

Supporting Information

Theoretical Study of the Mechanism of Oxoiron(IV) Formation from H₂O₂ and a Nonheme Iron(II) Complex: O–O Cleavage Involving Proton-Coupled Electron Transfer

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Gaussian 09, revision B.01; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Comperts, R.; Startmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W., Gonzalez, C.; Pople, J. A.; Gaussian, Inc.: Wallingford CT, 2009.

Table S1. Energy data for Model-1, B3LYP/B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-1506.525942	0.0	0.697957	0.0
³ RC	-1506.507964	11.3	0.699599	12.3
⁵ TS1	-1506.517033	5.6	0.698531	6.0
³ TS1	-1506.498054	17.5	0.699654	18.6
⁵ Int	-1506.525304	0.4	0.698772	0.9
³ Int	-1506.505390	12.9	0.700676	14.6
⁵ TSoo	-1506.512649	8.3	0.697080	7.8
³ TSoo	-1506.493225	20.5	0.698241	20.7
⁵ Int-oh	-1506.518215	4.8	0.696880	4.2
⁵ TSoh	-1506.515321	6.7	0.692955	3.5
⁵ P	-1506.532296	-4.0	0.698453	-3.7
³ P	-1506.537018	-6.9	0.701329	-4.8

Table S2. Energy data for Model-1, B3LYP/B2//B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-2646.838900	0.0	0.697957	0.0
³ RC	-2646.824363	9.1	0.699599	10.2
⁵ TS1	-2646.826193	8.0	0.698531	8.3
³ TS1	-2646.812394	16.6	0.699654	17.7
⁵ Int	-2646.832140	4.2	0.698772	4.8
³ Int	-2646.818035	13.1	0.700676	14.8
⁵ TSoo	-2646.823070	9.9	0.697080	9.4
³ TSoo	-2646.809877	18.2	0.698241	18.4
⁵ Int-oh	-2646.830911	5.0	0.696880	4.3
⁵ TSoh	-2646.830866	5.0	0.692955	1.9
⁵ P	-2646.851472	-7.9	0.698453	-7.6
³ P	-2646.858451	-12.3	0.701329	-10.2

Table S3. Energy data for Model-1, B3LYP(SCRf)/B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-1506.722272	0.0	0.697715	0.0
³ RC	-1506.701732	12.9	0.700469	14.6
⁵ TS1	-1506.702781	12.2	0.698509	12.7
³ TS1	-1506.681323	25.7	0.700638	27.5
⁵ TShooh	-1506.676486	28.7	0.696841	28.2
³ TShooh	-1506.657606	40.6	0.699536	41.7
⁵ Int	-1506.708651	8.5	0.699323	9.6
³ Int	-1506.687827	21.6	0.700765	23.5
⁵ Int-ho-oh	-1506.676486	28.7	0.696841	28.2
³ Int-ho-oh	-1506.657606	40.6	0.699536	41.7
⁵ TSoo	-1506.694805	17.2	0.697088	16.8
³ TSoo	-1506.674994	29.7	0.698022	29.9
⁵ TShat	-1506.692004	19.0	0.691031	14.8
³ TShat	-1506.677056	28.4	0.693974	26.0
⁵ Int-oh	-1506.700144	13.9	0.695752	12.7
⁵ P	-1506.732126	-6.2	0.699638	-5.0
³ P	-1506.737825	-9.8	0.702525	-6.7

Table S4. Energy data for Model-1, B3LYP(SCRf)/B2//B3LYP(SCRf)/B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-2647.037555	0.0	0.697715	0.0
³ RC	-2647.020129	10.9	0.700469	12.7
⁵ TS1	-2647.013686	15.0	0.698509	15.5
³ TS1	-2646.995873	26.2	0.700638	28.0
⁵ TShooh	-2646.992552	28.2	0.696841	27.7
³ TShooh	-2646.977480	37.7	0.699536	38.8
⁵ Int	-2647.016662	13.1	0.699323	14.1
³ Int	-2647.002309	22.1	0.700765	24.0
⁵ Int-ho-oh	-2647.016200	13.4	0.695496	12.0
³ Int-ho-oh	-2647.000929	23.0	0.696506	22.2
⁵ TSoo	-2647.006800	19.3	0.697088	18.9
³ TSoo	-2646.994016	27.3	0.698022	27.5
⁵ TShat	-2647.010592	16.9	0.691031	12.7
³ TShat	-2646.999714	23.7	0.693974	21.4
⁵ Int-oh	-2647.015575	13.8	0.695752	12.6
⁵ P	-2647.053198	-9.8	0.699638	-8.6
³ P	-2647.061063	-14.8	0.702525	-11.7

Table S5. Energy data for Model-2, B3LYP(SCRf)/B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-1312.549890	0.0	0.599194	0.0
³ RC	-1312.529500	12.8	0.601103	14.0
⁵ TS1	-1312.491666	36.5	0.596243	34.7
³ TS1	-1312.467013	52.0	0.598646	51.7
⁵ TShooh	-1312.508871	25.7	0.597943	25.0
³ TShooh	-1312.489703	37.8	0.599080	37.7
⁵ Int	-1312.506820	27.0	0.598521	26.6
³ Int	-1312.483221	41.8	0.600823	42.9
⁵ Int-ho-oh1	-1312.519604	19.0	0.595813	16.9
³ Int-ho-oh1	-1312.504709	28.4	0.597657	27.4
⁵ Int-ho-oh2	-1312.525651	15.2	0.596515	13.5
³ Int-ho-oh2	-1312.507088	26.9	0.597686	25.9
⁵ TSoo	-1312.506325	27.3	0.597977	26.6
³ TSoo	-1312.482809	42.1	0.599845	42.5
⁵ TShat	-1312.520046	18.7	0.592529	14.5
³ TShat	-1312.506058	27.5	0.595829	25.4
⁵ P	-1312.561710	-7.4	0.601206	-6.2
³ P	-1312.567711	-11.2	0.603665	-8.4

Table S6. Energy data for Model-2, B3LYP(SCRf)/B2//B3LYP(SCRf)/B1

	E (Eh)	ΔE (kcal/mol)	ZPE (Eh)	$\Delta (E+ZPE)$ (kcal/mol)
⁵ RC	-2452.806587	0.0	0.599194	0.0
³ RC	-2452.789007	11.0	0.601103	12.2
⁵ TS1	-2452.741480	40.9	0.596243	39.0
³ TS1	-2452.721333	53.5	0.598646	53.2
⁵ TShooh	-2452.764937	26.1	0.597943	25.4
³ TShooh	-2452.750034	35.5	0.599080	35.4
⁵ Int	-2452.757585	30.7	0.598521	30.3
³ Int	-2452.738485	42.7	0.600823	43.8
⁵ Int-ho-oh1	-2452.778342	17.7	0.595813	15.6
³ Int-ho-oh1	-2452.767604	24.5	0.597657	23.5
⁵ Int-ho-oh2	-2452.778200	17.8	0.596515	16.1
³ Int-ho-oh2	-2452.765210	26.0	0.597686	25.0
⁵ TSoo	-2452.757753	30.6	0.597977	29.9
³ TSoo	-2452.738357	42.8	0.599845	43.2
⁵ TShat	-2452.780151	16.6	0.592529	12.4
³ TShat	-2452.769658	23.2	0.595829	21.1
⁵ P	-2452.823697	-10.7	0.601206	-9.5
³ P	-2452.831597	-15.7	0.603665	-12.9

Table S7. Free energy data for Model-1, B3LYP(SCRf)/B1 (298.15K, 1atom)

	G (Eh)	ΔG (kcal/mol)
⁵ RC	-1506.101153	0.0
³ RC	-1506.072875	17.7
⁵ TS1	-1506.073377	17.4
³ TS1	-1506.050107	32.0
⁵ TShooh	-1506.049873	32.2
³ TShooh	-1506.026998	46.5
⁵ Int	-1506.079933	13.3
³ Int	-1506.058315	26.9
⁵ Int-ho-oh	-1506.075335	16.2
³ Int-ho-oh	-1506.055946	28.4
⁵ TSoo	-1506.067743	21.0
³ TSoo	-1506.051737	31.0
⁵ Int-oh	-1506.076568	15.4
⁵ TShat	-1506.072353	18.1
³ TShat	-1506.054125	29.5
⁵ P	-1506.105234	-2.6
³ P	-1506.108007	-4.3

Table S8. Free energy data for Model-2, B3LYP(SCRf)/B1 (298.15K, 1atom)

	G (Eh)	ΔG (kcal/mol)
⁵ RC	-1312.021566	0.0
³ RC	-1311.997217	15.3
⁵ TS1	-1311.960253	38.5
³ TS1	-1311.934055	54.9
⁵ TShooh	-1311.975818	28.7
³ TShooh	-1311.956813	40.6
⁵ Int	-1311.974859	29.3
³ Int	-1311.949614	45.2
⁵ Int-ho-oh1	-1311.992024	18.5
³ Int-ho-oh1	-1311.972203	31.0
⁵ Int-ho-oh2	-1311.995686	16.2
³ Int-ho-oh2	-1311.978077	27.3
⁵ TSoo	-1311.97408	29.8
³ TSoo	-1311.947747	46.3
⁵ TShat	-1311.995589	16.3
³ TShat	-1311.978317	27.1
⁵ P	-1312.028665	-4.5
³ P	-1312.02933	-4.9

