72546200	-0.84967800
H	3.48552000	1.37552200	-3.91863500	H	-0.63377300	-4.56471900	0.44221200

Model1-**IM**(IS-AF)

C	-1.75680400	2.79602600	-1.01164800	C	1.22233100	2.46201400	1.00826900
O	-2.10549200	1.59031100	-0.58900700	O	1.51101900	1.65649300	0.02534200
O	-1.83787200	3.75235600	-0.23694300	O	0.68261500	2.15681000	2.08374600
C	-0.11385800	-2.67348700	-1.00311400	C	3.32677300	-1.69855800	1.42078200
O	0.98979300	-2.11517200	-0.75442600	C	3.62421900	-1.84835900	2.75626700
O	-1.24883100	-2.09449400	-1.12159900	N	2.74925200	-1.02426500	3.45033400
C	-4.03154500	-1.64474700	0.52133200	H	2.71252700	-0.88268100	4.45209300
C	-4.72970100	-1.47148800	1.69439300	C	1.94959400	-0.40643900	2.55472600
N	-4.19279200	-0.34580000	2.30261500	N	2.27424900	-0.78913700	1.32312300
H	-4.47872700	0.07782000	3.17790000	H	4.37671500	-2.44863500	3.24754700
C	-3.20988500	0.14288600	1.52029900	H	1.18096200	0.32200200	2.78118400
N	-3.08352100	-0.62409400	0.43233700	Fe	1.18759400	-0.18763300	-0.22883600
H	-5.54526500	-2.03750800	2.12189600	Fe	-1.58308600	-0.17552200	-0.81531800
H	-2.64452300	1.04355800	1.77105300	O	-0.27639500	-0.27970300	0.62539100
C	3.71816900	0.50661900	-1.52620400	O	-2.06950800	2.79860300	2.50211300
O	2.59840000	-0.19841900	-1.49508600	H	-2.14860000	3.23981500	1.63039700
O	4.38012500	0.83114000	-0.54583000	H	-1.10834100	2.62788100	2.56707800

O	0.00137400	0.29116700	-1.75465600	H	3.42582200	1.57757800	-3.36999300
C	-0.11272900	-4.18362400	-1.16612200	H	2.39523700	3.97216500	-0.02943700
C	4.14472400	0.86268100	-2.94891600	H	0.69618000	4.40892100	0.30522600
C	-1.33751000	2.98599300	-2.45722400	H	1.87476100	4.41383500	1.63576900
C	1.58855800	3.91156400	0.70630200	H	-0.46414100	2.36226800	-2.66803000
C	-4.26028800	-2.70641900	-0.51162100	H	-2.15183300	2.67748000	-3.12465400
C	4.02343500	-2.35697900	0.27089500	H	-1.10786700	4.04038600	-2.62962700
H	-3.33507200	-3.24323000	-0.73827700	H	-0.34626800	-4.63580500	-0.19315700
H	-5.00892500	-3.41813600	-0.14646200	H	-0.87801900	-4.49551400	-1.88311300
H	-4.63306100	-2.27553600	-1.44912200	H	0.87531900	-4.53025100	-1.48060500
H	4.63610500	-3.18644600	0.64363000	C	-2.72708400	-0.26832500	-2.49718400
H	3.30507900	-2.73607200	-0.45951400	H	-2.79494800	-1.32262900	-2.76753400
H	4.67700800	-1.63639700	-0.23105200	H	-2.19887100	0.32320500	-3.24784700
H	5.14275200	1.30977300	-2.94226400	H	-3.69138900	0.17367000	-2.23762600
H	4.13345100	-0.02983200	-3.58637100	H	0.24417800	-0.33544500	-2.45967700
Model1H-RC(HS-FM)							
C	-3.02810900	2.04331500	0.74096900	C	-3.22038100	-1.71242100	1.39476200
O	-3.01224900	1.61527600	-0.48230600	N	-3.20799300	-1.06609900	0.23348800
O	-2.33246200	1.46854400	1.61059300	H	-6.08640700	-2.68982100	0.21908700
C	-0.40005600	-1.21705700	-2.53021200	H	-2.44790000	-1.67016200	2.15293200
O	0.71476400	-1.03172900	-1.97697700	C	3.64316600	1.64180000	-1.20775700
O	-1.53372800	-0.82785300	-2.06936300	O	2.49742800	1.01854000	-1.40271100
C	-4.39465700	-1.36854200	-0.42809600	O	4.51704400	1.25972800	-0.42975900
C	-5.12366800	-2.22219300	0.37026200	C	2.14746300	1.10543600	2.55128300
N	-4.36502700	-2.42411800	1.51552200	O	1.62261600	1.04891300	1.36493100
H	-4.61360600	-2.99647600	2.31338300	O	1.72032300	0.44996900	3.52462000

C	3.47590000	-2.28958000	-0.34709300	H	3.66934900	2.62888100	-3.12743000
C	3.95256000	-3.27758200	0.48649300	H	3.02438600	3.61335100	-1.81145400
N	3.24742400	-3.15371600	1.67643800	C	-3.88068600	3.25273400	1.04877000
H	3.36660200	-3.71224000	2.51267000	H	-3.36764400	4.14390700	0.66522400
C	2.37844700	-2.12468300	1.54004300	H	-4.84722800	3.17972200	0.53865400
N	2.48787900	-1.58408000	0.33189600	H	-4.01985700	3.35575400	2.12823900
H	4.71891300	-4.02553700	0.33954400	C	-4.75067800	-0.82215400	-1.77716100
H	1.72012600	-1.78536600	2.32799600	H	-4.79132700	0.27274700	-1.75090400
Fe	1.27317300	0.09848400	-0.27475800	H	-3.99448200	-1.10373500	-2.51771100
Fe	-1.64413000	0.20169700	-0.35025800	H	-5.72588600	-1.20743800	-2.09458100
O	-0.42210300	-0.87197400	0.59711000	C	3.32769300	2.04866600	2.70034100
O	-0.83837100	-0.36344300	3.19834200	H	4.09112800	1.78835300	1.95816400
H	-1.33170400	0.45642400	3.00542900	H	2.99758900	3.07201200	2.47961300
H	0.08582300	-0.07215800	3.43073200	H	3.73088200	2.00091200	3.71546900
O	-0.39698500	1.24574400	-0.75594000	C	-0.44034500	-1.94520100	-3.86366600
H	-0.51113300	-0.71243900	1.58374900	H	-1.27114900	-2.65844200	-3.88080500
C	-0.75219200	4.94094500	-1.40416400	H	-0.61449700	-1.20817800	-4.65817400
H	-0.62559400	5.45629000	-0.44471000	H	0.50769000	-2.45536600	-4.05197900
H	-0.65053000	3.86021700	-1.25932600	C	3.92747600	-1.94984500	-1.73354200
H	-1.74384100	5.16512400	-1.81457300	H	3.06951200	-1.84408200	-2.40489800
H	0.01486500	5.29014400	-2.10485800	H	4.46775400	-0.99662700	-1.72332000
C	3.80618400	2.88823700	-2.07047400	H	4.59472500	-2.73176100	-2.11425800
H	4.79342400	3.33239100	-1.91575400				

Model1H-TS1(HS-FM)

C	-3.05396400	2.31597900	0.30893500	O	-2.33546300	1.76477000	1.19597100
O	-3.09043000	1.80107100	-0.86545300	C	-0.44806800	-1.44976900	-2.31539500

O	0.66603500	-1.22132900	-1.78146100	O	-0.45235200	-0.58208700	0.72400400
O	-1.57016800	-0.92972300	-1.95784300	O	-0.92309700	0.31357500	3.22983800
C	-4.56773600	-1.30630000	-0.24414500	H	-1.38377800	1.09904300	2.88049900
C	-5.29294600	-2.02840500	0.67936300	H	0.00660300	0.60707200	3.42747900
N	-4.53641800	-2.02879900	1.84438300	O	-0.21138100	1.32869900	-0.95410100
H	-4.78072300	-2.46779400	2.72385100	H	-0.54130100	-0.28969600	1.67409600
C	-3.40040600	-1.32778500	1.60683000	C	0.23100500	3.10198800	-2.68036800
N	-3.39031100	-0.88027300	0.35666800	H	0.55207000	3.97300000	-2.10409800
H	-6.24944700	-2.52699800	0.60702500	H	-0.00480500	2.21573000	-1.82159700
H	-2.62821300	-1.15210100	2.34722800	H	-0.72222500	3.24017200	-3.19701600
C	3.85833300	1.18386100	-1.32100700	H	1.01899100	2.66757200	-3.29835000
O	2.61470000	0.78717200	-1.48865300	C	4.35799100	2.09628100	-2.44020100
O	4.58205400	0.85796600	-0.37943100	H	5.41897200	2.32143700	-2.30089700
C	2.19435100	1.50240100	2.42589400	H	4.19887900	1.61703900	-3.41403000
O	1.71090200	1.30137700	1.23965800	H	3.78112000	3.03015300	-2.43665300
O	1.68576100	1.04045600	3.46897200	C	-3.83553300	3.57505800	0.60280500
C	3.27785700	-2.42611700	0.06476300	H	-3.20766400	4.44050600	0.35261700
C	3.67435200	-3.29411300	1.05886500	H	-4.73815900	3.61924400	-0.01427800
N	3.01059800	-2.89140500	2.20989300	H	-4.08773900	3.62988100	1.66600000
H	3.09088400	-3.30202200	3.13189900	C	-4.91043000	-0.98355800	-1.66713800
C	2.24273200	-1.82144100	1.89338600	H	-4.95745100	0.10222200	-1.81434200
N	2.37805300	-1.51639500	0.60849900	H	-4.14076900	-1.37166400	-2.34415000
H	4.36008500	-4.12958000	1.04445800	H	-5.87810200	-1.42086200	-1.93688100
H	1.63576800	-1.28543100	2.61045900	C	3.44010400	2.37021300	2.48147000
Fe	1.27447100	0.15768900	-0.25247300	H	4.19972100	1.94354800	1.81652100
Fe	-1.71341400	0.31339700	-0.40698900	H	3.19753400	3.37045900	2.09957000

H	3.80972600	2.44670800	3.50765100	C	3.73260700	-2.39027400	-1.36150100
C	-0.51652400	-2.43706900	-3.46953500	H	2.87740400	-2.29170700	-2.03684700
H	-0.94120500	-3.38028600	-3.10178600	H	4.39191900	-1.52949100	-1.51992800
H	-1.18099000	-2.05506000	-4.25177200	H	4.28600200	-3.30511500	-1.60361300
H	0.48113900	-2.62738600	-3.87333900				

Model1H-**IM**(HS-FM)

C	-3.04945700	1.29213300	1.89712100	C	3.40287600	-1.57257000	-1.73051200
O	-3.10763500	1.78042100	0.71192800	C	3.83116700	-2.88241200	-1.73806100
O	-2.32220000	0.27257100	2.10091700	N	3.16105000	-3.51335900	-0.69842200
C	-0.43335500	0.66967400	-2.61224600	H	3.25766000	-4.47989400	-0.41264900
O	0.68551300	0.46541800	-2.08244100	C	2.35871700	-2.59730100	-0.10519600
O	-1.55445500	0.75930900	-1.98023300	N	2.47828200	-1.41835000	-0.70375200
C	-4.52451000	-0.89226800	-1.09287900	H	4.54270300	-3.39656600	-2.36876600
C	-5.22804600	-2.07007100	-0.95926800	H	1.73646700	-2.81105000	0.75328700
N	-4.45240300	-2.88939500	-0.14882900	Fe	1.31516400	0.29790000	-0.01952400
H	-4.67843000	-3.82933600	0.15346200	Fe	-1.70465100	0.41580300	-0.02733300
C	-3.32651000	-2.20977900	0.18006600	O	-0.38246900	-0.96704600	0.10518100
N	-3.34064800	-1.00318200	-0.37512700	O	-0.83954300	-2.19984400	2.47156400
H	-6.18237900	-2.38321900	-1.35914800	H	-1.29294800	-1.40456500	2.80698700
H	-2.54465200	-2.60130900	0.82130200	H	0.09755800	-2.14000200	2.80023100
C	3.78038300	1.96480600	0.02395900	O	-0.18466700	1.59611400	0.39687000
O	2.56479600	1.70923500	-0.41343500	H	-0.46163800	-1.48340700	0.95320300
O	4.58454000	1.11390000	0.40558700	C	-1.03394500	4.69600700	-0.17146100
C	2.29381800	-0.79492100	2.74071200	H	-1.93336200	4.11809100	0.02429100
O	1.78804900	-0.04086300	1.81432100	H	-0.12358600	2.51159200	0.06711800
O	1.78677100	-1.87569900	3.10658800	H	-0.75272900	4.94033100	-1.19241700

H	-0.46766100	5.11656500	0.65535300	C	3.56141700	-0.26450700	3.38818100
C	4.13050100	3.45105000	-0.00201800	H	4.28361600	-0.00683800	2.60534000
H	5.17659500	3.60067000	0.27928100	H	3.32404300	0.66169100	3.92795500
H	3.94471900	3.86239300	-1.00170600	H	3.97315300	-0.99946300	4.08531100
H	3.47953100	3.98990700	0.69854100	C	-0.51703200	0.81247300	-4.12324900
C	-3.81033900	1.94738700	3.02495200	H	-0.96291700	-0.10015000	-4.53969500
H	-3.15878600	2.69760200	3.49245800	H	-1.17175700	1.65063800	-4.38535900
H	-4.70157600	2.45557300	2.64473400	H	0.47777100	0.95443500	-4.55293200
H	-4.07835800	1.20757500	3.78530000	C	3.84694200	-0.45112800	-2.61792400
C	-4.89400400	0.34625500	-1.85178300	H	2.98399800	0.11279500	-2.98467200
H	-4.95511300	1.20696700	-1.17476000	H	4.48759300	0.23684800	-2.05490800
H	-4.13174400	0.57710900	-2.60483200	H	4.41500000	-0.84532600	-3.46866800
H	-5.86140200	0.21697200	-2.34956400				

Model1H-TS2(HS-FM)

C	-3.09002600	1.60440300	-1.67829100	H	-6.21501700	-0.98173000	2.47045500
O	-3.19115000	0.35437600	-1.92854700	H	-2.59537800	1.23655200	2.35278600
O	-2.24324000	1.99341200	-0.81271900	C	3.91991100	-0.24922900	-1.62701300
C	-0.40972500	-2.75147500	-0.35672800	O	2.69867700	-0.70387900	-1.45048900
O	0.69766800	-2.16939000	-0.20988300	O	4.54331000	0.43860500	-0.81662500
O	-1.53159900	-2.16307500	-0.56136800	C	2.02925600	2.87013500	0.07034600
C	-4.54904600	-0.94551500	0.96508500	O	1.56879100	1.78278500	-0.47222700
C	-5.26255100	-0.62819500	2.10085800	O	1.58826900	3.36012900	1.13105700
N	-4.49901700	0.31172700	2.78132600	C	3.32571200	-1.31232900	2.00222600
H	-4.73354500	0.76096400	3.65829300	C	3.78538000	-0.96327800	3.25303100
C	-3.37002100	0.53470700	2.06381100	N	3.15603200	0.23125700	3.57526200
N	-3.37072600	-0.20827900	0.96287800	H	3.28531700	0.77694900	4.41831000

C	2.34408600	0.56525400	2.54404900	C	-3.99041600	2.59197700	-2.38494800
N	2.42027800	-0.34518000	1.58069200	H	-3.51479600	3.57584200	-2.43715000
H	4.49360300	-1.44446700	3.91279300	H	-4.24417100	2.22921400	-3.38562100
H	1.75520300	1.47247100	2.51036900	H	-4.92182000	2.68915200	-1.81096400
Fe	1.27432600	-0.14095100	-0.25387100	C	-4.90085000	-1.90662400	-0.13016200
Fe	-1.73440100	-0.18230900	-0.51134000	H	-4.93558700	-1.39043500	-1.09685800
O	-0.41457900	0.11895100	0.90867500	H	-4.14331500	-2.69544200	-0.20905900
O	-1.00350700	2.70502300	1.69237000	H	-5.87562100	-2.36811700	0.06311700
H	-1.44919900	2.83613400	0.83407300	C	3.16842200	3.53926900	-0.67935500
H	-0.07972800	3.04096300	1.55803800	H	4.01830800	2.84651400	-0.69910000
O	-0.18493100	0.03263700	-1.77096800	H	2.87070100	3.72054400	-1.71970300
H	-0.52327300	1.02456100	1.29422200	H	3.44610900	4.48072000	-0.19773000
C	0.25066400	-0.96351100	-3.79704400	C	-0.44866900	-4.26723200	-0.26449600
H	-0.60029900	-1.63098700	-3.71620400	H	-0.76922400	-4.54624700	0.74810000
H	-0.09233600	0.94744600	-2.09058900	H	-1.17935600	-4.67213400	-0.97183900
H	1.22354200	-1.27194700	-3.43219800	H	0.54253300	-4.68980200	-0.44900200
H	0.16692200	-0.08692800	-4.43401500	C	3.72251500	-2.49469500	1.17293400
C	4.53576300	-0.67025300	-2.96136600	H	2.84235100	-2.98057600	0.74103400
H	5.57717000	-0.34178700	-3.01975300	H	4.36749400	-2.17483900	0.34672900
H	4.47737900	-1.75970600	-3.07615000	H	4.27398300	-3.21684700	1.78617000
H	3.96393300	-0.22500400	-3.78602300				

Model1H-P(HS-FM)

C	-2.72495200	2.86974500	-0.38959700	O	0.74465800	-0.91414800	-1.94014600
O	-3.06642100	1.78206800	-0.99417100	O	-1.49541500	-1.05242100	-2.22707400
O	-1.64652600	3.01963600	0.24242300	C	-4.63950200	-1.74397800	0.11869900
C	-0.28965200	-1.30922700	-2.55233500	C	-5.32320800	-2.10102900	1.26050800

N	-4.67355600	-1.46166200	2.30915000	O	0.43703300	1.96921100	-1.12048400
H	-4.91981100	-1.50972000	3.29064000	H	-0.67281100	0.29820400	1.29186300
C	-3.63780100	-0.75304500	1.79534400	C	1.17622400	3.08084300	-1.64580600
N	-3.59102800	-0.90577700	0.47427100	H	0.48745600	3.78779700	-2.12712300
H	-6.18706900	-2.73322900	1.41147000	H	-0.28366500	2.31418400	-0.52468900
H	-2.95094700	-0.14643300	2.38124100	H	1.87827900	2.68378400	-2.38131100
C	4.20858700	0.74626200	-0.95653200	H	1.73278800	3.59073200	-0.84805100
O	2.94634100	0.59891400	-1.28850200	C	5.01348500	1.55653000	-1.97334300
O	4.73667000	0.27865700	0.05470100	H	6.07407600	1.55422100	-1.70682000
C	2.10680200	1.33244700	2.54466200	H	4.87540200	1.14150000	-2.97924200
O	1.81005200	1.27468900	1.28414300	H	4.64569300	2.59087400	-1.99316900
O	1.30050600	1.05813900	3.46029300	C	-3.72325900	4.01404500	-0.47697600
C	2.86772300	-2.67413800	0.22770300	H	-3.91115900	4.25252100	-1.53090700
C	2.98016400	-3.60054000	1.24193800	H	-4.67955700	3.69919200	-0.04151000
N	2.24089800	-3.10004600	2.30533400	H	-3.34741500	4.89718300	0.04552900
H	2.12532700	-3.52608400	3.21652000	C	-4.90341500	-2.12185400	-1.30775300
C	1.70295800	-1.91856500	1.91778000	H	-5.22042500	-1.24657100	-1.89030200
N	2.06058900	-1.63385600	0.67172300	H	-3.99551700	-2.51774000	-1.77826200
H	3.51842200	-4.53634300	1.29701600	H	-5.69271300	-2.87897500	-1.36911700
H	1.08872000	-1.29692800	2.55572600	C	3.52107500	1.78888200	2.86276400
Fe	1.34116400	0.18806000	-0.27501000	H	4.23040000	1.21974400	2.25193300
Fe	-2.11477000	0.07298900	-0.69244300	H	3.62381600	2.84545800	2.58095100
O	-0.49600700	-0.13588100	0.42266300	H	3.73016600	1.67812600	3.93046400
O	-1.29473500	1.26581700	2.67419800	C	-0.07387100	-2.18877200	-3.77574900
H	-1.34556500	2.07740600	2.13373200	H	0.21311300	-3.19461100	-3.44140700
H	-0.37908700	1.24508400	3.06376000	H	-0.98716500	-2.25908900	-4.37258900

H	0.74986500	-1.79218100	-4.37833100	H	4.36143000	-2.01612900	-1.14770900
C	3.50845800	-2.70384700	-1.12557100	H	3.86633300	-3.71477500	-1.35340500
H	2.79892900	-2.38505800	-1.89524300				
Model1H-RC(HS-AF)							
C	-3.02176900	2.05627900	0.71685700	N	3.24117200	-3.20482200	1.61271700
O	-3.00281900	1.63418000	-0.50636600	H	3.34869400	-3.78849600	2.43315700
O	-2.33382700	1.46706200	1.58589100	C	2.37056000	-2.17461400	1.49295000
C	-0.40126000	-1.21939400	-2.51928400	N	2.49745000	-1.59685800	0.30427400
O	0.71322800	-1.05159000	-1.95876200	H	4.73713900	-4.03095500	0.27378600
O	-1.53419000	-0.82729100	-2.05975700	H	1.69610200	-1.86278900	2.27860800
C	-4.41040800	-1.34412100	-0.44288800	Fe	1.26709900	0.09549900	-0.27376900
C	-5.15071900	-2.19280100	0.35035800	Fe	-1.64260500	0.20181000	-0.33514800
N	-4.40208000	-2.39866300	1.50161500	O	-0.43753300	-0.88470900	0.62108400
H	-4.66026600	-2.96908900	2.29781000	O	-0.86362200	-0.35787300	3.21833200
C	-3.25224800	-1.69411700	1.38927500	H	-1.33715900	0.47371800	3.02795500
N	-3.22712400	-1.04858600	0.22768700	H	0.07010900	-0.09323800	3.44336100
H	-6.11499100	-2.65485400	0.19193200	O	-0.37167600	1.21192800	-0.71631000
H	-2.48503800	-1.65556000	2.15302200	H	-0.53349300	-0.70962100	1.60382900
C	3.60019400	1.69362500	-1.20329200	C	-0.62744700	4.92732100	-1.32118100
O	2.47212300	1.03827600	-1.40123200	H	-0.51378400	5.42493700	-0.35086400
O	4.50603600	1.30562200	-0.46644900	H	-0.55114800	3.84263800	-1.19113400
C	2.16943100	1.03542000	2.56112600	H	-1.60410400	5.17788200	-1.75165300
O	1.64875200	1.01967500	1.37179700	H	0.16314200	5.27137700	-1.99788800
O	1.72300900	0.37221300	3.52004900	C	3.69667200	2.98521300	-2.00723800
C	3.49844500	-2.27863100	-0.37958800	H	4.66949700	3.45965600	-1.85106800
C	3.96614800	-3.28987100	0.43111700	H	3.54680400	2.77132100	-3.07259000

H	2.89339000	3.66561500	-1.69748800	H	3.06090700	2.98469900	2.55179000
C	-3.86166300	3.27200700	1.03282100	H	3.77975500	1.85647500	3.74349000
H	-3.32995600	4.16231400	0.67330400	C	-0.43952000	-1.93168200	-3.86128200
H	-4.82110600	3.22161500	0.50700600	H	-1.27711100	-2.63644200	-3.89235200
H	-4.01567800	3.35892800	2.11174000	H	-0.60094700	-1.18363700	-4.64817900
C	-4.75225100	-0.79688200	-1.79524800	H	0.50493200	-2.44867100	-4.04889800
H	-4.78423800	0.29831800	-1.77082600	C	3.96696100	-1.89598800	-1.74914800
H	-3.99265100	-1.08535300	-2.52963300	H	3.11770600	-1.78846900	-2.43150400
H	-5.72805400	-1.17500400	-2.11942300	H	4.48928500	-0.93372500	-1.70602100
C	3.37145400	1.94755600	2.73335500	H	4.65346600	-2.65660200	-2.13877500
H	4.12468600	1.69962500	1.97681800				

Model1H-TS1(HS-AF)

C	-3.12622300	2.30809500	0.34635200	C	3.86122200	1.20083100	-1.28660400
O	-3.14154500	1.80961400	-0.83799800	O	2.60962700	0.83626500	-1.47191500
O	-2.39997900	1.76412200	1.22907000	O	4.57264600	0.83118500	-0.35187900
C	-0.45337700	-1.35674600	-2.36150200	C	2.21333600	1.44876100	2.46850700
O	0.65896400	-1.14609200	-1.81707400	O	1.75053900	1.28042200	1.27004100
O	-1.57756400	-0.84685100	-1.99472700	O	1.68453800	0.96536700	3.49209300
C	-4.53563400	-1.35076200	-0.25287400	C	3.26042600	-2.44186600	0.01111400
C	-5.23642200	-2.10460900	0.66401500	C	3.65785500	-3.33110500	0.98596000
N	-4.47500300	-2.09903400	1.82575400	N	3.00570200	-2.94507900	2.14919800
H	-4.70326200	-2.55555100	2.70058700	H	3.08951900	-3.37371400	3.06266500
C	-3.35988400	-1.36379100	1.59292600	C	2.24325300	-1.86388300	1.85842900
N	-3.36741800	-0.89998700	0.34853700	N	2.37136500	-1.53616700	0.57833700
H	-6.17906600	-2.62853000	0.58891100	H	4.33773400	-4.17073700	0.95112700
H	-2.59052700	-1.17536900	2.33324000	H	1.64626800	-1.33571800	2.58986600

Fe	1.28350000	0.17113100	-0.23718700	H	-4.92702900	3.46733800	0.15306200
Fe	-1.73804200	0.35821900	-0.41445000	H	-4.07165100	3.66806300	1.72476300
O	-0.44266000	-0.53844700	0.69211100	C	-4.89531700	-1.01926300	-1.66973800
O	-0.93064400	0.28010300	3.22054900	H	-4.97404100	0.06653700	-1.80288000
H	-1.39155700	1.07717900	2.89967200	H	-4.11905800	-1.37616500	-2.35615300
H	0.00053400	0.56220800	3.42870300	H	-5.85193600	-1.48014800	-1.93970500
O	-0.24971100	1.39201000	-0.88798900	C	3.46359700	2.30674200	2.56537800
H	-0.54178800	-0.27411400	1.64937900	H	4.22602000	1.90021500	1.89114300
C	0.37532100	3.05861800	-2.66385400	H	3.22891900	3.32158600	2.21857200
H	0.66532900	3.95015100	-2.10313700	H	3.82548500	2.34458800	3.59645800
H	0.02263300	2.21083800	-1.75848700	C	-0.51880200	-2.30908900	-3.54504200
H	-0.52774700	3.18273700	-3.26706400	H	-0.96825100	-3.25418900	-3.21342200
H	1.20198000	2.55997400	-3.17109000	H	-1.16200100	-1.89169700	-4.32717800
C	4.38743700	2.13594000	-2.37440200	H	0.48215400	-2.50589900	-3.93737300
H	5.45538200	2.32165000	-2.23040800	C	3.70517900	-2.38118400	-1.41743200
H	4.21090000	1.69824000	-3.36463700	H	2.84575500	-2.26492400	-2.08465700
H	3.84215100	3.08777500	-2.33463700	H	4.36791300	-1.52083700	-1.56391100
C	-3.95150500	3.53742400	0.64580700	H	4.25198700	-3.29392100	-1.68133000
H	-3.43364900	4.41495400	0.23721100				

Model1H-**IM**(HS-AF)

C	-3.07071900	1.34687800	1.85048300	C	-4.50859300	-0.96003900	-1.07029600
O	-3.11557200	1.79430700	0.64705400	C	-5.20086800	-2.13970700	-0.89991700
O	-2.34907700	0.33455000	2.09753300	N	-4.42215700	-2.92218800	-0.05659700
C	-0.43188100	0.59672300	-2.62749300	H	-4.64065100	-3.85332200	0.27691400
O	0.68699400	0.40924900	-2.09240600	C	-3.30538000	-2.22018400	0.25536800
O	-1.55532900	0.69658000	-2.00019900	N	-3.32821200	-1.03386900	-0.34192200

H	-6.14946400	-2.47640500	-1.29426300	H	-0.13095300	2.51057900	0.03461700
H	-2.52389000	-2.58021400	0.91533000	H	-0.84783100	4.99927700	-1.30396100
C	3.77736600	1.98004500	-0.02980300	H	-0.56975700	5.21229500	0.54095900
O	2.56429100	1.70098900	-0.46045000	C	4.10671100	3.47036500	-0.07851400
O	4.59409100	1.14584200	0.36158200	H	5.15067600	3.63882700	0.20000600
C	2.31599600	-0.72248500	2.75506800	H	3.91508600	3.86346000	-1.08443000
O	1.81633100	0.01617200	1.81347800	H	3.44829500	4.01089900	0.61374200
O	1.79734800	-1.78753700	3.14997900	C	-3.84450300	2.04629500	2.94246100
C	3.40498800	-1.61507800	-1.69010100	H	-3.23571400	2.87808600	3.32105600
C	3.82918200	-2.92610400	-1.66793600	H	-4.77629200	2.46171900	2.54593500
N	3.15643900	-3.53161400	-0.61489800	H	-4.04549300	1.36020900	3.77030900
H	3.25003800	-4.49177300	-0.30745700	C	-4.88601000	0.24791300	-1.87332200
C	2.35664300	-2.59998600	-0.04288800	H	-4.96555300	1.12972700	-1.22592700
N	2.48040500	-1.43499300	-0.66744100	H	-4.11884700	0.46421100	-2.62565800
H	4.53940100	-3.45647800	-2.28657200	H	-5.84640800	0.08960800	-2.37620500
H	1.73310800	-2.79221000	0.81971500	C	3.59343200	-0.19258600	3.38386100
Fe	1.32126900	0.29890200	-0.02444900	H	4.31145200	0.04729300	2.59162300
Fe	-1.71445200	0.41364400	-0.03965600	H	3.36769200	0.74364200	3.91123800
O	-0.37264300	-0.94217900	0.14813100	H	4.00463200	-0.91967400	4.08952600
O	-0.83327200	-2.11484700	2.54391700	C	-0.51504200	0.70518900	-4.14144900
H	-1.28654900	-1.31206400	2.86074900	H	-0.98326700	-0.20577000	-4.53624800
H	0.10551900	-2.04736600	2.86677900	H	-1.15114300	1.55208000	-4.42141400
O	-0.18933900	1.59502400	0.36210100	H	0.48169800	0.81586600	-4.57568000
H	-0.45218900	-1.43598500	1.00935600	C	3.85199600	-0.51563700	-2.60312100
C	-1.11438900	4.75289600	-0.27968000	H	2.98993100	0.03537700	-2.99112700
H	-1.97376100	4.11934600	-0.07577400	H	4.48588700	0.18916300	-2.05348900

H 4.42761400 -0.93015200 -3.43901500

Model1H-TS2(HS-AF)

C -3.13674000 1.70481200 -1.58160900

O -3.22746800 0.46929400 -1.90400800

O -2.28852100 2.05564200 -0.70334600

C -0.40570700 -2.71868600 -0.52673800

O 0.70253600 -2.13786700 -0.36309000

O -1.53155800 -2.13224800 -0.69494200

C -4.53512300 -1.01830500 0.93373900

C -5.23302500 -0.78088100 2.09837300

N -4.47062100 0.12749500 2.82159100

H -4.69535800 0.51880500 3.72831800

C -3.35762700 0.41013700 2.09964900

N -3.36724400 -0.26502200 0.95609400

H -6.17405200 -1.16989200 2.46160900

H -2.58756100 1.10473900 2.41696900

C 3.92927900 -0.12600600 -1.61523200

O 2.70991300 -0.60151300 -1.47665200

O 4.53959900 0.51631500 -0.75957400

C 2.02291400 2.87215700 0.23658900

O 1.58028400 1.80611800 -0.36110300

O 1.58792300 3.28834100 1.32999100

C 3.33303100 -1.44081200 1.90382000

C 3.80694200 -1.16333000 3.16713600

N 3.19402900 0.01917000 3.55779700

H 3.33601200 0.51741600 4.42778200

C 2.37702800 0.41659800 2.55377400

N 2.43520300 -0.44276300 1.54310800

H 4.51515700 -1.68655300 3.79404700

H 1.79823600 1.33115600 2.57285700

Fe 1.27634600 -0.11742000 -0.25821500

Fe -1.75914700 -0.14840000 -0.54441100

O -0.40309800 0.06586400 0.88081800

O -1.01836200 2.59964600 1.82880400

H -1.46328700 2.78188200 0.97933100

H -0.09652800 2.94688900 1.72323400

O -0.22018700 0.16072000 -1.76692600

H -0.51772000 0.94496900 1.32038400

C 0.33303900 -0.84709300 -3.79398900

H -0.51696500 -1.51876500 -3.74251600

H -0.13282900 1.07946700 -2.07305700

H 1.29277100 -1.14382300 -3.38759400

H 0.26069100 0.03845300 -4.41967200

C 4.55792500 -0.45959100 -2.96793400

H 5.59840600 -0.12434800 -2.99586100

H 4.50465400 -1.53960500 -3.15265700

H 3.99156300 0.03563600 -3.76746000

C -4.05633100 2.71832400 -2.22525300

H -3.59370700 3.70976300 -2.22665400

H -4.31473300 2.40845400 -3.24240300

H	-4.98359700	2.77139800	-1.63891400	C	-0.42569700	-4.23798900	-0.49968600
C	-4.89374700	-1.91485900	-0.21289700	H	-0.61931700	-4.56369400	0.53119000
H	-4.95979700	-1.33885300	-1.14361200	H	-1.22916300	-4.62242900	-1.13509100
H	-4.12375800	-2.68189000	-0.35799500	H	0.54184400	-4.63993900	-0.81333800
H	-5.85544400	-2.40671200	-0.02909100	C	3.70939700	-2.58156700	1.00907100
C	3.13296100	3.60957100	-0.49239500	H	2.82131400	-3.02076200	0.54489500
H	3.99984800	2.94136700	-0.56046000	H	4.36691600	-2.22994900	0.20568000
H	2.81478000	3.83832300	-1.51715600	H	4.24082700	-3.35047100	1.58179900
H	3.39444600	4.53074200	0.03527200				

Model1H-P(HS-AF)

C	-2.52499800	2.94461300	-0.53568300	O	4.71391400	-0.01528500	0.10792800
O	-2.90878000	1.79624300	-0.95585900	C	2.18849500	1.43388200	2.46348700
O	-1.39910300	3.18388900	-0.01315100	O	1.92422900	1.33272200	1.19733200
C	-0.36127600	-1.34748700	-2.59213700	O	1.34101200	1.27047200	3.36712000
O	0.62946400	-0.97038700	-1.91445100	C	2.56771700	-2.77082200	0.41579400
O	-1.59152400	-1.07522000	-2.33603300	C	2.58688200	-3.63743800	1.48723200
C	-4.61401200	-1.71779900	0.24262700	N	1.87401300	-3.01235300	2.50161800
C	-5.33792500	-1.88472800	1.40408100	H	1.70994600	-3.36873900	3.43501700
N	-4.68902500	-1.12800900	2.36910500	C	1.44122500	-1.81829000	2.03034400
H	-4.96191300	-1.02272400	3.33887600	N	1.84112500	-1.64241400	0.77676700
C	-3.61300500	-0.53671700	1.78915800	H	3.04483300	-4.60875500	1.61089600
N	-3.54217000	-0.87620700	0.50476900	H	0.87172600	-1.10862500	2.61557500
H	-6.23006300	-2.45733900	1.61592100	Fe	1.32401100	0.19799400	-0.27326700
H	-2.92595700	0.12819000	2.30652300	Fe	-2.05286300	-0.01042000	-0.73459600
C	4.23616300	0.43785700	-0.93402600	O	-0.51859200	0.07095200	0.44821500
O	2.97222400	0.35451200	-1.28409600	O	-1.23073900	1.64570800	2.55288500