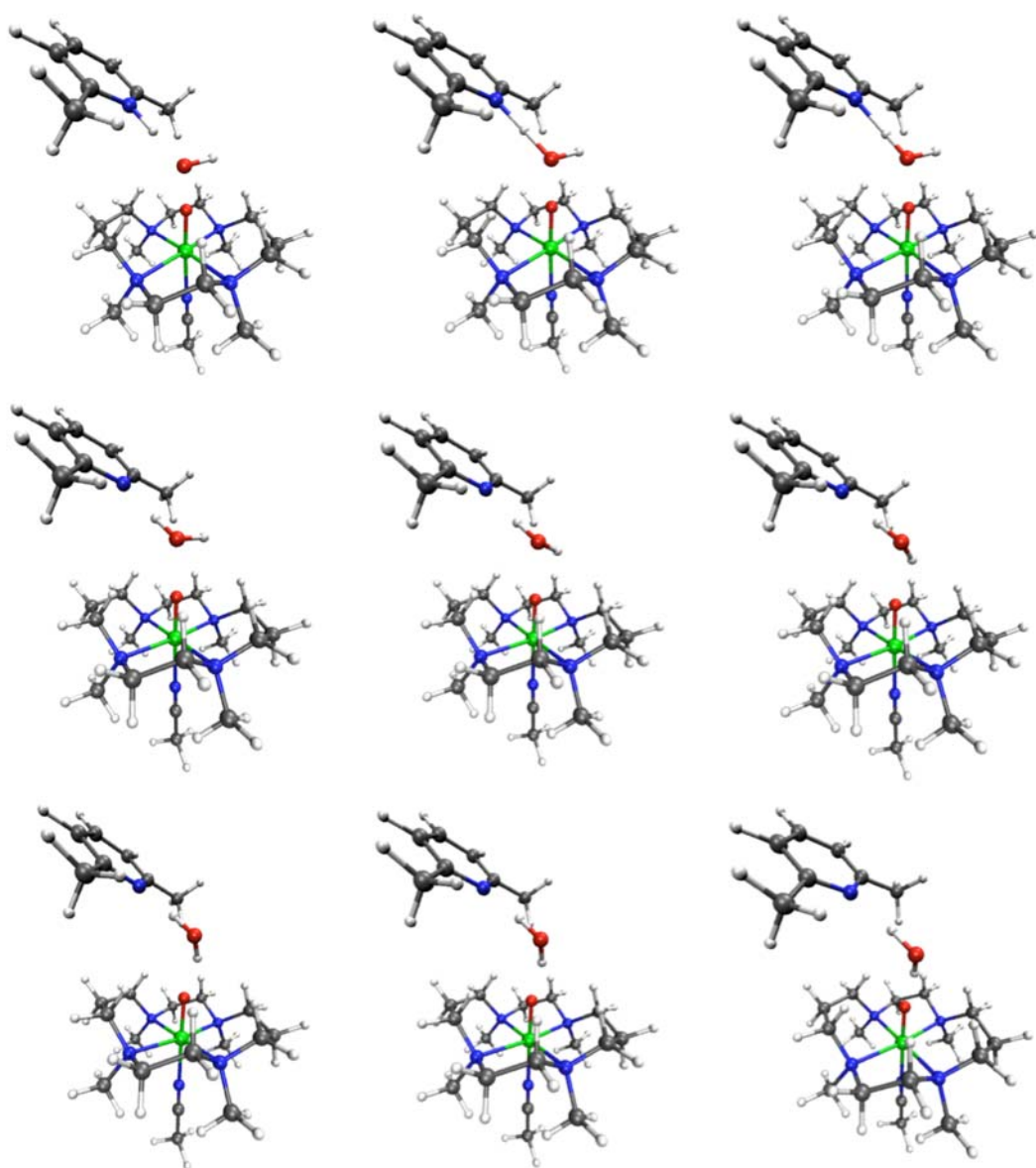


Figure S1. Geometric change during PCET obtained by IRC calculations (B3LYP(SCRF)/B1).

XYZ coordinates of optimized geometries (in Å)

			C	-1.265488	-5.967714	-0.692725
			H	-1.636974	-5.030941	-0.267429
			H	-1.061895	-5.793434	-1.757600
			H	-2.056001	-6.720846	-0.632881
=== Model-1, 5RC (gas-phase) ===						
Fe	0.126629	1.062156	0.009457			
N	-1.273998	1.058728	1.745292			
N	1.706074	1.249004	1.625156			
N	1.614414	0.284806	-1.447867			
N	-1.370475	0.109697	-1.387523			
C	-0.391401	0.698108	2.899363			
H	-0.912247	0.897143	3.846942			
H	-0.209883	-0.377522	2.842797			
C	0.923997	1.461752	2.883672			
H	1.524977	1.162303	3.753888			
H	0.745175	2.535384	2.983247			
C	2.425722	-0.067738	1.703411			
H	3.137635	-0.019240	2.540997			
H	1.689989	-0.839628	1.947961			
C	3.184287	-0.491618	0.439680			
H	3.719367	-1.409738	0.711894			
H	3.972167	0.224480	0.187494			
C	2.342261	-0.856560	-0.789622			
H	1.598277	-1.606901	-0.501782			
H	3.000401	-1.314418	-1.542819			
C	0.799020	-0.232954	-2.595204			
H	0.623077	0.603853	-3.275639			
H	1.379512	-0.977955	-3.156490			
C	-0.521016	-0.850360	-2.157247			
H	-0.343325	-1.713086	-1.511615			
H	-1.061229	-1.206560	-3.046439			
C	-2.484355	-0.669730	-0.748923			
H	-2.053670	-1.600327	-0.368882			
H	-3.206348	-0.937398	-1.533404			
C	-3.202578	0.042747	0.397535			
H	-3.551104	1.040611	0.108471			
H	-4.115986	-0.529030	0.601478			
C	-2.403822	0.069736	1.701388			
H	-1.968755	-0.919400	1.867092			
H	-3.071589	0.283358	2.547738			
C	-1.839477	2.422739	1.941958			
H	-2.413354	2.467327	2.877202			
H	-1.044937	3.168574	1.980326			
H	-2.504104	2.675203	1.114189			
C	2.685519	2.363101	1.529846			
H	3.318253	2.401054	2.427067			
H	2.152421	3.311265	1.433569			
H	3.331886	2.241950	0.662838			
C	2.587335	1.259952	-2.011291			
H	3.235155	1.658827	-1.234074			
H	2.047210	2.089989	-2.470828			
H	3.215187	0.779447	-2.773337			
C	-1.958896	1.125878	-2.299844			
H	-1.176562	1.709887	-2.786704			
H	-2.590475	1.812652	-1.733391			
H	-2.572208	0.642582	-3.072458			
N	0.065853	3.128023	-0.626350			
C	0.037850	4.233981	-0.972881			
C	0.001311	5.624115	-1.407643			
H	1.019892	6.021878	-1.468815			
H	-0.571685	6.223496	-0.692221			
H	-0.470477	5.697028	-2.393138			
O	-0.136941	-2.984013	0.503416			
O	-0.032355	-2.636731	1.914106			
H	0.296982	-3.930465	0.485802			
H	-0.684094	-3.238769	2.320937			
N	0.789060	-5.480869	0.541041			
C	1.937793	-5.834931	1.158749			
C	2.314892	-7.173057	1.275578			
C	1.487812	-8.160232	0.741670			
C	0.308641	-7.785299	0.104605			
C	-0.015927	-6.428578	0.015863			
C	2.794989	-4.719795	1.702645			
H	3.304581	-4.194283	0.883508			
H	2.183705	-3.988400	2.241235			
H	3.563854	-5.103630	2.377917			
H	3.238641	-7.433598	1.781552			
H	1.758282	-9.208622	0.826147			
H	-0.358467	-8.529371	-0.318340			
=== Model-1, 3RC (gas-phase) ===						
Fe	0.132410	0.903126	0.069502			
N	-1.232667	1.057396	1.704946			
N	1.631211	1.245226	1.559902			
N	1.547950	0.271394	-1.397479			
N	-1.314325	0.084951	-1.267757			
C	-0.399899	0.795853	2.921504			
H	-0.947737	1.087840	3.828079			
H	-0.226830	-0.281356	2.970551			
C	0.909377	1.544767	2.840325			
H	1.545829	1.292326	3.698512			
H	0.740679	2.623372	2.878839			
C	2.367333	-0.061429	1.705001			
H	3.075477	0.038794	2.539776			
H	1.637978	-0.827518	1.983757			
C	3.132711	-0.526394	0.462726			
H	3.638212	-1.455028	0.754576			
H	3.941916	0.165174	0.210142			
C	2.290632	-0.879059	-0.766912			
H	1.554138	-1.639421	-0.487438			
H	2.948860	-1.315263	-1.531714			
C	0.762658	-0.237729	-2.570197			
H	0.578592	0.608350	-3.236272			
H	1.361372	-0.962541	-3.137332			
C	-0.538870	-0.864414	-2.127968			
H	-0.356066	-1.760924	-1.532352			
H	-1.134880	-1.157572	-3.003224			
C	-2.435135	-0.715157	-0.660444			
H	-1.996573	-1.640565	-0.277286			
H	-3.126873	-0.983610	-1.470402			
C	-3.189617	-0.024119	0.467193			
H	-3.600761	0.944729	0.165630			
H	-4.062248	-0.647721	0.696014			
C	-2.363447	0.067558	1.742807			
H	-1.921307	-0.911465	1.945329			
H	-3.004780	0.328022	2.595599			
C	-1.808630	2.431937	1.775342			
H	-2.444569	2.529965	2.664493			
H	-1.016354	3.177480	1.819430			
H	-2.410683	2.630572	0.888456			
C	2.607873	2.358833	1.384977			
H	3.217892	2.465814	2.290922			
H	2.068820	3.289421	1.204976			
H	3.275155	2.175358	0.549152			
C	2.515673	1.256092	-1.959315			
H	3.200780	1.616850	-1.199359			
H	1.970680	2.106944	-2.369381			
H	3.104579	0.787376	-2.757994			
C	-1.909092	1.161386	-2.112244			
H	-1.130042	1.724290	-2.624246			
H	-2.473545	1.855373	-1.489239			
H	-2.585096	0.724628	-2.858363			
N	0.105583	3.098024	-0.634601			
C	0.084550	4.200234	-0.995865			
C	0.057395	5.586637	-1.449152			
H	1.077233	5.980647	-1.509743			
H	-0.518395	6.199433	-0.747852			
H	-0.406516	5.649281	-2.438925			
O	-0.136156	-2.987475	0.567381			
O	-0.010433	-2.634483	1.975038			
H	0.306600	-3.930186	0.539241			
H	-0.657613	-3.233616	2.393323			
N	0.810466	-5.476543	0.538018			
C	1.929396	-5.866024	1.187188			
C	2.299706	-7.210419	1.249607			
C	1.498328	-8.164989	0.626210			
C	0.349417	-7.752981	-0.043683			
C	0.029704	-6.393306	-0.073374			
C	2.766330	-4.785876	1.825308			
H	3.353267	-4.255655	1.062665			
H	2.133262	-4.050750	2.332222			

H	3.470339	-5.205101	2.548637
H	3.199036	-7.500131	1.783001
H	1.764073	-9.217193	0.666782
H	-0.297667	-8.471574	-0.535908
C	-1.186680	-5.889198	-0.809485
H	-1.633983	-5.034575	-0.292953
H	-0.916033	-5.562159	-1.822310
H	-1.941981	-6.672850	-0.910998

=== Model-1, 5TS1 (gas-phase) ===

Fe	0.195957	0.733153	0.114404
N	-1.307765	0.984496	1.723184
N	1.673176	1.324953	1.700500
N	1.809751	0.235101	-1.362431
N	-1.178069	-0.115197	-1.420623
C	-0.461296	0.685258	2.919977
H	-1.019283	0.903140	3.843299
H	-0.229216	-0.380277	2.900662
C	0.838202	1.486398	2.938583
H	1.420644	1.192569	3.822453
H	0.624006	2.551832	3.050707
C	2.604618	0.157294	1.841027
H	3.303351	0.372549	2.664279
H	2.002821	-0.704252	2.132218
C	3.435475	-0.184668	0.591034
H	4.116993	-0.984770	0.907025
H	4.098335	0.643739	0.321385
C	2.705021	-0.734805	-0.647098
H	2.072672	-1.568851	-0.335780
H	3.459597	-1.098200	-1.362291
C	1.081766	-0.444536	-2.483950
H	0.911087	0.302152	-3.262698
H	1.722431	-1.216887	-2.931856
C	-0.247891	-1.080439	-2.077789
H	-0.071351	-1.888236	-1.366645
H	-0.715242	-1.509909	-2.977833
C	-2.325773	-0.860094	-0.810457
H	-1.904229	-1.753178	-0.349352
H	-3.007923	-1.169685	-1.616153
C	-3.109659	-0.093033	0.262686
H	-3.417826	0.897392	-0.090691
H	-4.046751	-0.642152	0.416697
C	-2.417944	-0.014196	1.631561
H	-1.988692	-0.991181	1.859510
H	-3.161058	0.216528	2.408537
C	-1.893170	2.344395	1.833856
H	-2.514805	2.423359	2.736526
H	-1.107093	3.097827	1.879874
H	-2.513512	2.557937	0.962037
C	2.456143	2.577221	1.536744
H	3.079801	2.762045	2.422387
H	1.777615	3.420738	1.400717
H	3.107893	2.519301	0.667137
C	2.619773	1.325894	-1.965095
H	3.201102	1.845358	-1.206040
H	1.961333	2.050435	-2.447183
H	3.315387	0.924265	-2.715079
C	-1.703527	0.855941	-2.411675
H	-0.894171	1.442391	-2.847048
H	-2.394027	1.546304	-1.924422
H	-2.239271	0.335105	-3.217747
N	-0.003105	2.878158	-0.643313
C	-0.101918	3.970185	-1.020020
C	-0.226854	5.344975	-1.491132
H	0.765760	5.793350	-1.603066
H	-0.804023	5.936350	-0.772834
H	-0.737021	5.365699	-2.459609
O	0.162308	-1.918070	0.751732
O	0.483982	-2.243439	2.161195
H	0.495351	-3.566248	0.419295
H	-0.357160	-2.607010	2.489658
N	0.657211	-4.620312	0.349309
C	1.863180	-5.123197	0.727978
C	2.070966	-6.496690	0.633057
C	1.053776	-7.321653	0.158022
C	-0.171204	-6.766259	-0.213670
C	-0.363161	-5.393830	-0.111803
C	2.904589	-4.169185	1.228865

H	3.359432	-3.624227	0.392246
H	2.453260	-3.442336	1.909964
H	3.699609	-4.712338	1.743924
H	3.026886	-6.907773	0.937273
H	1.210743	-8.393458	0.083728
H	-0.980479	-7.389886	-0.576126
C	-1.650933	-4.717866	-0.482039
H	-2.004163	-4.073178	0.328694
H	-1.525168	-4.095081	-1.375077
H	-2.422096	-5.460500	-0.695623

=== Model-1, 3TS1 (gas-phase) ===

Fe	0.248601	0.608741	0.159786
N	-1.253767	0.839124	1.589107
N	1.552350	1.292359	1.687090
N	1.807462	0.296651	-1.243504
N	-1.012378	-0.120773	-1.350390
C	-0.523185	0.593574	2.871916
H	-1.175151	0.812944	3.729616
H	-0.255785	-0.465013	2.894852
C	0.725450	1.445805	2.936037
H	1.323277	1.179032	3.815782
H	0.468053	2.501484	3.040213
C	2.559362	0.192429	1.901991
H	3.212315	0.492374	2.734050
H	2.004746	-0.695691	2.211504
C	3.438350	-0.140783	0.691402
H	4.109051	-0.942887	1.023940
H	4.105410	0.690504	0.442561
C	2.729571	-0.677383	-0.557806
H	2.116512	-1.539198	-0.277494
H	3.489997	-0.996037	-1.285583
C	1.189202	-0.362913	-2.445315
H	1.018116	0.408796	-3.198282
H	1.894926	-1.078688	-2.885048
C	-0.111651	-1.052045	-2.094664
H	0.073202	-1.904976	-1.439345
H	-0.604331	-1.412832	-3.009306
C	-2.200454	-0.917760	-0.899733
H	-1.810611	-1.849400	-0.487395
H	-2.803425	-1.155792	-1.787012
C	-3.067848	-0.249558	0.162253
H	-3.462021	0.715707	-0.171682
H	-3.950655	-0.886062	0.298584
C	-2.375171	-0.152854	1.518760
H	-1.943704	-1.126718	1.758069
H	-3.104785	0.104910	2.298699
C	-1.824842	2.216949	1.573391
H	-2.480166	2.364246	2.441928
H	-1.032512	2.963125	1.585548
H	-2.404611	2.370111	0.663697
C	2.257549	2.595182	1.501111
H	2.774203	2.872356	2.428721
H	1.535842	3.368936	1.238482
H	2.997162	2.532863	0.709432
C	2.577951	1.458837	-1.777472
H	3.209237	1.902140	-1.014686
H	1.883934	2.219761	-2.135683
H	3.224009	1.129565	-2.601278
C	-1.484724	0.976823	-2.242861
H	-0.657506	1.616554	-2.544526
H	-2.202411	1.600239	-1.709574
H	-1.971752	0.558837	-3.133991
N	0.019066	3.575584	-0.856748
C	-0.105861	4.674157	-1.213219
C	-0.261746	6.055857	-1.660402
H	0.719832	6.522766	-1.789067
H	-0.831127	6.628483	-0.921446
H	-0.794815	6.084562	-2.615963
O	0.179641	-2.210812	0.812366
O	0.705766	-2.381096	2.186927
H	0.446662	-3.737553	0.486097
H	-0.036427	-2.814602	2.643611
N	0.590824	-4.818560	0.401389
C	1.842328	-5.328910	0.546839
C	2.021532	-6.704173	0.435280
C	0.923376	-7.526800	0.183696
C	-0.346318	-6.966382	0.053392

C	-0.502013	-5.588148	0.165539
C	2.960448	-4.370114	0.830095
H	3.248530	-3.833117	-0.082463
H	2.644240	-3.635846	1.577145
H	3.839979	-4.906613	1.192391
H	3.015343	-7.120877	0.554446
H	1.055841	-8.601225	0.099803
H	-1.216592	-7.587707	-0.127400
C	-1.830497	-4.899156	0.034739
H	-1.827491	-3.949290	0.574655
H	-2.055575	-4.693825	-1.019663
H	-2.632167	-5.533483	0.421755

=== Model-1, 5Int (gas-phase) ===

Fe	0.035141	0.665619	-0.005626
N	-1.276290	1.006894	1.759972
N	1.726472	1.005284	1.447922
N	1.432880	0.315279	-1.749275
N	-1.570791	0.305850	-1.534392
C	-0.371745	0.466365	2.818990
H	-0.795780	0.654587	3.817732
H	-0.302779	-0.610348	2.678047
C	1.036057	1.074080	2.779595
H	1.647743	0.579573	3.547213
H	0.985092	2.127847	3.062728
C	2.563959	-0.229434	1.322602
H	3.373502	-0.178155	2.068847
H	1.927398	-1.076265	1.577330
C	3.216665	-0.460802	-0.057538
H	3.864257	-1.337932	0.072778
H	3.911102	0.352242	-0.291882
C	2.334057	-0.788325	-1.280357
H	1.690472	-1.634626	-1.040664
H	3.000064	-1.069974	-2.111031
C	0.530307	-0.148517	-2.859058
H	0.402542	0.692480	-3.544631
H	1.025627	-0.941217	-3.436765
C	-0.845805	-0.657778	-2.413905
H	-0.733013	-1.578609	-1.843343
H	-1.436353	-0.875841	-3.317960
C	-2.753498	-0.356960	-0.902891
H	-2.445149	-1.366009	-0.625243
H	-3.553156	-0.442978	-1.653836
C	-3.313952	0.351102	0.343338
H	-3.510587	1.410333	0.142928
H	-4.302065	-0.088413	0.528009
C	-2.516815	0.178098	1.648622
H	-2.220048	-0.868897	1.738083
H	-3.170048	0.405560	2.504012
C	-1.653663	2.405111	2.077257
H	-2.175707	2.455428	3.043449
H	-0.767373	3.037887	2.120303
H	-2.311665	2.802779	1.303251
C	2.589543	2.208809	1.342155
H	3.312033	2.244595	2.170009
H	1.972231	3.107563	1.370575
H	3.144598	2.209015	0.405986
C	2.249778	1.431100	-2.290447
H	2.950280	1.799114	-1.543386
H	1.598341	2.256412	-2.580427
H	2.824428	1.104135	-3.168629
C	-2.030132	1.473537	-2.320618
H	-1.180444	1.999407	-2.756366
H	-2.560967	2.174717	-1.674745
H	-2.706808	1.157950	-3.127976
N	0.020232	3.009333	-0.508109
C	0.007837	4.142369	-0.755413
C	-0.008904	5.568026	-1.067778
H	1.005728	5.916182	-1.286308
H	-0.401948	6.134652	-0.217559
H	-0.642960	5.754180	-1.940559
O	-0.155730	-1.466446	0.212297
O	0.094078	-2.314876	1.409244
H	0.730272	-3.968137	1.060234
H	-0.816483	-2.493394	1.705840
N	1.051703	-4.952819	0.935229
C	1.883047	-5.477828	1.873554
C	2.310916	-6.790578	1.704724