H	-1.22623800	2.42113100	1.95759400	H	-3.91111500	4.11021400	-1.70551000
H	-0.32296400	1.59223800	2.95484400	H	-4.39804200	3.87164900	-0.02493300
O	0.58887900	1.94949600	-1.24785300	H	-3.09006400	5.03328000	-0.40101400
H	-0.69537600	0.59941700	1.26782700	C	-4.86392100	-2.28669100	-1.12182000
C	3.22646600	-2.93996000	-0.91824700	H	-5.07201100	-1.48793100	-1.84581000
H	2.55022000	-2.64088800	-1.72493700	H	-3.98758800	-2.83749300	-1.48499000
H	4.11804300	-2.30572500	-0.97390900	H	-5.72216200	-2.96715100	-1.10577600
H	3.52732600	-3.98435400	-1.06175600	C	-0.11007700	-2.22320100	-3.80978700
C	5.10842700	1.14940400	-1.96839700	H	-0.25146900	-3.27387700	-3.52234400
H	6.16372100	1.07447600	-1.69150200	H	-0.83201600	-1.99163600	-4.59905200
H	4.94553300	0.71598800	-2.96262900	H	0.91360900	-2.09340500	-4.17092000
H	4.82169800	2.20798300	-2.02180200	C	1.42608300	2.98891600	-1.77226500
C	3.62568100	1.79802200	2.79799800	H	1.98883400	3.47897800	-0.96636400
H	4.30229500	1.13782200	2.24430900	H	0.80666400	3.73006700	-2.29406000
H	3.82017300	2.82394200	2.45771800	H	2.12310700	2.52512700	-2.47322500
H	3.79712200	1.73609700	3.87625900	H	-0.14838100	2.36791700	-0.70612700
C	-3.53772600	4.07465300	-0.67541800				

Model1H-RC(IS-AF)

C	2.92090800	2.08432300	1.27495500	N	4.50029100	0.40358500	-2.56237700
O	2.38142600	0.90132000	1.38398200	H	4.80702500	0.91918400	-3.37858900
O	2.79365900	2.85385800	0.31241900	C	3.27997800	0.51254400	-1.98472700
C	0.28147600	-2.76024800	-0.66996800	N	3.21137200	-0.27664900	-0.92002100
O	-0.83985700	-2.21566100	-0.59849400	H	6.26757100	-0.76088900	-2.08034500
O	1.40640800	-2.19555500	-0.37676100	H	2.49323000	1.16367800	-2.34397100
C	4.43507600	-0.92018100	-0.79586800	C	-3.65257400	-0.50905800	1.65840300
C	5.25096700	-0.49929700	-1.82251200	O	-2.44166900	-0.94747600	1.37300800

O	-4.25129900	0.40093300	1.08925600	C	-3.93947000	-2.14106800	-1.32842600
C	-1.79077700	2.84577200	0.62575600	H	-3.05872900	-2.72836100	-1.05832900
O	-1.34921100	1.64932100	0.82311000	H	-4.54473300	-1.99558900	-0.42598700
O	-1.50048300	3.54787500	-0.37344800	H	-4.54134800	-2.69786100	-2.05619300
C	-3.54280700	-0.81696900	-1.90565900	C	-4.25889300	-1.26738000	2.83965400
C	-4.10692200	-0.17827900	-2.98739600	H	-5.32233100	-1.02751000	2.92786100
N	-3.44913500	1.03638500	-3.10979800	H	-4.11545100	-2.34745100	2.72121500
H	-3.63563600	1.76417800	-3.78862600	H	-3.73974200	-0.96670100	3.75857800
C	-2.51504200	1.10611100	-2.13454900	C	-2.71173100	3.39254200	1.70369600
N	-2.54273100	0.00377200	-1.39185000	H	-2.95668900	4.44054900	1.51052700
H	-4.90887200	-0.47625100	-3.64788100	H	-3.62104100	2.77967900	1.71477300
H	-1.88630600	1.96984400	-1.96435500	H	-2.23243900	3.28789100	2.68455400
Fe	-1.21946900	-0.19865000	0.16983000	C	3.74479000	2.48098600	2.49369500
Fe	1.54536200	-0.42048000	0.33212500	H	4.26003400	3.42612500	2.30457000
O	0.37713000	0.23477100	-0.92722800	H	3.07486000	2.59138800	3.35519000
O	0.77761600	2.68262600	-1.47550200	H	4.46744900	1.69417600	2.73910900
H	1.51051600	2.89437700	-0.84425400	C	4.72137800	-1.89421300	0.30667400
H	-0.04367000	3.12425400	-1.11366400	H	4.64466000	-1.40910800	1.28880000
O	0.27721700	-0.62671600	1.38015900	H	4.00470700	-2.72386700	0.28399800
H	0.50275200	1.25521900	-1.08690600	H	5.73286600	-2.30192400	0.20663400
H	0.57492200	-1.87067500	3.77333400	C	0.37974300	-4.21334700	-1.10415100
C	0.91246000	-2.38420000	4.67978100	H	1.36806700	-4.43497100	-1.51679800
H	1.08262000	-3.44521500	4.46227500	H	0.21616000	-4.84927100	-0.22431800
H	0.14650000	-2.29233500	5.45810000	H	-0.40267200	-4.43592100	-1.83583500
H	1.84506800	-1.92949700	5.03386900				

Model1H-TS1(IS-AF)

C	-2.26917800	2.87901900	0.03820700	H	4.22207100	-2.96579200	3.16766600
O	-2.34057300	1.89859700	-0.80903800	H	1.05148100	-0.17179600	2.85915100
O	-2.00759500	2.79672100	1.25033200	Fe	1.28063000	-0.11455500	-0.38757600
C	-0.37327900	-2.45240400	-1.13290200	Fe	-1.73827700	0.07094500	-0.90358200
O	0.76550400	-1.93053300	-1.00098100	O	-0.40474100	0.01353700	0.51846700
O	-1.49655800	-1.84631500	-1.11057900	O	-0.16117500	1.55929400	2.80799400
C	-4.25819700	-1.50605300	0.43515700	H	-0.81837400	2.21415400	2.49897400
C	-4.88858000	-1.50214000	1.65984600	H	0.71583600	1.93260000	2.53384900
N	-4.31095200	-0.47472300	2.38937800	O	-0.59230400	0.43140000	-2.09314500
H	-4.53858900	-0.19772000	3.33674800	H	-0.41338400	0.68163700	1.25335900
C	-3.36665700	0.10858700	1.61713500	H	-1.72227800	0.27814800	-2.63062100
N	-3.30326600	-0.48776600	0.42904400	C	-3.07425100	0.01365300	-2.69520700
H	-5.67929000	-2.12562000	2.05295100	H	-3.13236800	-0.98374900	-3.13801600
H	-2.76950300	0.96082400	1.91540800	H	-3.09698000	0.80537800	-3.45913000
C	3.84249300	0.31785300	-1.59257800	H	-3.91682300	0.20694500	-2.03151100
O	2.66067700	-0.27282200	-1.63779400	C	3.99959900	-2.54457500	0.18354400
O	4.35899500	0.81304600	-0.59505400	H	3.29487300	-2.79572500	-0.61517600
C	2.11705700	2.57013200	0.49383500	H	4.70570700	-1.80362600	-0.20742600
O	1.56046200	1.75087500	-0.35867100	H	4.56167800	-3.44296700	0.46472200
O	2.13305700	2.43025800	1.72673200	C	4.53211100	0.30986900	-2.95501900
C	3.27736200	-1.99968700	1.37792000	H	5.55613100	0.68109700	-2.85716700
C	3.50526400	-2.30426000	2.70170200	H	4.53194200	-0.70213800	-3.37697100
N	2.59482100	-1.55285200	3.43093100	H	3.97000600	0.95105400	-3.64577100
H	2.50304200	-1.51965200	4.43867500	C	2.77484000	3.77618000	-0.15918000
C	1.85203500	-0.83308700	2.55661600	H	2.86228900	4.59509100	0.56068400
N	2.23968000	-1.07417800	1.30891300	H	3.77807800	3.46627000	-0.47696400

H	2.21684600	4.09220700	-1.04670100	H	-3.63655100	-2.83875700	-1.12851700
C	-2.57555600	4.23276300	-0.59586400	H	-5.21382600	-3.22737200	-0.38949700
H	-2.68726300	4.99570100	0.17918000	C	-0.41733700	-3.95360000	-1.36544700
H	-1.74706100	4.50456900	-1.26196000	H	-1.44515700	-4.31193400	-1.46267600
H	-3.48253500	4.17130100	-1.20761400	H	0.14609800	-4.18700000	-2.27646000
C	-4.55715700	-2.41491200	-0.72001600	H	0.07891600	-4.46043300	-0.52984800
H	-5.06759800	-1.87868000	-1.52970300				

Model1H-**IM**(IS-AF)

C	-2.10520800	2.91352700	-0.17458300	O	1.45353300	1.73832200	-0.47564400
O	-1.99283500	1.88930000	-0.97025100	O	2.00940800	2.68272000	1.50580200
O	-2.15936700	2.88889600	1.06592400	C	3.28545100	-1.91695300	1.46381600
C	-0.45615700	-2.58815200	-0.99017000	C	3.62050800	-2.05986600	2.79206500
O	0.68328400	-2.12660900	-0.75774300	N	2.80473400	-1.18258700	3.49115000
O	-1.55997100	-1.92726400	-1.03584900	H	2.80022200	-1.02136300	4.49064300
C	-4.31379300	-1.41039500	0.45773800	C	2.00906600	-0.55045000	2.59606100
C	-4.98033300	-1.31580600	1.65853200	N	2.27460100	-0.96477300	1.36234900
N	-4.41399900	-0.24740700	2.33549900	H	4.35343000	-2.68838200	3.27822100
H	-4.66859900	0.09710300	3.25337700	H	1.25870100	0.17296900	2.88097900
C	-3.44080100	0.27466500	1.55754700	Fe	1.19898800	-0.18490600	-0.34183000
N	-3.34626100	-0.40189500	0.41465500	Fe	-1.76090800	-0.01957200	-0.86052700
H	-5.79013700	-1.90408400	2.06652300	O	-0.42022500	-0.03774300	0.64217700
H	-2.85018900	1.14694400	1.80564000	O	-0.19749300	1.76383900	2.67807300
C	3.76598300	0.10867500	-1.56393200	H	-0.89469400	2.36644200	2.35147100
O	2.57035900	-0.44899900	-1.58881500	H	0.65036000	2.15366600	2.32650400
O	4.26353100	0.70959300	-0.61481900	O	-0.31379500	0.19560700	-1.96349700
C	2.03777400	2.63842300	0.26242700	H	-0.39996500	0.63394300	1.37957200

H -0.18532600	1.15943700	-2.05991500	H -2.75410600	4.17017800	-1.82220500
C -3.04670300	-0.03411500	-2.44457900	H -2.51121700	5.03321600	-0.26069600
H -3.09253400	-1.07355200	-2.76897400	C 2.79435500	3.70381900	-0.51808100
H -2.56207800	0.61952900	-3.16822400	H 3.77677200	3.28451600	-0.76722500
H -3.99641100	0.36318600	-2.08334200	H 2.28013200	3.94350500	-1.45535400
C -4.60199200	-2.39492700	-0.63639600	H 2.92902700	4.60126700	0.09264200
H -5.06127000	-1.90471000	-1.50363700	C 4.50541000	-0.07962200	-2.88823600
H -3.68536500	-2.88436100	-0.97387600	H 4.49197700	-1.13485600	-3.18588600
H -5.30331700	-3.15257300	-0.26923400	H 3.98873700	0.48615300	-3.67389700
C -0.59770200	-4.08018700	-1.24921100	H 5.53524400	0.27651200	-2.79480900
H -1.37198400	-4.50187300	-0.59813200	C 3.88060900	-2.64591100	0.29745200
H -0.91191800	-4.23516300	-2.28881400	H 3.10470800	-2.92529300	-0.42089300
H 0.35526100	-4.58596400	-1.07690000	H 4.61211700	-2.01440400	-0.21938000
C -2.13834400	4.24460200	-0.91972900	H 4.39474100	-3.54949700	0.64606600
H -1.11610300	4.49530800	-1.23174700			

Model2-RC-nonet (HS-FM)

Fe -1.42846400	0.03512500	0.17782300	C -0.61060600	-0.36012800	-4.10826100
Fe 1.28614400	0.13082100	-0.12855700	C -0.43507700	-0.25527900	-2.59971100
H -3.79575400	3.66728500	-0.59848300	O -1.49434700	-0.27210300	-1.89251900
C -4.33184700	3.10425500	0.17532200	O 0.74499400	-0.13873200	-2.15550300
C -3.36217500	2.14240300	0.84423200	H 0.33760800	-0.61035500	-4.59130800
O -2.94066000	1.18712500	0.04659200	H -0.95379200	0.61225700	-4.48419200
O -3.03019600	2.27901100	2.02883100	H -5.33635700	-1.81651000	-1.82615400
H -4.74657100	3.79350000	0.91527700	C -4.46101300	-1.27755100	-1.44692000
H -5.13580500	2.54772100	-0.32038800	C -3.82507000	-2.05293400	-0.33442800
H -1.37845000	-1.10265900	-4.35117200	N -2.67885100	-1.64615400	0.33995800

C	-4.24309700	-3.24484400	0.21700700	C	4.94045100	-0.37483400	-0.26130900
C	-2.41574300	-2.55611600	1.26937800	C	4.04328900	-1.52576800	-0.59625200
N	-3.33692100	-3.54592300	1.22630600	N	2.65473500	-1.46861000	-0.55526400
H	-3.36793400	-4.34448400	1.84851200	C	4.40510100	-2.80053200	-0.97840800
H	-3.74732000	-1.11464700	-2.26019800	C	2.19368100	-2.66214100	-0.89890100
H	-4.77302700	-0.28843300	-1.09434900	N	3.22149500	-3.50316800	-1.16596200
H	-5.08797300	-3.87799600	-0.01461300	H	3.13289000	-4.46976600	-1.45433400
H	-1.59848600	-2.50637000	1.97504700	H	5.98720800	-0.69872900	-0.28795300
H	2.45259800	4.42413700	0.65733100	H	4.80325800	0.45715100	-0.95971400
C	1.99857600	3.44062900	0.50901800	H	4.70916800	0.01057700	0.73769900
C	2.90920800	2.59238100	-0.35720100	H	5.37743800	-3.24887900	-1.12708700
O	4.02134900	2.94997300	-0.71854900	H	1.14703200	-2.92878600	-0.95522400
O	2.43183000	1.40932500	-0.76297300	O	-1.60857100	0.05537900	2.31283200
H	1.85290300	2.94588700	1.47587400	H	-0.68428200	0.09224200	2.70524400
H	1.01167900	3.53595500	0.04388500	H	-2.06653300	0.92568400	2.46515800
H	3.75671700	0.84113000	3.68833200	O	-0.24327500	1.29771500	0.07330100
C	3.14208700	-0.06263500	3.77701300	O	0.05242900	-1.07884600	0.33104100
C	1.90684300	0.06753700	2.88936100	C	-1.20328500	4.24104500	-2.36125200
O	0.77395400	-0.03753200	3.39117300	H	-0.27459700	4.38077100	-2.92578000
O	2.17762100	0.30449600	1.64347600	H	-1.35718700	5.10185300	-1.70031200
H	3.75150200	-0.90815900	3.43395100	H	-2.04479600	4.16136900	-3.05940600
H	2.84801200	-0.21448000	4.81874400	H	-1.13100400	3.32569600	-1.76433900
Model2-TS1-nonet (HS-FM)							
Fe	1.46224100	-0.14507600	0.12057600	C	4.33052200	-3.26055600	-0.56620500
Fe	-1.48604000	-0.12778800	-0.24755700	C	3.36883000	-2.41826800	0.26161200
H	3.78199500	-3.74123500	-1.38559600	O	2.82990500	-1.42949800	-0.39574300

O	3.15270200	-2.69739000	1.45475000	O	-2.78656100	-1.11423400	-1.17768200
H	4.79792600	-4.02295800	0.06200500	H	-4.01110100	-4.05746400	-0.25923800
H	5.09805500	-2.62022100	-1.01701800	H	-2.63041900	-3.18453000	0.49219400
H	1.46424500	0.67493700	-4.39263200	H	-3.72446200	-1.76497800	3.28937500
C	0.65173100	1.22889900	-3.91128500	C	-3.01138800	-1.04630700	3.70974600
C	0.43699700	0.71946900	-2.49255200	C	-1.84126200	-0.85458400	2.75007900
O	1.49271100	0.44602200	-1.82510400	O	-0.67614600	-0.97754100	3.17455100
O	-0.74936600	0.61496300	-2.07565500	O	-2.18607600	-0.56623600	1.53761800
H	0.94656700	2.28591400	-3.86806400	H	-3.54001300	-0.09187600	3.82916400
H	-0.27118600	1.14146200	-4.49027600	H	-2.65447000	-1.39189100	4.68324300
H	5.54793800	1.61136600	-1.80010600	C	-4.92120800	1.09923500	0.18170400
C	4.56751000	1.21765500	-1.50909800	C	-3.83772100	2.12135500	0.03290500
C	4.19892500	1.70736500	-0.14171100	N	-2.49318300	1.79972700	-0.12348600
N	3.06355300	1.29107700	0.54180400	C	-3.95633700	3.49492000	0.03417500
C	4.87753900	2.60886700	0.65138700	C	-1.82323200	2.94087400	-0.20984100
C	3.05510700	1.91770800	1.70988500	N	-2.66975300	3.99553600	-0.12073200
N	4.13495000	2.73013700	1.81874700	H	-2.40247300	4.97126800	-0.16069200
H	4.36642200	3.29618600	2.62605800	H	-5.89218700	1.59581300	0.29110500
H	3.82090800	1.52775600	-2.24812800	H	-4.96145400	0.42303800	-0.67918700
H	4.59421900	0.12309900	-1.52873700	H	-4.74143800	0.47761700	1.06702500
H	5.79830900	3.15160000	0.48892300	H	-4.82241200	4.13507700	0.12688100
H	2.30924200	1.78247700	2.48121000	H	-0.75071500	3.02542700	-0.31958900
H	-2.47790100	-3.82075000	-1.14945000	O	1.64265900	-0.68260900	2.06769900
C	-3.18011700	-3.36945500	-0.43759100	H	0.71631900	-0.82461400	2.45847500
C	-3.70531400	-2.05387600	-1.00268600	H	2.15697500	-1.54711100	2.04667000
O	-4.88292900	-1.89033200	-1.30054200	O	0.02202300	-1.41892000	-0.23208700

O	0.24334100	0.93311700	0.51723700	H	0.40245600	-4.08161600	-1.57553200
C	0.38225600	-3.11067500	-2.07684800	H	1.33831300	-2.82619400	-2.52178400
H	-0.47067200	-2.97999800	-2.74709200	H	0.20568700	-2.28297500	-1.17446200
Model2- IM -undecet (HS-FM)							
Fe	1.57886000	-0.21621800	0.06598700	N	3.71498900	3.07235000	1.77511200
Fe	-1.34902400	-0.09030900	-0.07389700	H	3.82819200	3.69843300	2.56325900
H	3.97707600	-3.84358100	-1.24000000	H	3.73249400	1.58288000	-2.22174300
C	4.52262800	-3.33179500	-0.43738300	H	4.75017400	0.41777000	-1.38222700
C	3.55838300	-2.45173900	0.34411100	H	5.36223600	3.67108100	0.49343100
O	3.01253000	-1.49016500	-0.35236100	H	2.01495800	1.90048800	2.41338000
O	3.33597400	-2.66728000	1.54843600	H	-3.32575600	-4.09925100	0.31092600
H	4.98530900	-4.06916900	0.22334100	C	-2.58691200	-3.37801200	-0.04971900
H	5.29356200	-2.71195100	-0.91082800	C	-3.30474000	-2.23561400	-0.75610000
H	1.06671900	2.21037900	-3.86057000	O	-4.45202600	-2.35374200	-1.17230000
C	0.56361800	1.23597200	-3.90514000	O	-2.61404400	-1.12104500	-0.98089700
C	0.38183500	0.69969200	-2.49241200	H	-1.96125300	-3.01715800	0.76956900
O	1.45852400	0.44628300	-1.84175500	H	-1.93297600	-3.88342200	-0.77356900
O	-0.78880000	0.53744800	-2.06026400	H	-3.67451300	-1.53990700	3.57843900
H	-0.40244100	1.34217200	-4.40445400	C	-2.92679900	-0.79613600	3.87743000
H	1.21073300	0.55884700	-4.47465400	C	-1.80221300	-0.74944600	2.84644300
H	5.39900900	2.03711300	-1.76095500	O	-0.62218700	-0.88367500	3.21712000
C	4.50512800	1.48415500	-1.45178800	O	-2.21660200	-0.58019600	1.62955000
C	4.00870700	1.99298600	-0.13272000	H	-3.42888800	0.17917900	3.90954600
N	2.91401400	1.44628500	0.52561100	H	-2.52710600	-1.03840200	4.86555800
C	4.51801400	3.01252900	0.64266600	C	-4.97830200	0.74876000	-0.03830900
C	2.76732700	2.11011500	1.66503600	C	-3.98002400	1.85656300	-0.16476200

N	-2.60264100	1.66754300	-0.16219800	O	1.70390500	-0.67055100	2.06750900
C	-4.22639100	3.20940400	-0.27257800	H	0.79044900	-0.81497800	2.47247400
C	-2.03726200	2.86164400	-0.25962200	H	2.25768000	-1.50541100	2.10451000
N	-2.98412200	3.82826100	-0.33376100	O	0.04247100	-1.49089500	-0.20446500
H	-2.80808200	4.82198300	-0.41455600	O	-0.07455000	0.86014400	0.57306600
H	-5.99182500	1.16425200	0.00363600	C	-0.02497700	-2.94081700	-3.20894600
H	-4.91129800	0.04505400	-0.87408200	H	-0.87771100	-2.26897600	-3.26263400
H	-4.79189200	0.17287900	0.87556100	H	-0.18054100	-4.01621000	-3.21995200
H	-5.15436400	3.76287500	-0.30642700	H	0.98635600	-2.54502700	-3.25917000
H	-0.97106300	3.04190600	-0.26654700	H	-0.01632400	-2.04541500	-1.00531200

Model2-TS2-undecet (HS-FM)

Fe	-1.58145500	-0.11469600	0.13690000	H	-1.07583800	2.12307400	4.05243200
Fe	1.31737100	-0.15801700	0.07000300	H	-1.60804300	4.61454700	-0.02722400
H	-4.48103900	-3.26747700	1.97525400	C	-1.61320100	3.54321900	0.20321100
C	-5.02633900	-2.49539500	1.41716300	C	-2.76857700	2.87074500	-0.47339300
C	-4.08506400	-1.85891000	0.40556200	N	-2.91420200	1.48956100	-0.53044900
O	-3.13410800	-1.14249400	0.90501100	C	-3.84277100	3.44975200	-1.11420700
O	-4.25955300	-2.05113100	-0.82313400	C	-4.04218500	1.24113400	-1.18582200
H	-5.88256100	-2.95111000	0.91298100	N	-4.63770500	2.40058700	-1.55581100
H	-5.36057700	-1.74426900	2.14195700	H	-5.50384100	2.47510000	-2.07559500
H	0.72321600	2.04884700	4.13951600	H	-0.66975200	3.09261700	-0.12337800
C	-0.19193700	1.49190700	3.91858100	H	-1.67817900	3.42086200	1.29146600
C	-0.14716200	0.92509200	2.50795500	H	-4.09959200	4.48587400	-1.28486600
O	-1.27721000	0.70259600	1.94807200	H	-4.43926600	0.25775500	-1.40685200
O	0.98197300	0.68959100	1.99873800	H	5.26081100	-3.23217700	0.95879400
H	-0.26526900	0.65348000	4.62374500	C	4.23006400	-2.96567400	1.20890700

C	3.84680900	-1.65257000	0.52561900	N	3.52865700	2.88981500	-1.75549800
O	4.60122700	-1.07586400	-0.25118200	H	3.68261200	3.44068000	-2.59089000
O	2.64882600	-1.23291700	0.89420800	H	4.76855000	2.45588600	2.07431100
H	3.54991000	-3.75955900	0.87508400	H	3.25564300	1.53113600	2.31242500
H	4.11471700	-2.87260700	2.29547700	H	4.69102200	0.72898300	1.65041100
H	2.89315400	-2.24402000	-3.67221400	H	5.06438800	3.65793500	-0.42638400
C	1.83496300	-2.51759100	-3.62993900	H	1.86940200	1.64762200	-2.36922900
C	1.21723800	-2.06767500	-2.31284600	O	-1.99143300	-1.08433300	-1.70132600
O	0.20444300	-2.69072600	-1.87064100	H	-2.84948400	-1.58477000	-1.54555700
O	1.75999100	-1.06195400	-1.74474200	H	-1.26829900	-1.72732600	-1.91592100
H	1.30998600	-2.01419300	-4.45336500	O	-0.08295800	-1.46769700	0.52851000
H	1.70583800	-3.59679400	-3.75641400	O	-0.00566200	0.78896200	-0.60986800
C	4.12637500	1.66771600	1.66434500	H	-0.00961800	-2.12484800	-0.22072000
C	3.70077600	2.02192700	0.27388900	C	-0.80889200	-3.32944700	2.14629500
N	2.66238400	1.39383800	-0.40052500	H	0.16605800	-3.18451200	2.59798200
C	4.24385300	2.96853500	-0.56677300	H	-1.63918700	-2.68831200	2.42009700
C	2.58427700	1.93172800	-1.60965500	H	-0.94618100	-4.10772300	1.40065100

Model2-**P**-undecet (HS-FM)

Fe	-1.62844600	-0.07343800	0.04566600	H	-5.10686100	-2.04814500	2.38289600
Fe	1.47733800	-0.12628800	0.07102500	H	0.35118400	2.57932000	3.69685000
H	-4.12555500	-3.49016000	2.10891000	C	-0.10515500	1.58726500	3.80716200
C	-4.77606400	-2.75694200	1.61493900	C	-0.12016200	0.89326200	2.45293300
C	-3.97570800	-2.02576800	0.54424000	O	-1.25292900	0.64902400	1.92939600
O	-3.03819900	-1.25945100	0.97187700	O	1.00660000	0.60291100	1.94687000
O	-4.26055900	-2.20268700	-0.67133200	H	0.51997800	1.01686600	4.50346100
H	-5.63360100	-3.27264900	1.17452600	H	-1.11800200	1.68945800	4.20487500

H	-1.78100700	4.57922400	-0.21010800	H	1.04393700	-1.75425400	-4.49297800
C	-1.74834700	3.51933200	0.06626500	H	1.58423200	-3.35886100	-3.97216800
C	-2.98312300	2.81540200	-0.40761700	C	4.28957000	1.76003100	1.52832800
N	-3.09846500	1.43119100	-0.41565100	C	3.76352500	2.17457300	0.19027000
C	-4.16094700	3.35295200	-0.88000300	N	2.70954200	1.52640500	-0.44060600
C	-4.30739200	1.13765400	-0.87962600	C	4.19873600	3.18900900	-0.63431200
N	-4.98545600	2.27386300	-1.17125100	C	2.51303700	2.12505200	-1.60849100
H	-5.92423900	2.31542700	-1.54930800	N	3.39727600	3.13741700	-1.76957900
H	-0.85885600	3.05040600	-0.36930700	H	3.45926200	3.74135700	-2.57993000
H	-1.65711300	3.44649700	1.15747500	H	5.01580400	2.49401000	1.89596800
H	-4.47190300	4.37787900	-1.02626600	H	3.47200400	1.66641900	2.25210000
H	-4.70050500	0.13810100	-1.02400200	H	4.77634900	0.78278300	1.43688000
H	5.18958500	-3.52001300	1.00393400	H	4.99394500	3.91169600	-0.51738600
C	4.14994300	-3.23170100	1.18232100	H	1.75030400	1.84999300	-2.32467600
C	3.89909200	-1.80793800	0.68542800	O	-2.18209000	-1.07853600	-1.75561300
O	4.77825300	-1.15988200	0.11602000	H	-2.99001100	-1.63129800	-1.50544800
O	2.68805800	-1.36747300	0.94697900	H	-1.45564700	-1.67118800	-2.04895800
H	3.48093900	-3.92630300	0.65756800	O	-0.19063800	-1.76231000	0.45241400
H	3.92020400	-3.30069000	2.25306600	O	-0.10116500	0.64203600	-0.66097600
H	2.72085000	-1.96329500	-3.92402400	H	-0.02743700	-2.22703700	-0.45120200
C	1.68652800	-2.28643600	-3.77844800	C	-0.21185700	-2.70151100	1.54211800
C	1.21660100	-1.96258500	-2.36920900	H	0.81727900	-2.96200300	1.81185100
O	0.20384200	-2.59189100	-1.91719100	H	-0.71292300	-2.21857600	2.38467900
O	1.85397200	-1.06870400	-1.73037500	H	-0.77450600	-3.59842700	1.25402800
Model2-RC(HS-AF)							
Fe	-1.38698400	0.01180800	0.20014900	Fe	1.29604000	0.10804000	-0.12539700

H	-3.67796000	3.73840300	-0.47794300	H	2.50349700	4.39579400	0.56874300
C	-4.21409900	3.17233700	0.29325000	C	2.05175800	3.40758000	0.44746900
C	-3.26324500	2.16708700	0.92553700	C	2.95412300	2.54557500	-0.41534200
O	-2.83457700	1.25516600	0.08514600	O	4.05502100	2.90770800	-0.80659500
O	-2.95470600	2.23752500	2.12330500	O	2.48902600	1.34389500	-0.76967500
H	-4.59972600	3.85334100	1.05610900	H	1.92094800	2.93316500	1.42684500
H	-5.04140900	2.64839100	-0.20012800	H	1.05809500	3.49182400	-0.00592900
H	-1.47025100	-1.02210000	-4.35508200	H	3.75193900	0.90248000	3.70090300
C	-0.70203200	-0.27848800	-4.11489400	C	3.15259800	-0.00587800	3.83553900
C	-0.46995100	-0.22613700	-2.61031300	C	1.93114400	0.04445100	2.92049700
O	-1.51418600	-0.21310400	-1.87441900	O	0.79248300	-0.06688600	3.41622000
O	0.72287200	-0.18271600	-2.19789000	O	2.21147100	0.21428800	1.67042200
H	0.22955700	-0.50217100	-4.64118900	H	3.78357400	-0.85897400	3.55591600
H	-1.07250300	0.70097400	-4.44312500	H	2.84418700	-0.09946700	4.87997100
H	-5.40870500	-1.57185300	-1.83674600	C	4.92753300	-0.44487100	-0.18641500
C	-4.50915400	-1.08661200	-1.44178000	C	4.01196000	-1.56357500	-0.57619600
C	-3.91762700	-1.91941900	-0.34650800	N	2.62324000	-1.48064200	-0.56944100
N	-2.74828200	-1.59497900	0.33331900	C	4.35743900	-2.83247200	-0.99037700
C	-4.40484800	-3.09563900	0.18172900	C	2.14810500	-2.65304000	-0.96579500
C	-2.53898700	-2.53794500	1.24324100	N	3.16592800	-3.50452200	-1.23207600
N	-3.51728700	-3.47043900	1.18252000	H	3.06583900	-4.45852500	-1.55637200
H	-3.59458500	-4.27887900	1.78777100	H	5.96435200	-0.80044700	-0.18008900
H	-3.78414200	-0.93922600	-2.24770200	H	4.84095500	0.40054400	-0.87692200
H	-4.77322400	-0.09163800	-1.06705900	H	4.66761500	-0.07084000	0.80940900
H	-5.28602200	-3.67270100	-0.06103000	H	5.32459200	-3.29493200	-1.12879700
H	-1.72070700	-2.55046900	1.94943700	H	1.09910000	-2.89631400	-1.06353500

O	-1.55275300	0.00707800	2.31165600	C	-1.18303600	4.11731800	-2.47744900
H	-0.62692300	0.02910100	2.71582300	H	-0.22950600	4.11084000	-3.01714400
H	-2.01683200	0.86969700	2.49633500	H	-1.21227200	4.98445800	-1.80761300
O	-0.11911200	1.23731700	0.09459700	H	-2.00856600	4.18348400	-3.19566600
O	0.01103300	-1.10947800	0.30103000	H	-1.27424100	3.19608000	-1.89253700

Model2-TS1(HS-AF)

Fe	1.47009400	-0.16670400	0.09943200	C	4.68949400	2.73570700	0.76043300
Fe	-1.47132700	-0.13183500	-0.26533100	C	2.89881200	1.90868400	1.77491700
H	4.15363200	-3.32608500	-1.63676200	N	3.93249700	2.77166300	1.92425900
C	4.56269900	-3.03285900	-0.66314500	H	4.12792800	3.31575300	2.75588400
C	3.48898500	-2.34860500	0.17365900	H	3.72760800	1.73851700	-2.19290900
O	2.89235600	-1.36195600	-0.43978900	H	4.54013700	0.32989000	-1.52817200
O	3.25097100	-2.73101800	1.33151600	H	5.58115200	3.33233400	0.62773400
H	4.94902300	-3.90797800	-0.13463400	H	2.15736500	1.69988200	2.53360500
H	5.38192300	-2.32711900	-0.85087300	H	-2.54056400	-3.80894300	-1.30702100
H	-0.22649200	0.92804600	-4.56283500	C	-3.22454900	-3.36708700	-0.57150700
C	0.60261600	1.26865100	-3.93561700	C	-3.71491400	-2.01418000	-1.07779000
C	0.42345500	0.75557300	-2.51261400	O	-4.89013200	-1.80794900	-1.36018300
O	1.48633700	0.49761200	-1.85535100	O	-2.77164300	-1.09612500	-1.21929000
O	-0.76042300	0.64208300	-2.08433000	H	-4.07369800	-4.03834000	-0.41648200
H	1.56132600	0.94095300	-4.34796400	H	-2.66590600	-3.23685700	0.36230300
H	0.58612200	2.36685100	-3.91995500	H	-3.74599000	-1.88867500	3.20643300
H	5.44324700	1.86326700	-1.71100700	C	-3.02331300	-1.19179900	3.64686000
C	4.47360200	1.42043900	-1.45686000	C	-1.85512000	-0.97950500	2.68798500
C	4.06720300	1.83157100	-0.07445100	O	-0.69021800	-1.13743100	3.09767100
N	2.95040100	1.32973800	0.58281400	O	-2.20690100	-0.63864300	1.48953200

H -3.54207400	-0.23699800	3.80166400	H -4.79644900	4.13040000	0.22885500
H -2.66542000	-1.57419700	4.60625800	H -0.74164900	3.00478900	-0.31675600
C -4.91141700	1.09467400	0.24750300	O 1.68044700	-0.77260300	2.07391600
C -3.82507200	2.11257400	0.09280100	H 0.75174600	-0.95013100	2.42840100
N -2.48581000	1.78598200	-0.09343500	H 2.19962200	-1.62477400	2.01939600
C -3.93589500	3.48678400	0.11190600	O 0.04214000	-1.40267100	-0.28231800
C -1.81158300	2.92416600	-0.18147200	O 0.19657400	0.83174700	0.53574100
N -2.64989900	3.98250800	-0.06322200	C 0.64558600	-3.37131400	-1.72795600
H -2.37868100	4.95724100	-0.10052300	H -0.27181800	-3.58972400	-2.27879800
H -5.87568200	1.59524100	0.39273800	H 0.94465200	-4.14831700	-1.02122500
H -4.97800000	0.43865700	-0.62750700	H 1.45762600	-2.98096600	-2.34325400
H -4.71222200	0.45179600	1.11296100	H 0.31367300	-2.36692100	-0.98393700

Model2-**IM**(HS-AF)

Fe 1.56649300	-0.22596700	0.05796000	O -0.78232800	0.54712500	-2.07145900
Fe -1.34657300	-0.08856000	-0.07473600	H -0.38462100	1.32363300	-4.42420700
H 4.02235600	-3.81126100	-1.27341100	H 1.23003700	0.54095500	-4.48226200
C 4.55556600	-3.30531000	-0.45889900	H 5.39183800	2.04823100	-1.74273600
C 3.57609200	-2.44399700	0.32497900	C 4.48730900	1.50442000	-1.44852300
O 3.02316800	-1.48241300	-0.36278900	C 3.99592700	1.99262700	-0.11978000
O 3.35000300	-2.67613700	1.52662800	N 2.90162100	1.43827700	0.53277200
H 5.01930600	-4.04707300	0.19617000	C 4.51059600	2.99805300	0.67053000
H 5.32509800	-2.67216600	-0.91688900	C 2.76100400	2.08334300	1.68350400
H 1.08076900	2.19519400	-3.87724000	N 3.71151700	3.04139700	1.80648700
C 0.57898700	1.21991100	-3.91961900	H 3.83019100	3.65281900	2.60525800
C 0.39010500	0.69151600	-2.50456000	H 3.71969600	1.63366100	-2.21903900
O 1.46427500	0.42669900	-1.85411200	H 4.71210400	0.43250300	-1.40145700

H	5.35629500	3.65653300	0.52945000	C	-4.17907300	3.24019400	-0.25137300
H	2.01213100	1.86195900	2.43199100	C	-1.99446600	2.86609300	-0.25326800
H	-3.39454900	-4.04521500	0.34018400	N	-2.92993100	3.84389300	-0.32088800
C	-2.63958300	-3.35497700	-0.04696000	H	-2.74234600	4.83531600	-0.40418600
C	-3.33324700	-2.20234400	-0.76066100	H	-5.96752300	1.21798700	0.04083800
O	-4.47941200	-2.30304500	-1.18423900	H	-4.91161400	0.08994300	-0.85494900
O	-2.62216600	-1.10028300	-0.98571400	H	-4.77151200	0.20578600	0.89437300
H	-1.98522900	-3.00240800	0.75300500	H	-5.10043400	3.80491500	-0.27890300
H	-2.01897300	-3.89444800	-0.77546700	H	-0.92638800	3.03412100	-0.26994700
H	-3.67487100	-1.55778900	3.57668800	O	1.70391200	-0.70255900	2.05110500
C	-2.92340700	-0.81850100	3.87753500	H	0.79344000	-0.85315600	2.45841100
C	-1.80308100	-0.76926300	2.84196000	H	2.26580700	-1.53389700	2.08016200
O	-0.62246300	-0.91749800	3.20544900	O	0.03438700	-1.49987200	-0.21760200
O	-2.22098100	-0.58261800	1.62872800	O	-0.06080900	0.82581200	0.56704600
H	-3.42226800	0.15812800	3.91852800	C	-0.12424300	-2.94746700	-3.16818600
H	-2.52054400	-1.06919400	4.86227100	H	-0.96711400	-2.26471900	-3.23689800
C	-4.96019700	0.78920500	-0.01413400	H	-0.29678300	-4.01936700	-3.12175300
C	-3.94883000	1.88440000	-0.14545200	H	0.89119400	-2.57370900	-3.27440800
N	-2.57374400	1.67882100	-0.15162600	H	-0.04709600	-2.03538300	-1.03150100
Model2-TS2(HS-AF)							
Fe	-1.58015300	-0.11691300	0.14477500	O	-4.27611100	-1.99745800	-0.85669400
Fe	1.30909700	-0.14989100	0.07226000	H	-5.91341800	-2.91148800	0.86007700
H	-4.51205600	-3.26816500	1.90920200	H	-5.37655100	-1.74159100	2.11875700
C	-5.05183400	-2.47654500	1.37347300	H	0.73907600	2.04756000	4.13074900
C	-4.10652400	-1.82422800	0.37628000	C	-0.16744300	1.46991400	3.92731500
O	-3.15710300	-1.11658600	0.88891300	C	-0.14134900	0.91162100	2.51312000

O	-1.27402400	0.70322300	1.95950500	O	0.18349700	-2.66538000	-1.90732000
O	0.98567400	0.66809500	1.99731200	O	1.74313400	-1.04456500	-1.72673400
H	-0.20150600	0.62511200	4.62778700	H	1.35067000	-1.96667200	-4.45499400
H	-1.06311600	2.07806300	4.08561500	H	1.73086900	-3.55589200	-3.76496300
H	-1.55042900	4.63723000	0.03608700	C	4.12022600	1.64534200	1.67995400
C	-1.55959800	3.56186000	0.24667100	C	3.70153100	2.01010300	0.29009200
C	-2.71942500	2.90693900	-0.43975100	N	2.65972200	1.39530900	-0.39154100
N	-2.87625000	1.52813700	-0.51612000	C	4.25700800	2.95529200	-0.54419900
C	-3.78918200	3.50486800	-1.07071000	C	2.59233800	1.93938500	-1.59867700
C	-4.00750500	1.29938500	-1.17284600	N	3.54648200	2.88896700	-1.73605500
N	-4.59371500	2.46912500	-1.52581800	H	3.70977200	3.44178700	-2.56843200
H	-5.46074000	2.55833800	-2.04177000	H	4.76257000	2.42916600	2.09783100
H	-0.61733900	3.11600200	-0.08946900	H	3.24676000	1.50577000	2.32349900
H	-1.62274500	3.41966800	1.33250600	H	4.68302200	0.70551700	1.66210800
H	-4.03742100	4.54556600	-1.22558500	H	5.08363000	3.63594800	-0.39717100
H	-4.41468700	0.32286100	-1.40572200	H	1.88119500	1.66382200	-2.36492300
H	5.20580600	-3.26634700	0.93660300	O	-1.99870700	-1.04156600	-1.71084900
C	4.17907100	-2.98673300	1.18874400	H	-2.86460200	-1.53323700	-1.56217900
C	3.81561100	-1.66434100	0.51516100	H	-1.28386900	-1.69160400	-1.93040600
O	4.57541400	-1.09044600	-0.25757500	O	-0.13173300	-1.46654500	0.52472700
O	2.62276600	-1.22937500	0.88866000	O	0.00449200	0.76991500	-0.58388000
H	3.48712500	-3.76806300	0.84975000	H	-0.05437300	-2.13006600	-0.21345200
H	4.06461900	-2.89944900	2.27583000	C	-0.81699300	-3.68793200	2.02678700
H	2.91542200	-2.20395000	-3.63871900	H	0.15781500	-3.52241900	2.47286100
C	1.85664800	-2.47801900	-3.62465000	H	-1.64435200	-3.03454700	2.28201100
C	1.20621600	-2.04357000	-2.31794300	H	-0.93854000	-4.44735900	1.25888400

Model2-P(HS-AF)

Fe	1.57415500	-0.15944400	-0.06896600	H	0.74181100	3.01908400	-1.97085800
Fe	-1.67128800	-0.36398200	0.02094600	H	2.83072000	5.13591300	0.20790300
H	5.30944900	-2.84038800	-1.17783100	H	4.22803400	1.23501900	1.12521600
C	5.57538200	-1.80527200	-0.92412100	H	-4.68981700	-3.17156600	-1.92245200
C	4.46517000	-1.21814600	-0.05971600	C	-3.67666600	-3.43953000	-1.61053400
O	3.44934100	-0.74710100	-0.68789600	C	-2.96115800	-2.24001400	-1.02818900
O	4.59328300	-1.23375000	1.19368400	O	-3.57779500	-1.16566500	-0.76611400
H	6.52273300	-1.81763000	-0.37704500	O	-1.70662600	-2.31795100	-0.77841400
H	5.67228500	-1.24579700	-1.86034600	H	-3.72790200	-4.22783300	-0.84861300
H	-1.04217800	0.96598300	-4.36817200	H	-3.10908300	-3.83725900	-2.45965300
C	-0.12172000	0.46424200	-4.05623900	H	-2.94125400	-2.23898500	3.97888700
C	-0.12449400	0.21041800	-2.55430000	C	-1.84819300	-2.18438200	3.96219700
O	1.01690400	0.00346400	-2.02058300	C	-1.34518100	-1.90523700	2.54785900
O	-1.24626900	0.20149500	-1.96829100	O	-0.23084300	-2.37324000	2.20175700
H	-0.06255100	-0.50537000	-4.56835800	O	-2.11778500	-1.17639400	1.82325400
H	0.75972900	1.04573500	-4.34516800	H	-1.53944300	-1.35657700	4.61547700
H	0.36723100	4.38064900	-0.89276200	H	-1.40780500	-3.10847900	4.34792700
C	0.65280900	3.32288600	-0.92000400	C	-4.31885800	1.78318200	-1.48114800
C	1.94562300	3.11079500	-0.19327000	C	-3.76149600	2.16218300	-0.14337600
N	2.43784300	1.85029200	0.11574400	N	-2.74795100	1.44936300	0.48419900
C	2.84190100	4.05604600	0.25873500	C	-4.11376000	3.22012400	0.66794500
C	3.59680300	2.02481300	0.73690200	C	-2.49419800	2.05448300	1.63654200
N	3.88140400	3.34629000	0.84506000	N	-3.30068300	3.13270300	1.79169700
H	4.70538800	3.73474200	1.28752400	H	-3.30679400	3.75392200	2.59140900
H	-0.14242600	2.72096800	-0.46849000	H	-5.05379200	2.52655700	-1.81031600

H	-3.51560600	1.71574800	-2.22401000	O	1.22535400	-2.26027500	0.02033700
H	-4.79051900	0.79655400	-1.43216100	O	-0.06293900	0.25468000	0.55559200
H	-4.85160400	4.00042800	0.54432000	H	0.50719800	-2.44765600	0.69046000
H	-1.74786200	1.73849500	2.35343900	C	1.30207400	-3.23916400	-1.02123300
O	2.21941100	-0.50418700	1.97043800	H	0.32862600	-3.35172000	-1.50973900
H	3.13411000	-0.91494200	1.84998200	H	2.04744600	-2.88468900	-1.73866300
H	1.59708700	-1.17289600	2.31917200	H	1.62741800	-4.20262300	-0.60383500

Model2H-RC(HS-FM)

Fe	-1.48952500	0.03337900	0.16028600	C	-4.07636200	-1.75945200	-0.53172500
Fe	1.44420700	0.13474400	-0.19787900	N	-2.92503100	-1.52412900	0.21391400
H	-3.53263700	3.87703400	-0.45661100	C	-4.67061500	-2.90741400	-0.05376600
C	-4.11001400	3.35129200	0.31378600	C	-2.83086000	-2.49508500	1.11225400
C	-3.23884300	2.26531300	0.92415000	N	-3.86589600	-3.35776500	0.98446100
O	-2.95371000	1.28580100	0.10619100	H	-4.02663900	-4.17102400	1.56613500
O	-2.85953000	2.33688600	2.10542400	H	-3.80409300	-0.83240900	-2.44650800
H	-4.42625200	4.05791500	1.08527400	H	-4.70199800	0.14408700	-1.29040000
H	-4.98376000	2.90522800	-0.17552200	H	-5.57291900	-3.42020500	-0.35592900
H	-1.45668400	-0.93905000	-4.34487400	H	-2.05581200	-2.58479800	1.85933400
C	-0.56077200	-0.36864600	-4.08103000	H	2.95957800	4.50517900	0.62089000
C	-0.39965100	-0.28628000	-2.57170400	C	2.34718000	3.64482400	0.33697100
O	-1.46424900	-0.27575500	-1.87366300	C	3.20223600	2.61217700	-0.38499900
O	0.77757900	-0.21314500	-2.11207500	O	4.39505300	2.77370500	-0.61309800
H	0.33085900	-0.80709700	-4.53793400	O	2.54559600	1.52571300	-0.77210000
H	-0.67845400	0.65215200	-4.46781200	H	1.89676900	3.18947900	1.22692200
H	-5.49328700	-1.26557200	-2.05202900	H	1.52522700	3.96636900	-0.31383500
C	-4.55076200	-0.87971300	-1.64766800	H	2.47405700	1.21794800	4.26332800

C	2.62378200	0.15717600	4.02384900	H	4.84456800	-0.16917100	0.92624700
C	1.74857000	-0.20601800	2.83350000	H	5.46662900	-3.41678300	-0.89842900
O	0.73918000	-0.94182400	3.00226800	H	1.24296600	-2.97594100	-0.94274200
O	2.10438900	0.29673300	1.70611000	O	-1.76128400	-0.01900400	2.34468300
H	3.68107400	0.02848200	3.76685500	H	-2.10815400	0.91435900	2.47546300
H	2.36333100	-0.45071100	4.89414400	H	-0.88865200	-0.11674500	2.78499000
C	5.05865100	-0.51133200	-0.09363200	O	-0.30398300	1.22847300	0.13136000
C	4.15679300	-1.64730100	-0.46570600	O	-0.06628100	-1.26064600	0.40479600
N	2.76967800	-1.54685900	-0.49904300	H	0.15687700	-1.32721900	1.37158800
C	4.50191100	-2.93767900	-0.80740600	C	-0.94691300	4.22970000	-2.27654500
C	2.29320000	-2.73565500	-0.84467800	H	-0.04409200	4.30656600	-2.89293400
N	3.30886600	-3.60991800	-1.04386100	H	-1.05055600	5.13851400	-1.67242500
H	3.20716400	-4.57979700	-1.31655000	H	-1.82285700	4.12218600	-2.92712800
H	6.10552600	-0.83167400	-0.14414600	H	-0.86596900	3.35691700	-1.61992800
H	4.91586300	0.35432600	-0.74936200				

Model2H-TS1(HS-FM)

Fe	-1.56607100	0.16277300	0.04156400	C	-0.48889400	-1.44099200	-3.85092700
Fe	1.49513000	0.11753100	-0.19826200	C	-0.33553300	-0.88651200	-2.44299700
H	-3.76516200	3.88821500	-1.40712000	O	-1.41984700	-0.61554300	-1.81921700
C	-4.35271500	3.43326300	-0.59998400	O	0.82967200	-0.73856300	-1.98526200
C	-3.45662100	2.51865700	0.22233600	H	0.48637700	-1.53972500	-4.33339600
O	-2.95328300	1.51173600	-0.42521700	H	-1.13632900	-0.77890600	-4.43733700
O	-3.25063700	2.76192300	1.43022600	H	-5.50629400	-1.62504100	-2.05654000
H	-4.78186600	4.21571700	0.03086600	C	-4.54923800	-1.22752900	-1.70028800
H	-5.15185400	2.84672300	-1.06905100	C	-4.24128000	-1.76024200	-0.33393800
H	-0.97886300	-2.42184300	-3.80221000	N	-3.15040300	-1.33961500	0.41782200

C	-4.94320400	-2.69479700	0.39749600	C	4.06509400	-1.95194500	-0.00235800
C	-3.19432300	-1.99626300	1.56849600	N	2.69557800	-1.71168800	-0.01657200
N	-4.26098200	-2.83289600	1.59946900	C	4.26610000	-3.31426100	0.06714800
H	-4.52191700	-3.42643600	2.37747800	C	2.08944700	-2.88985300	0.04463000
H	-3.75955300	-1.49711600	-2.40971000	N	3.00238700	-3.89079900	0.09431300
H	-4.59769900	-0.13304200	-1.67911200	H	2.79132400	-4.87966800	0.14568300
H	-5.84414200	-3.24883300	0.17350700	H	6.10077400	-1.30332200	0.01250200
H	-2.49917800	-1.86995500	2.38712400	H	5.01920400	-0.26921200	-0.95768900
H	4.07497700	4.09987500	-0.27177000	H	4.96668100	-0.18062000	0.80157300
C	3.27121700	3.35889300	-0.24465400	H	5.17390000	-3.90037800	0.09882400
C	3.66460400	2.13416200	-1.06503100	H	1.01682500	-3.02885800	0.06684800
O	4.74316000	2.05315500	-1.64345500	O	-1.87694100	0.67376000	2.07791600
O	2.75821600	1.17211400	-1.10803700	H	-2.35966700	1.56234100	2.02253600
H	3.07281100	3.05026300	0.78837700	H	-1.02592500	0.75326400	2.56814400
H	2.34671600	3.79759900	-0.63793900	O	-0.06522700	1.36806100	-0.26978700
H	2.43592400	2.41355900	3.81533100	O	-0.07146200	-0.96990800	0.70769000
C	2.55566300	1.32415000	3.88631000	H	0.10347600	-0.78862600	1.66374200
C	1.69637500	0.66949100	2.81265800	C	-0.22264900	3.25213000	-1.93940200
O	0.58904100	0.16220200	3.13283900	H	0.67314300	3.15608000	-2.55711600
O	2.17568900	0.70028500	1.62098900	H	-0.26605200	4.18162000	-1.36578500
H	3.61403600	1.09595900	3.72224900	H	-1.14859700	3.02611500	-2.47328700
H	2.23953300	0.99904700	4.88115600	H	-0.12481600	2.34454600	-1.09325000
C	5.09655400	-0.86769200	-0.04369400				
Model2H- IM (HS-FM)							
Fe	-1.54461500	0.11295400	0.11796900	H	-3.78163900	3.96073300	-0.96420800
Fe	1.52165500	0.12442000	-0.18076200	C	-4.35055800	3.42630300	-0.19327200

C	-3.43686500	2.44142100	0.52199200	C	3.50500000	2.33498600	-0.88781700
O	-2.92231500	1.51728600	-0.23257000	O	4.67883400	2.35900700	-1.24121900
O	-3.23074100	2.55520600	1.74850600	O	2.72705200	1.27780300	-1.05826300
H	-4.77190600	4.14154200	0.51753000	H	2.33299400	3.23806700	0.68605200
H	-5.15648400	2.88242100	-0.70098800	H	2.04089800	3.91912300	-0.92120800
H	-1.00544500	-2.15754900	-3.90756000	H	2.59078800	2.13099600	3.89983900
C	-0.52712700	-1.16968800	-3.90939100	C	2.64728800	1.03556600	3.94813800
C	-0.34909200	-0.69851700	-2.47424700	C	1.77063500	0.45126400	2.84854600
O	-1.42229200	-0.45859600	-1.81876400	O	0.67382400	-0.08733300	3.14913800
O	0.82286500	-0.57981800	-2.02632700	O	2.23206700	0.56770100	1.65379000
H	0.43840400	-1.22993600	-4.41721300	H	3.69400300	0.75503300	3.78759600
H	-1.19442200	-0.48298600	-4.44273400	H	2.30529800	0.70173200	4.93130400
H	-5.52209500	-1.46528700	-2.08807300	C	5.12369700	-0.73605300	-0.01587100
C	-4.57252100	-1.08204400	-1.69793500	C	4.14218700	-1.85974900	-0.14034200
C	-4.23031400	-1.75891500	-0.40565000	N	2.76444800	-1.67404000	-0.17942900
N	-3.12474400	-1.41485000	0.36356800	C	4.39827900	-3.21275500	-0.21211300
C	-4.91088300	-2.77275500	0.23451900	C	2.20694700	-2.87399200	-0.26698500
C	-3.13965400	-2.19348500	1.43651100	N	3.15982400	-3.83790700	-0.29313800
N	-4.20138700	-3.03571400	1.39922200	H	2.99001400	-4.83408500	-0.35514900
H	-4.44141700	-3.71296500	2.11299400	H	6.14531900	-1.13195200	0.01543600
H	-3.78453800	-1.24331300	-2.44127700	H	5.03970000	-0.02720700	-0.84659700
H	-4.65408500	0.00071800	-1.55019800	H	4.93872800	-0.16732600	0.90361100
H	-5.81356500	-3.30596500	-0.02937500	H	5.32850000	-3.76347100	-0.21076000
H	-2.42581300	-2.15325900	2.24780000	H	1.14125000	-3.05734000	-0.29531700
H	3.55284800	4.32950700	-0.05934900	O	-1.82000000	0.43625300	2.18598300
C	2.82062000	3.53946100	-0.24778300	H	-2.31573100	1.31895800	2.21804600

H -0.95427600	0.48947900	2.65601900	H 0.15817700	2.98162000	-3.14368300
O -0.04685600	1.40521300	-0.08608400	H -0.67422100	4.44292700	-2.30561600
O -0.02869800	-1.06379600	0.63957700	H -1.59093700	2.80768200	-2.46772800
H 0.16284400	-0.98124300	1.60375100	H -0.12228000	2.12977300	-0.73467300
C -0.68944600	3.39862400	-2.60619400			

Model2H-TS2(HS-FM)

Fe -1.63809	0.13541	0.02683	C -5.04206	-2.65481	0.40489
Fe 1.43567	0.11644	-0.21872	C -3.24488	-2.05157	1.55581
H -3.90375	3.82008	-1.3098	N -4.33173	-2.86279	1.58041
C -4.07717	3.70652	-0.23308	H -4.58472	-3.4872	2.33656
C -3.08201	2.71386	0.35181	H -3.87617	-1.3031	-2.36136
O -3.03171	1.56308	-0.23835	H -4.73611	-0.00369	-1.53795
O -2.38845	3.0318	1.34759	H -5.96181	-3.17727	0.18157
H -3.99431	4.67428	0.26815	H -2.52566	-1.98308	2.36076
H -5.09387	3.31334	-0.1058	H 3.82758	4.19175	0.14613
H 0.45083	-1.17428	-4.47053	C 3.04705	3.43526	0.02711
C -0.527	-1.13462	-3.9847	C 3.5708	2.2682	-0.80691
C -0.39487	-0.65989	-2.54623	O 4.70144	2.26523	-1.28376
O -1.4814	-0.46109	-1.90638	O 2.71474	1.27879	-0.98451
O 0.76876	-0.49676	-2.07977	H 2.72616	3.06511	1.00806
H -1.19554	-0.46137	-4.53359	H 2.17465	3.88341	-0.46469
H -0.98579	-2.13155	-3.99414	H 3.02514	1.59408	3.88087
H -5.6175	-1.48566	-2.00616	C 2.70272	0.54836	3.94539
C -4.66543	-1.09367	-1.63098	C 1.68751	0.24996	2.85022
C -4.3365	-1.70494	-0.30285	O 0.59576	-0.30069	3.14759
N -3.21488	-1.34555	0.43497	O 2.0408	0.59048	1.66028

H	3.5919	-0.07563	3.7886	H	1.0371	-3.03675	-0.29567
H	2.27955	0.34135	4.93161	O	-1.77745	0.58893	2.14302
C	5.06947	-0.79736	-0.043	H	-1.94954	1.57266	2.09018
C	4.06095	-1.89785	-0.15827	H	-0.92252	0.42075	2.60922
N	2.68622	-1.68572	-0.18211	O	-0.15836	1.47888	-0.28398
C	4.29174	-3.25474	-0.24057	O	-0.09314	-1.08	0.51381
C	2.10676	-2.8762	-0.27344	H	0.06552	-1.06579	1.48309
N	3.04177	-3.85648	-0.31511	C	-0.20421	2.84237	-2.0978
H	2.85285	-4.84882	-0.38401	H	-0.2874	3.79852	-1.58778
H	6.08099	-1.21867	-0.01486	H	0.76604	2.50675	-2.44541
H	5.00011	-0.09199	-0.87785	H	-1.10604	2.37923	-2.48157
H	4.90748	-0.21907	0.87517	H	-0.16908	2.22754	0.3364
H	5.21204	-3.82184	-0.25198				

Model2H-P(HS-FM)

Fe	1.94670600	-0.17814200	-0.06041500	O	1.46739400	0.56798200	-1.96662100
Fe	-1.54176900	-0.07063100	-0.17929800	O	-0.79012600	0.41772800	-1.99825200
H	3.48701600	-4.08950000	-1.98729300	H	-0.08721300	0.27463000	-4.60077100
C	3.39597200	-4.17123300	-0.89789600	H	1.29763200	1.37872000	-4.34620000
C	2.51490500	-3.04896300	-0.37055100	H	4.84128300	3.09823900	-1.95665000
O	2.82764600	-1.86048700	-0.73395600	C	4.10896100	2.35858800	-1.61390900
O	1.54334400	-3.32229700	0.39401700	C	4.42203400	1.93032300	-0.21244900
H	2.98830000	-5.14703600	-0.62241100	N	3.66341800	0.99166700	0.47926500
H	4.40473700	-4.06247500	-0.47958700	C	5.45873700	2.34335600	0.59646700
H	-0.39480200	1.93903500	-4.10737000	C	4.23145800	0.83926600	1.67145000
C	0.30155500	1.10032300	-3.99183000	N	5.31974500	1.63982300	1.78570900
C	0.34294000	0.66327000	-2.53271400	H	5.92256700	1.70115300	2.59738400

H	3.10556300	2.79446900	-1.67843300	C	-3.29869400	3.95303500	0.29979200
H	4.12367100	1.50064600	-2.29550700	C	-1.32261200	2.96263500	0.12458100
H	6.25964300	3.05013300	0.42943300	N	-1.92796400	4.16959000	0.23812200
H	3.88029100	0.15751400	2.43609400	H	-1.45520100	5.06374300	0.28422400
H	-5.08539000	-3.19951500	0.03741300	H	-5.60350900	2.51935400	0.39214500
C	-4.10601000	-2.72952000	-0.08905500	H	-4.92668800	1.24929800	-0.66313100
C	-4.26143600	-1.40136900	-0.82404600	H	-4.76380200	1.11087000	1.08365200
O	-5.33966200	-1.03203500	-1.27998200	H	-4.01152700	4.75963200	0.39929200
O	-3.15554700	-0.68791200	-0.94642500	H	-0.25323600	2.80724400	0.07879300
H	-3.62927700	-2.55813400	0.88195200	O	2.07417300	-1.18894500	2.13428000
H	-3.45081600	-3.39790100	-0.66080500	H	1.87733500	-2.08331400	1.77671600
H	-2.76386000	-2.15785600	3.82150200	H	1.26512400	-0.93178200	2.62979000
C	-2.50577300	-1.10430200	3.98863900	O	-0.71192600	-2.09727400	-0.49978100
C	-1.59940700	-0.62883700	2.86085100	O	0.21451300	0.50102400	0.60454200
O	-0.40887800	-0.30982000	3.11556400	H	0.10046000	0.37943900	1.57783900
O	-2.14182700	-0.59450000	1.69428000	H	0.08095000	-2.46708500	-0.02802800
H	-3.44208800	-0.53445400	3.97872600	C	-0.80747400	-2.75381300	-1.77271300
H	-2.00716800	-0.99843000	4.95560700	H	-1.66856300	-2.33032300	-2.29312900
C	-4.76517000	1.82705800	0.25272700	H	0.09820600	-2.58193400	-2.37042700
C	-3.47730700	2.58853300	0.21326100	H	-0.95051000	-3.83302400	-1.62923900
N	-2.22611300	1.99019400	0.10176400				

Model2H-RC(HS-AF)

Fe	-1.48237700	0.01927500	0.17614500	C	-3.19311800	2.29052500	0.91252900
Fe	1.43379400	0.13217500	-0.19596600	O	-2.92147300	1.30453800	0.09893900
H	-3.44897400	3.90694100	-0.47123700	O	-2.81953400	2.35745900	2.09632800
C	-4.04046800	3.39182300	0.29560500	H	-4.34911500	4.10448900	1.06461400

H	-4.91882100	2.96137700	-0.19935900	H	1.50865600	3.96672000	-0.27760500
H	-1.45990500	-0.93638400	-4.34083800	H	2.46102400	1.22601800	4.25601300
C	-0.55997600	-0.37459000	-4.07216100	C	2.62084500	0.16526100	4.02259300
C	-0.39933000	-0.30635300	-2.56221300	C	1.75121400	-0.21075600	2.83207700
O	-1.46337700	-0.28645400	-1.86467600	O	0.72742500	-0.92478900	3.00890000
O	0.77964000	-0.25622400	-2.10210700	O	2.12682800	0.25767300	1.69723100
H	0.32872300	-0.81578000	-4.53202100	H	3.67986700	0.04309700	3.77048500
H	-0.67037600	0.65018000	-4.45046700	H	2.36059500	-0.43867000	4.89574100
H	-5.51927100	-1.18205600	-2.05154800	C	5.05935800	-0.50336100	-0.11875000
C	-4.57653100	-0.80844800	-1.63634100	C	4.16031400	-1.64677300	-0.47482400
C	-4.11242600	-1.70954200	-0.53322500	N	2.77318400	-1.55024000	-0.50341400
N	-2.95413800	-1.50315000	0.21002800	C	4.50877300	-2.93953100	-0.80438200
C	-4.72236400	-2.85471200	-0.06866300	C	2.29947000	-2.74380400	-0.83476400
C	-2.87064900	-2.48846000	1.09373600	N	3.31684400	-3.61797100	-1.02853700
N	-3.91993200	-3.33254700	0.95912100	H	3.21692200	-4.59088500	-1.29071600
H	-4.09028600	-4.15192100	1.52935100	H	6.10752600	-0.81919000	-0.17134500
H	-3.82527300	-0.75270300	-2.43037100	H	4.90930700	0.35478300	-0.78267300
H	-4.72350200	0.21022000	-1.26321600	H	4.84832000	-0.15186900	0.89851300
H	-5.63337400	-3.34966900	-0.37441000	H	5.47460400	-3.41659900	-0.89455200
H	-2.09109600	-2.60219800	1.83284300	H	1.24970600	-2.98890600	-0.92653900
H	2.95188300	4.49271500	0.64989100	O	-1.77912900	-0.02377900	2.35694700
C	2.33719400	3.63592800	0.36020200	H	-2.11137800	0.91641000	2.47864400
C	3.18524900	2.61491600	-0.38669500	H	-0.90702000	-0.12601800	2.79847600
O	4.37296200	2.78558700	-0.63311000	O	-0.26156200	1.17065000	0.16453400
O	2.52738200	1.52942500	-0.77435400	O	-0.09223900	-1.29839100	0.42825000
H	1.89636200	3.16753000	1.24817800	H	0.14922100	-1.32704200	1.39361100

C	-0.89081800	4.17357800	-2.32623900	H	-1.75915600	4.07536900	-2.98827600
H	0.02236500	4.22827300	-2.92945900	H	-0.83490700	3.30580200	-1.66050300
H	-0.98698100	5.08985500	-1.73224600				

Model2H-TS1(HS-AF)

Fe	1.58697200	-0.18614800	0.03769100	N	4.24912300	2.81077000	1.63930100
Fe	-1.50327500	-0.11075600	-0.18570400	H	4.50709500	3.39329800	2.42655300
H	3.75637900	-3.87518300	-1.50424800	H	3.74412600	1.53484300	-2.38971700
C	4.35493800	-3.44060000	-0.69398500	H	4.60815600	0.17265000	-1.68646000
C	3.47295100	-2.53721800	0.15547500	H	5.82150900	3.26856500	0.21425100
O	2.97571500	-1.51036700	-0.46634900	H	2.50190000	1.81444400	2.41773500
O	3.27271800	-2.80512400	1.35859000	H	-4.15242900	-4.05771400	-0.21618800
H	4.78441800	-4.23852000	-0.08306600	C	-3.33398500	-3.33313300	-0.18553900
H	5.15347000	-2.85002500	-1.15894100	C	-3.68210800	-2.11905300	-1.04060200
H	0.96396000	2.43298600	-3.78971600	O	-4.75119000	-2.02088600	-1.63361100
C	0.48132900	1.44852900	-3.83926400	O	-2.74766600	-1.18406300	-1.09823000
C	0.33533900	0.89030700	-2.43177200	H	-3.15502300	-3.00471600	0.84485200
O	1.42310900	0.62840300	-1.81114900	H	-2.40935600	-3.79901700	-0.54542200
O	-0.82886200	0.73274000	-1.97335200	H	-2.41380600	-2.46502900	3.80604500
H	-0.49574000	1.54104500	-4.31939900	C	-2.54015100	-1.37690000	3.88625700
H	1.13253700	0.79270700	-4.42855200	C	-1.68977100	-0.70931700	2.81354500
H	5.49059300	1.68519400	-2.04309800	O	-0.56754100	-0.23085400	3.12660500
C	4.54184900	1.26642300	-1.68900100	O	-2.19044100	-0.69975100	1.63019300
C	4.23276300	1.77176100	-0.31250200	H	-3.60064200	-1.15296700	3.73119800
N	3.14976800	1.32607600	0.43653400	H	-2.21873400	-1.05968000	4.88206400
C	4.92746800	2.70114100	0.43221400	C	-5.08819900	0.92587400	-0.08647100
C	3.19159700	1.96315100	1.59833500	C	-4.04266100	1.99481700	-0.01287800

N	-2.67708300	1.73381300	-0.00073400	H	2.39227800	-1.61191600	1.99123400
C	-4.22471900	3.35932500	0.06569800	H	1.05955000	-0.82216100	2.55449900
C	-2.05467300	2.90209800	0.08501100	O	0.11000700	-1.37171800	-0.24654900
N	-2.95345600	3.91631700	0.12515400	O	0.07828500	0.92201100	0.72296400
H	-2.72885800	4.90133100	0.19143600	H	-0.08794700	0.72002200	1.67762400
H	-6.08726400	1.37612800	-0.06601700	C	0.01465200	-3.14920600	-2.03032600
H	-4.98877000	0.32284700	-0.99529000	H	-0.90348800	-2.91811000	-2.57314700
H	-4.99855500	0.23988700	0.76500100	H	0.00355000	-4.11266600	-1.51473300
H	-5.12405800	3.95890300	0.08356400	H	0.92916100	-2.96363600	-2.59877000
H	-0.98073200	3.02472200	0.12918100	H	0.06570800	-2.27483400	-1.09547700
O	1.91295400	-0.72422900	2.07268700				

Model2H-**IM**(HS-AF)

Fe	-1.56415600	0.12289400	0.12229300	H	0.44117600	-1.22046300	-4.40733100
Fe	1.51996200	0.11639700	-0.16371400	H	-1.15365700	-0.39908800	-4.44747000
H	-3.69027100	4.01280700	-0.98110900	H	-5.52779900	-1.43367300	-2.10411500
C	-4.28667200	3.49228900	-0.22146500	C	-4.58026300	-1.05314600	-1.70650300
C	-3.40985200	2.48441300	0.50730900	C	-4.24862000	-1.73387700	-0.41349500
O	-2.91228200	1.54444500	-0.24004300	N	-3.14677200	-1.39518000	0.36360900
O	-3.21405100	2.59430400	1.73546200	C	-4.93732100	-2.74564600	0.22107300
H	-4.70211400	4.21713300	0.48305300	C	-3.17194700	-2.17487800	1.43577600
H	-5.09655900	2.96937800	-0.74458800	N	-4.23666100	-3.01269600	1.39020100
H	-1.05331000	-2.08761700	-3.93300100	H	-4.48412000	-3.68980200	2.10158700
C	-0.52852300	-1.12406300	-3.91326900	H	-3.78729000	-1.21384800	-2.44458300
C	-0.35300800	-0.67731300	-2.46993700	H	-4.66118500	0.02943800	-1.55673100
O	-1.42824000	-0.44731600	-1.81421800	H	-5.84052700	-3.27470800	-0.04923300
O	0.81842600	-0.56530800	-2.01872700	H	-2.46379100	-2.13781400	2.25214600

H	3.58135700	4.30917200	0.01050300	N	3.12397800	-3.85619500	-0.30931900
C	2.84320400	3.52449600	-0.17712500	H	2.94624700	-4.85070400	-0.37584200
C	3.51240100	2.32669500	-0.84494400	H	6.13181500	-1.17356200	-0.00845300
O	4.68374800	2.34650400	-1.20622900	H	5.02594200	-0.05432300	-0.85103200
O	2.72337700	1.27964600	-1.02979500	H	4.94027000	-0.20831600	0.89893200
H	2.37139700	3.21093700	0.76090700	H	5.29363100	-3.79854200	-0.24165600
H	2.05303000	3.91663200	-0.83096500	H	1.11132700	-3.06059000	-0.29358300
H	2.55879300	2.10325800	3.93774200	O	-1.84896300	0.44412600	2.19569000
C	2.62654700	1.00786800	3.97286800	H	-2.32948500	1.33464900	2.21970400
C	1.75849200	0.42912800	2.86352400	H	-0.98114300	0.49444100	2.66166500
O	0.65126900	-0.09469400	3.15168600	O	-0.04655700	1.39577100	-0.04755300
O	2.23729500	0.53516000	1.67444500	O	-0.04371100	-1.04567200	0.64074700
H	3.67644600	0.73928900	3.81372700	H	0.14191200	-0.96639700	1.60691200
H	2.28296700	0.66033100	4.95079300	C	-0.43437400	3.23766500	-2.80059700
C	5.11268600	-0.77055900	-0.02696200	H	0.46573200	2.68525300	-3.05721100
C	4.12228400	-1.88643000	-0.15149100	H	-0.41640100	4.32418300	-2.79201200
N	2.74581100	-1.69020400	-0.18017300	H	-1.37282800	2.71014800	-2.65090700
C	4.36761200	-3.24086900	-0.23307700	H	-0.10662500	2.15282900	-0.65767700
C	2.17854000	-2.88540300	-0.27088000				

Model2H-TS2(HS-AF)