C	1.880027	-7.519544	0.595959
C	1.022324	-6.936212	-0.338442
C	0.599103	-5.624757	-0.156943
C	2.280569	-4.613760	3.035224
H	3.371474	-4.545741	3.104887
H	1.871128	-3.604321	2.947713
H	1.923382	-5.052853	3.973717
H	2.975437	-7.231252	2.439861
H	2.212275	-8.544283	0.459778
H	0.677293	-7.491554	-1.203597
C	-0.347766	-4.908498	-1.075180
H	-0.324270	-3.826541	-0.912719
H	-0.100214	-5.121014	-2.119362
H	-1.373313	-5.261290	-0.907355

=== Model-1, 3Int (gas-phase) ===

Fe	0.019300	0.215467	0.070691
N	-1.187916	0.706083	1.706847
N	1.630917	0.689866	1.362367
N	1.275378	-0.012421	-1.648303
N	-1.551845	-0.002189	-1.288026
C	-0.345669	0.250010	2.852747
H	-0.799293	0.552088	3.808707
H	-0.307106	-0.838139	2.814824
C	1.058298	0.820309	2.751310
H	1.716085	0.327575	3.477234
H	1.049937	1.880462	3.010763
C	2.553290	-0.494442	1.287775
H	3.370299	-0.340180	2.008619
H	1.974769	-1.361774	1.607642
C	3.180585	-0.756736	-0.092282
H	3.826156	-1.635220	0.036459
H	3.871205	0.049696	-0.358115
C	2.253546	-1.090606	-1.272840
H	1.658206	-1.970140	-1.025018
H	2.879227	-1.312849	-2.149985
C	0.381288	-0.484375	-2.767483
H	0.244991	0.349727	-3.458549
H	0.878980	-1.279980	-3.335048
C	-0.970434	-0.967139	-2.269691
H	-0.868383	-1.917858	-1.745994
H	-1.650726	-1.103812	-3.123709
C	-2.789831	-0.620773	-0.716603
H	-2.526436	-1.644888	-0.444484
H	-3.552403	-0.661848	-1.507323
C	-3.362229	0.086013	0.512203
H	-3.629037	1.125866	0.297728
H	-4.313676	-0.407421	0.745845
C	-2.491995	-0.025089	1.764505
H	-2.260583	-1.079450	1.935499
H	-3.052342	0.333723	2.639651
C	-1.445743	2.170410	1.802883
H	-1.915370	2.414979	2.765554
H	-0.519442	2.732816	1.698348
H	-2.108380	2.486008	0.997979
C	2.399952	1.949334	1.123659
H	3.071741	2.143947	1.969533
H	1.711513	2.786725	1.000233
H	3.006915	1.877673	0.228081
C	2.007948	1.172530	-2.189266
H	2.829870	1.458352	-1.541365
H	1.329497	2.023045	-2.273940
H	2.428383	0.935165	-3.174785
C	-1.906731	1.276450	-1.964596
H	-1.014454	1.782249	-2.330517
H	-2.393701	1.950199	-1.260442
H	-2.589944	1.088283	-2.804178
N	0.132203	3.932069	-0.819526
C	0.121967	5.066244	-1.069856
C	0.109416	6.492601	-1.385009
H	1.119710	6.832722	-1.632964
H	-0.254559	7.065286	-0.526246
H	-0.546807	6.684047	-2.239760
O	-0.142639	-1.910256	0.325716
O	0.073658	-2.669376	1.590393
H	0.700111	-4.313079	1.270591
H	-0.843740	-2.823676	1.878304
N	1.045374	-5.290022	1.134054

C	1.860440	-5.817640	2.084799	H	-0.794597	-2.645142	1.458268
C	2.326187	-7.115134	1.899104	N	1.133113	-5.025674	1.015243
C	1.946335	-7.827903	0.761470	C	1.734212	-5.523848	2.127229
C	1.102516	-7.243345	-0.184580	C	2.169231	-6.845166	2.100575
C	0.642076	-5.946749	0.013772	C	1.978941	-7.611034	0.950123
C	2.194925	-4.973863	3.280820	C	1.351625	-7.055789	-0.166075
H	3.276926	-4.955835	3.445884	C	0.919337	-5.734929	-0.122704
H	1.838810	-3.947271	3.163525	C	1.894284	-4.614631	3.311504
H	1.736848	-5.396995	4.182647	H	2.953537	-4.379455	3.469694
H	2.979977	-7.556600	2.643295	H	1.347124	-3.679083	3.170225
H	2.308153	-8.840656	0.611570	H	1.532545	-5.106122	4.220305
H	0.797353	-7.786039	-1.072423	H	2.649344	-7.264233	2.978104
C	-0.293862	-5.230428	-0.915157	H	2.315738	-8.642992	0.924654
H	-0.273676	-4.148236	-0.748569	H	1.190603	-7.640047	-1.065524
H	-0.033510	-5.443028	-1.956138	C	0.217536	-5.046353	-1.258544
H	-1.320810	-5.585477	-0.759549	H	-0.015768	-4.007229	-1.011450
				H	0.840298	-5.065296	-2.159609
				H	-0.715872	-5.567511	-1.499473

=== Model-1, 5TSoo (gas-phase) ===

Fe	-0.006746	0.607255	-0.036681
N	-1.223436	0.996444	1.779757
N	1.745658	0.929701	1.353922
N	1.306014	0.354440	-1.864689
N	-1.657930	0.407931	-1.538182
C	-0.304961	0.364948	2.778628
H	-0.693588	0.513220	3.797585
H	-0.275009	-0.704153	2.569983
C	1.117143	0.934773	2.720484
H	1.745525	0.371409	3.423288
H	1.114964	1.968636	3.073372
C	2.569256	-0.305441	1.138758
H	3.411092	-0.284571	1.849110
H	1.937746	-1.158552	1.384694
C	3.160339	-0.481273	-0.275576
H	3.811773	-1.362398	-0.207386
H	3.844237	0.340361	-0.511400
C	2.227256	-0.764722	-1.470888
H	1.597831	-1.624401	-1.242319
H	2.858853	-1.009537	-2.338819
C	0.366056	-0.074188	-2.959754
H	0.244959	0.776869	-3.633717
H	0.827567	-0.872826	-3.555418
C	-1.014388	-0.549371	-2.488620
H	-0.925486	-1.501423	-1.967913
H	-1.648058	-0.692105	-3.377369
C	-2.839619	-0.230553	-0.875668
H	-2.561154	-1.258974	-0.640258
H	-3.667219	-0.264263	-1.599129
C	-3.327897	0.462612	0.408629
H	-3.487066	1.534297	0.243478
H	-4.327161	0.058068	0.611662
C	-2.500245	0.218823	1.682524
H	-2.241155	-0.840001	1.738550
H	-3.116993	0.452566	2.562334
C	-1.529787	2.392912	2.170019
H	-1.996769	2.421722	3.164407
H	-0.619497	2.991672	2.188264
H	-2.214394	2.842960	1.449628
C	2.610286	2.133104	1.262874
H	3.376113	2.121339	2.051167
H	2.003446	3.032752	1.372889
H	3.114370	2.179652	0.299255
C	2.103309	1.492029	-2.391718
H	2.817676	1.842727	-1.649862
H	1.440977	2.320579	-2.644166
H	2.658968	1.192474	-3.291230
C	-2.105531	1.620033	-2.265032
H	-1.257494	2.126029	-2.726218
H	-2.578261	2.318862	-1.574059
H	-2.829814	1.353165	-3.047398
N	-0.000042	2.999931	-0.482611
C	0.016876	4.146088	-0.658566
C	0.035536	5.588198	-0.882109
H	1.055164	5.921433	-1.100754
H	-0.324657	6.111357	0.009589
H	-0.610405	5.845257	-1.727842
O	-0.189596	-1.179175	0.128388
O	0.153731	-2.464685	1.337883
H	0.792961	-4.026815	1.045394

=== Model-1, 3TSoo (gas-phase) ===

Fe	-0.014765	0.169794	0.040400
N	-1.186953	0.710852	1.699782
N	1.620592	0.656176	1.292535
N	1.214147	0.033739	-1.722923
N	-1.590628	0.047438	-1.293902
C	-0.328358	0.190561	2.808561
H	-0.761331	0.458029	3.783475
H	-0.301566	-0.895441	2.716705
C	1.079158	0.746781	2.700371
H	1.744650	0.215190	3.389658
H	1.094701	1.796838	2.998347
C	2.559270	-0.514701	1.174436
H	3.392201	-0.352371	1.874267
H	2.001059	-1.394507	1.495116
C	3.155566	-0.741231	-0.224826
H	3.805244	-1.620974	-0.131659
H	3.838347	0.072586	-0.489150
C	2.205721	-1.049811	-1.393570
H	1.622459	-1.941168	-1.163082
H	2.813170	-1.240814	-2.290268
C	0.296638	-0.417190	-2.834187
H	0.157806	0.426132	-3.513262
H	0.779706	-1.210103	-3.416792
C	-1.054483	-0.893572	-2.325379
H	-0.964956	-1.865473	-1.841394
H	-1.757524	-0.976023	-3.166866
C	-2.840158	-0.551634	-0.724849
H	-2.603196	-1.589077	-0.480820
H	-3.606390	-0.551674	-1.512449
C	-3.384922	0.142212	0.523264
H	-3.640203	1.189150	0.329808
H	-4.340013	-0.342694	0.759297
C	-2.499502	-0.006246	1.759949
H	-2.273967	-1.064876	1.904438
H	-3.041388	0.344770	2.649318
C	-1.414605	2.174829	1.847475
H	-1.843949	2.397301	2.833717
H	-0.483612	2.725743	1.725817
H	-2.102339	2.524545	1.078208
C	2.364499	1.931811	1.060007
H	3.051017	2.118972	1.895231
H	1.663734	2.762816	0.967146
H	2.954013	1.884613	0.151478
C	1.932325	1.234691	-2.250502
H	2.776700	1.496193	-1.621943
H	1.256383	2.090549	-2.287701
H	2.318719	1.024615	-3.255576
C	-1.908573	1.367606	-1.911165
H	-1.004388	1.863547	-2.260132
H	-2.373585	2.022756	-1.176359
H	-2.599412	1.233257	-2.753975
N	0.115585	3.984117	-0.795454
C	0.126992	5.125489	-1.010941
C	0.141782	6.560793	-1.281920
H	1.085927	6.844829	-1.757131
H	0.034441	7.121727	-0.348225
H	-0.683428	6.826993	-1.949782
O	-0.145404	-1.594569	0.299693