Fe	-1.65670900	0.15348200	0.01904500	O	-2.44047700	3.07107000	1.24385400
Fe	1.45079900	0.10268700	-0.20260600	H	-4.04636000	4.67446300	0.10644500
H	-3.94910900	3.77327800	-1.44500400	H	-5.13765500	3.29681700	-0.22721800
C	-4.12295000	3.69156300	-0.36551500	H	0.49985200	-1.30375300	-4.41554400
C	-3.12355900	2.72215600	0.25091800	C	-0.48480400	-1.25055600	-3.94495400
O	-3.05981900	1.55750100	-0.30917700	C	-0.37564800	-0.72757400	-2.52061300

O	-1.46903500	-0.52175400	-1.90005800	O	0.57579300	-0.17734000	3.16067600
O	0.78450000	-0.53543600	-2.05100900	O	2.05850100	0.61952600	1.65627000
H	-1.14638100	-0.59712700	-4.52545500	H	3.61662100	0.15035600	3.77426000
H	-0.94212100	-2.24803200	-3.92843500	H	2.27846900	0.43148200	4.93514500
H	-5.57156900	-1.60817100	-2.00909300	C	5.08215500	-0.81379400	-0.06084700
C	-4.63274100	-1.18612300	-1.63305300	C	4.06649500	-1.91080200	-0.13781500
C	-4.31707500	-1.74157800	-0.27744100	N	2.69269000	-1.69187900	-0.14801300
N	-3.21321600	-1.33737000	0.46415200	C	4.28800800	-3.27056800	-0.19090200
C	-5.02229100	-2.67257200	0.45532300	C	2.10464200	-2.88081400	-0.20221900
C	-3.25393000	-1.99863200	1.61165100	N	3.03367700	-3.86651800	-0.23341700
N	-4.32997800	-2.82388700	1.65011800	H	2.83827400	-4.85915900	-0.27501700
H	-4.58806900	-3.42092500	2.42633000	H	6.09197200	-1.23969500	-0.04556100
H	-3.82711100	-1.40819800	-2.34133000	H	4.99951100	-0.12133200	-0.90512700
H	-4.72346500	-0.09474900	-1.58213300	H	4.94118400	-0.21993800	0.85083300
H	-5.93148400	-3.21560400	0.23787200	H	5.20482600	-3.84324200	-0.20121000
H	-2.55132600	-1.88664000	2.42627100	H	1.03375100	-3.03469100	-0.20562500
H	3.83095600	4.19561700	0.08365800	O	-1.82432700	0.65471800	2.13563600
C	3.05285300	3.43374500	-0.01478400	H	-2.00514200	1.63342900	2.04259000
C	3.57736600	2.25236300	-0.82681800	H	-0.96428900	0.52108400	2.60046100
O	4.70702500	2.23985800	-1.30490200	O	-0.18307300	1.47199600	-0.28213700
O	2.72122100	1.25861500	-0.98551600	O	-0.07887000	-1.03363900	0.54649500
H	2.73913600	3.08250000	0.97527900	H	0.05884300	-0.98920300	1.51792500
H	2.17536500	3.86731500	-0.51038100	C	-0.11666000	2.75240900	-2.18775400
H	2.90906100	1.76169700	3.91088900	H	-0.18354300	3.73323000	-1.72444200
C	2.67833000	0.69013100	3.95147400	H	0.85112300	2.36700900	-2.48611700
C	1.67921200	0.34172200	2.85626900	H	-1.02348000	2.29347400	-2.56459900

H -0.21430700 2.25852400 0.28842700

Model2H-P(HS-AF)

Fe	1.94914800	-0.18840200	-0.06418400	H	3.06442400	2.82304200	-1.61274200
Fe	-1.54015100	-0.07823100	-0.16435100	H	4.09518700	1.56525800	-2.27947800
H	3.44241400	-4.06185300	-2.09841900	H	6.25053000	3.04133500	0.46198100
C	3.36009300	-4.16990100	-1.01065700	H	3.90868400	0.08362100	2.41692800
C	2.49527300	-3.05253300	-0.44723100	H	-5.17286500	-3.11505900	0.10229300
O	2.81480600	-1.85870300	-0.78590900	C	-4.19133100	-2.63847300	0.02863200
O	1.53030000	-3.33538900	0.32239400	C	-4.29930200	-1.35187200	-0.78447000
H	2.94523000	-5.14822400	-0.75561900	O	-5.35691100	-0.98762500	-1.29061000
H	4.37351400	-4.08158300	-0.59878200	O	-3.17778600	-0.66471600	-0.90882400
H	-0.44014400	1.90907300	-4.11046800	H	-3.79929200	-2.40360800	1.02432700
C	0.28638800	1.09782600	-3.98574000	H	-3.47974400	-3.32546600	-0.44460700
C	0.33296100	0.66763000	-2.52470600	H	-2.75107200	-2.15073500	3.86055200
O	1.45792600	0.60396400	-1.95419800	C	-2.47701200	-1.10012400	4.02102200
O	-0.79545400	0.39470700	-1.99405600	C	-1.58465300	-0.63925300	2.87640800
H	-0.06596300	0.25515800	-4.59373900	O	-0.37967400	-0.35315200	3.10846400
H	1.27424200	1.41116300	-4.33406800	O	-2.14849700	-0.58125800	1.72247200
H	4.79305000	3.16183900	-1.89746700	H	-3.40578500	-0.51816200	4.02676500
C	4.07487800	2.40117600	-1.57118600	H	-1.95975100	-1.00001800	4.97879000
C	4.40781500	1.93427100	-0.18683000	C	-4.72678500	1.90831000	0.17877200
N	3.66174600	0.97318400	0.48789700	C	-3.41687000	2.63242800	0.17889200
C	5.45416300	2.32729900	0.61955500	N	-2.17933900	2.00026900	0.10723000
C	4.24687600	0.78825700	1.66734000	C	-3.20435500	3.99189000	0.26898400
N	5.33394500	1.58903600	1.78960400	C	-1.25144600	2.94851600	0.15627100
H	5.94751800	1.62932300	2.59452600	N	-1.82724500	4.17164100	0.24951600

H	-1.33225300	5.05293200	0.30830300	O	-0.76185800	-2.12095800	-0.49878900
H	-5.54902500	2.62642200	0.27764900	O	0.21849500	0.43927600	0.61066900
H	-4.87026600	1.32321400	-0.73524100	H	0.10998100	0.30089800	1.58554400
H	-4.77843700	1.20385500	1.01802000	H	0.05140100	-2.48550300	-0.05939700
H	-3.89813200	4.81742600	0.34523300	C	-0.90736000	-2.78050000	-1.76562600
H	-0.18560900	2.76557100	0.13914100	H	-1.78175300	-2.35014300	-2.25718600
O	2.09356300	-1.25073600	2.10458900	H	-0.02167200	-2.61831100	-2.39512700
H	1.88290100	-2.13262500	1.72339400	H	-1.05497000	-3.85802200	-1.61395600
H	1.29473700	-1.00022400	2.61884200				

Model3H-Q (HS-FM)

C	-3.65255000	1.93102600	-0.71161900	O	3.52419300	-0.54778500	-1.29946000
O	-3.69324000	0.83146700	-1.37202100	C	2.39049400	2.90758200	0.73492300
O	-2.62772300	2.20412400	-0.02472500	O	2.36617200	1.80400100	0.06665900
C	-0.20775800	-2.24265300	-1.45061900	O	1.74573800	3.12334900	1.78376700
O	0.89341600	-1.74894100	-1.06103400	C	2.97919300	-1.97305700	1.75646500
O	-1.34691400	-1.68559200	-1.39334400	C	3.29402100	-1.95054900	3.09838900
C	-3.80877800	-1.62259900	0.80782700	N	2.86241400	-0.71974600	3.57541000
C	-4.15505500	-1.88728300	2.11502600	H	2.96004700	-0.36762700	4.51995900
N	-3.34082900	-1.08072700	2.89873100	C	2.31220400	-0.03959000	2.54092800
H	-3.34409800	-1.01703800	3.90919900	N	2.36257700	-0.76997100	1.43156700
C	-2.53825700	-0.36457200	2.07253600	H	3.78082700	-2.68127700	3.72897700
N	-2.79374800	-0.67073800	0.80625500	H	1.92212300	0.96993700	2.61324900
H	-4.88944500	-2.55920500	2.53665400	Fe	1.61853400	0.06711000	-0.42994500
H	-1.82056000	0.37283600	2.41257500	Fe	-1.81399000	0.21847700	-0.88017600
C	3.12423800	-0.02833100	-2.38774900	O	-0.17572800	0.46142400	0.20175200
O	1.95590700	0.49329400	-2.41731200	O	-0.79798800	2.27041300	2.15130700

H	-1.42429100	2.70759500	1.54395600	H	-5.16981800	-2.93556700	-0.19592000
H	0.06936300	2.74049800	2.09202800	C	3.30455000	3.98189700	0.15963000
O	-1.19282600	0.84575900	-2.23308800	H	4.31507500	3.57647800	0.02948300
C	3.99901500	0.01110500	-3.61722500	H	2.93754600	4.26767400	-0.83406900
H	4.78442800	-0.74760500	-3.55432000	H	3.32857700	4.85808100	0.81282100
H	3.39063600	-0.13143900	-4.51622600	C	-0.16057000	-3.63387200	-2.06639000
H	4.46806600	1.00166600	-3.68211900	H	-1.11713500	-4.14918400	-1.93963800
C	-4.82180500	2.88590500	-0.80452400	H	0.02978900	-3.52219300	-3.14203400
H	-4.89215800	3.49270200	0.10326700	H	0.65693600	-4.21984800	-1.63573600
H	-4.65234600	3.55666800	-1.65698600	C	3.24632900	-3.05951700	0.76030200
H	-5.75378800	2.33999500	-0.98005300	H	2.30920900	-3.44276100	0.34195000
C	-4.39183100	-2.20499400	-0.44429900	H	3.83701900	-2.66904500	-0.07510100
H	-4.82947700	-1.41436400	-1.06466500	H	3.78948300	-3.88304900	1.23761100
H	-3.61493000	-2.69572200	-1.04025200	H	-0.31076800	1.13969900	0.91321900

Model3H-TS1(HS-FM)

C	3.77754200	-1.09584400	1.51861400	N	2.63893500	1.20705700	-0.30582100
O	3.91819800	-1.27475500	0.26919500	H	4.44151300	3.76099100	-1.40668100
O	2.62651600	-0.77372400	1.97114500	H	1.59312900	2.16371100	1.30644700
C	0.21355900	-0.19974400	-2.55574100	C	-3.23020900	-1.81389100	-1.26999900
O	-0.87938400	0.07679900	-1.96893000	O	-2.09475200	-2.19026300	-0.81025900
O	1.26704900	-0.64092400	-2.00944700	O	-3.56046500	-0.59544600	-1.14285100
C	3.58316100	1.69456200	-1.20079400	C	-2.43775600	-0.74231700	2.89227600
C	3.79238900	3.03276900	-0.94033700	O	-2.52449700	-0.70871900	1.60253400
N	2.96481000	3.34570700	0.13000300	O	-1.77223300	0.05609700	3.58423700
H	2.87786200	4.24652500	0.58381100	C	-2.78189600	2.74068800	-0.76802000
C	2.29106200	2.21755100	0.47877500	C	-3.07296800	3.88724500	-0.06069100

N	-2.74311500	3.61893600	1.26170900	C	4.94148900	-1.28815300	2.46392900
H	-2.85309400	4.24198700	2.05258900	H	4.92084100	-0.52735800	3.25158000
C	-2.27556300	2.34965300	1.32816700	H	4.84196700	-2.27100800	2.94270900
N	-2.28093100	1.79461300	0.11981300	H	5.88968500	-1.25508500	1.92023900
H	-3.48308000	4.83586500	-0.37771800	C	4.23945200	0.83077900	-2.23569500
H	-1.97096100	1.85549100	2.24488900	H	4.78251900	0.00937300	-1.75364800
Fe	-1.67439700	-0.27202100	-0.10725400	H	3.49052500	0.38095200	-2.89737500
Fe	1.82905100	-0.92422300	-0.05364000	H	4.94217100	1.41844400	-2.83746100
O	0.10709500	-0.14824500	0.62705000	C	-3.24432800	-1.85073300	3.55645800
O	0.72359000	1.01610800	3.04179300	H	-4.27075900	-1.84825900	3.17178900
H	1.42986300	0.34620000	3.12443500	H	-2.79825400	-2.81808100	3.29200600
H	-0.09195800	0.65527100	3.45915200	H	-3.24244200	-1.73085500	4.64308800
O	1.50482800	-2.64648600	-0.02708600	C	0.27378200	0.03762000	-4.05973400
C	0.38006100	-4.52727100	-1.22376200	H	0.75944400	-0.81342600	-4.54910600
H	0.88110700	-4.59608700	-2.19229100	H	-0.72669200	0.19383300	-4.47167500
H	0.97589000	-3.54583200	-0.61828000	H	0.88803700	0.92639800	-4.25552500
H	-0.65138600	-4.17300800	-1.26201200	C	-2.96767900	2.48191000	-2.23176800
H	0.54644400	-5.38924700	-0.57371100	H	-2.00379400	2.30850700	-2.72260600
C	-4.13589900	-2.81576300	-1.94604800	H	-3.57325700	1.58172800	-2.38120900
H	-5.08642800	-2.35149100	-2.22161100	H	-3.46308900	3.33712800	-2.70537100
H	-3.63942600	-3.20569900	-2.84337300	H	0.22127600	0.26565900	1.51941700
H	-4.31129500	-3.66238900	-1.27201200				

Model3H-**IM**(HS-FM)

C	-3.76930500	1.22181200	0.81377300	C	0.03457500	-1.24605100	-2.34221300
O	-3.86622900	0.77213900	-0.37481400	O	1.13395700	-0.96294000	-1.76405500
O	-2.64204400	1.14965100	1.40735100	O	-1.10963700	-0.81529600	-2.02124000

C	-3.42300100	-2.56143900	-0.25502400	H	-1.42210500	0.75350500	2.93402800
C	-3.60122600	-3.62121400	0.60952000	H	0.09925400	0.71282200	3.38993500
N	-2.80111900	-3.35133300	1.71204100	O	-1.51096200	1.94579900	-1.34820800
H	-2.70620300	-3.92061600	2.54391600	C	-3.49930400	4.77097200	-0.89369000
C	-2.17416500	-2.16549000	1.49120200	H	-3.15687500	5.53326000	-0.19765100
N	-2.52619400	-1.66662400	0.31411600	H	-0.59262900	2.14846800	-1.60737000
H	-4.21243800	-4.51022500	0.53760300	H	-4.41389800	4.94159700	-1.45667900
H	-1.50464100	-1.69537900	2.20264700	H	-2.90562400	3.87567900	-1.06724800
C	2.58841100	1.77683900	-2.09785200	C	3.08965200	2.71398100	-3.16801400
O	1.38737600	1.88592400	-1.66143700	H	4.02719400	2.34611100	-3.59353500
O	3.32973700	0.88240900	-1.58912900	H	2.33013600	2.83117100	-3.94861400
C	2.22974500	2.07154600	2.26262100	H	3.26031500	3.70133800	-2.71982100
O	2.32599500	1.62708100	1.05199100	C	-4.95879400	1.86815100	1.48185100
O	1.73989000	1.43530900	3.21926000	H	-4.86696600	1.81969400	2.57124100
C	3.71531600	-2.18462100	0.15243500	H	-4.98185900	2.92305400	1.17687600
C	4.23526900	-2.89060600	1.21552400	H	-5.88810700	1.39596800	1.14788900
N	3.69484800	-2.31945900	2.36066600	C	-4.06237600	-2.32481300	-1.59023700
H	3.88361700	-2.58875200	3.31869000	H	-4.63120300	-1.38748900	-1.57795000
C	2.88381000	-1.30412700	1.98146800	H	-3.30046800	-2.23563500	-2.37320400
N	2.86998300	-1.20060800	0.65508600	H	-4.73947600	-3.14852100	-1.84348600
H	4.92864900	-3.71917900	1.25002900	C	2.78447500	3.47485700	2.47066300
H	2.35721400	-0.64731100	2.66689300	H	3.79825800	3.54059100	2.05884200
Fe	1.69120100	0.33716600	-0.27993800	H	2.16060700	4.18888200	1.91797500
Fe	-1.79858300	0.35777900	-0.47716400	H	2.78624700	3.73430900	3.53259600
O	-0.05944900	0.10659500	0.49880800	C	0.11109100	-2.21611800	-3.51347900
O	-0.67913500	0.15859400	3.15591900	H	-0.73865900	-2.07087100	-4.18637900

H	1.05510800	-2.09091200	-4.05251300	H	4.34714000	-1.42916000	-1.74786400
H	0.07341600	-3.24181900	-3.12228800	H	4.74559600	-3.14694900	-1.45571100
C	3.98984800	-2.36715900	-1.30891900	H	-0.17804200	0.14707600	1.48356400
H	3.07560900	-2.64437000	-1.84447600				

Model3H-TS2(HS-FM)

C	3.72004100	1.75403400	-0.41736900	C	-3.83642100	-2.97432700	-1.88758500
O	3.83059800	1.11595600	0.67849700	N	-3.32473200	-2.15070000	-2.88241700
O	2.61852700	1.70736000	-1.05918900	H	-3.46016000	-2.25131000	-3.88112100
C	0.09333700	-1.62813900	2.10593200	C	-2.62652600	-1.15566300	-2.28658700
O	-1.01516100	-1.38057100	1.52392400	N	-2.65848400	-1.30248300	-0.96471900
O	1.17391800	-0.99652700	1.94609200	H	-4.44428800	-3.84128700	-2.10526000
C	3.73791200	-2.17640900	0.02104000	H	-2.14595200	-0.33658100	-2.81286600
C	4.05780300	-3.05369400	-0.99387600	Fe	-1.65571600	0.12326200	0.29492500
N	3.26408600	-2.69067900	-2.07436700	Fe	1.80917300	0.46879400	0.62396400
H	3.25568000	-3.12229900	-2.99018000	O	0.11472200	0.21391200	-0.45383400
C	2.50285700	-1.63041300	-1.69430800	O	0.84736000	0.79027400	-3.04238100
N	2.76334500	-1.29947800	-0.43702100	H	1.51994900	1.38895800	-2.66116800
H	4.76074200	-3.87408300	-1.03781600	H	0.02829200	1.31129200	-3.19359600
H	1.80483200	-1.12176300	-2.34976400	O	1.31587100	1.86351200	1.73940000
C	-2.74116200	1.08821900	2.32156800	C	0.61531000	4.07816800	0.79952300
O	-1.54231200	1.38823400	1.97605500	H	-0.42404900	3.76651400	0.78576900
O	-3.38044300	0.25746100	1.60973800	H	0.39623100	1.84043400	2.06495100
C	-2.27576500	2.25153400	-1.88472100	H	1.24764200	3.88903100	-0.06027000
O	-2.39217900	1.61111500	-0.76721900	H	1.00948300	4.61405800	1.65638900
O	-1.69405400	1.81697700	-2.90140700	C	-3.35867500	1.73777400	3.53546000
C	-3.41580500	-2.43708800	-0.69038800	H	-2.64947100	1.71870200	4.37037800

H -3.57088200	2.78962200	3.30463200	H -2.31867100	4.30965000	-1.28028700
H -4.28932500	1.23404700	3.80989400	H -2.96887400	4.02268100	-2.91911900
C 4.87569400	2.58701000	-0.92696900	C 0.10378700	-2.81349000	3.06230300
H 4.83148700	3.57298900	-0.44571600	H 0.24291900	-3.73396900	2.47931800
H 5.82893200	2.12231000	-0.65592400	H 0.92848000	-2.72455600	3.77492400
H 4.80619900	2.72575400	-2.01015700	H -0.85289500	-2.88785900	3.58888600
C 4.30712200	-2.09416000	1.40546400	C -3.70497800	-2.91921200	0.69811300
H 4.77254600	-1.11424700	1.56514500	H -2.77970700	-3.20679300	1.20853900
H 3.51539600	-2.20667700	2.15519700	H -4.16258900	-2.11925900	1.29034100
H 5.05948700	-2.87584000	1.56048800	H -4.38304900	-3.77937800	0.66462900
C -2.92129100	3.63180500	-1.89913600	H 0.25072900	0.43676500	-1.40912400
H -3.92270600	3.58571600	-1.45673900			

Model3H-P(HS-FM)

C 3.74449500	-1.65735000	0.84518300	H 1.85440600	1.59605200	2.15747700
O 3.72290000	-1.31000800	-0.39224400	C -2.73363500	-1.72152100	-1.93998700
O 2.73529300	-1.50522000	1.58495100	O -1.52908700	-1.89733300	-1.52533500
C -0.01167500	1.00712000	-2.47498000	O -3.39609300	-0.75359200	-1.47279800
O -1.09064200	0.92905600	-1.79230800	C -2.33397300	-1.71694300	2.43037100
O 1.08567900	0.45843100	-2.18874700	O -2.44967800	-1.40144500	1.18328500
C 3.68398900	2.23947900	-0.43149300	O -1.69158600	-1.06672300	3.28268600
C 4.00605200	3.30048800	0.38834600	C -3.47392400	2.47348000	0.12299700
N 3.25535700	3.12653700	1.54448300	C -3.86601100	3.30927700	1.14618900
H 3.25940500	3.72295500	2.36259700	N -3.29807800	2.79434700	2.30488000
C 2.51880500	1.99297700	1.39736000	H -3.40094700	3.15990100	3.24374300
N 2.75213700	1.43926500	0.21522800	C -2.59555300	1.68552800	1.97151300
H 4.68327500	4.13265000	0.25422300	N -2.67842900	1.46801200	0.66223800

H	-4.48761100	4.19366200	1.14604800	H	5.51419600	-2.88290700	0.65639700
H	-2.07798200	1.04537800	2.67902300	H	5.72768500	-1.40888500	1.61227400
Fe	-1.67971100	-0.22324200	-0.21350100	C	4.21174700	1.90168900	-1.79348600
Fe	1.85208400	-0.45493200	-0.49505600	H	4.72209200	0.93048200	-1.77276900
O	0.08939800	-0.18999500	0.49316100	H	3.39118700	1.82430600	-2.51662100
O	0.88192000	-0.10484700	3.14475600	H	4.91921500	2.66520500	-2.13650100
H	1.55783100	-0.77285800	2.91095200	C	-3.07514200	-2.98790800	2.83406200
H	0.06531700	-0.57130900	3.42537300	H	-4.11977200	-2.92851300	2.50647500
O	1.17250100	-2.38278200	-1.44449500	H	-2.62227800	-3.84648000	2.32188300
C	1.40536400	-3.66185700	-0.84551700	H	-3.02409300	-3.13724600	3.91592500
H	1.02441900	-4.46458000	-1.49323100	C	-0.07813600	1.86385600	-3.73351500
H	0.20840200	-2.29282800	-1.60536600	H	-0.06516400	2.92291800	-3.44288000
H	0.93719600	-3.73612600	0.14593900	H	0.77949700	1.66373700	-4.38149600
H	2.48774100	-3.77417600	-0.74133600	H	-1.01468100	1.67805200	-4.27017600
C	-3.32429600	-2.68170700	-2.94482400	C	-3.82192400	2.55246000	-1.33192700
H	-2.60972500	-2.86318600	-3.75552500	H	-2.92141400	2.70408200	-1.93660100
H	-3.51457800	-3.64158600	-2.44756400	H	-4.27592900	1.61280000	-1.66555900
H	-4.26415300	-2.29098000	-3.34363200	H	-4.52202500	3.37673200	-1.50892800
C	5.03603800	-2.23499900	1.39880100	H	0.24300700	-0.18646700	1.47049800
H	4.84871000	-2.78413800	2.32619100				
Model3H-Q (HS-AF)							
C	-3.68172300	2.01859000	-0.36635200	O	-1.26506600	-1.50701600	-1.52565400
O	-3.87883000	1.04994500	-1.16385400	C	-3.82722900	-1.76348000	0.64182100
O	-2.55228200	2.11688200	0.22399800	C	-4.14524800	-2.19595600	1.91186000
C	-0.17389100	-2.14942500	-1.50734100	N	-3.32809500	-1.47793900	2.77571900
O	0.93695100	-1.72975800	-1.05360300	H	-3.31163700	-1.54357100	3.78599100

C	-2.55441500	-0.64957600	2.02713900	C	3.74471700	0.24874800	-3.79487800
N	-2.83066000	-0.80092700	0.73843200	H	4.56808100	-0.47053000	-3.82388300
H	-4.86248100	-2.92550500	2.26147800	H	3.06737400	0.10035200	-4.64226300
H	-1.83437400	0.04741600	2.44143300	H	4.15564800	1.26409000	-3.86899800
C	2.98234900	0.13094200	-2.49848200	C	-4.75337600	3.06031800	-0.13718000
O	1.80503800	0.62732100	-2.40184700	H	-4.77143100	3.36352200	0.91520500
O	3.48349900	-0.43150200	-1.47493300	H	-4.51143700	3.94616600	-0.73877000
C	2.44185000	2.83962800	0.90677200	H	-5.73142000	2.68158700	-0.44665000
O	2.43732300	1.78713600	0.15881300	C	-4.41506500	-2.18401400	-0.67112200
O	1.79685200	2.96491600	1.97020200	H	-4.86998200	-1.32276900	-1.17461300
C	3.09213000	-2.05394600	1.59921400	H	-3.63520600	-2.57673000	-1.33367500
C	3.42253300	-2.12039200	2.93560300	H	-5.17964900	-2.95459100	-0.52171400
N	2.96691700	-0.93887000	3.50592300	C	3.33015200	3.97210000	0.40878900
H	3.06654400	-0.65488600	4.47302200	H	4.33964800	3.59289400	0.21105900
C	2.38922900	-0.19832400	2.53057500	H	2.92995400	4.34592500	-0.54213900
N	2.44294500	-0.84483200	1.36945200	H	3.36449200	4.78442700	1.13943400
H	3.93631500	-2.88176900	3.50557300	C	-0.20872900	-3.56083800	-2.07762700
H	1.98085600	0.79539000	2.67895400	H	-0.86119200	-4.18637300	-1.45543200
Fe	1.65824600	0.08737700	-0.41979100	H	-0.64207500	-3.53244000	-3.08380300
Fe	-1.82225600	0.36535500	-0.88604500	H	0.79357800	-3.99527500	-2.11342200
O	-0.14417400	0.55123100	0.10692500	C	3.37740100	-3.05678800	0.52357100
O	-0.70769000	1.99838400	2.31460000	H	2.44642500	-3.45863500	0.10978700
H	-1.38039800	2.49177100	1.80619600	H	3.91853000	-2.58225400	-0.30196500
H	0.13555200	2.51308500	2.29671400	H	3.97779400	-3.88001300	0.92701400
O	-1.59198000	1.14317000	-2.50403600	H	-0.26422600	1.11447200	0.92144400
Model3H-TS1(HS-AF)							

C	3.77988900	-1.10576100	1.52138700	H	-3.40080600	4.86636000	-0.28364300
O	3.92968100	-1.26677300	0.27116200	H	-1.94462400	1.80996200	2.28104800
O	2.62117700	-0.80713700	1.97131500	Fe	-1.65830300	-0.26658700	-0.12413700
C	0.24014300	-0.17726800	-2.55977100	Fe	1.83363700	-0.94661700	-0.05725700
O	-0.84675100	0.12106300	-1.97013100	O	0.11068700	-0.20961000	0.61783600
O	1.28011900	-0.65383800	-2.01827600	O	0.67519900	0.92012200	3.03659700
C	3.56044100	1.70851300	-1.16681300	H	1.39453700	0.26687000	3.13746100
C	3.75352200	3.04549000	-0.88820000	H	-0.14026300	0.55270000	3.45143700
N	2.91445600	3.33662500	0.17933800	O	1.55147900	-2.67808600	-0.05446000
H	2.81470500	4.23090100	0.64332700	C	0.34114800	-4.50100500	-1.25649200
C	2.25014300	2.19715900	0.50889000	H	0.82635900	-4.57449800	-2.23279000
N	2.61458500	1.20002000	-0.28520500	H	0.97507700	-3.55375600	-0.64993900
H	4.39833200	3.78620700	-1.34062800	H	-0.67931500	-4.11449300	-1.27824800
H	1.54670900	2.12583400	1.33048200	H	0.48685900	-5.37757200	-0.62097400
C	-3.24065000	-1.75377300	-1.32639500	C	-4.17061200	-2.73623800	-1.99816100
O	-2.10970400	-2.15539100	-0.87418100	H	-3.61911400	-3.32551100	-2.73958100
O	-3.55375800	-0.53407500	-1.17837600	H	-4.55763400	-3.43243300	-1.24325800
C	-2.48293500	-0.79263500	2.85789500	H	-5.00632600	-2.21348900	-2.47107100
O	-2.53419000	-0.73192600	1.56808600	C	4.94117500	-1.29185000	2.47120000
O	-1.80919700	-0.03194100	3.58462000	H	4.85895300	-2.28569300	2.93018800
C	-2.71863900	2.77362500	-0.71736700	H	5.89198500	-1.22931600	1.93467700
C	-3.00296300	3.90642700	0.01438400	H	4.89993600	-0.54687800	3.27299500
N	-2.68741400	3.60366100	1.33279100	C	4.23302600	0.86534400	-2.20818000
H	-2.79807500	4.20879600	2.13737700	H	4.77451900	0.03877400	-1.73341300
C	-2.23433900	2.32810700	1.37314600	H	3.49420100	0.42343200	-2.88629400
N	-2.23487100	1.80147900	0.15213000	H	4.93948800	1.46664600	-2.79179700

C	-3.34427500	-1.88453000	3.47970400	H	0.61604200	1.13275600	-4.21530300
H	-4.35918200	-1.84016700	3.06801000	C	-2.90023900	2.55106700	-2.18752500
H	-2.92396300	-2.86183100	3.20970100	H	-1.93834900	2.36138300	-2.67583900
H	-3.36783300	-1.78399400	4.56802600	H	-3.52859000	1.67076600	-2.35997600
C	0.29963900	0.09253500	-4.05797800	H	-3.36967600	3.42908200	-2.64562900
H	1.03058200	-0.56548600	-4.53664900	H	0.22357900	0.18970600	1.52076900
H	-0.68886200	-0.03476100	-4.50947600				

Model3H-**IM**(HS-AF)

C	3.77106600	1.21957600	-0.83230400	O	-2.33740100	1.61135600	-1.04962000
O	3.87195800	0.77166500	0.35644600	O	-1.77205200	1.45976200	-3.22626500
O	2.64092600	1.14968500	-1.42077300	C	-3.67472300	-2.20820600	-0.14500200
C	-0.01312300	-1.23158200	2.35515800	C	-4.19295000	-2.91729900	-1.20693900
O	-1.11487600	-0.95963100	1.77574800	N	-3.66039700	-2.34172400	-2.35344400
O	1.12880400	-0.79700200	2.03043700	H	-3.85103300	-2.61122800	-3.31104600
C	3.41156600	-2.55706300	0.24068700	C	-2.85576000	-1.32062200	-1.97604000
C	3.57923800	-3.61893900	-0.62342600	N	-2.83821100	-1.21765500	-0.64975100
N	2.77126400	-3.34845600	-1.71999800	H	-4.88066800	-3.75064000	-1.23969600
H	2.66773400	-3.91918300	-2.54985300	H	-2.33765000	-0.65994400	-2.66371300
C	2.15016500	-2.16009100	-1.49619000	Fe	-1.68011600	0.33519700	0.28634700
N	2.51312100	-1.66025600	-0.32290000	Fe	1.80201000	0.36827300	0.47093800
H	4.18804900	-4.50984800	-0.55477100	O	0.06630700	0.13379800	-0.47659300
H	1.47658100	-1.68910500	-2.20310100	O	0.63102200	0.18374600	-3.11991800
C	-2.59438000	1.76997000	2.09982000	H	1.38476700	0.77725500	-2.93399600
O	-1.39485900	1.88931800	1.66017200	H	-0.15022900	0.73585500	-3.35630400
O	-3.32966100	0.86768100	1.59716900	O	1.52699800	1.96257000	1.33660200
C	-2.28015700	2.06499100	-2.25843100	C	3.52742600	4.77515000	0.86405900

H	3.18465600	5.53632500	0.16695500	H	4.73927200	-3.14636400	1.81873600
H	0.60663300	2.16989300	1.58390700	C	-2.90931300	3.43869900	-2.45245900
H	4.44635100	4.94341300	1.42068800	H	-3.92730800	3.44264000	-2.04558800
H	2.92992300	3.88391700	1.04532400	H	-2.32911200	4.17903700	-1.88717100
C	-3.09958100	2.70700700	3.16857200	H	-2.92101700	3.71061000	-3.51117100
H	-4.03638800	2.33678300	3.59365700	C	-0.08388700	-2.19205300	3.53468400
H	-2.34116000	2.82699000	3.94987400	H	0.77119500	-2.04408000	4.20017300
H	-3.27224500	3.69363500	2.71956300	H	-1.02358200	-2.05898900	4.07949600
C	4.95935700	1.86116600	-1.50711900	H	-0.05332600	-3.22116700	3.15188100
H	4.86262100	1.81058400	-2.59600100	C	-3.94416100	-2.39351000	1.31694200
H	4.98672500	2.91667500	-1.20459500	H	-3.02871800	-2.67372100	1.84885500
H	5.88883400	1.38713900	-1.17621800	H	-4.29787100	-1.45566700	1.75899300
C	4.06317800	-2.32046600	1.56996400	H	-4.70087600	-3.17222900	1.46451200
H	4.63528400	-1.38528900	1.55095100	H	0.18336800	0.17592800	-1.46545700
H	3.30843900	-2.22675600	2.35924700				

Model3H-TS2(HS-AF)

C	3.71543200	1.76144400	-0.44529400	C	2.48998800	-1.63391200	-1.69342100
O	3.83340700	1.12946300	0.65303500	N	2.75735900	-1.29273900	-0.44038200
O	2.61055200	1.70905400	-1.08110300	H	4.75518800	-3.86879000	-1.03303700
C	0.11022600	-1.61046800	2.12632800	H	1.78696200	-1.13174900	-2.34839900
O	-0.99999500	-1.37039200	1.54329200	C	-2.74411200	1.09579400	2.31544200
O	1.19049100	-0.98063300	1.95894300	O	-1.54761500	1.40259200	1.96519900
C	3.73615400	-2.16453400	0.01869300	O	-3.37872400	0.25370400	1.61378200
C	4.05124400	-3.04916000	-0.99133300	C	-2.32471200	2.22621200	-1.90124700
N	3.25054500	-2.69592400	-2.06987400	O	-2.40114200	1.59013800	-0.77880500
H	3.23704000	-3.13522000	-2.98196300	O	-1.73097400	1.81402900	-2.92086500

C	-3.38067300	-2.45867900	-0.67094100	H	-4.29595100	1.25365200	3.79892000
C	-3.79679600	-3.00773700	-1.86439000	C	4.86628100	2.59458600	-0.96564800
N	-3.28919000	-2.18890900	-2.86515500	H	4.82319100	3.58250500	-0.48828600
H	-3.42360900	-2.29769400	-3.86314100	H	5.82210800	2.13292900	-0.69850200
C	-2.59754500	-1.18517600	-2.27628600	H	4.78996500	2.72866700	-2.04897400
N	-2.62964800	-1.32174900	-0.95339700	C	4.31397600	-2.07087700	1.39879100
H	-4.39952900	-3.87981900	-2.07577400	H	4.78206600	-1.09041600	1.54681800
H	-2.12342700	-0.36719500	-2.80951600	H	3.52645300	-2.17502800	2.15405300
Fe	-1.64503500	0.12285500	0.29948600	H	5.06588200	-2.85255700	1.55602800
Fe	1.81068800	0.47994200	0.61484200	C	-3.03872200	3.57245000	-1.92063600
O	0.11818600	0.22647800	-0.43160500	H	-4.04543500	3.47081200	-1.49961500
O	0.79873400	0.78244700	-3.01114300	H	-2.48602300	4.27568100	-1.28409600
H	1.48153500	1.39133900	-2.66589100	H	-3.08667700	3.96731000	-2.93898400
H	-0.02279400	1.29973400	-3.17032700	C	0.12061300	-2.78501800	3.09614500
O	1.32396700	1.87977000	1.72708400	H	0.23411200	-3.71452100	2.52199700
C	0.65098800	4.09802700	0.79684500	H	0.95866500	-2.70035600	3.79347400
H	-0.39605000	3.81243900	0.79280700	H	-0.82786500	-2.83831600	3.64011100
H	0.40102000	1.86318600	2.04303200	C	-3.67047000	-2.93121000	0.72071300
H	1.26727100	3.90187500	-0.07295600	H	-2.74468100	-3.20592000	1.23711400
H	1.06617900	4.62429200	1.64965300	H	-4.13725300	-2.13014500	1.30425300
C	-3.36255600	1.75262600	3.52520700	H	-4.34095700	-3.79749100	0.69208000
H	-2.65574800	1.73284600	4.36224400	H	0.25572000	0.44621300	-1.39117600
H	-3.56880000	2.80483500	3.29084600				

Model3H-P(HS-AF)

C	3.74708400	-1.66412300	0.80938300	O	2.71921900	-1.52327300	1.53135700
O	3.74670900	-1.29944800	-0.41986100	C	-0.01776100	1.01401800	-2.47589700

O	-1.10308600	0.93170300	-1.79620900	O	0.08499000	-0.17769200	0.49179800
O	1.07477700	0.46288000	-2.19171700	O	0.88809900	-0.13426700	3.11582800
C	3.68306200	2.23102700	-0.43138200	H	1.56358600	-0.80175900	2.87700200
C	4.02127300	3.29233700	0.38195800	H	0.07563700	-0.60002500	3.40981400
N	3.28909200	3.12220300	1.55010600	O	1.16695400	-2.37939600	-1.43181200
H	3.30724400	3.72039200	2.36666900	C	1.39982800	-3.66691400	-0.85187000
C	2.54748600	1.98964500	1.41568600	H	1.01979000	-4.46056800	-1.51126400
N	2.75970600	1.43383100	0.23098700	H	0.20517500	-2.28932400	-1.60276000
H	4.69899200	4.12206900	0.23578700	H	0.93201900	-3.75600000	0.13850700
H	1.89316200	1.59653700	2.18617600	H	2.48224400	-3.78034700	-0.74912800
C	-2.75018500	-1.71704000	-1.92578500	C	-3.33842600	-2.68618900	-2.92326000
O	-1.54160300	-1.88669300	-1.51531500	H	-2.63106900	-2.85592100	-3.74289000
O	-3.41367600	-0.75006100	-1.46138600	H	-3.50723300	-3.64934300	-2.42468000
C	-2.33680100	-1.71208900	2.42477100	H	-4.28869400	-2.30937500	-3.31053100
O	-2.44910300	-1.39368300	1.17805100	C	5.02539400	-2.24654200	1.38766200
O	-1.68913600	-1.06891100	3.27847000	H	4.81181800	-2.83710800	2.28358900
C	-3.46331700	2.47767200	0.12744200	H	5.54201400	-2.85515700	0.63804800
C	-3.85096100	3.31314100	1.15249800	H	5.69426100	-1.42040100	1.66460500
N	-3.27824100	2.79823400	2.30886700	C	4.18959800	1.89064300	-1.80082700
H	-3.37715500	3.16393700	3.24812000	H	4.69900300	0.91890800	-1.78590200
C	-2.57716800	1.68962500	1.97291800	H	3.35788200	1.81246400	-2.51092500
N	-2.66548100	1.47226600	0.66381100	H	4.89240200	2.65319800	-2.15551500
H	-4.47257700	4.19749500	1.15493200	C	-3.08941700	-2.97707900	2.82577300
H	-2.05770200	1.04896600	2.67849700	H	-4.13237700	-2.90952800	2.49458500
Fe	-1.67022700	-0.21603000	-0.21562400	H	-2.64143600	-3.83915900	2.31517900
Fe	1.84276400	-0.46170800	-0.47039200	H	-3.04305600	-3.12688700	3.90777500

C	-0.08851000	1.88037400	-3.72791000	H	-2.92167500	2.70648300	-1.93516700
H	-0.11822400	2.93668900	-3.42896900	H	-4.27665100	1.61799300	-1.65627500
H	0.78666700	1.71353000	-4.36161900	H	-4.51869300	3.38242300	-1.49842300
H	-1.00830000	1.66763300	-4.28374400	H	0.24556300	-0.17408800	1.47113900
C	-3.81905000	2.55690000	-1.32553100				
Model4H-RC(HS-FM)							
C	-4.01441100	-1.10383200	-1.07099900	C	2.60904800	2.71818600	0.48480900
O	-3.90939400	-0.84460200	0.18652400	C	2.87284300	3.78834500	-0.34840600
O	-3.02758700	-1.02485000	-1.84062900	N	2.50374400	3.37105700	-1.62284000
C	-0.25871400	0.27437200	2.64216100	H	2.61736800	3.88637700	-2.48598600
O	0.82511700	0.07117700	2.05338500	C	2.05103600	2.08839200	-1.51764800
O	-1.44102400	0.21438500	2.14140000	N	2.09731100	1.67265000	-0.26513000
C	-3.35355400	2.38361700	0.41196600	H	3.28352300	4.76993000	-0.15325200
C	-3.43340200	3.53222700	-0.34685900	H	1.73414800	1.48137300	-2.35602100
N	-2.60821000	3.31925600	-1.44559000	Fe	1.66122100	-0.67244900	0.18276400
H	-2.43434700	3.96015800	-2.20880600	Fe	-1.90926000	-0.52075100	0.31735200
C	-2.05981900	2.08232100	-1.32550900	O	-0.25962100	-0.17802600	-0.52069400
N	-2.48952600	1.49804000	-0.21624300	O	-0.67324400	-0.00321000	-3.29889200
H	-3.98324800	4.45143700	-0.19922700	H	-1.44924400	-0.58067200	-3.18522200
H	-1.39362900	1.63652300	-2.05701200	H	0.10042300	-0.59395400	-3.54418900
C	4.64907000	-0.99672800	0.79599400	O	-1.62646300	-2.07842200	0.70334700
O	3.43806800	-0.57659600	1.02317500	H	-0.29736700	-0.17785800	-1.50776000
O	5.09395800	-1.45233100	-0.26213700	C	-3.48147800	-4.43162800	2.74204100
C	2.05831700	-1.73780300	-2.65341000	H	-3.71066400	-5.31056000	2.12737700
O	2.05667700	-0.78157800	-1.78098000	H	-2.97895700	-3.67607100	2.12882500
O	1.39659600	-1.67484400	-3.71904700	H	-4.41211400	-4.01537300	3.14659700

H	-2.82367800	-4.72802100	3.56772500	H	3.89234700	-2.63489200	-1.98448500
C	5.55891500	-0.87392100	2.03068900	H	2.42997900	-3.47840700	-1.49616200
H	6.57836600	-1.19206900	1.78979700	H	2.97447800	-3.61917700	-3.20627200
H	5.56648200	0.16338200	2.39097300	C	-0.21204000	0.62139900	4.13118400
H	5.15584000	-1.49728400	2.83936300	H	-0.96320200	1.38084900	4.37663100
C	-5.37776200	-1.54406100	-1.57999900	H	-0.45280800	-0.28509400	4.70216100
H	-5.48297400	-2.62204200	-1.39948900	H	0.78879600	0.95946900	4.41501800
H	-6.17839600	-1.03083100	-1.03632300	C	2.82004300	2.61555800	1.96620700
H	-5.46022700	-1.35993400	-2.65566000	H	1.86605800	2.67747900	2.50499000
C	-4.05028900	2.06092000	1.69907100	H	3.26087500	1.64192100	2.20387300
H	-4.68478100	1.17563800	1.57287000	H	3.47577800	3.42169800	2.31975200
H	-3.31773400	1.82157800	2.47750300	O	1.24189800	-2.43447500	0.54295700
H	-4.66824700	2.90711000	2.02305900	H	0.26944400	-2.55295900	0.56191400
C	2.90613800	-2.95678700	-2.33699400				

Model4H-TS1(HS-FM)

C	-3.97345700	-1.42071500	-0.73376200	N	-2.66312700	1.39319000	-0.32064500
O	-4.01182400	-1.03820200	0.48042700	H	-4.22056300	4.29939900	-0.65168100
O	-2.89289700	-1.35222300	-1.39590200	H	-1.56228900	1.34471600	-2.15991600
C	-0.23218300	0.74285600	2.55796400	C	4.68145800	-0.71673600	0.93172300
O	0.85877800	0.54143400	1.98220800	O	3.48747100	-0.20626400	1.02915700
O	-1.40648700	0.43913400	2.13026400	O	5.09764100	-1.47926000	0.05429900
C	-3.54090800	2.33026700	0.19859500	C	2.05208200	-2.15184200	-2.30196200
C	-3.64941300	3.38179500	-0.68918800	O	2.07148300	-1.04916000	-1.62549300
N	-2.82145200	3.05793000	-1.75868300	O	1.36397300	-2.28967700	-3.34355500
H	-2.65612300	3.61331200	-2.58802700	C	2.49688000	2.86217900	-0.15428200
C	-2.24794200	1.85284800	-1.49015300	C	2.66112000	3.75530300	-1.19575400

N	2.26194500	3.07307700	-2.34058900	C	-5.22174300	-1.98597000	-1.39040800
H	2.30412900	3.40999400	-3.29354900	H	-5.10562800	-3.07318500	-1.48957900
C	1.89023900	1.81692500	-1.95875700	H	-6.11008800	-1.77381300	-0.78774400
N	2.01565700	1.66360400	-0.65321900	H	-5.33485300	-1.57124700	-2.39871400
H	3.02090600	4.77522400	-1.22109300	C	-4.22082600	2.13709800	1.52070300
H	1.56724000	1.04259300	-2.64265400	H	-4.83147200	1.22632300	1.50029600
Fe	1.69978300	-0.56158200	0.28391900	H	-3.47499200	2.00500600	2.31303800
Fe	-1.86383500	-0.61922300	0.47252500	H	-4.85905600	2.99687900	1.75897800
O	-0.25249600	-0.29818900	-0.45939400	C	2.91113600	-3.29126100	-1.78194700
O	-0.70817300	-0.54944100	-3.22138100	H	3.90038600	-2.90945500	-1.50639300
H	-1.46978100	-1.09776500	-2.95936300	H	2.45191800	-3.65134800	-0.85182300
H	0.06066100	-1.17763200	-3.36202800	H	2.96996600	-4.10151700	-2.51632800
O	-1.50233800	-2.25495900	1.15809300	C	-0.20813600	1.41236300	3.93353300
H	-0.28513100	-0.40213300	-1.43993000	H	-0.97086700	2.19828700	3.98893200
C	-2.81609800	-3.72206200	2.69659600	H	-0.45272800	0.65830300	4.69313600
H	-2.71812700	-4.71816000	2.25906300	H	0.78330400	1.82288500	4.14477600
H	-2.13863200	-2.93014600	1.88709700	C	2.77445800	3.06905600	1.30477600
H	-3.82599700	-3.30817000	2.65486100	H	1.83929300	3.14077200	1.87364400
H	-2.32276300	-3.61118900	3.66483600	H	3.31998600	2.20459200	1.69733900
C	5.61271700	-0.26373200	2.07014400	H	3.35691500	3.98610300	1.46192300
H	6.61832900	-0.67312000	1.92969000	O	1.36679300	-2.21312300	1.02920400
H	5.65761000	0.83293700	2.10560300	H	0.40819400	-2.41752500	1.10018600
H	5.20274100	-0.60541600	3.02948000				
Model4H- IM (HS-FM)							
C	-3.92837300	-1.39062800	-0.87872100	O	-2.83421900	-1.31056700	-1.51504200
O	-3.99430400	-1.01800800	0.33953700	C	-0.29928600	0.69059300	2.53898000

O	0.80760500	0.50239400	1.99261200	O	-0.19041300	-0.30569600	-0.51864100
O	-1.46064700	0.39685100	2.06484200	O	-0.54126600	-0.54329000	-3.29146600
C	-3.47147400	2.37180600	0.05855500	H	-1.31500900	-1.08801000	-3.06069400
C	-3.53822900	3.42680400	-0.82934200	H	0.22815500	-1.17750200	-3.40157800
N	-2.68072600	3.09478400	-1.87257500	O	-1.52729700	-2.32225700	1.07358200
H	-2.48093000	3.65040700	-2.69416500	H	-0.17419100	-0.38976300	-1.50100300
C	-2.13160300	1.88188900	-1.58877200	C	-4.34577200	-3.01317900	3.14882100
N	-2.58965600	1.42443000	-0.43439300	H	-4.42486300	-4.08907800	3.01426000
H	-4.09867900	4.35148900	-0.80770600	H	-2.10796100	-2.58462500	1.80723800
H	-1.43083900	1.36758700	-2.23769100	H	-4.46874000	-2.34367500	2.30112800
C	4.66182500	-0.80771600	1.10356100	H	-4.09382500	-2.61592100	4.12881700
O	3.47557200	-0.27202800	1.14751100	C	5.55728600	-0.35734600	2.27134200
O	5.09602000	-1.59003400	0.25279000	H	6.55587900	-0.79694000	2.18118900
C	2.15793400	-2.18894000	-2.25718900	H	5.63209400	0.73821100	2.28627100
O	2.17424400	-1.09027600	-1.57414700	H	5.09849700	-0.66699400	3.21934700
O	1.51411600	-2.30471900	-3.32950000	C	-5.15974300	-1.96590200	-1.55633200
C	2.57296800	2.81242700	-0.05591700	H	-5.16379800	-3.05365300	-1.40433400
C	2.79990300	3.70971400	-1.08195400	H	-6.07249600	-1.55246100	-1.11481100
N	2.45656300	3.03715600	-2.25032200	H	-5.12897000	-1.77231000	-2.63352600
H	2.55140900	3.37912000	-3.19768200	C	-4.19703100	2.18464700	1.35709500
C	2.05425300	1.78233700	-1.89596400	H	-4.82862300	1.28917700	1.31064600
N	2.10853600	1.62084700	-0.58655100	H	-3.47976900	2.02836600	2.17100000
H	3.16887100	4.72667100	-1.08212800	H	-4.82211900	3.05733600	1.58282400
H	1.76227700	1.01430600	-2.60058200	C	2.96351400	-3.35233200	-1.70560000
Fe	1.72089200	-0.60765300	0.31925500	H	3.94451800	-2.99551000	-1.37313000
Fe	-1.83155000	-0.61498000	0.36093100	H	2.44710200	-3.71255700	-0.80602300

H	3.04382200	-4.15599300	-2.44517800	H	1.81200700	3.08105800	1.93658500
C	-0.32089500	1.32452400	3.93093100	H	3.29629900	2.13967600	1.83167500
H	-1.09632700	2.09772000	3.98777400	H	3.35268300	3.92234900	1.60985600
H	-0.57223200	0.54711100	4.66447600	O	1.32508600	-2.24877600	1.04879400
H	0.65891600	1.74256800	4.17838000	H	0.36155700	-2.44482100	1.08565800
C	2.77529000	3.00894100	1.41686900				

Model4H-RC(HS-AF)

C	-4.00751500	-1.09584700	-1.09036600	O	1.42084200	-1.72624800	-3.70147400
O	-3.91097800	-0.83080500	0.16641600	C	2.60473200	2.71014700	0.47990100
O	-3.01347900	-1.02664000	-1.85162700	C	2.89573400	3.76755900	-0.36058500
C	-0.27927700	0.27732700	2.64423000	N	2.54607700	3.33916300	-1.63677100
O	0.80731900	0.06386800	2.06468400	H	2.68352700	3.84214200	-2.50372800
O	-1.45863600	0.21798900	2.13543900	C	2.07772100	2.06247000	-1.52489200
C	-3.34434200	2.39764600	0.37872100	N	2.09591400	1.66117300	-0.26709200
C	-3.40953100	3.54318300	-0.38622900	H	3.31349800	4.74691900	-0.16925100
N	-2.57398100	3.32022700	-1.47514100	H	1.77076300	1.44881500	-2.36215600
H	-2.38736500	3.95701300	-2.23880000	Fe	1.64180400	-0.68762000	0.19514700
C	-2.03400700	2.08078500	-1.34319600	Fe	-1.91119300	-0.51759200	0.30976200
N	-2.47884700	1.50420300	-0.23597500	O	-0.25580000	-0.17604400	-0.51335100
H	-3.95523800	4.46642300	-0.24865300	O	-0.64187200	-0.04031300	-3.28952800
H	-1.36197400	1.62783200	-2.06465700	H	-1.42502600	-0.60903600	-3.18135700
C	4.63926500	-0.96308300	0.80706300	H	0.12662000	-0.63804100	-3.53351500
O	3.41910200	-0.57526700	1.03882400	O	-1.64061400	-2.07642900	0.69768800
O	5.09454600	-1.40031200	-0.25485900	H	-0.27713800	-0.19892900	-1.50192800
C	2.07220800	-1.77573200	-2.62883700	C	-3.51916300	-4.36191800	2.80032200
O	2.05155800	-0.81339400	-1.76349600	H	-3.76303300	-5.25057300	2.20560100

H	-3.00841800	-3.62687200	2.16924700	C	2.93005400	-2.98284300	-2.29468100
H	-4.44234600	-3.92384800	3.19884600	H	3.90991200	-2.64570200	-1.93837800
H	-2.86264800	-4.64969900	3.63007300	H	2.45331500	-3.50191700	-1.45260900
C	5.54791200	-0.82711200	2.04155300	H	3.01244400	-3.65245500	-3.15717600
H	6.57346000	-1.12325100	1.79837600	C	-0.24171500	0.63676200	4.13037500
H	5.53477000	0.20881400	2.40570400	H	-0.99219800	1.40056600	4.36413200
H	5.15853300	-1.46145700	2.84838700	H	-0.48905300	-0.26400200	4.70758700
C	-5.36899300	-1.53038600	-1.60881500	H	0.75823500	0.97435700	4.41786100
H	-5.48099000	-2.60737900	-1.42652000	C	2.78610500	2.62302700	1.96625400
H	-6.17123400	-1.01172300	-1.07277100	H	1.82330100	2.70657400	2.48637500
H	-5.44205800	-1.34863300	-2.68555100	H	3.20773100	1.64606200	2.22404600
C	-4.05555800	2.08469100	1.66031100	H	3.44716800	3.42366500	2.32242800
H	-4.69533100	1.20359300	1.53152700	O	1.23294900	-2.44922600	0.56751600
H	-3.33196000	1.84267500	2.44629800	H	0.26164000	-2.57378000	0.58540500
H	-4.67021000	2.93649800	1.97575100				

Model4H-TS1(HS-AF)

C	-3.97731400	-1.39984700	-0.75109600	C	-2.20500800	1.85611700	-1.49869100
O	-4.02624100	-1.01298000	0.46091000	N	-2.63750300	1.40125100	-0.33353500
O	-2.88831500	-1.34256400	-1.40103700	H	-4.15613800	4.32615300	-0.67934200
C	-0.24504100	0.74269400	2.56437700	H	-1.51900100	1.33988000	-2.16176100
O	0.84825900	0.53559300	1.99507300	C	4.67405400	-0.69279100	0.93173900
O	-1.41849400	0.44177800	2.13190100	O	3.47204600	-0.20397900	1.03669000
C	-3.50915700	2.34888200	0.17716200	O	5.09999000	-1.44430600	0.04925600
C	-3.59581500	3.40171200	-0.71139900	C	2.06017900	-2.17730700	-2.27899200
N	-2.76113400	3.06801000	-1.77257400	O	2.06795900	-1.07153300	-1.60781500
H	-2.57954300	3.62213200	-2.59934500	O	1.37820100	-2.32414500	-3.32361200

C	2.48102900	2.85374300	-0.16181000	H	5.20264600	-0.58170000	3.02786500
C	2.66360000	3.73654500	-1.20904400	C	-5.22209400	-1.95770000	-1.42052700
N	2.28010500	3.04455500	-2.35336400	H	-5.11746700	-3.04732100	-1.50530000
H	2.33982400	3.37154500	-3.30885100	H	-6.11674700	-1.72857300	-0.83358700
C	1.89946200	1.79286200	-1.96523500	H	-5.31521000	-1.55336500	-2.43502900
N	2.00423000	1.65165400	-0.65655800	C	-4.20514300	2.16393800	1.49205600
H	3.02685800	4.75513100	-1.23856800	H	-4.82837900	1.26192300	1.46445400
H	1.58532200	1.01279100	-2.64674100	H	-3.46924600	2.02038600	2.29160400
Fe	1.68406400	-0.57311000	0.29709300	H	-4.83349300	3.03245800	1.72482400
Fe	-1.87158900	-0.61523300	0.47141800	C	2.92559200	-3.30747000	-1.74987900
O	-0.24797500	-0.31815100	-0.43922800	H	3.91428000	-2.91743500	-1.48367900
O	-0.68035400	-0.57010700	-3.19766400	H	2.47249600	-3.65863800	-0.81339700
H	-1.45139100	-1.11067300	-2.94729500	H	2.98537800	-4.12563000	-2.47534500
H	0.08198100	-1.20605600	-3.34105200	C	-0.22474600	1.41468400	3.93876800
O	-1.52902400	-2.25326900	1.16120500	H	-0.99687500	2.19110400	3.99646500
H	-0.26852400	-0.42629200	-1.42109800	H	-0.45669300	0.65804600	4.69984500
C	-2.85833800	-3.72390900	2.68158600	H	0.76255700	1.83696400	4.14640300
H	-2.75981100	-4.71774100	2.23900600	C	2.73724100	3.07368500	1.29924400
H	-2.17590800	-2.92901800	1.88268400	H	1.79393000	3.15339000	1.85346800
H	-3.86776400	-3.30894600	2.63735000	H	3.27477500	2.21170900	1.70795300
H	-2.37110600	-3.62050800	3.65376300	H	3.31968300	3.99074600	1.45642000
C	5.60248900	-0.22894000	2.06825600	O	1.36661600	-2.22516800	1.05381000
H	6.61438000	-0.62037900	1.92170700	H	0.40891700	-2.43237400	1.11413400
H	5.62873500	0.86818400	2.10834700				
Model4H-IM(HS-AF)							
C	-3.92938300	-1.37149600	-0.89748400	O	-4.00539400	-0.99321900	0.31832000

O	-2.82728500	-1.30453300	-1.52168800	Fe	1.70354300	-0.61803300	0.33294700
C	-0.31405200	0.69795700	2.54377600	Fe	-1.83863800	-0.61325000	0.36234300
O	0.79539800	0.50422300	2.00470600	O	-0.18367300	-0.33473000	-0.49323700
O	-1.47380100	0.40122400	2.06682100	O	-0.51062600	-0.57057800	-3.26045900
C	-3.43098600	2.38944900	0.03251400	H	-1.29448700	-1.10678000	-3.04417800
C	-3.47291700	3.44432400	-0.85692000	H	0.25183400	-1.21329200	-3.37410500
N	-2.60842800	3.09945800	-1.89011200	O	-1.55481600	-2.32226800	1.08036700
H	-2.39040100	3.65213300	-2.70903800	H	-0.15666700	-0.42279100	-1.47675100
C	-2.07935200	1.87948100	-1.59926200	C	-4.41091600	-2.98155500	3.12659700
N	-2.55667400	1.42942600	-0.44967200	H	-4.50218300	-4.05637800	2.99115800
H	-4.02066700	4.37670200	-0.84226100	H	-2.14910100	-2.57599900	1.80614400
H	-1.37881900	1.35492500	-2.24012300	H	-4.51578100	-2.31070800	2.27753900
C	4.65014400	-0.78607500	1.11414200	H	-4.16327000	-2.58747700	4.10896600
O	3.45820700	-0.26369000	1.15511600	C	5.54121100	-0.31814400	2.27852200
O	5.09311800	-1.56930700	0.26850100	H	6.54467600	-0.74703900	2.19070400
C	2.16563600	-2.22110300	-2.22752800	H	5.60362400	0.77827400	2.28624100
O	2.17355200	-1.11721100	-1.55342500	H	5.08644700	-0.62673200	3.22882200
O	1.52795200	-2.34725600	-3.30267100	C	-5.15809100	-1.93818500	-1.58699600
C	2.55538200	2.80602800	-0.07504200	H	-5.16999800	-3.02613100	-1.43684000
C	2.80229000	3.68922400	-1.10870300	H	-6.07231500	-1.51973200	-1.15338900
N	2.47630000	3.00258200	-2.27384900	H	-5.11619800	-1.74340000	-2.66362800
H	2.59021400	3.33113600	-3.22386400	C	-4.17448900	2.21401800	1.32252400
C	2.06438200	1.75346500	-1.90978400	H	-4.82139100	1.32997200	1.26824100
N	2.09591300	1.60899300	-0.59769100	H	-3.46928800	2.04433600	2.14417500
H	3.17486200	4.70485300	-1.11596600	H	-4.78653000	3.09750200	1.54191700
H	1.78235900	0.97700200	-2.60922800	C	2.97349700	-3.37643100	-1.66292800

H	3.95399900	-3.01289600	-1.33613600	C	2.73447700	3.02053800	1.39824100
H	2.45913700	-3.72654100	-0.75821600	H	1.76327300	3.10278900	1.90152600
H	3.05517500	-4.18879300	-2.39276700	H	3.24571000	2.15479700	1.83211800
C	-0.34098400	1.34134000	3.93130100	H	3.31200000	3.93433100	1.58906400
H	-1.12982000	2.10078300	3.98739700	O	1.32048000	-2.25631900	1.07977000
H	-0.57405400	0.56383400	4.67084100	H	0.35772400	-2.45396000	1.10687800
H	0.63262600	1.77773600	4.17168600				

Model5-Q (HS-FM)

C	-0.40079300	-2.59850200	0.06684300	C	3.53393500	-0.68511900	3.09519100
O	0.68815200	-1.99713100	-0.11180200	N	2.57052300	0.22122500	3.51406400
O	-1.54731800	-2.00398500	0.19308800	H	2.46919700	0.60163600	4.44879200
C	-4.79341100	-0.50433700	-0.58212200	C	1.78384500	0.52029700	2.45910500
C	-5.98131000	0.09067700	-0.22867300	N	2.19340800	-0.14977100	1.38124500
N	-5.65982500	1.12232900	0.64405100	H	4.29584000	-1.07111800	3.75773900
H	-6.31525400	1.75755200	1.08867100	H	0.93440900	1.18935600	2.50088400
C	-4.32419800	1.14431800	0.80843600	Fe	1.25179000	-0.02493700	-0.48655200
N	-3.76616400	0.17060600	0.08122400	Fe	-1.76437400	-0.10172800	-0.02634000
H	-6.99969200	-0.12735200	-0.51873000	O	-1.24999200	0.92986600	1.16336000
H	-3.78456700	1.84310600	1.43442000	O	-0.58655400	0.13063500	-1.21524400
C	3.54190900	0.23708100	-2.23639300	C	4.05631900	-1.79140600	0.81227100
O	2.35439000	-0.32465300	-1.92489300	H	3.38463400	-2.48205500	0.28949000
O	4.22042800	0.81983400	-1.40688500	H	4.57449900	-1.18040000	0.06471700
C	0.47743200	2.92045700	-0.03190600	H	4.80166300	-2.37796100	1.35909800
O	1.24902500	1.95217000	-0.29088800	C	3.92223700	0.04638300	-3.68923000
O	-0.65201900	2.85744100	0.55308800	H	4.90023100	0.49488700	-3.87890700
C	3.29540800	-0.91650300	1.75955700	H	3.94460000	-1.02342000	-3.92968300

H	3.16493500	0.50885600	-4.33386600	H	-4.01023600	-2.46426300	-0.99021400
C	0.92594400	4.31580400	-0.44309700	H	-5.49528300	-2.05520700	-1.87675000
H	1.94675200	4.47429500	-0.07884600	C	-0.42234300	-4.10716900	0.13664300
H	0.94640800	4.35374600	-1.53888700	H	-0.86143900	-4.49347400	-0.79245700
H	0.25393400	5.08534800	-0.05725000	H	0.59068100	-4.50048000	0.24397700
C	-4.54572900	-1.65808700	-1.50535400	H	-1.05737200	-4.43670300	0.96542800
H	-3.94671700	-1.35054900	-2.37276200				

Model5-TS1 (HS-FM)

C	0.24859300	-2.72769200	-0.52467300	C	-3.97884100	-0.10202500	-2.96204800
O	-0.76003500	-2.02635300	-0.26732400	N	-3.01166100	0.77895300	-3.42396600
O	1.46556400	-2.26913300	-0.51669100	H	-3.01605600	1.26438600	-4.31410100
C	4.85921300	-0.38824700	-0.02665000	C	-2.04713700	0.87498200	-2.48419200
C	5.87088400	0.49374900	-0.32486900	N	-2.34888600	0.10786400	-1.43706700
N	5.25691600	1.67515300	-0.71922300	H	-4.86162600	-0.34890400	-3.53494100
H	5.72714500	2.52667100	-1.00977000	H	-1.14964600	1.46921100	-2.58809600
C	3.92202300	1.50599800	-0.66099700	Fe	-1.08689000	-0.00185300	0.25604200
N	3.64452000	0.26491300	-0.24364300	Fe	1.72924200	-0.40922100	-0.09362000
H	6.94565100	0.38195000	-0.29146200	O	0.55066200	0.46195700	-1.09286700
H	3.18483400	2.25869100	-0.91494600	O	0.70864900	-0.23141100	1.39500900
C	-3.31223400	0.27212700	2.17351500	C	-4.25068200	-1.46432300	-0.78366700
O	-2.24373900	-0.36555800	1.66448400	H	-3.55099200	-2.21493300	-0.40010300
O	-4.01917900	1.01033400	1.50742800	H	-4.67206400	-0.91808400	0.06665300
C	-0.18056000	2.81033600	0.11303300	H	-5.06509400	-1.97785100	-1.30560100
O	-1.03693100	1.98987500	0.55311600	C	-3.55692100	-0.03975600	3.63877200
O	0.78729600	2.51530400	-0.66670000	H	-4.47352900	0.45052800	3.97522400
C	-3.56226200	-0.51836900	-1.71774800	H	-3.63623100	-1.12405100	3.78351000

H	-2.70974200	0.31407700	4.23977100	C	0.08960300	-4.18683000	-0.88093300
C	-0.29935500	4.26278100	0.54103900	H	0.78836800	-4.79193600	-0.29321400
H	-1.32986400	4.59395300	0.37267800	H	-0.93806700	-4.51364700	-0.70990700
H	-0.10147000	4.32419500	1.61801600	H	0.34725700	-4.32275100	-1.93896200
H	0.40107200	4.90195500	-0.00177900	C	0.56344600	-0.75431500	3.85850400
C	4.93978200	-1.80586400	0.45236800	H	1.40351300	-1.42192300	4.06574000
H	4.52903000	-1.90574300	1.46579900	H	0.65823800	-0.49440700	2.62213000
H	4.38029000	-2.47979200	-0.20800000	H	-0.41668900	-1.22747000	3.93899800
H	5.98159200	-2.13942700	0.47843500	H	0.63507800	0.21962000	4.34789000

Model5-**IM**-r (HS-FM)

C	-0.61548300	1.74026400	1.77016300	O	-1.26514000	-1.13020400	-1.81335200
O	0.54886000	1.29017300	1.59977000	C	2.93590700	2.32622800	-0.95501500
O	-1.66858600	1.35613300	1.11464300	C	4.12919800	2.46753400	-1.62475400
C	-4.61284900	0.60495400	-0.29152700	N	4.66860400	1.19357200	-1.73287700
C	-5.74146700	-0.18024600	-0.33631300	H	5.55093600	0.94618000	-2.16762400
N	-5.30434300	-1.48794500	-0.49110300	C	3.82448000	0.32237200	-1.14368100
H	-5.89099600	-2.31300800	-0.56294300	N	2.76174200	0.97289700	-0.65995600
C	-3.95797900	-1.48238500	-0.54419200	H	4.62469700	3.34476500	-2.01654300
N	-3.50326300	-0.23305000	-0.42089600	H	3.99158100	-0.74633100	-1.05178000
H	-6.78956700	0.07899900	-0.28196700	Fe	1.21809100	-0.15634800	0.23641200
H	-3.34446500	-2.36376900	-0.67366000	Fe	-1.50018000	0.17276600	-0.40631800
C	3.20217700	-2.11630300	1.31283800	O	-0.19124300	1.03383000	-0.95983100
O	2.26745100	-1.16646700	1.40218800	O	-0.53688700	-1.10105200	0.73900600
O	3.78485200	-2.38084400	0.26761100	C	1.96873000	3.40152700	-0.56506300
C	-0.08577400	-1.59775600	-2.08756100	H	0.97596600	3.20686300	-0.98641500
O	0.97162200	-1.31467000	-1.46552300	H	1.87065300	3.46091700	0.52572500

H	2.32119400	4.37084500	-0.93243000	H	-4.02063600	2.53139600	-1.04722500
C	3.47623300	-2.82249700	2.62631400	H	-5.52002800	2.52972600	-0.10288100
H	4.27741000	-3.55397200	2.49807800	C	-0.84425900	2.81598600	2.80822700
H	3.75602100	-2.08880000	3.39185900	H	-0.83289300	3.79105500	2.30268400
H	2.56538800	-3.32757500	2.97112900	H	-1.82279400	2.69511700	3.28214400
C	-0.00970100	-2.57988100	-3.23463800	H	-0.04498700	2.79907800	3.55312900
H	0.84245900	-2.32439300	-3.87284900	C	-0.70637600	-1.58682800	3.80213900
H	0.17439100	-3.58102300	-2.82466300	H	-1.44107200	-0.89684200	4.21101000
H	-0.93554200	-2.58445700	-3.81429100	H	-0.70495000	-1.11232900	1.70911300
C	-4.51777200	2.09539400	-0.17062300	H	0.34447700	-1.30754900	3.78876500
H	-3.94806300	2.38363700	0.71867200	H	-0.98186400	-2.62909600	3.66035300

Model5-**IM**-n (HS-FM)

C	-0.40335700	-2.60367100	-0.51321600	C	0.39769900	2.85323400	-0.00336300
O	0.67608300	-1.99015300	-0.34874100	O	1.37256500	2.06318600	-0.17995600
O	-1.54702400	-2.01930100	-0.72309700	O	-0.78882800	2.49301300	0.29544000
C	-4.62496600	-0.46738200	0.41040000	C	3.17301600	-1.12098700	1.94743000
C	-5.43544000	0.19251600	1.30521600	C	3.37237900	-0.96031500	3.30004300
N	-4.73902100	1.32082800	1.71055700	N	2.43045900	-0.03506400	3.72742100
H	-5.06093000	2.02005300	2.37191100	H	2.31214000	0.30843100	4.67391100
C	-3.54405600	1.33495300	1.08753600	C	1.69205200	0.33551900	2.65950500
N	-3.44304800	0.26784200	0.28987200	N	2.11470600	-0.29804700	1.56695800
H	-6.42013600	-0.04945900	1.68011400	H	4.09223200	-1.40864000	3.97029500
H	-2.77846400	2.08830400	1.21852400	H	0.86510200	1.03100900	2.69980400
C	3.81513000	0.40365600	-1.68519600	Fe	1.23527200	0.05653400	-0.31570200
O	2.61266000	-0.18069900	-1.54801700	Fe	-1.72360400	-0.08887200	-0.74244500
O	4.43570900	0.86344800	-0.73980200	O	-0.63382500	0.37489400	0.63688900

O	-0.22133900	0.30443600	-1.82207200	C	-4.89174500	-1.75438800	-0.31079300
C	3.93145900	-1.99399400	0.99707500	H	-5.08237100	-1.59267300	-1.37959900
H	3.24767100	-2.59019800	0.38302200	H	-4.04100600	-2.43837100	-0.22275800
H	4.54695000	-1.38001500	0.33140000	H	-5.77619800	-2.24032600	0.11276300
H	4.58774400	-2.67152300	1.55339500	C	-0.43297300	-4.11468900	-0.46236100
C	4.32019900	0.40746000	-3.11614700	H	-0.91615200	-4.42712500	0.47243800
H	5.32002200	0.84600200	-3.15824600	H	-1.03113100	-4.50794100	-1.29103500
H	4.34175500	-0.61695300	-3.50732300	H	0.58163800	-4.51719600	-0.49582800
H	3.63525700	0.98586400	-3.74892400	C	-2.81435700	0.28510500	-2.48023700
C	0.65300100	4.34116200	-0.16747400	H	-3.87087900	0.12887400	-2.26827800
H	1.54648300	4.61315500	0.40492600	H	-0.10945000	-0.00693700	-2.73474900
H	0.86417400	4.53936700	-1.22536900	H	-2.41963000	-0.42256500	-3.21345600
H	-0.20571100	4.93547800	0.15366200	H	-2.57041600	1.32560100	-2.70810300