O	0.252898	-2.806583	1.569431	H	-0.817865	5.985527	-1.314467
H	0.796786	-4.356101	1.248709	O	-0.009151	-0.977076	-0.044973
H	-0.684304	-2.949571	1.785775	O	0.059682	-2.782056	1.151190
N	1.113750	-5.367599	1.180733	H	0.722836	-4.261820	1.176167
C	1.786892	-5.892484	2.236889	H	-0.805094	-2.868494	0.715572
C	2.191765	-7.221950	2.162798	N	1.067408	-5.264801	1.315660
C	1.898738	-7.969030	1.021858	C	0.914692	-5.821060	2.544099
C	1.200053	-7.386857	-0.036854	C	1.353194	-7.128764	2.732615
C	0.800186	-6.058261	0.055130	C	1.929244	-7.822497	1.668636
C	2.053310	-5.002441	3.416975	C	2.061897	-7.209324	0.421954
H	3.129672	-4.823063	3.522818	C	1.616118	-5.903036	0.252056
H	1.547316	-4.039608	3.309353	C	0.281959	-4.986913	3.620833
H	1.713267	-5.482873	4.340277	H	0.999003	-4.801937	4.429005
H	2.728902	-7.661420	2.996215	H	-0.055648	-4.026039	3.223648
H	2.211423	-9.006951	0.958742	H	-0.571526	-5.514987	4.059261
H	0.959633	-7.956093	-0.928219	H	1.239188	-7.592724	3.706263
C	0.026896	-5.340769	-1.015016	H	2.272407	-8.842983	1.809654
H	-0.129811	-4.290181	-0.755567	H	2.503511	-7.736421	-0.416791
H	0.557885	-5.396894	-1.971431	C	1.696695	-5.151655	-1.046791
H	-0.950216	-5.816074	-1.159617	H	1.305087	-4.136990	-0.936631

=== Model-1, 5Int-oh (gas-phase) ===

Fe	0.018808	0.721470	-0.193033
N	-0.946009	0.889461	1.806417
N	1.936933	0.938767	0.997155
N	1.108676	0.633693	-2.174101
N	-1.791335	0.576054	-1.479646
C	0.105359	0.193979	2.617970
H	-0.152048	0.249361	3.686527
H	0.112941	-0.853788	2.312552
C	1.489784	0.817422	2.428925
H	2.221889	0.227874	2.996617
H	1.505516	1.822410	2.857431
C	2.727741	-0.269996	0.581131
H	3.646908	-0.296321	1.186481
H	2.125345	-1.145549	0.824031
C	3.143496	-0.318816	-0.902402
H	3.796477	-1.196959	-0.989226
H	3.795183	0.525881	-1.148596
C	2.071626	-0.507050	-1.993510
H	1.475926	-1.391659	-1.768518
H	2.589503	-0.666652	-2.951454
C	0.042504	0.283000	-3.176477
H	-0.190297	1.191903	-3.736050
H	0.438175	-0.434944	-3.906851
C	-1.240793	-0.288863	-2.569946
H	-1.044528	-1.266734	-2.132014
H	-1.983284	-0.406800	-3.372891
C	-2.854742	-0.165994	-0.725844
H	-2.513669	-1.197576	-0.621596
H	-3.765259	-0.177847	-1.341809
C	-3.192327	0.391388	0.666553
H	-3.403088	1.466290	0.622863
H	-4.144813	-0.070017	0.954897
C	-2.195996	0.062404	1.791205
H	-1.886506	-0.980475	1.705621
H	-2.698738	0.183393	2.761548
C	-1.246269	2.225840	2.371605
H	-1.606746	2.134440	3.405444
H	-0.355887	2.855110	2.365391
H	-2.015101	2.721343	1.776479
C	2.788113	2.152161	0.904917
H	3.642394	2.078626	1.592052
H	2.202061	3.034728	1.165088
H	3.174226	2.282452	-0.104357
C	1.833331	1.820152	-2.698792
H	2.636002	2.114727	-2.025769
H	1.143821	2.659381	-2.797373
H	2.270480	1.601904	-3.682776
C	-2.368815	1.818993	-2.046985
H	-1.600542	2.401426	-2.555514
H	-2.787090	2.433472	-1.248593
H	-3.167206	1.580070	-2.762731
N	-0.046817	3.059355	-0.387129
C	-0.073311	4.216126	-0.456704
C	-0.106554	5.671856	-0.543509
H	0.886566	6.055151	-0.799503
H	-0.414776	6.097380	0.417068

=== Model-1, 5TSoh (gas-phase) ===

Fe	0.001911	0.783261	-0.234976
N	-0.957098	0.821469	1.767445
N	1.924705	0.876145	0.960759
N	1.097578	0.690449	-2.210550
N	-1.802380	0.630650	-1.519413
C	0.092241	0.091387	2.554342
H	-0.168829	0.112072	3.622598
H	0.097929	-0.946993	2.214657
C	1.475707	0.718953	2.388236
H	2.206014	0.111810	2.938828
H	1.493399	1.712289	2.843253
C	2.689775	-0.338776	0.509662
H	3.604554	-0.400425	1.118073
H	2.070188	-1.209994	0.725638
C	3.110657	-0.349460	-0.971370
H	3.740847	-1.240821	-1.084827
H	3.783523	0.486045	-1.190685
C	2.036234	-0.477944	-2.066488
H	1.423948	-1.359101	-1.874870
H	2.548424	-0.614827	-3.030257
C	0.028321	0.393215	-3.226024
H	-0.199273	1.327486	-3.744503
H	0.418936	-0.295117	-3.986590
C	-1.254249	-0.197012	-2.640157
H	-1.063492	-1.192445	-2.240878
H	-1.999138	-0.283708	-3.443990
C	-2.865310	-0.142048	-0.792713
H	-2.521664	-1.175871	-0.724621
H	-3.772004	-0.134328	-1.413435
C	-3.206531	0.363699	0.616630
H	-3.420777	1.438833	0.613847
H	-4.156978	-0.111756	0.887702
C	-2.207035	-0.007344	1.722968
H	-1.896733	-1.046315	1.598966
H	-2.702969	0.077108	2.699998
C	-1.260052	2.135038	2.386445
H	-1.627243	1.998283	3.412343
H	-0.368878	2.762658	2.416130
H	-2.026105	2.655521	1.809104
C	2.802719	2.073601	0.906480
H	3.657063	1.954488	1.586385
H	2.239425	2.959500	1.203605
H	3.187624	2.230789	-0.099281
C	1.849545	1.876563	-2.699654
H	2.662906	2.128200	-2.022436
H	1.180360	2.735029	-2.770499
H	2.276331	1.677910	-3.691850
C	-2.383572	1.892741	-2.042876
H	-1.618096	2.492883	-2.534929
H	-2.802802	2.478074	-1.223296
H	-3.182851	1.675360	-2.763756
N	-0.036496	3.007768	-0.340812
C	-0.046576	4.165773	-0.374757
C	-0.059217	5.622723	-0.416679

H	0.931702	5.997829	-0.693346	C	0.202312	3.925194	0.010757
H	-0.329643	6.022684	0.566230	C	0.380008	5.349889	0.254065
H	-0.790105	5.969823	-1.154573	H	1.376324	5.663818	-0.075608
O	-0.026252	-0.872774	-0.129508	H	0.274759	5.561691	1.323669
O	0.120923	-2.881049	1.069832	H	-0.374961	5.920442	-0.297650
H	0.637261	-4.056098	1.189784	O	-0.446938	-0.830959	-0.781913
H	-0.725873	-3.009975	0.612024	O	0.574991	-3.462512	0.700238
N	1.057359	-5.183518	1.383325	H	0.952276	-4.196511	1.276761
C	0.939389	-5.716424	2.621854	H	0.050786	-3.940739	0.039495
C	1.401808	-7.010732	2.856767	N	1.512702	-5.613779	2.185344
C	1.979889	-7.731631	1.813586	C	0.732123	-6.152316	3.143481
C	2.084341	-7.153949	0.549022	C	1.100730	-7.322399	3.813436
C	1.606148	-5.860734	0.348948	C	2.302002	-7.942690	3.479866
C	0.315055	-4.869352	3.697534	C	3.101818	-7.381351	2.487027
H	1.071953	-4.562328	4.429551	C	2.676942	-6.209289	1.855950
H	-0.137115	-3.972067	3.269155	C	-0.556967	-5.437529	3.471493
H	-0.448267	-5.436088	4.240303	H	-0.500938	-4.963429	4.459726
H	1.305543	-7.441548	3.847783	H	-0.761928	-4.661956	2.729113
H	2.343940	-8.740381	1.984043	H	-1.401361	-6.134810	3.497979
H	2.526014	-7.697497	-0.279666	H	0.451296	-7.738222	4.577668
C	1.656660	-5.173299	-0.990087	H	2.608251	-8.855497	3.982594
H	1.312377	-4.139678	-0.907085	H	4.040609	-7.843807	2.198345
H	2.676147	-5.180648	-1.390457	C	3.511243	-5.550313	0.783983
H	1.021564	-5.697271	-1.714119	H	2.910354	-4.831137	0.221007
				H	4.361586	-5.014349	1.225728
				H	3.923105	-6.289934	0.089685