Model5-**TS2**-r (HS-FM)

C	-4.25037100	-1.26521700	-0.56261000	N	2.48411000	0.41201000	-1.22366900
N	-3.64141400	-0.08657300	-0.38652600	C	3.48715600	1.37837800	-1.24319200
C	-4.60212000	0.90886500	-0.58922300	C	4.27963200	1.13699900	-2.34208000
C	-5.79638200	0.29226500	-0.88175200	N	3.74717800	0.02385900	-2.97396100
N	-5.55015100	-1.07257800	-0.85826500	C	2.67505900	-0.38777800	-2.26840700
Fe	-1.62794800	0.01034600	0.06466600	C	3.64970000	2.46539500	-0.22555300
O	-0.24993700	0.37071800	-1.06248300	O	-0.32365200	-0.47917200	1.52082500
Fe	1.05308700	0.00416700	0.13262400	O	0.81457000	1.88717000	0.77142900
O	0.90119700	-1.87072100	-0.42644200	C	-0.31294400	2.45887300	0.93892100
C	-0.20666900	-2.50008400	-0.50094400	O	-1.45669500	1.88718700	0.84982500
O	-1.36866000	-2.00461500	-0.30602900	O	2.31458100	-0.28612700	1.43642000
C	-4.31060400	2.37622000	-0.51203900	C	3.39496500	-1.08731900	1.41785200

O	3.78387900	-1.70684000	0.44308900	H	4.26824300	-0.11596400	3.14492500
C	-1.53760200	-1.67712600	3.23276900	H	3.42147700	-1.62697300	3.50127700
C	-0.29289400	3.93716000	1.26337400	H	-0.70857400	-4.56085200	-0.17272500
C	4.07915300	-1.13075100	2.77665300	H	-0.56252500	-4.10164100	-1.87589000
C	-0.12153200	-3.96471200	-0.88032500	H	0.91637900	-4.30413700	-0.88750000
H	-6.22553900	-1.80806500	-1.04001900	H	-3.90444100	2.65181300	0.46662000
H	-6.77175300	0.70259700	-1.10296000	H	-3.57496600	2.67102800	-1.27093100
H	-3.76793500	-2.23132300	-0.49589300	H	-5.22836800	2.94644200	-0.68663600
H	4.11339100	-0.43133200	-3.80251800	H	-0.47281700	4.49515500	0.33467100
H	5.15626900	1.65135000	-2.70979900	H	-1.09668000	4.18143900	1.96440100
H	2.08399900	-1.25934400	-2.50594400	H	0.67771800	4.23406400	1.66788300
H	2.84434100	3.20431200	-0.29930400	H	-2.21655600	-0.90461400	3.58568400
H	3.62942800	2.05810600	0.79034500	H	-0.16615300	0.19198100	2.20931000
H	4.60583200	2.97517100	-0.38353300	H	-0.61372700	-1.86351300	3.77078500
H	5.01734300	-1.68512600	2.69544100	H	-1.88561100	-2.41277600	2.51596700
Model5-TS2-n (HS-FM)							
C	-4.16340300	1.13728300	0.88692900	O	-1.46046100	2.06532500	0.21920400
N	-3.60452500	0.03532600	0.37465800	C	-4.32467700	-2.39919500	0.02708300
C	-4.55206800	-0.98817800	0.47709700	N	2.49940000	-0.68149800	1.18943800
C	-5.68498300	-0.46494700	1.05717400	C	3.65774900	-1.43171400	1.00665100
N	-5.41679400	0.87179200	1.30567600	C	4.22652200	-1.63221400	2.24417100
Fe	-1.61376800	0.07050300	-0.28356900	N	3.41049800	-0.98910500	3.16235200
O	-0.17566800	-0.23382800	0.98398500	C	2.37916100	-0.43513300	2.49231300
Fe	1.12705900	0.15139000	-0.09526100	C	4.15148000	-1.92184700	-0.31971300
O	0.80081900	2.07944400	0.28118900	O	-0.30875700	0.61892800	-1.71829800
C	-0.33171200	2.63537000	0.42391400	O	0.83443200	-1.73016600	-1.02302800

C	-0.26169700	-2.35679000	-1.10095400	H	4.87894600	-2.72675100	-0.16953100
O	-1.41953100	-1.80840700	-0.95139900	H	5.17751800	2.23673100	-2.11029600
O	2.44559200	0.57468600	-1.33822100	H	4.40710000	0.87357900	-2.99546900
C	3.49283600	1.37233200	-1.09222300	H	3.61190800	2.45190800	-2.94421200
O	3.81516600	1.75804400	0.02116700	H	-0.80083400	4.69299000	0.06427200
C	-2.24390900	0.91344800	-2.51103700	H	-0.95875400	4.19622900	1.75615900
C	-0.22988200	-3.84309700	-1.38082200	H	0.67199100	4.43938000	1.04829600
C	4.23117100	1.75372600	-2.36682000	H	-4.10497500	-2.45037900	-1.04512900
C	-0.34317700	4.08655100	0.85551700	H	-3.47861300	-2.85289700	0.55488700
H	-6.04677000	1.54214300	1.73418200	H	-5.22009900	-2.99672500	0.22578500
H	-6.63080300	-0.92460300	1.30788300	H	-0.23666300	-4.37335400	-0.41880700
H	-3.67821100	2.10093100	0.96324400	H	-1.11520200	-4.15051200	-1.94483400
H	3.55358000	-0.94102100	4.16502700	H	0.68478400	-4.11440700	-1.91438400
H	5.12217100	-2.16308700	2.53480900	H	-2.88921200	0.03420800	-2.52531000
H	1.57386300	0.11848200	2.95493000	H	-0.03431100	-0.05112800	-2.36982800
H	3.32422600	-2.29679900	-0.92951900	H	-1.69185200	1.09888800	-3.42621900
H	4.64662700	-1.11944000	-0.87820000	H	-2.60521500	1.80503800	-2.00553200

Model5-**P** (HS-FM)

C	4.40373700	-0.45536700	-0.51705500	O	-1.01801600	0.59643700	-1.98706100
N	3.25066800	-0.93576400	-0.05036400	C	0.11679000	0.88591500	-2.46735900
C	3.45946400	-2.27790600	0.26863500	O	1.21343400	0.91095700	-1.79762400
C	4.76823500	-2.58670100	-0.02478300	C	2.39780600	-3.15449500	0.85838500
N	5.34266700	-1.42421700	-0.51870100	N	-2.87977800	-1.40607900	-0.29151500
Fe	1.48673500	0.16740400	0.03070800	C	-4.25809600	-1.43391800	-0.08124200
O	0.12868400	-1.02097700	-0.14661600	C	-4.71691000	-2.67905600	-0.44635800
Fe	-1.42673400	0.06065100	-0.03631900	N	-3.60800700	-3.39573800	-0.87621700

C	-2.52379300	-2.60076500	-0.76667600	H	-4.64950500	0.03528300	1.43760500
C	-5.03733300	-0.27506200	0.46027900	H	-4.97091000	0.59209100	-0.20519700
O	2.65315700	1.99310000	0.42947900	H	-6.08959900	-0.55475300	0.57420600
O	-1.12956200	0.08677300	2.00112800	H	-2.83189800	4.11168300	1.24915900
C	-0.02311300	0.26840700	2.58758800	H	-1.23518000	4.64596500	0.62987800
O	1.10173300	0.45322300	1.99133600	H	-2.60537500	4.35530800	-0.48465600
O	-0.49504000	2.20904500	0.26566200	H	-0.72012400	0.99708800	-4.45272500
C	-1.70995600	2.57015300	0.27392800	H	0.36424800	2.34200400	-4.01283000
O	-2.63091800	1.68444000	0.13766000	H	1.06264400	0.76214500	-4.39679000
C	2.55161200	3.24630300	-0.29601900	H	2.15627600	-2.83761300	1.88118100
C	-0.01439500	0.30804700	4.10129500	H	1.47531400	-3.09349200	0.27195400
C	-2.10714000	4.01717600	0.43242000	H	2.74154400	-4.19329200	0.89304100
C	0.20413600	1.25891500	-3.93264400	H	0.93158800	-0.07827000	4.49187400
H	6.30264400	-1.31252700	-0.82749900	H	-0.11376900	1.35356800	4.42276900
H	5.32306600	-3.50850800	0.07985300	H	-0.86102500	-0.25486000	4.50274500
H	4.57772000	0.56104300	-0.84289700	H	3.25974000	3.96910800	0.12635600
H	-3.60491100	-4.35240500	-1.21307200	H	2.41908000	2.14842800	1.36228900
H	-5.71173500	-3.10180300	-0.43417200	H	1.52580800	3.62350700	-0.24900500
H	-1.51274700	-2.89002400	-1.02178100	H	2.81418900	3.02962300	-1.33289000
Model5-Q (HS-AF)							
C	-0.44175100	-2.56186600	-0.01179400	H	-6.40388500	1.61937600	1.01137900
O	0.67895800	-2.03130400	-0.22091400	C	-4.37434400	1.12276600	0.78149900
O	-1.53278700	-1.89826100	0.21124800	N	-3.74019900	0.20730500	0.04185000
C	-4.70604000	-0.49576400	-0.68201800	H	-6.92997100	-0.23632500	-0.68751800
C	-5.93566900	0.02282900	-0.35139400	H	-3.89267400	1.82431900	1.44993200
N	-5.70056300	1.03604300	0.56903900	C	3.57004100	0.01777800	-2.15546100

O	2.27976200	-0.33698200	-2.04012900	H	4.39826500	-1.39788400	0.36022300
O	4.22253700	0.40292200	-1.19375500	H	4.48123700	-2.54769600	1.71627900
C	0.82113800	3.01686900	-0.14591400	C	4.10800600	-0.11574900	-3.56356900
O	1.49302400	1.97427300	-0.31742000	H	5.16144400	0.17271900	-3.58873100
O	-0.32238300	3.09979000	0.43362800	H	3.99204000	-1.15062800	-3.90769000
C	3.01064400	-1.01494600	1.94393600	H	3.52744200	0.51945900	-4.24350100
C	3.13467300	-0.76647700	3.29195500	C	1.35520500	4.35614700	-0.63366800
N	2.18929800	0.20078400	3.60108900	H	2.38615300	4.45579100	-0.27599600
H	2.01961100	0.60514000	4.51557000	H	1.36353100	4.32986900	-1.72999200
C	1.52391700	0.51947200	2.47095900	H	0.74553800	5.19492000	-0.28829700
N	1.99473800	-0.19602400	1.44838500	C	-4.36906200	-1.59918200	-1.63757500
H	3.80673600	-1.17970800	4.03090500	H	-3.73683800	-1.23390000	-2.45760200
H	0.70957800	1.23109300	2.42124800	H	-3.83199900	-2.40711100	-1.12737700
Fe	1.26670800	-0.05552400	-0.51520500	H	-5.28332200	-2.01131400	-2.07534800
Fe	-1.73335200	0.02061700	0.01964100	C	-0.56531700	-4.06787500	-0.02015600
O	-1.38492600	1.19753500	1.16399200	H	-1.05577400	-4.37298200	-0.95394100
O	-0.49743200	0.27552500	-1.10758100	H	0.42056200	-4.53488800	0.03121000
C	3.80373000	-1.95663100	1.09162500	H	-1.19694800	-4.39888500	0.81051500
H	3.14402200	-2.64276100	0.54776400				

Model5-TS1 (HS-AF)

C	-0.37933900	2.56644500	-0.06210800	H	-6.30438500	-1.94287100	-1.15721800
O	0.72991400	1.99875700	0.16031600	C	-4.32225700	-1.36002700	-0.76354000
O	-1.48394500	1.94723600	-0.29057100	N	-3.77555700	-0.23478300	-0.28950800
C	-4.82132600	0.65790200	-0.03775500	H	-7.02430000	0.38190100	-0.33057400
C	-6.00078600	0.03701500	-0.37676500	H	-3.77385500	-2.24926000	-1.04431000
N	-5.66092200	-1.22897400	-0.83096600	C	3.35156000	-0.87919400	1.92032600

O	2.29160200	-0.09640700	1.64545500	C	3.71635200	-0.89703400	3.39344300
O	3.95621700	-1.49660000	1.05940000	H	4.60524400	-1.51287400	3.54914000
C	-0.28547800	-2.62022700	-0.23026700	H	3.90179100	0.12440900	3.74773500
O	0.81398600	-2.01551600	-0.08218700	H	2.88003600	-1.30131500	3.97728000
O	-1.42474300	-2.04156500	-0.39237300	C	-0.28701800	-4.13369500	-0.20449000
C	3.80037000	0.93989200	-1.38094200	H	0.73378400	-4.51660100	-0.26712700
C	4.43763700	0.68457400	-2.57335400	H	-0.73929900	-4.46676100	0.73857600
N	3.63896200	-0.22115300	-3.25636000	H	-0.89923800	-4.52524000	-1.02386900
H	3.82630000	-0.61829900	-4.17033900	C	-4.62033900	2.03385700	0.51929100
C	2.55706400	-0.48541000	-2.49409200	H	-4.16084100	1.99355000	1.51542600
N	2.62162500	0.19762200	-1.35305200	H	-3.96701000	2.62958700	-0.12687800
H	5.36891900	1.05682900	-2.97654300	H	-5.58447900	2.54345900	0.61145100
H	1.75715100	-1.15195400	-2.78520600	C	-0.42546000	4.07823200	-0.08860600
Fe	1.17229000	-0.00323800	0.16034600	H	-1.35953100	4.44190600	0.35023300
Fe	-1.72689200	-0.04818100	-0.07814400	H	0.43802100	4.49692700	0.43367400
O	-0.31603900	-0.01215100	-1.38511300	H	-0.39780700	4.40448200	-1.13677100
O	-0.67300800	-0.12046400	1.36282900	C	-0.25992700	0.58241500	3.76505800
C	4.24301200	1.83676000	-0.26660200	H	-0.95611100	1.40271400	3.95898100
H	3.42249900	2.47859000	0.07242100	H	-0.48300300	0.23742000	2.60110200
H	4.59100000	1.24593600	0.58785700	H	0.78970200	0.88076700	3.74979900
H	5.06943800	2.47214000	-0.60176600	H	-0.45940000	-0.31288200	4.35925400
Model5- IM -r (HS-AF)							
C	-0.61478100	1.70657500	1.79218100	C	-5.74414200	-0.16860700	-0.36017600
O	0.54619300	1.24669400	1.62550100	N	-5.31053900	-1.47724300	-0.51818200
O	-1.66708600	1.33533700	1.12660000	H	-5.89962600	-2.30021900	-0.59461400
C	-4.61329600	0.61273500	-0.30802700	C	-3.96419100	-1.47627800	-0.56575600

N	-3.50606000	-0.22860400	-0.43620900	H	1.81687100	3.46386200	0.52285900
H	-6.79162600	0.09368500	-0.30855900	H	2.27178400	4.38088200	-0.92885100
H	-3.35269800	-2.35926700	-0.69440000	C	3.45773500	-2.85988500	2.58988200
C	3.24408400	-2.12602700	1.28077700	H	4.26307100	-3.59015100	2.48215600
O	2.30001900	-1.18391700	1.34293600	H	3.70490800	-2.14250800	3.38176300
O	3.87866000	-2.36291700	0.25954200	H	2.53169700	-3.36946900	2.88356500
C	-0.08086200	-1.59059400	-2.10233500	C	-0.00598500	-2.55734400	-3.26218300
O	0.97452100	-1.32116000	-1.47239000	H	0.86354400	-2.31399100	-3.88121500
O	-1.26136500	-1.12342700	-1.82599700	H	0.14586600	-3.56825800	-2.86276300
C	2.91662500	2.34549600	-0.94490700	H	-0.92148100	-2.53284200	-3.85770100
C	4.11400100	2.50570900	-1.60292100	C	-4.51233500	2.10217300	-0.18008800
N	4.67761900	1.24143200	-1.69934000	H	-3.94059300	2.38369000	0.71016700
H	5.56906600	1.00813500	-2.12318900	H	-4.01487200	2.54063000	-1.05534200
C	3.84398600	0.35747900	-1.11416900	H	-5.51266300	2.54031400	-0.10879800
N	2.76410900	0.99048400	-0.64518500	C	-0.84215100	2.77506800	2.83694600
H	4.59786600	3.39029500	-1.99274300	H	-0.85161900	3.75249500	2.33597900
H	4.03144300	-0.70747800	-1.01402800	H	-1.81293100	2.63892900	3.32292900
Fe	1.21805100	-0.15865700	0.22780300	H	-0.03350300	2.76439600	3.57166900
Fe	-1.50123200	0.16817300	-0.40723700	C	-0.79365900	-1.54730200	3.92139700
O	-0.17719100	1.00851300	-0.93265900	H	-1.49870400	-0.84965900	4.36685800
O	-0.53981600	-1.13447000	0.72603700	H	-0.71914400	-1.11470100	1.68940400
C	1.92865300	3.40623000	-0.56680700	H	0.26185600	-1.28951000	3.87577100
H	0.94368800	3.19893100	-1.00021800	H	-1.09898700	-2.57786600	3.75756200
Model5- IM -n (HS-AF)							
C	-0.43593900	-2.45161700	-0.77787900	O	-1.53579800	-1.78275000	-0.76687500
O	0.71452300	-1.94779100	-0.63303000	C	-4.62290300	-0.67698200	0.36699600

C	-5.47540700	-0.34322500	1.39472100	C	3.93275300	-2.24792000	0.49710800
N	-4.86861800	0.69247200	2.08775200	H	3.09576200	-2.80458200	0.06215900
H	-5.23860000	1.16769800	2.90443100	H	4.41996700	-1.68637700	-0.30778400
C	-3.68946900	0.96687300	1.49415300	H	4.65695400	-2.96086500	0.90467900
N	-3.50592600	0.15692000	0.44919800	C	4.40614700	0.89127600	-2.94099600
H	-6.43556200	-0.75000500	1.67989800	H	5.38237700	1.37946200	-2.89094500
H	-2.99798300	1.73126700	1.82043600	H	4.50646000	-0.11082000	-3.37501300
C	3.79927900	0.80032600	-1.55305200	H	3.73875000	1.46525800	-3.59609700
O	2.63137000	0.13503700	-1.53035900	C	-0.03486000	4.17257800	0.22548000
O	4.31054400	1.27147700	-0.54978900	H	0.86442500	4.48223300	0.76458800
C	-0.11005700	2.66186600	0.15703600	H	0.03730600	4.55477500	-0.80161900
O	0.97113300	2.00872900	0.17307200	H	-0.93536200	4.59088700	0.68361600
O	-1.28549100	2.14129500	0.06869100	C	-4.80796300	-1.73588300	-0.67702500
C	3.46236500	-1.32095500	1.57484300	H	-4.94091600	-1.29813000	-1.67454300
C	3.96607800	-1.16725600	2.84590900	H	-3.94190100	-2.40433100	-0.71288000
N	3.20935400	-0.17222600	3.44742200	H	-5.70086800	-2.32736800	-0.45161100
H	3.33257700	0.19204900	4.38551100	C	-0.54882600	-3.95010500	-0.96175500
C	2.28136200	0.24334300	2.55933200	H	-0.71404100	-4.40503100	0.02414400
N	2.40265900	-0.42992200	1.41806200	H	-1.40267000	-4.20027300	-1.59799100
H	4.78226200	-1.66246100	3.35286000	H	0.37757700	-4.35360700	-1.37817900
H	1.55415200	1.01805500	2.75916000	C	-2.88297500	0.79273800	-2.30988600
Fe	1.24898800	0.01832800	-0.28771000	H	-3.85259100	1.12237200	-1.94162500
Fe	-1.71333500	0.23207000	-0.58963100	H	-0.12315700	-0.03543200	-2.59221800
O	-0.51481700	-0.05546300	0.89908400	H	-2.89822400	-0.14246400	-2.87462900
O	-0.20817200	0.45553000	-1.75917500	H	-2.25983600	1.57779300	-2.73538700

Model5-TS2-r (HS-AF)

C -4.07505200	-1.13329900	-1.11179800	C -0.65327500	3.04861700	2.83595300
N -3.52425500	-0.07676600	-0.50164400	C 3.82222100	-2.04981700	2.70410500
C -4.53332100	0.87971900	-0.34614700	C 0.07327600	-3.27554200	-2.48120100
C -5.69408900	0.36207100	-0.87211100	H -6.01790800	-1.55003600	-1.79984300
N -5.38125700	-0.90370000	-1.34497500	H -6.68684200	0.78270800	-0.95065200
Fe -1.51201700	-0.10455500	0.02686500	H -3.54563800	-2.03287200	-1.39518400
O -0.08529300	0.74196100	-0.78559700	H 5.24355800	0.92142000	-2.72324400
Fe 1.19648300	0.01469900	0.15657200	H 4.22628500	3.28707900	-2.66663900
O 1.05434200	-1.64208600	-1.04905600	H 3.88992900	-0.72905100	-1.30387900
C -0.02721600	-2.13564900	-1.48955700	H 0.72223700	3.11719600	-1.29771000
O -1.20484700	-1.73099000	-1.17360400	H 1.69793900	3.47289800	0.13960400
C -4.32493600	2.22958000	0.26904700	H 2.02846100	4.32566200	-1.38597900
N 2.63868200	0.97455100	-0.92955900	H 4.69157900	-2.70622300	2.61775300
C 2.70781600	2.30397700	-1.35027900	H 4.06338100	-1.17372000	3.31632100
C 3.81731300	2.42831300	-2.15312700	H 3.00465800	-2.58687900	3.20096900
N 4.40093600	1.17081300	-2.21647700	H -0.70112100	-4.02272700	-2.27988300
C 3.67086000	0.31953200	-1.46964200	H -0.09706300	-2.87673600	-3.48999200
C 1.73127900	3.36607800	-0.95084300	H 1.06581200	-3.73023400	-2.44259100
O -0.28320400	-1.08094700	1.20589000	H -3.96559800	2.14721300	1.29954700
O 0.68626100	1.45806700	1.64789600	H -3.58303000	2.80863200	-0.29497800
C -0.48444600	1.85980900	1.91422500	H -5.26738700	2.78627900	0.26499200
O -1.56356600	1.32141300	1.45538700	H -1.00162100	3.90678500	2.24645200
O 2.42000200	-0.68011600	1.37021600	H -1.42010400	2.83394200	3.58808900
C 3.37192000	-1.61577300	1.31821000	H 0.29390100	3.30170200	3.31755300
O 3.84152400	-2.07078900	0.28408200	H -2.32367500	-2.54173500	3.08998600
C -1.38738200	-3.02922000	2.83127500	H -0.18041900	-0.78034100	2.12622300

H -0.57472900 -3.04988000 3.55204100	H -1.30901500 -3.61159800 1.91992200
Model5-P (HS-AF)	
C 4.05754700 -0.90359500 0.86081300	O -2.00992800 1.88207200 0.35454700
N 3.06012900 -1.01955900 -0.01481600	C 3.58459200 2.38426600 -0.80856500
C 3.33197100 -2.12809600 -0.81318000	C 0.13990700 -0.06209300 4.19785600
C 4.52540900 -2.67257700 -0.39484900	C -1.27243000 4.12894200 0.72028400
N 4.96339300 -1.88547100 0.66126400	C -0.10956400 1.01395900 -3.94978400
Fe 1.35608300 0.19510600 0.05855500	H 5.81300100 -2.02006100 1.19894800
O 0.02571900 -1.01664100 -0.06001500	H 5.08283600 -3.52747700 -0.75125200
Fe -1.46644900 -0.02550600 0.09326500	H 4.13328400 -0.14275700 1.62653700
O -1.19079800 0.53660300 -1.87827600	H -4.72561800 -3.87670800 0.66697900
C -0.07729600 0.72927100 -2.46170700	H -6.26449100 -2.15122400 -0.45507700
O 1.06326600 0.73170700 -1.88193600	H -2.35586600 -2.98455200 0.96822400
C 2.42786900 -2.57327200 -1.92117000	H -4.55254400 1.25087900 -0.36592700
N -3.13882800 -1.20615500 0.04238500	H -4.11965900 0.60068600 -1.95387500
C -4.41054500 -0.89362200 -0.43865800	H -5.79139900 0.45245800 -1.36308400
C -5.22046300 -1.98570900 -0.22914300	H -1.48423400 4.25563900 1.79018200
N -4.42800000 -2.95083200 0.37777400	H -0.40613600 4.74208600 0.45843800
C -3.18495600 -2.44896700 0.52410700	H -2.15716300 4.45761300 0.16649800
C -4.73858600 0.42716700 -1.06506900	H -0.86129500 0.38549900 -4.43732600
O 2.76702100 1.87845400 0.27001000	H -0.40437300 2.06095300 -4.09949000
O -1.07261400 0.02358800 2.13688200	H 0.87469800 0.85851800 -4.39876000
C 0.06882700 0.08994400 2.69170100	H 1.41244600 -2.74255800 -1.54473200
O 1.17565500 0.26802700 2.07421900	H 2.36816300 -1.80839900 -2.70536000
O 0.19116900 2.24721000 0.36038600	H 2.80238300 -3.49969100 -2.36819300
C -1.00157500 2.66459300 0.45418000	H 0.52062400 -1.06507100 4.43185500

H	0.84402100	0.66457900	4.61589100	H	2.07042200	2.53710100	0.47637800
H	-0.84883800	0.05774800	4.64701200	H	2.97399300	2.60672000	-1.69066800
H	4.12164300	3.28069600	-0.47624700	H	4.30661500	1.60240200	-1.05797900
Model5H-Q (HS-FM)							
C	-0.24657100	2.90646600	-0.02746200	N	2.40286700	0.04870200	-1.06593200
O	0.75018500	2.15861800	0.04076900	H	5.11121800	0.92673900	-2.72914500
O	-1.47982100	2.45906600	-0.05522800	H	1.64845500	-1.48444300	-2.37755500
C	-4.82830900	0.40000400	0.16041800	Fe	0.91068800	-0.05924700	0.30020400
C	-5.80610300	-0.54055800	-0.05622400	Fe	-1.73765200	0.58279000	0.02207700
N	-5.15266300	-1.71042700	-0.42059400	O	-0.43866600	-0.07769700	-1.21635100
H	-5.59264400	-2.59621100	-0.65073500	O	-0.55326500	0.03622800	1.33486400
C	-3.82673600	-1.48423700	-0.42296300	C	3.95649500	1.86617300	-0.11612700
N	-3.59203800	-0.20966400	-0.07527900	H	3.10427400	2.44967800	0.23902500
H	-6.88269300	-0.47643900	0.01833700	H	4.42147800	1.37030800	0.74352200
H	-3.06598100	-2.21789500	-0.67256300	H	4.69724200	2.54496300	-0.55203700
C	3.10789000	-0.67000000	2.05855500	C	3.41419600	-0.52212500	3.53894100
O	2.03922100	0.09426600	1.70870000	H	4.33275800	-1.06490800	3.77482300
O	3.73282700	-1.36118400	1.28210300	H	3.51511400	0.53680900	3.80199600
C	0.05235600	-2.91027400	-0.20849400	H	2.57757500	-0.92705500	4.12092700
O	0.93921900	-2.07236600	0.20186900	C	0.19121900	-4.33363000	0.28654300
O	-0.89428600	-2.58799000	-0.98377600	H	1.24223800	-4.63889400	0.25986200
C	3.53669100	0.86033500	-1.14284000	H	-0.13257600	-4.37387800	1.33488500
C	4.19640900	0.53658000	-2.30581600	H	-0.42440300	-5.01231900	-0.30917500
N	3.46486900	-0.47320900	-2.91118500	C	-4.95854800	1.83171900	0.58315200
H	3.68666600	-0.93742600	-3.78543900	H	-4.48676100	2.00208300	1.55978100
C	2.39447500	-0.74056100	-2.14051200	H	-4.48887800	2.50751900	-0.14235400

H	-6.01448000	2.10533800	0.66845800	H	-0.62074300	4.85519300	0.76910700
C	-0.09878500	4.40754000	-0.08508100	H	0.95560400	4.69066800	-0.06889300
H	-0.57744700	4.78593400	-0.99601600	H	-0.63758100	-1.08183600	-1.31132000
Model5H-TS1-r (HS-FM)							
C	0.18381700	-2.82257500	0.17820100	N	-2.42178900	-0.22987700	-1.37720400
O	-0.77372300	-2.01699600	0.23415100	H	-5.01804700	-1.25222100	-3.14936400
O	1.43036300	-2.45043700	0.07889400	H	-1.42966000	0.97786700	-2.85781600
C	4.90054700	-0.44434200	-0.07930200	Fe	-1.08290900	0.08663300	0.21645200
C	5.86589700	0.47335400	-0.41903700	Fe	1.77368500	-0.57490000	-0.05326300
N	5.19316900	1.61710500	-0.82809200	O	0.62770400	0.01926800	-1.34556600
H	5.61921000	2.48099500	-1.14947200	O	0.78403300	0.12370600	1.27967700
C	3.86869300	1.39508000	-0.73866100	C	-4.15817900	-1.75348600	-0.28824900
N	3.65450800	0.15141300	-0.28601600	H	-3.38361600	-2.35937900	0.19303900
H	6.94496000	0.40877700	-0.40511600	H	-4.57620600	-1.07054500	0.45906200
H	3.09778900	2.11425300	-0.99901100	H	-4.95810700	-2.41468600	-0.63791300
C	-3.23455500	0.77887300	2.06882500	C	-3.47165200	0.85940700	3.56607400
O	-2.15070200	0.05264600	1.74139600	H	-4.38937600	1.41718600	3.76706300
O	-3.95875100	1.29766200	1.23516400	H	-3.54643700	-0.15014300	3.98825900
C	-0.17212600	2.89012000	-0.54709600	H	-2.62349800	1.35864700	4.05105900
O	-0.98198900	2.02506800	-0.03268700	C	-0.46331500	4.34021300	-0.22439000
O	0.80644500	2.57811600	-1.27713800	H	-1.52342900	4.55156000	-0.40184100
C	-3.59706600	-0.97808200	-1.43942900	H	-0.27495200	4.51419900	0.84269200
C	-4.12274700	-0.84165400	-2.70414100	H	0.16609900	5.00384900	-0.82200900
N	-3.26215000	-0.00343200	-3.39739500	C	5.05156800	-1.84621600	0.42815900
H	-3.36336700	0.30168700	-4.35909200	H	4.63603200	-1.95096700	1.43894700
C	-2.25356100	0.34014400	-2.56938700	H	4.53778700	-2.56321900	-0.22441400

H	6.10939800	-2.12264600	0.46962000	H	1.63069000	-0.03397700	4.18417600
C	-0.06042400	-4.31151700	0.21419600	H	0.76743100	0.28108900	2.58122400
H	0.58397300	-4.77467300	0.96954700	H	-0.19736700	-0.10074700	4.08910800
H	-1.11040200	-4.52319800	0.42588900	H	0.66925500	1.50593300	3.95502300
H	0.21438700	-4.73999000	-0.75788500	H	0.73153900	1.03044000	-1.46704200
C	0.71518600	0.42503200	3.80143400				

Model5H-**IM**-n(HS-FM)

C	-0.21579700	-2.75820100	-0.08870800	N	2.79363200	0.25727700	3.58747500
O	0.78353100	-2.01748600	-0.15300800	H	2.76417600	0.65104300	4.52135700
O	-1.44258100	-2.34422200	-0.29959600	C	1.94787000	0.56274300	2.58068200
C	-4.69247100	-0.26435600	0.54193500	N	2.26741000	-0.12476300	1.48561200
C	-5.51234600	0.72574400	1.03238000	H	4.49652600	-1.07840000	3.73213300
N	-4.82243100	1.91772800	0.88231000	H	1.12846000	1.26256900	2.67277300
H	-5.14329000	2.83859000	1.16488300	Fe	1.18372800	0.10710900	-0.30854900
C	-3.62245300	1.65609600	0.32836800	Fe	-1.79044500	-0.50050500	-0.61001700
N	-3.51329100	0.34166900	0.10195100	O	-0.72301500	0.21038900	0.76023200
H	-6.50008300	0.67579600	1.46907800	O	-0.41131800	0.13663200	-1.73191700
H	-2.85161800	2.39877700	0.15238700	C	4.06464900	-1.81088600	0.82222400
C	3.55841800	0.40119600	-1.98771600	H	3.34380900	-2.44306600	0.29326500
O	2.38680200	-0.19454600	-1.71107100	H	4.60714300	-1.21344900	0.08174800
O	4.24818400	0.93793200	-1.13474000	H	4.78162000	-2.45226900	1.34560800
C	0.39937900	3.00747600	0.06649800	C	3.93866900	0.31912800	-3.45539800
O	1.22793200	2.05848000	-0.22755900	H	4.93342100	0.74466000	-3.60778800
O	-0.71097100	2.81019700	0.62500600	H	3.91925300	-0.72470300	-3.79089100
C	3.37451200	-0.91152200	1.80002600	H	3.20637800	0.87216500	-4.05737500
C	3.70416700	-0.67717600	3.11605500	C	0.84568900	4.40608200	-0.30348300

H	1.87047400	4.57170400	0.04639400	H	-0.64401900	-4.82855700	-0.47293700
H	0.86092500	4.49785500	-1.39699900	H	0.97176700	-4.51767600	0.25117400
H	0.16967600	5.15356500	0.11864300	C	-2.84972900	-0.87817400	-2.37146100
C	-4.94394100	-1.74195200	0.48179000	H	-3.74955500	-1.39659400	-2.03900900
H	-5.27154300	-2.06192800	-0.51614300	H	-0.24312600	-0.17986000	-2.63479200
H	-4.04321900	-2.30954900	0.74242800	H	-2.18039000	-1.51679300	-2.95035800
H	-5.73405000	-2.01575100	1.18790300	H	-3.03711500	0.10147900	-2.81483200
C	-0.08026100	-4.22507300	0.24663500	H	-0.80980800	1.21347400	0.86658600
H	-0.51505000	-4.40393000	1.23830800				

Model5H-**IM**-r(HS-FM)

C	0.18140100	-2.76608700	-0.4074650	O	0.85836400	2.82385700	-0.7029160
O	-0.77007000	-1.98426800	-0.1905210	C	-3.59086600	-0.64168800	-1.6236760
O	1.43490900	-2.38971600	-0.4072680	C	-4.10892200	-0.27225900	-2.8441270
C	4.91378600	-0.37617600	-0.1638570	N	-3.24501800	0.68058900	-3.3636370
C	5.86962900	0.60502200	-0.27609400	H	-3.34132400	1.16074000	-4.2515190
N	5.18530500	1.80561700	-0.4119770	C	-2.24263000	0.86448100	-2.4791260
H	5.60241800	2.72504600	-0.5206720	N	-2.41765300	0.08276600	-1.4149030
C	3.86329500	1.55643000	-0.38332700	H	-5.00131300	-0.59234800	-3.3632680
N	3.66175400	0.23905500	-0.2326020	H	-1.41762300	1.54496200	-2.6364360
H	6.94928800	0.54992800	-0.2715930	Fe	-1.08506000	0.10551700	0.2157480
H	3.08419600	2.30793000	-0.4741830	Fe	1.78926100	-0.53162900	-0.1814880
C	-3.21528200	0.39159600	2.18559800	O	0.64446300	0.32486700	-1.3281570
O	-2.13194900	-0.25683600	1.7193670	O	0.74676200	-0.06080900	1.3067950
O	-3.95693700	1.04106500	1.4667670	C	-4.15793900	-1.61832800	-0.6407830
C	-0.14391400	2.98756800	0.04054600	H	-3.39081600	-2.31879600	-0.2945020
O	-0.99159800	2.04822700	0.3110590	H	-4.55906300	-1.08732800	0.2290040

H	-4.97080100	-2.18594400	-1.1058540	H	6.13953300	-2.12327100	-0.0055700
C	-3.42744600	0.20897400	3.67770000	C	-0.06704100	-4.22512500	-0.7019830
H	-4.33695800	0.72789700	3.9893900	H	0.62979800	-4.84892200	-0.1324470
H	-3.50735600	-0.85859200	3.9172110	H	-1.10083100	-4.49180700	-0.4723750
H	-2.56699900	0.60924000	4.2284470	H	0.12642400	-4.40499400	-1.7675260
C	-0.42577200	4.33106300	0.67804400	C	0.45610500	-1.42798100	4.03627700
H	-1.48050000	4.59257300	0.5410080	H	1.03899000	-2.34061400	3.9317720
H	-0.24996000	4.25503000	1.7588400	H	0.71558800	-0.51566400	2.1823230
H	0.22079100	5.10355300	0.25492200	H	-0.59565700	-1.43143900	3.7596030
C	5.07860500	-1.85594100	0.00513600	H	0.84269500	-0.62369300	4.6581260
H	4.65477400	-2.19738900	0.9585980	H	0.76352600	1.33330800	-1.2571980
H	4.58162100	-2.40707400	-0.8032010				

Model5H-TS2-r(HS-FM)

C	-0.10146800	2.88197500	0.41703900	O	3.79329400	-1.40156300	1.35248200
O	0.81665600	2.02931300	0.41306700	C	0.14562100	-2.80779500	-0.82896700
O	-1.36581600	2.56998000	0.33021700	O	0.93804400	-2.01077900	-0.18259900
C	-4.89212000	0.55183600	-0.01695000	O	-0.82073000	-2.41075700	-1.52807100
C	-5.85463200	-0.32678600	-0.45581100	C	3.71146800	1.01653000	-1.24946300
N	-5.17725800	-1.41970700	-0.97741400	C	4.28913500	0.97295400	-2.49801100
H	-5.59886100	-2.24544000	-1.39111600	N	3.43258400	0.23363000	-3.30048500
C	-3.85246600	-1.20459100	-0.85613500	H	3.56685700	0.01262400	-4.28105900
N	-3.64333700	-0.01535400	-0.27562400	C	2.37605400	-0.14353500	-2.55096200
H	-6.93388200	-0.26577200	-0.44075200	N	2.51020000	0.31067700	-1.30527900
H	-3.08021400	-1.89215200	-1.18821700	H	5.21699100	1.38761600	-2.86612000
C	3.04526100	-0.88509000	2.16910100	H	1.54346500	-0.71996800	-2.93047700
O	1.97978100	-0.14789900	1.81961800	Fe	1.07635600	-0.09414900	0.17243700

Fe	-1.76746600	0.72350000	0.01352800	C	-5.04869900	1.89178300	0.63594800
O	-0.53366000	0.15457500	-1.25854600	H	-4.64218000	1.88714700	1.65591000
O	-0.83582400	-0.18834600	1.40483300	H	-4.53089300	2.67527100	0.06801800
C	4.24062500	1.66665100	-0.00928500	H	-6.10675700	2.16358100	0.69830700
H	3.46748200	2.27056400	0.47733900	C	0.21325800	4.35428200	0.52200200
H	4.58052600	0.90416000	0.69954900	H	-0.41455300	4.81623900	1.29168800
H	5.08911100	2.31238700	-0.25856800	H	1.27082300	4.50693700	0.74673600
C	3.23523900	-0.98820200	3.67231900	H	-0.03271600	4.83646900	-0.43272900
H	4.12702400	-1.57831400	3.89635200	C	-0.98514800	-2.22181500	2.77008100
H	3.33213000	0.01528600	4.10465700	H	-1.91821300	-2.54465300	2.31967900
H	2.35546600	-1.45751000	4.13014400	H	-0.62361600	0.24764800	2.24864100
C	0.44937500	-4.28522400	-0.69172400	H	-1.00480700	-1.77533800	3.76089200
H	1.51938200	-4.45949000	-0.84810100	H	-0.04138500	-2.54060400	2.34297500
H	0.21734700	-4.60787700	0.33151200	H	-0.70444300	-0.80249300	-1.54132000
H	-0.14353500	-4.86820100	-1.40053100				

Model5H-P(HS-FM)

C	0.20507500	-2.39024900	0.83583400	H	3.53507500	0.34118400	-2.90064600
O	-0.85950800	-1.71015300	0.69621800	C	-1.65891300	0.74191200	2.59640000
O	1.37696100	-1.94749000	0.60202700	O	-0.54845600	0.94981200	1.98616100
C	4.89313900	-0.67547800	-0.13152400	O	-2.60254500	0.22320700	1.92180000
C	5.97812300	-0.63243400	-0.97744300	C	-1.49765100	2.95873000	-0.94563900
N	5.49685900	-0.20029900	-2.20434600	O	-2.08806300	1.95116300	-0.36539100
H	6.04264700	-0.06302600	-3.04866200	O	-0.36577800	2.88509500	-1.47255300
C	4.16658900	0.00380000	-2.08823100	C	-3.94930800	-1.64884500	-0.83586000
N	3.76480200	-0.27096000	-0.84657900	C	-4.62204000	-1.89792700	-2.01152300
H	7.02025100	-0.86949600	-0.81462200	N	-4.00899600	-1.12199100	-2.98462000

H -4.26736200 -1.07042000 -3.96393000	H -3.28325700 4.08335000 -1.35609800
C -3.00474800 -0.43299300 -2.40053400	H -2.40803700 4.60458800 0.08348400
N -2.93808500 -0.72775100 -1.10371800	H -1.75891900 5.01751100 -1.53406900
H -5.46516700 -2.53937400 -2.22644400	C 4.82685400 -1.08176200 1.30977100
H -2.35743300 0.25642400 -2.92677600	H 4.45737600 -0.25926400 1.93503500
Fe -1.49042100 0.15575900 0.15871600	H 4.15012800 -1.93500600 1.44335500
Fe 1.82645900 -0.15395200 -0.12401500	H 5.81905400 -1.36916600 1.67137100
O 0.14616300 0.40035600 -0.91994700	C 0.06370500 -3.82227400 1.30933000
O 2.01125400 1.30082000 1.37080300	H -0.51944900 -4.38929600 0.57346400
C -4.21154800 -2.21574800 0.52552100	H 1.04188800 -4.28965900 1.44185900
H -3.31785900 -2.71538400 0.91521500	H -0.49388300 -3.84186700 2.25287600
H -4.47885700 -1.42407900 1.23408500	C 2.39490700 2.67443000 1.11726200
H -5.03207100 -2.93907400 0.47866400	H 2.47632700 3.21391000 2.06766600
C -1.84378600 1.12610700 4.03860700	H 1.13597100 1.29051500 1.83449000
H -2.64579500 0.53659600 4.49065500	H 1.66775900 3.16863900 0.46137800
H -0.90932100 0.99987700 4.59403400	H 3.37555200 2.65293800 0.63390000
H -2.12726700 2.18615700 4.08377900	H 0.08310300 1.34972700 -1.26175800
C -2.28035100 4.25627200 -0.94908200	

Model5H-Q(HS-AF)

C -0.24542400 2.90967900 -0.05468100	C -3.82249900 -1.48331200 -0.39438000
O 0.74635900 2.15695300 0.01739100	N -3.58776100 -0.20450900 -0.06345100
O -1.48161400 2.46749400 -0.09369600	H -6.87722100 -0.47493400 0.05373800
C -4.82344700 0.40639200 0.17225400	H -3.06284100 -2.21907600 -0.64111600
C -5.80101000 -0.53836600 -0.02669500	C 3.12134300 -0.64566200 2.05255600
N -5.14800800 -1.71156100 -0.38069100	O 2.02759700 0.08977200 1.72634300
H -5.58806600 -2.60056200 -0.59799300	O 3.72015500 -1.36296900 1.27841700

C	0.05419800	-2.92803900	-0.20431100	H	4.67160400	2.55691100	-0.56025200
O	0.93187200	-2.08552500	0.21531600	C	3.49150300	-0.43874300	3.51213500
O	-0.89184100	-2.60871700	-0.98211600	H	4.43346000	-0.95105000	3.72261400
C	3.52506400	0.85863600	-1.14076800	H	3.57655100	0.63053500	3.73584100
C	4.18197900	0.53786000	-2.30624400	H	2.69410300	-0.84484800	4.14607900
N	3.45502900	-0.47814600	-2.90634200	C	0.20382200	-4.35325800	0.28098000
H	3.67581900	-0.94228300	-3.78081800	H	1.25758400	-4.64887600	0.25524200
C	2.39041700	-0.75157000	-2.12920200	H	-0.12238400	-4.40382300	1.32811400
N	2.39766300	0.03915900	-1.05583900	H	-0.40428000	-5.03264700	-0.32154500
H	5.09219200	0.93356400	-2.73432900	C	-4.95334500	1.84302400	0.57806000
H	1.64909900	-1.50149000	-2.36204800	H	-4.47796300	2.02573100	1.55071600
Fe	0.89894400	-0.07889100	0.31384600	H	-4.48720900	2.51035800	-0.15748300
Fe	-1.73688100	0.59380200	0.01350500	H	-6.00920100	2.11665700	0.66418800
O	-0.45594500	-0.10762400	-1.21456200	C	-0.09308900	4.41058600	-0.10650700
O	-0.56324300	0.04191400	1.30291300	H	-0.57928800	4.79593300	-1.01040100
C	3.94423400	1.86822800	-0.11728100	H	-0.60485800	4.85560500	0.75532300
H	3.08885000	2.44049400	0.24809000	H	0.96253100	4.68946500	-0.09817500
H	4.42587400	1.37733700	0.73622700	H	-0.65564700	-1.11843100	-1.29443800
Model5H-TS1(HS-AF)							
C	0.20344000	-2.81952400	0.03959200	C	3.87120100	1.45351500	-0.65254200
O	-0.75203700	-2.01503700	0.13529400	N	3.66979800	0.18194600	-0.27990000
O	1.45054300	-2.44470700	-0.04045200	H	6.95655700	0.46254200	-0.43907000
C	4.92121900	-0.41997400	-0.13460900	H	3.09368500	2.18519600	-0.85072800
C	5.87719500	0.52268100	-0.43005100	C	-3.22910500	0.63583800	2.08770600
N	5.19322200	1.68753600	-0.75084600	O	-2.13554300	-0.05928800	1.72847200
H	5.61026600	2.57290400	-1.02145100	O	-3.96233800	1.18011200	1.27785000

C	-0.20408600	2.93453100	-0.35318000	H	-3.51037500	-0.37634100	3.97090800
O	-1.01353800	2.03775500	0.10435900	H	-2.63563000	1.15809800	4.09087900
O	0.77914600	2.66840800	-1.09598100	C	-0.49815500	4.36164700	0.05533700
C	-3.59290700	-0.89985000	-1.52168800	H	-1.56429700	4.57313600	-0.07924400
C	-4.11898200	-0.68509600	-2.77532200	H	-0.27821200	4.47796200	1.12438200
N	-3.26328400	0.20123900	-3.41263700	H	0.11021500	5.06246100	-0.52133200
H	-3.36612900	0.56679600	-4.35286800	C	5.08604800	-1.85087700	0.27877400
C	-2.25682000	0.49646400	-2.56367400	H	4.69034500	-2.02137500	1.28861500
N	-2.42241100	-0.15013400	-1.41068800	H	4.56189700	-2.52685800	-0.40845000
H	-5.01151700	-1.07152200	-3.24689500	H	6.14523200	-2.12518200	0.28239500
H	-1.43641600	1.15685700	-2.80855600	C	-0.04408700	-4.30764200	0.00062900
Fe	-1.08236800	0.08372900	0.19498300	H	0.60536500	-4.81144100	0.72493200
Fe	1.79542600	-0.56354600	-0.05278100	H	-1.09292100	-4.52802700	0.20926600
O	0.60397900	0.12961700	-1.26061900	H	0.22145800	-4.68533900	-0.99490200
O	0.85498900	0.09932900	1.31372000	C	0.56333300	-0.01620400	3.82423800
C	-4.14761300	-1.75295600	-0.42370400	H	1.41558100	-0.59599700	4.18832300
H	-3.37125800	-2.39367400	0.00740800	H	0.72411400	0.03829600	2.58761500
H	-4.55684900	-1.12301100	0.37325400	H	-0.40155500	-0.51353100	3.93431500
H	-4.95242900	-2.38545200	-0.81288100	H	0.56802200	1.02800500	4.14546700
C	-3.46753400	0.65019800	3.58700600	H	0.71538600	1.14941300	-1.33164600
H	-4.40181800	1.17116800	3.80929000				

Model5H-**IM**-n(HS-AF)

C	-0.21733200	-2.75781000	-0.10871100	C	-5.50706400	0.74178500	1.04590300
O	0.78329400	-2.01735600	-0.17070800	N	-4.81374500	1.93088900	0.88938400
O	-1.44434500	-2.34056300	-0.30319600	H	-5.12969900	2.85352700	1.17167600
C	-4.69347300	-0.25244100	0.55315300	C	-3.61772000	1.66349200	0.32961200

N	-3.51452400	0.34821600	0.10557900	H	4.79379100	-2.44905900	1.33881200
H	-6.49249600	0.69637600	1.48825800	C	3.89053100	0.37072600	-3.47325500
H	-2.84544900	2.40313300	0.14764900	H	4.87643700	0.80796400	-3.64828300
C	3.55925100	0.41343500	-1.99229200	H	3.86838200	-0.66507000	-3.83279900
O	2.39749300	-0.19051100	-1.69157500	H	3.13414400	0.93147700	-4.03709600
O	4.27718400	0.92604200	-1.14818400	C	0.86933700	4.39840600	-0.28343200
C	0.42057500	2.99810900	0.07648700	H	1.89725100	4.55740200	0.06006700
O	1.24730400	2.04969800	-0.22213900	H	0.87606000	4.50024100	-1.37617800
O	-0.69188600	2.79928000	0.63142500	H	0.19876400	5.14413500	0.15034900
C	3.37498400	-0.92213900	1.80255300	C	-4.95089700	-1.72923400	0.49825100
C	3.70301700	-0.69444100	3.12020400	H	-5.29441600	-2.04877600	-0.49442100
N	2.78817100	0.23306900	3.59704300	H	-4.04836900	-2.29961800	0.74618600
H	2.75645500	0.62064000	4.53344400	H	-5.73138700	-1.99972700	1.21625900
C	1.94150800	0.54110300	2.59173600	C	-0.07896100	-4.22947800	0.20321600
N	2.26456300	-0.13819000	1.49257200	H	-0.53015700	-4.42950000	1.18331400
H	4.49670600	-1.09614800	3.73424900	H	-0.62720600	-4.82218800	-0.53725100
H	1.11902900	1.23688800	2.68765300	H	0.97433400	-4.51696500	0.21884600
Fe	1.18231400	0.09710800	-0.30347800	C	-2.87061400	-0.89633200	-2.35572900
Fe	-1.79663900	-0.49518100	-0.61475300	H	-3.75943800	-1.43135800	-2.02011900
O	-0.71300900	0.20958300	0.73796700	H	-0.28433100	-0.13850800	-2.65130500
O	-0.42930300	0.16068400	-1.73847700	H	-2.19199400	-1.52333700	-2.93697000
C	4.06865200	-1.81332800	0.81980400	H	-3.07830500	0.07888300	-2.80015000
H	3.35113800	-2.45118200	0.29296500	H	-0.79423900	1.21628000	0.84321000
H	4.60156600	-1.20944900	0.07768200				
Model5H- IM -r(HS-AF)							
C	0.19931700	-2.76206500	-0.42460400	O	-0.75427700	-1.98401800	-0.20240900

O	1.45125700	-2.38113800	-0.42363900	O	0.76515200	-0.05952300	1.32268400
C	4.92353400	-0.36075200	-0.18112300	C	-4.15188000	-1.62041900	-0.68131000
C	5.87488200	0.62544000	-0.28870100	H	-3.38463600	-2.32368600	-0.34095000
N	5.18514100	1.82497900	-0.40389400	H	-4.55717600	-1.10135000	0.19362700
H	5.59798000	2.74729900	-0.50405900	H	-4.96159200	-2.18360600	-1.15717500
C	3.86428000	1.57022300	-0.36780400	C	-3.41383600	0.18225300	3.66479700
N	3.66888000	0.25049300	-0.23216900	H	-4.31829100	0.70302700	3.98791900
H	6.95473400	0.57435500	-0.29340100	H	-3.49215700	-0.88454800	3.90843100
H	3.08234700	2.32046700	-0.44205900	H	-2.54490200	0.58241600	4.20201100
C	-3.22331300	0.35990600	2.16930700	C	-0.46573500	4.32713700	0.74055200
O	-2.14217100	-0.28292900	1.68994800	H	-1.52399900	4.57854400	0.61270100
O	-3.97961400	1.00053000	1.45799000	H	-0.28076500	4.24643900	1.81948800
C	-0.17451100	2.99038300	0.09365200	H	0.17023000	5.10837500	0.31746600
O	-1.01376400	2.04251800	0.35868600	C	5.09505400	-1.84183800	-0.03167200
O	0.82894500	2.84022800	-0.65206500	H	4.67934700	-2.19660100	0.92051200
C	-3.58278500	-0.62994600	-1.64897100	H	4.59429400	-2.38481400	-0.84318700
C	-4.09649400	-0.24581500	-2.86678600	H	6.15685400	-2.10503700	-0.05313000
N	-3.23153700	0.71416600	-3.37126500	C	-0.04487100	-4.22015000	-0.72633600
H	-3.32504300	1.20516500	-4.25350900	H	0.65008600	-4.84483300	-0.15538100
C	-2.23248600	0.88764700	-2.48091600	H	-1.07931200	-4.48965600	-0.50314800
N	-2.41095400	0.09271900	-1.42696600	H	0.15505600	-4.39567900	-1.79140200
H	-4.98636300	-0.56057300	-3.39347500	C	0.39040100	-1.53699000	4.02160900
H	-1.40700300	1.57032300	-2.62663400	H	0.96528000	-2.45380500	3.91037300
Fe	-1.07880100	0.10118300	0.20504100	H	0.72174600	-0.53744600	2.18375400
Fe	1.79897100	-0.52538900	-0.16759800	H	-0.64631900	-1.51229600	3.69398900
O	0.63140200	0.35374100	-1.27290000	H	0.76048500	-0.75996000	4.68660500

H 0.74917500 1.36499200 -1.18934300

Model5H-TS2-r(HS-AF)

C -0.12782300 2.86808500 0.49428100

O 0.79366700 2.01851600 0.46788300

O -1.39044200 2.55364200 0.40301100

C -4.90301100 0.54812200 -0.03369000

C -5.86084300 -0.32352100 -0.49646900

N -5.17821600 -1.41344600 -1.01709100

H -5.59524400 -2.23397700 -1.44542100

C -3.85483300 -1.20289300 -0.87200400

N -3.65190700 -0.02010900 -0.27716900

H -6.94000800 -0.25939100 -0.49843500

H -3.07960400 -1.88954300 -1.19849500

C 3.07036900 -0.92224600 2.13196200

O 2.01112300 -0.17378800 1.78718400

O 3.83137800 -1.41368200 1.31214500

C 0.18786100 -2.80067800 -0.86408300

O 0.97554700 -2.00865800 -0.20682100

O -0.79100700 -2.39994200 -1.54463900

C 3.69862100 1.06865900 -1.25206100

C 4.25736000 1.07173200 -2.50997900

N 3.38778100 0.36423000 -3.32709600

H 3.50711600 0.18072200 -4.31731900

C 2.34176200 -0.03982400 -2.57702400

N 2.49567200 0.36639900 -1.31690400

H 5.17982300 1.49989200 -2.87619200

H 1.50183200 -0.59971900 -2.96520700

Fe 1.08017000 -0.08991300 0.16087900

Fe -1.77775300 0.70666400 0.05758300

O -0.53541000 0.14421200 -1.20666300

O -0.85011300 -0.23069700 1.42599300

C 4.24549900 1.67367200 0.00309600

H 3.47996900 2.26137700 0.52084700

H 4.59294800 0.88628300 0.68028500

H 5.09168100 2.32666000 -0.23489300

C 3.23698300 -1.06954200 3.63415300

H 4.12072400 -1.67287400 3.85481300

H 3.33582300 -0.07911900 4.09532900

H 2.34663400 -1.54342300 4.06599900

C 0.51087500 -4.27674900 -0.76446700

H 1.58189300 -4.43366900 -0.93157900

H 0.28916500 -4.62612500 0.25222600

H -0.07963700 -4.84998300 -1.48313300

C -5.06662600 1.88220400 0.62942000

H -4.68233600 1.86509400 1.65784500

H -4.53217300 2.66830600 0.08091500

H -6.12433800 2.15921200 0.67166500

C 0.18327600 4.33828800 0.63352500

H -0.44394900 4.77994800 1.41551300

H 1.24096800 4.48829200 0.85944800

H	-0.06624600	4.84267500	-0.30874300	H	-0.96139300	-1.90289800	3.74438800
C	-0.94292000	-2.31941900	2.74062100	H	0.00287500	-2.59781500	2.29049000
H	-1.87391900	-2.64487000	2.28791400	H	-0.69939500	-0.81422600	-1.50223200
H	-0.64662200	0.18192500	2.28336400				

Model5H-P(HS-AF)

C	0.20923200	-2.38016100	0.89042100	C	-2.94851000	-0.45039100	-2.42643400
O	-0.85796500	-1.71074200	0.72215600	N	-2.90163700	-0.73923800	-1.12737400
O	1.38185200	-1.93483100	0.66213500	H	-5.41776500	-2.54836700	-2.27837800
C	4.88282200	-0.65458400	-0.14020700	H	-2.29185500	0.23484600	-2.94656800
C	5.96617300	-0.60833200	-0.98818300	Fe	-1.48306500	0.15327200	0.16021400
N	5.47806100	-0.19867900	-2.21984800	Fe	1.81374100	-0.16353000	-0.12876500
H	6.02108800	-0.06474900	-3.06644100	O	0.14747800	0.41594900	-0.88915700
C	4.14506100	-0.01124600	-2.10468400	O	1.99907100	1.28263400	1.38037600
N	3.74823200	-0.27452900	-0.85901900	C	-4.20332800	-2.21628300	0.48983700
H	7.01146600	-0.82967900	-0.82352700	H	-3.31842000	-2.72146500	0.89228600
H	3.50875700	0.30762800	-2.92080100	H	-4.47321100	-1.42033400	1.19252200
C	-1.69147100	0.75269000	2.59135300	H	-5.02862200	-2.93356800	0.43477000
O	-0.57259700	0.95660100	1.99460500	C	-1.89461000	1.14839500	4.02810600
O	-2.62595700	0.22864700	1.90876800	H	-2.70449200	0.56485200	4.47380200
C	-1.50518700	2.94882200	-0.94893300	H	-0.96806600	1.02354200	4.59698100
O	-2.10031800	1.95275400	-0.35969900	H	-2.17500500	2.20969400	4.06137900
O	-0.36636200	2.86567400	-1.46526400	C	-2.28084000	4.24975600	-0.98018100
C	-3.91973700	-1.65587100	-0.86992500	H	-3.28827700	4.07232900	-1.37343800
C	-4.57603100	-1.90828400	-2.05413600	H	-2.39664200	4.62470600	0.04450700
N	-3.94648700	-1.13882800	-3.02178300	H	-1.75985600	4.99344100	-1.58772000
H	-4.19061800	-1.09099700	-4.00493700	C	4.82468100	-1.04347400	1.30627800

H	4.44846100	-0.21743600	1.92268200	C	2.40814600	2.65096300	1.14493800
H	4.15670300	-1.90141900	1.45274600	H	2.49717800	3.17846500	2.10148300
H	5.82089400	-1.31651000	1.66801700	H	1.12253000	1.28165300	1.84013100
C	0.07147300	-3.80202600	1.39421200	H	1.69181300	3.16659900	0.49347000
H	-0.50499400	-4.38799300	0.66802700	H	3.38907000	2.61768000	0.66274400
H	1.05093400	-4.26167900	1.54330000	H	0.07697600	1.37401000	-1.22938700
H	-0.49163400	-3.80298500	2.33473100				

Model5H*-Q(HS-FM)

C	0.48277400	-1.85035000	1.45592400	C	-3.70366200	-2.40805300	-2.36960900
O	-0.63087800	-1.51965500	0.98601400	N	-3.05807800	-1.55704700	-3.25495200
O	1.57399400	-1.17190900	1.28582900	H	-3.13685700	-1.56864400	-4.26621100
C	4.34457300	-1.07907800	-0.79386500	C	-2.31238800	-0.69076900	-2.53693400
C	5.66247800	-0.82323000	-1.09062800	N	-2.44080000	-0.94308000	-1.23432100
N	5.90492600	0.48917500	-0.70780000	H	-4.37279100	-3.19019900	-2.69989900
H	6.78522700	0.98760600	-0.79389600	H	-1.70631900	0.09247600	-2.97385500
C	4.77027300	1.00469400	-0.20230700	Fe	-1.45639800	0.24032300	0.21390500
N	3.80300000	0.08128200	-0.23442700	Fe	1.92939800	0.47784100	0.39555500
H	6.42513100	-1.44964400	-1.53196400	O	0.39425200	0.62646700	-0.59334500
H	4.65357300	2.01351500	0.17090300	O	2.25220200	2.03237200	0.68671600
C	-2.15306900	0.81053800	2.48118800	C	-3.73422100	-2.59641100	0.21232000
O	-0.97450900	1.09325300	2.07656100	H	-2.86274400	-2.93918300	0.78105500
O	-2.91028200	0.18002600	1.65859000	H	-4.24817700	-1.84418500	0.82054100
C	-1.50242800	2.86303300	-1.23895900	H	-4.40899700	-3.44377500	0.05393300
O	-2.08482500	1.88622800	-0.59690800	C	-2.64797700	1.21362800	3.83976400
O	-0.31999300	2.79847500	-1.64047600	H	-3.21459600	0.39255900	4.29153800
C	-3.31575200	-2.02156800	-1.10607100	H	-1.81437200	1.51128900	4.48074100

H	-3.33284000	2.06384400	3.72431200	H	2.67003800	-2.15360400	-1.61636600
C	-2.34293000	4.09706800	-1.47005700	H	4.18341500	-3.07574300	-1.53368200
H	-3.34334700	3.81626500	-1.81613200	C	0.61615700	-3.12077500	2.26374400
H	-2.46192600	4.62278700	-0.51378300	H	1.10000400	-2.89457000	3.22076700
H	-1.85453600	4.76128400	-2.18678300	H	-0.36165600	-3.57661800	2.43221700
C	3.56564100	-2.33976500	-1.00996600	H	1.26556000	-3.82575000	1.72970100
H	3.24634900	-2.77023800	-0.05426200	H	0.25203700	1.55011800	-1.05546500
Model5H*-TS1-r(HS-FM)							
C	-0.21316100	-0.35369400	-2.5488060	C	3.61121200	-3.47576800	0.25030100
O	0.82624400	-0.36523100	-1.8415390	N	2.82595800	-3.49042900	1.3938180
O	-1.38414600	-0.02250000	-2.1174510	H	2.81042000	-4.21495500	2.1034200
C	-3.87454200	-1.87923200	0.1865970	C	2.09180200	-2.35693600	1.41322100
C	-5.18372100	-2.07299700	0.5601380	N	2.36129500	-1.61543100	0.3394200
N	-5.73952900	-0.80917300	0.7084880	H	4.29930100	-4.27363900	0.0083610
H	-6.69585900	-0.60212600	0.9788500	H	1.39327900	-2.10128500	2.1998650
C	-4.79426000	0.10984300	0.43398900	Fe	1.43148000	0.27240100	0.05149000
N	-3.65061800	-0.50437000	0.1143960	Fe	-1.94358900	0.49853200	-0.3469880
H	-5.75005500	-2.97861200	0.7268170	O	-0.46366700	-0.05536700	0.6822350
H	-4.93723200	1.18210600	0.4660380	O	-2.58873500	2.10234000	-0.2605100
C	2.38450100	2.26494100	-0.99912500	C	3.90229200	-1.78090900	-1.6845820
O	1.15585300	2.24384200	-0.6408570	H	3.11364800	-1.57682400	-2.4170120
O	3.06117000	1.19437700	-0.8142230	H	4.43993200	-0.84194100	-1.5138450
C	1.22859900	0.90432700	2.98103300	H	4.59692700	-2.51523000	-2.1051120
O	1.89260600	0.83935000	1.86275600	C	3.01779500	3.49607200	-1.58240500
O	0.06399100	0.46164000	3.11179300	H	3.78712400	3.21819400	-2.3090770
C	3.31886200	-2.30090600	-0.4067350	H	2.26086100	4.13780700	-2.0417670

H	3.50505600	4.05436000	-0.7719150	H	-0.20592600	0.18948300	-4.6078180
C	1.94979400	1.55905700	4.13861200	H	0.82681900	-1.21599500	-4.2308730
H	2.96267300	1.15185400	4.23035600	H	-0.96606500	-1.37273200	-4.2894460
H	2.04836900	2.63245900	3.93203300	H	-0.41607300	0.11621300	1.6966930
H	1.39066100	1.41816000	5.06653100	C	-1.54945600	4.40586200	0.18271800
C	-2.81169100	-2.88858100	-0.1218100	H	-2.07115000	3.35188500	-0.0223610
H	-2.52664800	-2.84557400	-1.1808320	H	-1.98346400	5.09182200	-0.5499480
H	-1.91214500	-2.70533400	0.4786600	H	-1.79871400	4.66860900	1.2144660
H	-3.17289600	-3.89903000	0.0926700	H	-0.48428100	4.21957800	0.0260840
C	-0.12569500	-0.72862800	-4.0112010				

Model5H*-**TS1**-n(HS-FM)

C	-0.44769600	1.19248400	1.99205200	O	2.11656200	-1.51026900	-1.25419300
O	0.70043900	1.03001800	1.51091500	O	0.48377400	-1.53348700	-2.79588800
O	-1.50715000	0.56106600	1.61435400	C	3.28201400	2.36341900	-0.37703600
C	-4.12923500	1.49700600	-0.28794400	C	3.58378000	3.20345900	-1.42578600
C	-5.31737900	1.55151500	-0.98044700	N	2.88812400	2.72152800	-2.52528600
N	-5.52710900	0.28405100	-1.50031800	H	2.89932700	3.11041000	-3.46201300
H	-6.31384500	-0.01209800	-2.06879800	C	2.19640900	1.62772100	-2.13988000
C	-4.49570500	-0.50012600	-1.13200500	N	2.40948100	1.38305900	-0.84681100
N	-3.62809600	0.19601500	-0.38972100	H	4.22331200	4.07336800	-1.47895100
H	-6.00717300	2.36829800	-1.14140700	H	1.56603700	1.04432700	-2.79980500
H	-4.38236500	-1.53848900	-1.41179800	Fe	1.52248700	-0.27724900	0.11979400
C	2.36092300	-1.63055600	1.98566500	Fe	-1.87637000	-0.76041700	0.26649900
O	1.16263800	-1.79694500	1.57328200	O	-0.33164200	-0.30494900	-0.69109700
O	3.05022300	-0.71139700	1.41760600	O	-2.26664000	-2.17213200	-0.58627500
C	1.58495400	-1.93977200	-2.36708300	C	3.77664200	2.41895900	1.03579100

H	2.93784200	2.48360900	1.73785400	H	-2.44723500	2.79490500	0.04734000
H	4.34502300	1.51660400	1.28658800	H	-4.03732100	3.53870400	0.31324900
H	4.42191800	3.29252000	1.17353200	C	-0.64470100	2.21579300	3.09159900
C	2.95805300	-2.48427600	3.06798300	H	-1.37235100	1.85518000	3.82495400
H	3.54565700	-1.86443900	3.75322600	H	0.30906700	2.44201500	3.57423000
H	2.17962100	-3.02920800	3.60812600	H	-1.04154000	3.13896300	2.64889700
H	3.64327200	-3.20587200	2.60436800	C	-2.14099400	-2.18496800	1.98622800
C	2.39064100	-2.97687500	-3.11795800	H	-2.85066500	-1.55144900	2.52293200
H	3.42957900	-2.64460500	-3.22159500	H	-2.29254900	-2.45259400	0.64608700
H	2.40261800	-3.90603200	-2.53408000	H	-1.11605000	-2.10591500	2.35372100
H	1.94677300	-3.16859500	-4.09756700	H	-2.47295700	-3.23511400	2.04285700
C	-3.45608500	2.61961300	0.43987900	H	-0.21513300	-0.79814700	-1.57667300
H	-3.37205400	2.40477300	1.51009900				

Model5H*-**IM**-r(HS-FM)

C	-0.23366900	-0.32252800	-2.54889400	O	1.21756100	2.22384600	-0.63073600
O	0.80925900	-0.37141000	-1.84826200	O	3.08544400	1.11010900	-0.81200200
O	-1.38970900	0.04365000	-2.10700500	C	1.25822300	0.83334200	2.98542200
C	-3.95080100	-1.82797500	0.16616900	O	1.91324900	0.77324300	1.86133900
C	-5.26734400	-1.97900800	0.53457100	O	0.08257100	0.42068800	3.11449000
N	-5.77581000	-0.69706600	0.69819300	C	3.22726400	-2.40133800	-0.42144800
H	-6.72412000	-0.45759700	0.96962200	C	3.46914500	-3.59414700	0.22364800
C	-4.79480700	0.18871800	0.43759500	N	2.67334600	-3.59285100	1.35994100
N	-3.67413800	-0.46318900	0.11182400	H	2.62359600	-4.32503800	2.06006100
H	-5.86791900	-2.86468600	0.68795700	C	1.98202800	-2.43291300	1.38698900
H	-4.89475500	1.26571900	0.48353800	N	2.28930300	-1.68936800	0.32474700
C	2.44689200	2.20501300	-0.98806700	H	4.12900000	-4.41440500	-0.02206600

H	1.28589500	-2.16064700	2.17024100	H	1.44336500	1.30725200	5.07833500
Fe	1.43126300	0.23220500	0.04814300	C	-2.92397000	-2.87078700	-0.15313700
Fe	-1.95038400	0.55435800	-0.33459000	H	-2.62989500	-2.82017200	-1.20939100
O	-0.47185600	-0.03297900	0.67765700	H	-2.02241500	-2.73071300	0.45605500
O	-2.54834800	2.22805300	-0.15666800	H	-3.32229500	-3.87126300	0.04154800
C	3.84090900	-1.88765600	-1.68760300	C	-0.16795300	-0.69131600	-4.01382000
H	3.06664000	-1.64192000	-2.42257300	H	-0.24036800	0.23032700	-4.60587800
H	4.41467000	-0.97358500	-1.49991400	H	0.77353700	-1.19386200	-4.24616200
H	4.50871500	-2.64329500	-2.11373900	H	-1.02199200	-1.32042300	-4.28509200
C	3.12545000	3.41700200	-1.56049800	H	-0.41810600	0.12077200	1.69439400
H	3.85874600	3.11756200	-2.31558500	C	-1.00209500	4.84021500	0.19397800
H	2.39139400	4.10827400	-1.98329100	H	-2.07083900	3.07900000	-0.01966400
H	3.66564700	3.92805200	-0.75245800	H	-1.48459100	5.40190800	-0.60271400
C	2.00501500	1.44312900	4.15122000	H	-1.24721100	5.07662300	1.22695800
H	3.00253300	0.99760200	4.23351900	H	-0.12492500	4.23578000	-0.02797300
H	2.14283000	2.51531900	3.96172800				

Model5H*-**IM**-n(HS-FM)

C	0.13050200	-2.46589000	0.36641000	H	5.96063000	-0.35089400	-2.69406100
O	-0.96657500	-1.85167000	0.40745500	H	4.01669400	2.08305800	0.19073200
O	1.28750400	-1.92262000	0.52241400	C	-1.69047500	0.19567700	2.75886700
C	4.14381600	-0.72614400	-1.43847500	O	-0.51132700	0.39084100	2.30927900
C	5.23456900	-0.05989000	-1.94787100	O	-2.62117400	-0.04097000	1.91244500
N	5.27749800	1.17016400	-1.30634700	C	-1.15106200	3.01736100	-0.58414700
H	5.95997000	1.90540000	-1.46032000	O	-1.74317900	2.08415800	0.11628400
C	4.24648800	1.23532100	-0.44190600	O	-0.18275900	2.79489100	-1.33811700
N	3.53900300	0.10152800	-0.49236000	C	-3.84704500	-1.11150400	-1.37258600