=== Model-1, 5P (gas-phase) ===

Fe	-0.194732	0.733646	-0.519964
N	-0.908979	0.379021	1.529724
N	1.819136	0.287003	0.343845
N	0.629677	0.937670	-2.618448
N	-2.143685	1.052469	-1.535375
C	0.112388	-0.612370	2.008327
H	-0.018804	-0.774325	3.087270
H	-0.049089	-1.565721	1.498801
C	1.538853	-0.129610	1.765028
H	2.228065	-0.933278	2.049530
H	1.768286	0.726163	2.404671
C	2.355342	-0.879264	-0.451287
H	3.329240	-1.143055	-0.014202
H	1.687153	-1.728005	-0.287009
C	2.578786	-0.619959	-1.951205
H	3.028098	-1.544051	-2.336308
H	3.352176	0.140473	-2.104013
C	1.375407	-0.348458	-2.869770
H	0.654639	-1.162674	-2.787103
H	1.737333	-0.321821	-3.907482
C	-0.582913	1.026959	-3.503060
H	-0.729191	2.079914	-3.754290
H	-0.387697	0.505562	-4.448604
C	-1.856203	0.460736	-2.880847
H	-1.772102	-0.618288	-2.751720
H	-2.696893	0.654824	-3.560881
C	-3.209757	0.238071	-0.854809
H	-2.995869	-0.812647	-1.060544
H	-4.168308	0.480448	-1.332712
C	-3.325691	0.432767	0.661520
H	-3.407140	1.492484	0.929509
H	-4.287821	-0.006029	0.951864
C	-2.257453	-0.283369	1.496662
H	-2.111252	-1.293347	1.109242
H	-2.605677	-0.375992	2.534088
C	-0.962316	1.555872	2.435359
H	-1.242142	1.237079	3.447422
H	0.008079	2.050482	2.482559
H	-1.702386	2.273942	2.078797
C	2.841136	1.366866	0.399894
H	3.742946	1.003716	0.909311
H	2.451409	2.223695	0.950992
H	3.122747	1.691129	-0.599144
C	1.501939	2.094729	-2.958006
H	2.422227	2.071770	-2.379901
H	0.978871	3.028544	-2.747537
H	1.764463	2.071104	-4.023656
C	-2.611787	2.456039	-1.673682
H	-1.852845	3.069836	-2.158877
H	-2.821941	2.877495	-0.689867
H	-3.530042	2.491107	-2.273746
N	0.061178	2.792218	-0.181284

=== Model-1, 3P (gas-phase) ===

Fe	-0.197150	0.708902	-0.556262
N	-0.937030	0.354077	1.388283
N	1.721737	0.268120	0.289950
N	0.614077	0.959852	-2.548270
N	-2.081528	1.063155	-1.492811
C	0.052960	-0.641351	1.928751
H	-0.130472	-0.786627	3.001827
H	-0.091080	-1.599528	1.423244
C	1.467469	-0.152861	1.718856
H	2.171908	-0.945104	1.994213
H	1.685862	0.705448	2.358402
C	2.287639	-0.902679	-0.483344
H	3.253237	-1.148113	-0.020294
H	1.624641	-1.755433	-0.323849
C	2.537909	-0.647024	-1.974424
H	2.956846	-1.582145	-2.366565
H	3.334954	0.090518	-2.117187
C	1.341408	-0.322351	-2.875779
H	0.610442	-1.129224	-2.831933
H	1.699193	-0.239138	-3.910939
C	-0.572504	1.118202	-3.464935
H	-0.699487	2.184751	-3.661961
H	-0.356876	0.644859	-4.430074
C	-1.840800	0.537762	-2.878150
H	-1.771231	-0.547224	-2.805461
H	-2.694867	0.783726	-3.522901
C	-3.198956	0.249891	-0.899148
H	-2.994435	-0.796279	-1.133828
H	-4.123725	0.534558	-1.417068
C	-3.374627	0.388015	0.608579
H	-3.505911	1.430578	0.918272
H	-4.319589	-0.107226	0.861881
C	-2.280869	-0.318869	1.400997
H	-2.137970	-1.323518	0.999760
H	-2.583558	-0.420040	2.451070
C	-1.000773	1.547172	2.279697
H	-1.310741	1.238724	3.285097
H	-0.027774	2.030799	2.347241
H	-1.723662	2.267236	1.895846
C	2.756430	1.341048	0.365749
H	3.633897	0.960013	0.901731
H	2.365288	2.202546	0.905623
H	3.075587	1.656746	-0.622328
C	1.512756	2.112469	-2.853965
H	2.446951	2.042711	-2.306241
H	1.019002	3.048647	-2.595852
H	1.745558	2.120472	-3.925766
C	-2.520444	2.486091	-1.559051
H	-1.760614	3.103690	-2.034669
H	-2.699404	2.867002	-0.553871

H	-3.449476	2.561930	-2.136608
N	0.090715	2.788688	-0.175536
C	0.245372	3.916695	0.035670
C	0.439434	5.335568	0.304507
H	1.473027	5.621446	0.081610
H	0.230696	5.548163	1.358588
H	-0.236834	5.931128	-0.318182
O	-0.459070	-0.848254	-0.855515
O	0.592385	-3.498858	0.706837
H	0.972889	-4.224721	1.291135
H	0.067931	-3.984659	0.051822
N	1.546463	-5.623529	2.220703
C	0.776030	-6.148375	3.194573
C	1.156657	-7.302832	3.884534
C	2.359682	-7.921848	3.554764
C	3.148987	-7.374862	2.545698
C	2.712123	-6.218114	1.894756
C	-0.515485	-5.435590	3.517512
H	-0.458625	-4.948008	4.499112
H	-0.727037	-4.671408	2.765219
H	-1.356279	-6.136682	3.556235
H	0.515230	-7.707831	4.661248
H	2.675373	-8.822637	4.073085
H	4.088823	-7.836851	2.259614
C	3.534334	-5.575969	0.803319
H	2.929602	-4.858651	0.242169
H	4.395544	-5.042121	1.226015
H	3.929819	-6.325779	0.110293

=== Model-1, 5RC ===

Fe	0.103924	1.034532	0.036512
N	-1.307809	1.150224	1.767856
N	1.681890	1.306892	1.633052
N	1.616187	0.202502	-1.393017
N	-1.377609	0.041856	-1.346288
C	-0.423680	0.817724	2.925038
H	-0.934895	1.049664	3.870423
H	-0.248688	-0.260556	2.900601
C	0.898211	1.569873	2.880419
H	1.496595	1.297592	3.760908
H	0.724428	2.646623	2.938716
C	2.424444	0.011963	1.772488
H	3.135766	0.112574	2.606098
H	1.701355	-0.759245	2.053864
C	3.192579	-0.455443	0.529736
H	3.745117	-1.349788	0.843126
H	3.963860	0.266519	0.245761
C	2.364276	-0.889461	-0.686125
H	1.634368	-1.640678	-0.368502
H	3.035615	-1.368110	-1.414498
C	0.803031	-0.385039	-2.505440
H	0.630166	0.405870	-3.238121
H	1.381292	-1.167975	-3.014575
C	-0.521103	-0.968437	-2.034618
H	-0.345784	-1.778524	-1.323705
H	-1.051546	-1.391342	-2.900173
C	-2.510329	-0.677669	-0.682522
H	-2.106163	-1.598790	-0.254202
H	-3.235008	-0.965485	-1.457728
C	-3.220021	0.102003	0.426271
H	-3.532740	1.096110	0.089347
H	-4.149360	-0.438066	0.643110
C	-2.436645	0.167081	1.739701
H	-2.012202	-0.819833	1.942713
H	-3.116902	0.406863	2.569285
C	-1.860748	2.522559	1.913695
H	-2.440109	2.601942	2.843784
H	-1.059713	3.261466	1.930466
H	-2.513208	2.752883	1.070786
C	2.637010	2.433387	1.473539
H	3.274314	2.525096	2.363844
H	2.083407	3.363209	1.332663
H	3.277664	2.281815	0.607418
C	2.564491	1.167169	-2.008365
H	3.211255	1.611995	-1.255837
H	2.003473	1.966407	-2.494958
H	3.193601	0.662438	-2.754046
C	-1.927996	1.017143	-2.321828

H	-1.127438	1.575693	-2.807117
H	-2.570847	1.732641	-1.806977
H	-2.518962	0.498553	-3.089550
N	0.102074	3.051985	-0.678341
C	0.074827	4.141817	-1.067748
C	0.041035	5.511246	-1.554574
H	1.045462	5.813708	-1.865375
H	-0.306585	6.176323	-0.758662
H	-0.638032	5.581887	-2.409226
O	-0.217389	-2.970124	0.835613
O	0.067210	-2.680199	2.231696
H	0.212441	-3.881459	0.727591
H	-0.726935	-3.037382	2.671055
N	0.798996	-5.499334	0.537717
C	1.952669	-5.911321	1.100039
C	2.369358	-7.243148	1.007947
C	1.572152	-8.155524	0.319642
C	0.381539	-7.718730	-0.257349
C	0.021171	-6.373607	-0.130898
C	2.770773	-4.869195	1.819046
H	3.284458	-4.220252	1.097617
H	2.126439	-4.229981	2.430377
H	3.531017	-5.329942	2.455566
H	3.299511	-7.553187	1.473051
H	1.872610	-9.196342	0.238858
H	-0.265057	-8.404862	-0.794725
C	-1.244076	-5.829063	-0.744968
H	-1.740364	-5.136280	-0.058301
H	-1.017399	-5.271935	-1.663195
H	-1.938732	-6.632446	-1.004171