C -4.36752500	-1.03870800	-2.64549100	C -1.72307600	4.41004700	-0.41753500
N -3.56204800	-0.15264000	-3.34690800	H -2.80828000	4.39025700	-0.56918100
H -3.67663500	0.12683000	-4.31521400	H -1.54645000	4.74964300	0.61088200
C -2.59443500	0.28785500	-2.51430500	H -1.25071600	5.10297200	-1.11774300
N -2.73585100	-0.27288700	-1.31364300	C 3.62925300	-2.08571600	-1.79942300
H -5.22262900	-1.52511000	-3.09356800	H 3.58244700	-2.73961000	-0.92118300
H -1.82376000	0.99541000	-2.79488000	H 2.61952500	-2.02182500	-2.22286300
Fe -1.42933100	0.17177800	0.27539000	H 4.28607300	-2.54897900	-2.54237000
Fe 1.83124300	-0.04952600	0.67057400	C 0.11682200	-3.96738300	0.16548100
O 0.35414200	0.34549600	-0.55913600	H -0.71580700	-4.25258800	-0.48373700
O 1.95354100	1.58145100	1.41882200	H 1.06726800	-4.31784000	-0.24523400
C -4.33452900	-1.90878400	-0.20177800	H -0.03518400	-4.44610400	1.14201900
H -3.54624400	-2.57325400	0.16967600	C 2.67126700	-0.75919300	2.44887300
H -4.62610400	-1.25165200	0.62552300	H 3.05667800	-1.73602800	2.15594500
H -5.20012700	-2.51312500	-0.49142300	H 1.23415000	1.76336300	2.05348000
C -2.00524200	0.25806300	4.22873100	H 1.80004500	-0.79456400	3.10559500
H -1.09064700	0.29879900	4.82556000	H 3.41763100	-0.01896900	2.73153600
H -2.60593000	1.15586600	4.42244700	H 0.36237700	1.28582600	-0.92125100
H -2.61226300	-0.60787500	4.51470800			
Model5H*- TS2 -r(HS-FM)					
C 0.17649000	-0.92760800	2.45741500	H 6.63197500	-0.21097100	-1.22123900
O -0.81295400	-0.86727500	1.68769700	C 4.74993000	0.29888300	-0.42876000
O 1.33768700	-0.42355900	2.18832200	N 3.65634700	-0.41471900	-0.14764200
C 3.92487300	-1.74012500	-0.48391300	H 5.79405100	-2.63775400	-1.33558400
C 5.20940800	-1.80414500	-0.97227100	H 4.85031500	1.36694900	-0.28410300
N 5.70738700	-0.50901300	-0.92730800	C -2.49159800	1.80993300	1.52765300

O	-1.25841000	1.94951400	1.21090600	H	-3.89127400	2.28624200	3.07745900
O	-3.10506300	0.79762600	1.04563700	H	-2.48338300	3.40466900	2.96942400
C	-1.21416400	1.79774900	-2.55711600	H	-3.79593600	3.47027800	1.76567600
O	-1.90178200	1.21901900	-1.60992900	C	-2.00751300	2.68903400	-3.48829300
O	0.01749300	1.64195800	-2.70117600	H	-2.91794100	2.17585300	-3.81668600
C	-3.17256700	-2.46643700	-0.26508900	H	-2.32004200	3.58621500	-2.93873700
C	-3.41137400	-3.43176600	-1.21817700	H	-1.39904800	2.98355900	-4.34663300
N	-2.62700400	-3.10213400	-2.31404200	C	2.91911200	-2.83509600	-0.30013900
H	-2.57963400	-3.60566800	-3.19312000	H	2.68418500	-2.97792100	0.76243100
C	-1.94616400	-1.97390400	-2.01764700	H	1.98508400	-2.59839400	-0.82506700
N	-2.24787200	-1.56294800	-0.78697500	H	3.30635300	-3.78046400	-0.69246700
H	-4.06213200	-4.29489200	-1.20852500	C	0.04634400	-1.61263100	3.79922400
H	-1.26216400	-1.48284900	-2.69771300	H	0.04529300	-0.84402900	4.58316100
Fe	-1.41238400	0.22547700	-0.00597800	H	-0.88334800	-2.18304100	3.85543800
Fe	1.94319300	0.45947800	0.59415400	H	0.91050300	-2.26025500	3.98029900
O	0.49456000	0.20434500	-0.62489500	H	0.47561900	0.76056400	-1.48061700
O	2.51563400	2.18438600	0.74338700	C	1.11302300	4.10787400	-0.18703900
C	-3.77992300	-2.33919700	1.09818400	H	2.46011000	2.72044100	1.55071500
H	-3.00209100	-2.31861200	1.86916700	H	1.70900500	4.93385500	0.19245200
H	-4.35018900	-1.40812100	1.18484900	H	1.28707900	3.74524500	-1.19484300
H	-4.44895100	-3.18433400	1.29003100	H	0.24583800	3.75863800	0.36526900
C	-3.20082100	2.80403300	2.40406200				
Model5H*- TS2 -n(HS-FM)							
C	0.16957500	1.90549900	-1.57511900	C	4.40000100	1.31626000	0.81734500
O	-0.86515200	1.20059000	-1.39097300	C	5.62044200	0.95632000	1.34171900
O	1.35840600	1.53499300	-1.27143900	N	5.70129000	-0.42425200	1.23062800

H	6.47500000	-1.00736600	1.53265300	H	-4.58584300	0.81798900	-1.33546800
C	4.56484000	-0.87151700	0.65908500	H	-5.03429200	2.53697900	-1.21701300
N	3.75366100	0.15602400	0.39071700	C	-2.24233000	-2.82090000	-3.11086100
H	6.41277900	1.55097800	1.77436900	H	-1.35681400	-3.26651500	-3.57159400
H	4.34262500	-1.91151100	0.45608700	H	-2.85547000	-3.61876500	-2.67202000
C	-1.85888300	-1.85828500	-2.02023800	H	-2.85486200	-2.31133500	-3.86187600
O	-0.68522300	-1.84039500	-1.51308500	C	-2.02867900	-3.39751900	2.86127200
O	-2.71702800	-1.03577800	-1.55108400	H	-3.07232600	-3.13712100	3.07039700
C	-1.32140300	-2.22753400	2.20874300	H	-2.03933800	-4.24332600	2.16208900
O	-1.94573800	-1.69587000	1.18999300	H	-1.51418100	-3.69007600	3.77956700
O	-0.22027200	-1.81813700	2.62881300	C	3.79359700	2.68157000	0.70248500
C	-3.78619400	1.84357300	0.37443300	H	3.55477300	2.92364800	-0.33932500
C	-4.30974100	2.56717200	1.42305600	H	2.86272500	2.74694800	1.27975900
N	-3.56423900	2.22694500	2.54276700	H	4.48836100	3.43532100	1.08602500
H	-3.69707600	2.58041200	3.48410400	C	0.00056400	3.27721000	-2.19479400
C	-2.62878800	1.32748900	2.16764900	H	-0.42275500	3.95304400	-1.44013500
N	-2.73233400	1.07498500	0.86409100	H	0.95828900	3.67824400	-2.53482500
H	-5.13222300	3.26746500	1.46415300	H	-0.71034500	3.22537900	-3.02578700
H	-1.90772700	0.88428300	2.84284400	C	2.17533800	-0.92878200	-2.55833700
Fe	-1.46053000	-0.31560600	-0.09812000	H	2.83855200	-0.06357000	-2.64090300
Fe	1.87471300	-0.18397800	-0.42123700	H	1.22220700	-2.42879200	-0.98473000
O	0.31028000	-0.11675600	0.73824100	H	1.14236500	-0.77178900	-2.86269300
O	2.08386600	-2.02584200	-0.74332300	H	2.62280700	-1.85861900	-2.88882000
C	-4.22684300	1.81522400	-1.05696700	H	0.29580200	-0.73530600	1.53881200
H	-3.39252700	2.05954800	-1.72379300				

Model5H*-P(HS-FM)

C	0.12088600	-1.94183600	1.72427000	Fe	1.84542200	-0.16963100	0.15831900
O	-0.92108100	-1.34926100	1.30137000	O	0.23056100	0.07507300	-0.88363000
O	1.31216600	-1.60733900	1.41934800	O	1.96645000	1.71245700	1.08784100
C	4.48338900	-1.03372700	-1.29357200	C	-4.30207300	-1.84789400	1.03272700
C	5.84223300	-1.04978700	-1.07478800	H	-3.46136800	-2.15327800	1.66534700
N	6.04265000	-0.44842300	0.15891800	H	-4.62267300	-0.85628500	1.37107200
H	6.93587400	-0.30527200	0.61864900	H	-5.12838100	-2.55219000	1.17332500
C	4.83891000	-0.08744600	0.65361300	C	-2.04554300	2.44069000	3.40889100
N	3.87015700	-0.42437400	-0.19952600	H	-2.90127600	2.04980800	3.96552000
H	6.65840400	-1.42671700	-1.67521800	H	-1.15791900	2.49015700	4.04731100
H	4.69821900	0.40195200	1.60931500	H	-2.28434500	3.46021400	3.07783700
C	-1.77781100	1.59394300	2.19515400	C	-2.12826900	3.67368500	-2.39260400
O	-0.62543400	1.58190600	1.62913600	H	-3.11490900	3.36666600	-2.75820800
O	-2.68915600	0.88074500	1.67035200	H	-2.29570100	4.36758900	-1.55932900
C	-1.36830800	2.46312300	-1.88957300	H	-1.56880800	4.17602200	-3.18523500
O	-2.00043800	1.73016700	-1.01535400	C	3.70650500	-1.55275400	-2.46513200
O	-0.21565300	2.20603200	-2.30049700	H	2.99616800	-2.33013300	-2.15491800
C	-3.89383200	-1.81555200	-0.40801500	H	3.13776500	-0.74963000	-2.95086600
C	-4.46191300	-2.47232300	-1.47709500	H	4.38146100	-1.98885200	-3.20829400
N	-3.72942700	-2.10346000	-2.59624100	C	-0.07278000	-3.13056100	2.64294800
H	-3.89115200	-2.41072300	-3.54910600	H	-0.76164300	-2.86428700	3.45213300
C	-2.75787100	-1.25263900	-2.20025400	H	-0.53453900	-3.94836000	2.07524000
N	-2.82669000	-1.05718700	-0.88498800	H	0.88227100	-3.46754400	3.05202900
H	-5.30535100	-3.14623400	-1.53162800	H	0.20480400	0.84357700	-1.54020800
H	-2.03420100	-0.80480200	-2.86892000	C	2.33130200	2.92481800	0.38292100
Fe	-1.47080100	0.21839800	0.11519500	H	1.06845800	1.83814900	1.48741500

H	2.39541600	3.75753000	1.09268200	H	1.60323700	3.15233000	-0.40493000
H	3.31494200	2.75781200	-0.06500800				
Model5H*-Q(HS-AF)							
C	0.47491800	-1.94853400	1.33679200	H	-4.58623500	-2.95490800	-2.70361900
O	-0.64480200	-1.59823800	0.89408800	H	-1.73499200	0.17026800	-2.95686600
O	1.55929400	-1.25061300	1.21062300	Fe	-1.42519200	0.22607500	0.23377600
C	4.31177900	-1.06572200	-0.85930800	Fe	1.89530000	0.44128200	0.38702300
C	5.62664100	-0.79196900	-1.15375800	O	0.37390600	0.59256000	-0.60925800
N	5.86184000	0.51022600	-0.73380300	O	2.21283800	1.99159100	0.70269500
H	6.73822700	1.01720400	-0.80891000	C	-3.86232000	-2.46574000	0.20885700
C	4.72578000	1.00306800	-0.20924600	H	-3.00502400	-2.89092600	0.74286400
N	3.76484900	0.07422100	-0.26399200	H	-4.30209200	-1.69604300	0.85239200
H	6.39146700	-1.40021000	-1.61623200	H	-4.60310800	-3.25515700	0.04625500
H	4.60329600	2.00001300	0.19272900	C	-2.36560100	1.12082800	3.95684000
C	-1.96403300	0.74267500	2.56063900	H	-2.95816500	0.31801700	4.40790400
O	-0.79626900	0.98514600	2.10157500	H	-1.48497400	1.34479500	4.56408800
O	-2.79335500	0.17821600	1.76109600	H	-3.00208800	2.01397700	3.90676300
C	-1.47060900	2.87982000	-1.14263200	C	-2.26167000	4.15241000	-1.33057700
O	-2.05435500	1.93161100	-0.46794600	H	-3.29595100	3.91972000	-1.60501300
O	-0.31352800	2.76373000	-1.61226400	H	-2.28843700	4.69033800	-0.37403000
C	-3.43604500	-1.88543100	-1.10465500	H	-1.79028100	4.78633500	-2.08515700
C	-3.86707800	-2.22047600	-2.36895100	C	3.54270900	-2.32609200	-1.10937000
N	-3.18728300	-1.38958400	-3.24759400	H	3.24029800	-2.79251700	-0.16521000
H	-3.28251100	-1.37522500	-4.25741500	H	2.63762000	-2.12859100	-1.69766100
C	-2.37969000	-0.58464300	-2.52500500	H	4.16154300	-3.03673300	-1.66586500
N	-2.50162200	-0.85736900	-1.22598400	C	0.62089400	-3.26893800	2.05790100

H	1.10734000	-3.10316000	3.02591800	H	1.27265900	-3.93223600	1.47551300
H	-0.35292600	-3.74224100	2.19924800	H	0.22316100	1.53395700	-1.06886700
Model5H*-TS1-r(HS-AF)							
C	-0.21589400	-0.36632800	-2.55601000	H	4.19725400	-4.34177800	0.11690300
O	0.82364900	-0.39386200	-1.84883300	H	1.31188500	-2.07787800	2.24050300
O	-1.37947500	-0.00472700	-2.12872800	Fe	1.41558300	0.25695700	0.04292600
C	-3.85770300	-1.86236100	0.19310200	Fe	-1.93445500	0.52110700	-0.35596000
C	-5.16449900	-2.05532900	0.57534600	O	-0.45234400	0.01734600	0.66858400
N	-5.71706800	-0.79114700	0.73157700	O	-2.58350500	2.12412800	-0.25635400
H	-6.67115500	-0.58323800	1.00910300	C	3.85349500	-1.88104600	-1.63144300
C	-4.77222700	0.12720200	0.45310900	H	3.07366300	-1.67462100	-2.37252000
N	-3.63191200	-0.48787100	0.12331600	H	4.40953500	-0.95042300	-1.47541900
H	-5.73116200	-2.96056300	0.74295700	H	4.53460500	-2.63834600	-2.03293800
H	-4.91302300	1.19965200	0.48963200	C	3.13165300	3.40962400	-1.60348700
C	2.45834700	2.20112100	-1.01721200	H	3.90854500	3.10466900	-2.31090600
O	1.22396600	2.22134500	-0.67211600	H	2.39932100	4.06296000	-2.08591100
O	3.09885200	1.11380700	-0.81591300	H	3.61497800	3.96751300	-0.79035100
C	1.22045700	0.98828900	2.94186400	C	1.93045700	1.62904700	4.11278900
O	1.91274100	0.85189200	1.85353000	H	2.92517300	1.18798000	4.23806600
O	0.02192000	0.62060200	3.04202600	H	2.07171700	2.69595000	3.89703700
C	3.25172200	-2.36300900	-0.34728300	H	1.33976200	1.52070200	5.02544600
C	3.52036200	-3.52813000	0.33685100	C	-2.79865500	-2.87250900	-0.12526800
N	2.72701400	-3.50587100	1.47444200	H	-2.51625500	-2.82348700	-1.18470700
H	2.69521900	-4.21451400	2.19935400	H	-1.89707400	-2.69640100	0.47446900
C	2.01083300	-2.36072300	1.46372000	H	-3.16182100	-3.88345300	0.08346800
N	2.29960800	-1.64648000	0.37669900	C	-0.13562700	-0.75659900	-4.01470800

H	-0.18819600	0.15858800	-4.61892500	H	-2.03650900	3.37248800	-0.06141700
H	0.80353400	-1.27198400	-4.22800100	H	-1.91006000	5.08978100	-0.64957300
H	-0.99324200	-1.37883100	-4.28995900	H	-1.71170600	4.72125700	1.12523100
H	-0.39778800	0.24511500	1.69454700	H	-0.42641100	4.19816000	-0.06446000
C	-1.48439300	4.41681200	0.09987100				

Model5H*-**TS1**-n(HS-AF)

C	0.46541300	1.06190900	-2.06786800	H	-2.65254500	3.28323600	3.41010300
O	-0.67656000	0.95983500	-1.55799200	C	-2.04830700	1.73546100	2.11341600
O	1.52074100	0.44024000	-1.66015400	N	-2.30257600	1.46580500	0.83305500
C	4.11849800	1.47709400	0.19345200	H	-3.97792500	4.25241900	1.43113300
C	5.29628100	1.57252700	0.89901100	H	-1.42921400	1.14280600	2.77552500
N	5.49663900	0.33889200	1.49773100	Fe	-1.51876000	-0.26806800	-0.10222800
H	6.27553600	0.07634000	2.09291100	Fe	1.88393800	-0.82193400	-0.25523300
C	4.47044500	-0.46595500	1.16212100	O	0.32023800	-0.37223900	0.66342500
N	3.61423100	0.18437700	0.36652200	O	2.30197600	-2.19274300	0.64903500
H	5.98503600	2.39710100	1.01957900	C	-3.66696900	2.51590700	-1.04558100
H	4.35297200	-1.48670400	1.49904600	H	-2.84403700	2.51542400	-1.76898900
C	-2.50562100	-1.60985800	-1.90127800	H	-4.28899400	1.63940400	-1.25705600
O	-1.30650100	-1.83450000	-1.51411000	H	-4.26725000	3.41959500	-1.19248700
O	-3.12340800	-0.63737400	-1.34390500	C	-3.17733100	-2.46054800	-2.94150200
C	-1.61419100	-1.87148100	2.41683900	H	-3.76815400	-1.83240800	-3.61609600
O	-2.16278700	-1.42784900	1.32025900	H	-2.44220100	-3.04619300	-3.49953100
O	-0.46525400	-1.53950100	2.78568400	H	-3.86933000	-3.14666800	-2.43585200
C	-3.14094200	2.47236100	0.35630800	C	-2.45358400	-2.83085600	3.23061500
C	-3.37959400	3.35314000	1.38791600	H	-3.46779100	-2.43512900	3.35289300
N	-2.68092600	2.86947700	2.48449700	H	-2.53695400	-3.77801300	2.68240400

H	-1.98936100	-3.01460000	4.20231700	H	1.16446100	2.90682300	-2.89856600
C	3.46245200	2.55540100	-0.61270400	C	1.98703700	-2.35756100	-1.90156300
H	3.38587400	2.27071900	-1.66697500	H	2.68439800	-1.78909100	-2.52083200
H	2.45235200	2.76781400	-0.24219500	H	2.22807100	-2.54661400	-0.56326400
H	4.05278600	3.47468100	-0.54154100	H	0.94413200	-2.25953500	-2.20926400
C	0.66496600	1.99313700	-3.24617100	H	2.27393700	-3.42254500	-1.91107200
H	1.31206500	1.52472600	-3.99461300	H	0.19544000	-0.85612100	1.56335500
H	-0.29837100	2.26170600	-3.68559300				

Model5H*-**TS1**-n(HS-AF)

C	0.46541300	1.06190900	-2.06786800	C	-3.14094200	2.47236100	0.35630800
O	-0.67656000	0.95983500	-1.55799200	C	-3.37959400	3.35314000	1.38791600
O	1.52074100	0.44024000	-1.66015400	N	-2.68092600	2.86947700	2.48449700
C	4.11849800	1.47709400	0.19345200	H	-2.65254500	3.28323600	3.41010300
C	5.29628100	1.57252700	0.89901100	C	-2.04830700	1.73546100	2.11341600
N	5.49663900	0.33889200	1.49773100	N	-2.30257600	1.46580500	0.83305500
H	6.27553600	0.07634000	2.09291100	H	-3.97792500	4.25241900	1.43113300
C	4.47044500	-0.46595500	1.16212100	H	-1.42921400	1.14280600	2.77552500
N	3.61423100	0.18437700	0.36652200	Fe	-1.51876000	-0.26806800	-0.10222800
H	5.98503600	2.39710100	1.01957900	Fe	1.88393800	-0.82193400	-0.25523300
H	4.35297200	-1.48670400	1.49904600	O	0.32023800	-0.37223900	0.66342500
C	-2.50562100	-1.60985800	-1.90127800	O	2.30197600	-2.19274300	0.64903500
O	-1.30650100	-1.83450000	-1.51411000	C	-3.66696900	2.51590700	-1.04558100
O	-3.12340800	-0.63737400	-1.34390500	H	-2.84403700	2.51542400	-1.76898900
C	-1.61419100	-1.87148100	2.41683900	H	-4.28899400	1.63940400	-1.25705600
O	-2.16278700	-1.42784900	1.32025900	H	-4.26725000	3.41959500	-1.19248700
O	-0.46525400	-1.53950100	2.78568400	C	-3.17733100	-2.46054800	-2.94150200

H -3.76815400 -1.83240800 -3.61609600	C 0.66496600 1.99313700 -3.24617100
H -2.44220100 -3.04619300 -3.49953100	H 1.31206500 1.52472600 -3.99461300
H -3.86933000 -3.14666800 -2.43585200	H -0.29837100 2.26170600 -3.68559300
C -2.45358400 -2.83085600 3.23061500	H 1.16446100 2.90682300 -2.89856600
H -3.46779100 -2.43512900 3.35289300	C 1.98703700 -2.35756100 -1.90156300
H -2.53695400 -3.77801300 2.68240400	H 2.68439800 -1.78909100 -2.52083200
H -1.98936100 -3.01460000 4.20231700	H 2.22807100 -2.54661400 -0.56326400
C 3.46245200 2.55540100 -0.61270400	H 0.94413200 -2.25953500 -2.20926400
H 3.38587400 2.27071900 -1.66697500	H 2.27393700 -3.42254500 -1.91107200
H 2.45235200 2.76781400 -0.24219500	H 0.19544000 -0.85612100 1.56335500
H 4.05278600 3.47468100 -0.54154100	

Model5H*-**IM**-r(HS-AF)

C -0.23029300 -0.45228400 -2.54254500	C 1.23522800 1.11296900 2.88965900
O 0.80681900 -0.47800700 -1.83135900	O 1.93522100 0.82811700 1.83493700
O -1.38510600 -0.04936400 -2.13099600	O 0.00231500 0.88204500 2.97581500
C -3.93761500 -1.79901400 0.26397300	C 3.13208900 -2.50193700 -0.26881900
C -5.25389300 -1.92705000 0.64210600	C 3.36227100 -3.64959100 0.45734000
N -5.76071600 -0.63734400 0.73151800	N 2.58627300 -3.55029400 1.60269100
H -6.70846000 -0.38127400 0.98940400	H 2.53614100 -4.22786700 2.35573800
C -4.77899300 0.23067500 0.41862800	C 1.91773400 -2.37769100 1.55569200
N -3.65939100 -0.44023000 0.12983200	N 2.21977900 -1.71870200 0.43767100
H -5.85519600 -2.80172400 0.84717300	H 4.00290600 -4.49804000 0.26169400
H -4.87747500 1.30869300 0.40195100	H 1.24359600 -2.03668000 2.33091600
C 2.55380800 2.07080500 -1.07371000	Fe 1.41512200 0.20672100 0.03902000
O 1.32152400 2.16296200 -0.73071700	Fe -1.94501900 0.55913500 -0.38702000
O 3.13814800 0.95910100 -0.84089900	O -0.46503300 0.09923300 0.65802800

O	-2.54905300	2.23981700	-0.30706700	H	-2.61381600	-2.86798400	-1.05074500
C	3.73806700	-2.09607700	-1.57708000	H	-2.01361100	-2.69153100	0.61103400
H	2.95907800	-1.88886600	-2.31861800	H	-3.31502900	-3.84784000	0.25157300
H	4.33183900	-1.18276300	-1.46360600	C	-0.15758700	-0.89813800	-3.98544500
H	4.38466500	-2.89525000	-1.95367100	H	-0.24053900	-0.01091500	-4.62648300
C	3.28771500	3.22651700	-1.69282600	H	0.78914900	-1.40285800	-4.18993500
H	4.04766300	2.86232800	-2.39056300	H	-1.00467500	-1.55029600	-4.22262100
H	2.59031800	3.90332800	-2.19429000	H	-0.41128500	0.41599500	1.66281400
H	3.79968800	3.78140100	-0.89530400	C	-0.91518800	4.81092500	-0.02331100
C	1.98026300	1.75660600	4.03688100	H	-2.05680000	3.08385000	-0.17982600
H	2.93299700	1.24332200	4.20473500	H	-1.39138000	5.36438900	-0.82952400
H	2.21183700	2.79491600	3.76611100	H	-1.14665600	5.07723200	1.00559000
H	1.36932500	1.74962000	4.94265500	H	-0.05237200	4.18328400	-0.23742000
C	-2.91275200	-2.86037500	0.00534000				

Model5H*-**IM**-n(HS-AF)

C	0.12499300	-2.48707600	0.23331800	C	-1.68263300	0.00647600	2.75825900
O	-0.97408400	-1.87528200	0.2760520	O	-0.50252000	0.22001700	2.3179570
O	1.27838600	-1.95025100	0.4279890	O	-2.61807600	-0.16011300	1.9015010
C	4.08278300	-0.63912800	-1.5216200	C	-1.12889000	3.04997000	-0.3712160
C	5.18257200	0.03674300	-1.99786500	O	-1.73520900	2.07513900	0.2547260
N	5.27455100	1.20691800	-1.2572940	O	-0.14472500	2.87383800	-1.1183690
H	5.97475100	1.93359000	-1.3651990	C	-3.84543400	-0.99967200	-1.4443670
C	4.26281400	1.22803200	-0.36784800	C	-4.36331500	-0.84701300	-2.7112590
N	3.52180000	0.12262400	-0.4967460	N	-3.54756400	0.06965300	-3.3591980
H	5.88486200	-0.21087700	-2.7815220	H	-3.65764000	0.40589300	-4.3098030
H	4.06884800	2.02721900	0.33594800	C	-2.57627500	0.45008900	-2.5015060

N	-2.72525500	-0.17796500	-1.3357130	H	-1.54718200	4.70282900	0.9235860
H	-5.22293100	-1.29724100	-3.1875990	H	-1.21158700	5.16563100	-0.7716300
H	-1.79799900	1.16451000	-2.7404400	C	3.51999400	-1.94854000	-1.9819930
Fe	-1.41865400	0.15482200	0.2814070	H	3.48957000	-2.67741400	-1.1641390
Fe	1.82655100	-0.08290700	0.6758080	H	2.49668800	-1.82304100	-2.3560440
O	0.35995500	0.38361400	-0.5203320	H	4.13572700	-2.35761300	-2.7891440
O	1.97896900	1.49777600	1.52331300	C	0.11456300	-3.98066700	-0.0208530
C	-4.34384100	-1.85937700	-0.3233240	H	-0.71522900	-4.24505700	-0.6822620
H	-3.56399400	-2.55392600	0.0088400	H	1.06738800	-4.31452000	-0.4400030
H	-4.62965400	-1.24945700	0.5412560	H	-0.03859400	-4.49369400	0.9379660
H	-5.21579700	-2.43530000	-0.6495550	C	2.69536500	-0.91121000	2.40637400
C	-1.99056600	-0.02760800	4.2305730	H	3.06824600	-1.86981900	2.0456290
H	-1.07348800	-0.07712800	4.8230700	H	1.29122400	1.64836700	2.19871400
H	-2.54241500	0.88357900	4.4951110	H	1.82847400	-0.97918500	3.0661110
H	-2.64074900	-0.87991700	4.4549660	H	3.44979200	-0.19319600	2.7224960
C	-1.70116300	4.43082600	-0.1282850	H	0.36696000	1.35370400	-0.8091690
H	-2.78270900	4.42469600	-0.3051430				

Model5H*-TS2-r(HS-AF)

C	-0.21154000	0.71927300	2.52241800	N	-3.61459700	0.37536400	-0.14887100
O	0.76754800	0.76848100	1.73845000	H	-5.70464200	2.71588000	-1.18786400
O	-1.35419000	0.18724500	2.22653000	H	-4.79957600	-1.37854500	-0.51975800
C	-3.87112600	1.72895000	-0.35678400	C	2.63344700	-1.76171000	1.41192800
C	-5.13407400	1.84734200	-0.88975900	O	1.40383600	-1.96953100	1.11274700
N	-5.63131500	0.55614300	-1.00100800	O	3.16633900	-0.69019000	0.96774900
H	-6.54255400	0.29268600	-1.36196700	C	1.28057700	-1.69522300	-2.61017500
C	-4.69416400	-0.30161700	-0.54841500	O	1.95418700	-1.09369200	-1.67121300

O	0.03356900	-1.62759900	-2.70887000	H	4.02423400	-3.36234900	1.54099000
C	2.96844400	2.61845200	-0.19239300	C	2.09771400	-2.50287300	-3.59442000
C	3.14338700	3.62516200	-1.11618300	H	2.97339600	-1.93021100	-3.91833500
N	2.37390500	3.28284300	-2.21860700	H	2.46662600	-3.40472200	-3.08903700
H	2.29303500	3.80831200	-3.08228000	H	1.48619800	-2.79457100	-4.45158400
C	1.76366000	2.10715000	-1.95453600	C	-2.87907000	2.79794600	-0.01395200
N	2.09651000	1.67733600	-0.73840600	H	-2.69836300	2.83303400	1.06803300
H	3.74176000	4.52481500	-1.08255900	H	-1.91875200	2.61508500	-0.51242900
H	1.10748900	1.59652800	-2.64739100	H	-3.24950700	3.77862900	-0.32812300
Fe	1.39976200	-0.19585800	-0.02127200	C	-0.09183700	1.29785800	3.91420800
Fe	-1.92966000	-0.58267100	0.56194700	H	-0.07699800	0.47017700	4.63515000
O	-0.48125800	-0.28541000	-0.61921800	H	0.82652600	1.88016900	4.01564700
O	-2.53241300	-2.30419800	0.57594000	H	-0.96817700	1.91284400	4.14502300
C	3.58866600	2.48809900	1.16475600	H	-0.43177800	-0.83118000	-1.49517500
H	2.81733000	2.42395500	1.94010300	C	-0.96576400	-4.18614400	-0.14482400
H	4.19337300	1.57744300	1.22950000	H	-2.61659000	-2.86134100	1.36661800
H	4.22629700	3.35432300	1.36904600	H	-1.51697000	-5.02937600	0.26398200
C	3.42336700	-2.74870900	2.22514100	H	-1.13799800	-3.88933200	-1.17415300
H	4.11298000	-2.22127600	2.89166900	H	-0.13053100	-3.76104800	0.40367000
H	2.75796000	-3.40456200	2.79291400				

Model5H*-**TS2**-n(HS-AF)

C	0.17502600	1.90062400	-1.58000800	N	5.71117200	-0.42670500	1.20117600
O	-0.86185800	1.19717800	-1.40051300	H	6.48856400	-1.00955000	1.49412500
O	1.36147700	1.53286800	-1.26298300	C	4.56841200	-0.87444200	0.64285800
C	4.40478900	1.31341700	0.80236200	N	3.75391700	0.15284800	0.38336800
C	5.63122300	0.95385300	1.31284400	H	6.42833500	1.54887300	1.73611900

H	4.34419200	-1.91442300	0.44197100	C	-2.29447600	-2.83386800	-3.07755700
C	-1.89775100	-1.86349200	-1.99863200	H	-1.41412600	-3.27182500	-3.55541800
O	-0.72053200	-1.85286000	-1.49712100	H	-2.88760800	-3.63763000	-2.62206500
O	-2.74438500	-1.02845100	-1.53265600	H	-2.92908600	-2.33452000	-3.81676800
C	-1.31852000	-2.22857700	2.20288000	C	-2.02668100	-3.38091300	2.88421900
O	-1.96147900	-1.68624800	1.20436900	H	-3.06115900	-3.10325200	3.11504000
O	-0.19338000	-1.84298300	2.58647600	H	-2.06575000	-4.23305100	2.19373300
C	-3.76370700	1.86424000	0.37818500	H	-1.49451300	-3.67281400	3.79261100
C	-4.27709400	2.59835300	1.42458000	C	3.79757000	2.67885900	0.69387400
N	-3.52709200	2.26221800	2.54239600	H	3.54618300	2.92008100	-0.34509800
H	-3.65261800	2.62318200	3.48187500	H	2.87370000	2.74524400	1.28223000
C	-2.59866000	1.35508000	2.16814500	H	4.49723500	3.43247900	1.06867500
N	-2.71098100	1.09343000	0.86719700	C	0.01153100	3.26809100	-2.21062500
H	-5.09545500	3.30348300	1.46520700	H	-0.41640100	3.94981500	-1.46388400
H	-1.87629200	0.91326800	2.84274700	H	0.97191800	3.66597400	-2.54692800
Fe	-1.45647400	-0.31455100	-0.09554200	H	-0.69377700	3.21081700	-3.04603700
Fe	1.87044700	-0.19155000	-0.41295100	C	2.12682700	-0.94494900	-2.56022600
O	0.30562600	-0.14197500	0.72064500	H	2.80805100	-0.09474900	-2.64932500
O	2.08430800	-2.03371900	-0.73778300	H	1.22458000	-2.44656100	-0.96648700
C	-4.21404000	1.82915000	-1.05005300	H	1.09164500	-0.76449500	-2.84301000
H	-3.38155200	2.05888800	-1.72423200	H	2.54748200	-1.88253400	-2.90388100
H	-4.58567400	0.83379200	-1.31821900	H	0.28937100	-0.77597600	1.51862000
H	-5.01458400	2.55855100	-1.21028000				
Model5H*-P(HS-AF)							
C	0.11837800	-1.87517200	1.81293800	O	1.31091800	-1.54366900	1.50702300
O	-0.92366700	-1.30854700	1.35624700	C	4.46624600	-1.05417800	-1.28439300

C	5.82586600	-1.06492500	-1.07003600	H	-3.45519100	-2.11830500	1.69626100
N	6.02910600	-0.44703800	0.15493800	H	-4.61960200	-0.83697200	1.35122000
H	6.92343100	-0.29705600	0.61032100	H	-5.11374600	-2.54070700	1.19498400
C	4.82624100	-0.08116300	0.64841400	C	-2.09433100	2.54071600	3.32518700
N	3.85527900	-0.43119900	-0.19686700	H	-2.96324500	2.17209500	3.87648000
H	6.64075100	-1.44833200	-1.66810700	H	-1.21866500	2.60297300	3.97890900
H	4.68759900	0.41998200	1.59830800	H	-2.31854300	3.55178600	2.95985800
C	-1.80884000	1.65665100	2.14228500	C	-2.11783600	3.59216500	-2.51818600
O	-0.64836300	1.63157900	1.59269200	H	-3.10203700	3.27140500	-2.87828800
O	-2.71062500	0.92415200	1.62859900	H	-2.29043600	4.32396200	-1.71904800
C	-1.36684600	2.40449800	-1.95228800	H	-1.54912300	4.05646600	-3.32722700
O	-2.00833400	1.70595600	-1.06096900	C	3.68671600	-1.58906200	-2.44703000
O	-0.20448900	2.13531900	-2.33501300	H	2.97283400	-2.35793700	-2.12379200
C	-3.86351200	-1.84182600	-0.39097700	H	3.12198500	-0.79149400	-2.94651000
C	-4.41784100	-2.52824200	-1.44859400	H	4.35932200	-2.04094200	-3.18286000
N	-3.67301300	-2.18816900	-2.56865000	C	-0.07502400	-3.02827700	2.77576900
H	-3.82336100	-2.52107800	-3.51474400	H	-0.79015600	-2.74395800	3.55528200
C	-2.70739000	-1.32531000	-2.18436400	H	-0.50439300	-3.87873400	2.23089100
N	-2.79171700	-1.09474300	-0.87566000	H	0.87597300	-3.32800800	3.22171000
H	-5.25948100	-3.20501700	-1.49478000	H	0.20339500	0.84130500	-1.53511000
H	-1.97739700	-0.89363900	-2.85678700	C	2.34137100	2.92645400	0.36173400
Fe	-1.46264300	0.21908300	0.10996700	H	1.05476300	1.86465500	1.46020200
Fe	1.83432800	-0.17340900	0.16888500	H	2.41237800	3.76443600	1.06474800
O	0.23439200	0.07902000	-0.85892500	H	3.32517200	2.74271100	-0.07926700
O	1.95555500	1.72545500	1.07295600	H	1.62140300	3.15812400	-0.43250500
C	-4.28955300	-1.83588000	1.04495700				