==== Model-1, 3RC ====

Fe	0.105190	0.914503	0.073492
N	-1.237439	1.137059	1.722196
N	1.630485	1.257645	1.535794
N	1.497745	0.230623	-1.401297
N	-1.370787	0.109162	-1.236704
C	-0.391487	0.871468	2.926687
H	-0.917930	1.184006	3.838715
H	-0.239048	-0.208336	2.983776
C	0.930559	1.592430	2.817562
H	1.571772	1.340143	3.671829
H	0.782003	2.673781	2.838470
C	2.343908	-0.056836	1.693218
H	3.059391	0.041003	2.521650
H	1.600836	-0.804039	1.986296
C	3.092679	-0.551441	0.452384
H	3.590998	-1.480235	0.755275
H	3.904686	0.129453	0.181717
C	2.240192	-0.914223	-0.767018
H	1.502835	-1.667859	-0.474410
H	2.890528	-1.361118	-1.531878
C	0.685841	-0.288458	-2.549693
H	0.507940	0.545107	-3.231641
H	1.260328	-1.039991	-3.106270
C	-0.621946	-0.876827	-2.076199
H	-0.447033	-1.759324	-1.457641
H	-1.231279	-1.183992	-2.936909
C	-2.502062	-0.647538	-0.603045
H	-2.084240	-1.575366	-0.203913
H	-3.210000	-0.915706	-1.398887
C	-3.225415	0.083152	0.519778
H	-3.607266	1.059103	0.204693
H	-4.111695	-0.512862	0.767398
C	-2.384934	0.173944	1.785749
H	-1.963577	-0.812005	1.997797
H	-3.012562	0.457463	2.641320
C	-1.778731	2.524781	1.775973
H	-2.403283	2.649733	2.669729
H	-0.968348	3.250721	1.800393
H	-2.382349	2.724395	0.890596
C	2.620391	2.351994	1.326253
H	3.250080	2.456754	2.219013
H	2.092738	3.288634	1.146929
H	3.265701	2.148559	0.478295
C	2.463920	1.196189	-1.995033
H	3.165229	1.561610	-1.252657
H	1.920921	2.046103	-2.408221

H	3.033108	0.705576	-2.794965
C	-1.947399	1.179305	-2.100269
H	-1.161306	1.718044	-2.625991
H	-2.495029	1.895828	-1.488315
H	-2.633975	0.737535	-2.833656
N	0.114098	3.031909	-0.651914
C	0.123614	4.129989	-1.020600
C	0.137681	5.510683	-1.481065
H	1.170291	5.866571	-1.543243
H	-0.417744	6.139484	-0.779159
H	-0.325884	5.576346	-2.469603
O	-0.222594	-3.024447	0.697858
O	-0.067205	-2.691361	2.104666
H	0.240273	-3.924713	0.649859
H	-0.877344	-3.076946	2.487428
N	0.868722	-5.537256	0.548309
C	1.944849	-5.937193	1.254427
C	2.366893	-7.270566	1.241181
C	1.657729	-8.197227	0.479904
C	0.548061	-7.772581	-0.248013
C	0.177534	-6.425495	-0.193694
C	2.674889	-4.880335	2.043106
H	3.275332	-4.250981	1.373213
H	1.965186	-4.224812	2.556973
H	3.350365	-5.327520	2.777294
H	3.232981	-7.570273	1.822311
H	1.963573	-9.239367	0.457953
H	-0.028131	-8.469926	-0.847452
C	-1.000359	-5.893226	-0.970649
H	-1.593507	-5.209766	-0.355017
H	-0.658305	-5.328340	-1.847368
H	-1.643891	-6.703218	-1.323759

=== Model-1, 5TS1 ===

Fe	0.201967	0.729490	0.119573
N	-1.308832	0.972928	1.724972
N	1.667333	1.328124	1.714256
N	1.832362	0.223263	-1.337255
N	-1.150280	-0.149153	-1.403559
C	-0.468941	0.690907	2.927552
H	-1.032689	0.917656	3.845372
H	-0.234036	-0.374132	2.921628
C	0.825386	1.499439	2.943927
H	1.405457	1.218758	3.833716
H	0.603879	2.564416	3.040405
C	2.596494	0.163232	1.868097
H	3.285253	0.380928	2.699417
H	1.991469	-0.698130	2.152257
C	3.441282	-0.181898	0.628881
H	4.119850	-0.980188	0.955170
H	4.101651	0.649428	0.362597
C	2.724774	-0.738881	-0.613670
H	2.096480	-1.576086	-0.305828
H	3.486779	-1.102243	-1.320440
C	1.113161	-0.464630	-2.459036
H	0.938642	0.279651	-3.238555
H	1.760616	-1.234740	-2.899755
C	-0.210894	-1.109778	-2.053796
H	-0.029022	-1.914132	-1.341271
H	-0.672618	-1.548591	-2.951333
C	-2.288729	-0.900961	-0.789157
H	-1.857456	-1.778025	-0.308939
H	-2.958920	-1.236414	-1.594370
C	-3.092089	-0.130174	0.265761
H	-3.406188	0.853029	-0.101181
H	-4.021194	-0.692577	0.419313
C	-2.413204	-0.029976	1.638812
H	-1.986639	-1.002955	1.886465
H	-3.163473	0.212052	2.405773
C	-1.896889	2.332418	1.809405
H	-2.528922	2.418872	2.704587
H	-1.113823	3.088523	1.853804
H	-2.505223	2.531913	0.926531
C	2.444626	2.580802	1.538544
H	3.066411	2.773941	2.424232
H	1.762360	3.419186	1.393030
H	3.096066	2.517289	0.669647
C	2.640015	1.314293	-1.939687

H	3.217774	1.837164	-1.180423
H	1.982169	2.036147	-2.425524
H	3.338239	0.907927	-2.684905
C	-1.684073	0.811201	-2.399990
H	-0.879940	1.395261	-2.846727
H	-2.371841	1.505367	-1.915076
H	-2.221741	0.275791	-3.195259
N	0.011359	2.808431	-0.640585
C	-0.095136	3.890260	-1.039474
C	-0.229830	5.250321	-1.538957
H	0.758188	5.652749	-1.780971
H	-0.697677	5.879382	-0.776111
H	-0.850281	5.253115	-2.439788
O	0.200652	-1.926586	0.810446
O	0.458288	-2.256917	2.231083
H	0.469290	-3.483229	0.441015
H	-0.400968	-2.615524	2.515225
N	0.628564	-4.551236	0.337846
C	1.846272	-5.058526	0.659009
C	2.061280	-6.426491	0.515101
C	1.033112	-7.242215	0.049510
C	-0.206156	-6.684299	-0.260245
C	-0.401251	-5.315709	-0.108945
C	2.897121	-4.114874	1.158481
H	3.320151	-3.538825	0.327346
H	2.462094	-3.413952	1.875952
H	3.709877	-4.671112	1.629890
H	3.029537	-6.838494	0.773982
H	1.193287	-8.309598	-0.064113
H	-1.024967	-7.300081	-0.612928
C	-1.705791	-4.641430	-0.413526
H	-2.030315	-4.015394	0.422887
H	-1.616341	-4.001917	-1.298246
H	-2.478025	-5.386877	-0.612173

=== Model-1, 3TS1 ===

Fe	0.238408	0.541099	0.189905
N	-1.244089	0.864995	1.643199
N	1.579165	1.237799	1.689763
N	1.778151	0.188166	-1.249599
N	-1.057903	-0.170914	-1.309815
C	-0.505526	0.617175	2.918656
H	-1.134861	0.884302	3.779825
H	-0.280960	-0.448720	2.963958
C	0.778840	1.417511	2.952867
H	1.381350	1.125126	3.821064
H	0.565740	2.481927	3.063203
C	2.580696	0.133818	1.888932
H	3.247390	0.428349	2.712251
H	2.024025	-0.749115	2.204531
C	3.444237	-0.197453	0.665670
H	4.131602	-0.987036	0.994176
H	4.092637	0.644077	0.402820
C	2.731803	-0.755253	-0.572049
H	2.143006	-1.625541	-0.279381
H	3.489988	-1.061227	-1.306891
C	1.130757	-0.508715	-2.415388
H	0.977475	0.231249	-3.202364
H	1.810183	-1.266438	-2.823316
C	-0.188268	-1.146271	-2.032662
H	-0.023593	-1.987540	-1.359515
H	-0.696724	-1.519348	-2.933273
C	-2.258946	-0.915475	-0.812578
H	-1.889460	-1.839832	-0.371057
H	-2.883432	-1.170562	-1.679764
C	-3.090632	-0.184704	0.236742
H	-3.436799	0.791607	-0.117171
H	-3.999872	-0.778938	0.387833
C	-2.395422	-0.088828	1.592346
H	-2.004201	-1.073229	1.853947
H	-3.116555	0.207091	2.366679
C	-1.776249	2.257088	1.625941
H	-2.431403	2.416826	2.492361
H	-0.963161	2.979438	1.649361
H	-2.345223	2.429250	0.712965
C	2.294609	2.528491	1.475428
H	2.865792	2.787945	2.376117
H	1.572108	3.315194	1.261968

H	2.985801	2.463367	0.641564	H	3.031876	2.916125	2.132545
C	2.530080	1.336311	-1.832260	H	1.686034	3.456229	1.097192
H	3.144227	1.829007	-1.085217	H	2.973050	2.453797	0.423185
H	1.827769	2.064717	-2.236080	C	2.312969	0.939048	-1.990274
H	3.190077	0.977907	-2.632891	H	2.893272	1.573925	-1.325767
C	-1.515203	0.899001	-2.240027	H	1.608795	1.565659	-2.535588
H	-0.673385	1.486818	-2.599765	H	2.996208	0.461079	-2.703456
H	-2.191109	1.575618	-1.717638	C	-1.838722	0.657509	-2.322607
H	-2.043491	0.454127	-3.093786	H	-0.978881	1.077236	-2.843401
N	0.079834	3.274092	-0.795569	H	-2.425585	1.480952	-1.916476
C	-0.084633	4.359040	-1.172950	H	-2.454021	0.101820	-3.042185
C	-0.292042	5.723494	-1.645172	N	-0.059800	2.573879	-0.787173
H	0.634697	6.114379	-2.075071	C	-0.126435	3.625511	-1.266725
H	-0.596142	6.363218	-0.811571	C	-0.208321	4.945365	-1.869861
H	-1.074205	5.738305	-2.409750	H	-1.048700	4.977785	-2.569465
O	0.224401	-2.002547	0.830134	H	0.719613	5.160290	-2.408014
O	0.523207	-2.316655	2.246454	H	-0.356861	5.697203	-1.089158
H	0.483270	-3.544548	0.462216	O	-0.106309	-1.164104	1.107734
H	-0.324058	-2.681649	2.556714	O	0.298414	-1.949087	-2.703337
N	0.632675	-4.616608	0.356112	H	0.368247	-1.902415	0.696744
C	1.860737	-5.130963	0.620626	H	-0.537715	-2.503314	2.786061
C	2.060219	-6.500516	0.470344	N	-1.789215	-3.734602	3.268619
C	1.005127	-7.310680	0.057500	C	-1.857484	-4.897814	2.591182
C	-0.244485	-6.745961	-0.192152	C	-2.699261	-5.935637	3.003684
C	-0.422562	-5.375437	-0.035892	C	-3.481167	-5.758559	4.142985
C	2.938412	-4.191935	1.069938	C	-3.396870	-4.557235	4.843309
H	3.330469	-3.622587	0.219182	C	-2.534445	-3.559080	4.378114
H	2.539014	-3.485214	1.802428	C	-0.987075	-5.028006	1.366665
H	3.766782	-4.751019	1.509809	H	-1.412931	-4.464262	0.526774
H	3.037121	-6.918324	0.683465	H	0.012475	-4.627078	1.562357
H	1.152795	-8.379396	-0.060492	H	-0.893754	-6.071249	1.053360
H	-1.083774	-7.357864	-0.501005	H	-2.731155	-6.863455	2.441727
C	-1.734835	-4.690555	-0.278597	H	-4.140544	-6.550621	4.486408
H	-1.971821	-3.996982	0.532813	H	-3.982800	-4.391199	5.741474
H	-1.707392	-4.119921	-1.213776	C	-2.399837	-2.238799	5.093917
H	-2.537082	-5.426708	-0.357641	H	-1.348808	-1.940686	5.159766
				H	-2.932199	-1.447003	4.552204
				H	-2.816682	-2.290433	6.103282

=== Model-1, 5TShooh ===

Fe	0.044874	0.617003	0.273679
N	-1.385496	1.289281	1.793983
N	1.588267	1.417168	1.675557
N	1.572212	-0.103886	-1.221770
N	-1.399161	-0.246715	-1.228123
C	-0.555309	1.079060	3.026076
H	-1.079524	1.487557	3.901001
H	-0.432116	0.005420	3.169063
C	0.815221	1.751770	2.927291
H	1.405336	1.474006	3.809062
H	0.703114	2.836981	2.956831
C	2.530613	0.269644	1.917798
H	3.269955	0.595964	2.663090
H	1.954740	-0.542657	2.361092
C	3.308511	-0.232046	0.685939
H	4.008529	-0.981923	1.074500
H	3.947310	0.560978	0.286591
C	2.569338	-0.938084	-0.466026
H	2.061186	-1.829976	-0.094240
H	3.323006	-1.295576	-1.180984
C	0.811709	-0.932136	-2.231890
H	0.736123	-0.337452	-3.142963
H	1.392186	-1.824937	-2.490776
C	-0.593250	-1.367121	-1.800625
H	-0.550969	-2.165024	-1.059458
H	-1.098721	-1.789018	-2.680674
C	-2.609981	-0.782192	-0.519811
H	-2.305203	-1.676717	0.024979
H	-3.341075	-1.087903	-1.280221
C	-3.282797	0.190196	0.461672
H	-3.498639	1.151461	-0.016525
H	-4.263788	-0.244192	0.688001
C	-2.583056	0.384829	1.816081
H	-2.255462	-0.584786	2.193326
H	-3.301846	0.795877	2.537659
C	-1.841001	2.702136	1.718557
H	-2.437057	2.946815	2.607151
H	-0.988727	3.378241	1.666990
H	-2.451094	2.855704	0.828669
C	2.365976	2.631208	1.307628

=== Model-1, 3TShooh ===

Fe	0.025404	0.705792	0.323780
N	-1.251707	1.570244	1.777700
N	1.594087	1.287963	1.656719
N	1.374929	-0.189960	-1.124035
N	-1.499667	0.077383	-1.042711
C	-0.497136	1.316005	3.049634
H	-0.985066	1.844487	3.879723
H	-0.540857	0.245060	3.247751
C	0.936816	1.785254	2.924679
H	1.515104	1.451728	3.793147
H	0.985988	2.874959	2.913342
C	2.378230	0.034910	1.949845
H	3.142772	0.294646	2.693919
H	1.695705	-0.677141	2.413926
C	3.097941	-0.594870	0.748178
H	3.663176	-1.443143	1.152370
H	3.859139	0.088538	0.360947
C	2.270091	-1.167665	-0.410801
H	1.663560	-2.010985	-0.073614
H	2.965533	-1.585664	-1.150147
C	0.510863	-0.908403	-2.138747
H	0.491107	-0.296117	-3.040767
H	0.979315	-1.858818	-2.415594
C	-0.906431	-1.155828	-1.653395
H	-0.940024	-1.943404	-0.902533
H	-1.521867	-1.485807	-2.501017
C	-2.785284	-0.309143	-0.369879
H	-2.597738	-1.227294	0.187762
H	-3.516938	-0.535799	-1.155840
C	-3.355399	0.739872	0.581846
H	-3.500533	1.705857	0.087432
H	-4.361565	0.398879	0.852806
C	-2.577203	0.876336	1.888649
H	-2.386417	-0.115486	2.299779
H	-3.177921	1.430770	2.621355
C	-1.490945	3.032327	1.612756
H	-2.058908	3.406567	2.473122

H	-0.548938	3.572008	1.546066	C	-1.634763	2.456030	2.059324
H	-2.057768	3.222530	0.702660	H	-2.171248	2.548124	3.015147
C	2.533455	2.367301	1.231517	H	-0.713723	3.035828	2.111840
H	3.249369	2.564086	2.038659	H	-2.251395	2.881302	1.266310
H	1.974857	3.276537	1.017716	C	2.602474	1.994104	1.381941
H	3.087072	2.085407	0.342265	H	3.323908	1.987307	2.212240
C	2.251603	0.727163	-1.918730	H	2.042403	2.929406	1.403876
H	2.984856	1.217808	-1.286190	H	3.157666	1.954886	0.446964
H	1.645948	1.486310	-2.407441	C	2.270270	1.204373	-2.244804
H	2.787613	0.144452	-2.677244	H	2.983793	1.531969	-1.491422
C	-1.812502	1.056285	-2.124545	H	1.677143	2.067421	-2.548710
H	-0.908346	1.347866	-2.653515	H	2.833196	0.832023	-3.113237
H	-2.262281	1.952921	-1.701999	C	-2.014800	1.497138	-2.330787
H	-2.514613	0.602909	-2.834576	H	-1.134767	1.968708	-2.768375
N	0.235096	2.792805	-0.853641	H	-2.506621	2.235354	-1.695729
C	0.319702	3.837951	-1.347067	H	-2.704180	1.209248	-3.138767
C	0.423767	5.150461	-1.967285	N	0.116335	2.853130	-0.490090
H	1.447796	5.523220	-1.873124	C	0.178291	3.980840	-0.747741
H	-0.259959	5.846647	-1.472815	C	0.256617	5.398373	-1.073210
H	0.161666	5.079880	-3.026971	H	1.299559	5.681067	-1.243338
O	-0.344940	-1.082221	1.219390	H	-0.145217	5.991386	-0.246562
O	-0.397555	-1.795400	2.854721	H	-0.323066	5.603716	-1.977841
H	0.227595	-1.815207	0.948746	O	-0.328608	-1.475707	0.248883
H	-1.143228	-2.440842	2.673318	O	-0.181460	-2.304612	1.472693
N	-2.306009	-3.867739	2.636592	H	0.631863	-3.808135	1.099711
C	-1.854768	-5.034205	2.133856	H	-1.101828	-2.590595	1.617755
C	-2.604965	-6.210906	2.228648	N	1.090577	-4.730108	0.908940
C	-3.847036	-6.170721	2.858332	C	2.023848	-5.172169	1.790820
C	-4.303783	-4.962693	3.380547	C	2.628340	-6.397947	1.541225
C	-3.503540	-3.822494	3.252876	C	2.269607	-7.123870	0.404204
C	-0.506997	-5.011938	1.456837	C	1.303717	-6.628499	-0.469806
H	-0.594341	-4.615748	0.436681	C	0.698000	-5.405354	-0.199547
H	0.186948	-4.368805	2.006430	C	2.353666	-4.294416	2.961088
H	-0.080026	-6.016002	1.385432	H	3.057671	-3.508683	2.660768
H	-2.214468	-7.137570	1.820397	H	1.459310	-3.807661	3.360654
H	-4.447401	-7.071532	2.949002	H	2.822542	-4.881316	3.753298
H	-5.261892	-4.898752	3.886300	H	3.373634	-6.772755	2.232575
C	-3.947062	-2.485395	3.790509	H	2.742816	-8.079492	0.202608
H	-3.102796	-1.949448	4.234835	H	1.009719	-7.182043	-1.353749
H	-4.350387	-1.859098	2.984225	C	-0.388335	-4.799631	-1.036218
H	-4.730576	-2.599245	4.544707	H	-0.437234	-3.715494	-0.900569
				H	-0.227895	-5.028854	-2.092665
				H	-1.358353	-5.223934	-0.747957

=== Model-1, 5Int ===

Fe	-0.024644	0.604960	0.020791
N	-1.335982	1.035555	1.769090
N	1.668600	0.847697	1.492262
N	1.379919	0.147185	-1.706614
N	-1.628834	0.314318	-1.531130
C	-0.477357	0.455186	2.843923
H	-0.897400	0.688996	3.834810
H	-0.479646	-0.626075	2.719845
C	0.966389	0.973269	2.812960
H	1.536441	0.447558	3.591827
H	0.979041	2.031408	3.083512
C	2.428220	-0.436105	1.388390
H	3.230351	-0.427841	2.144623
H	1.740537	-1.240132	1.644413
C	3.084086	-0.721748	0.020240
H	3.667245	-1.639841	0.169422
H	3.831962	0.044266	-0.208623
C	2.204231	-1.003296	-1.215862
H	1.511100	-1.810490	-0.984946
H	2.867667	-1.329232	-2.032902
C	0.462802	-0.268401	-2.821388
H	0.392452	0.575752	-3.511014
H	0.915194	-1.093977	-3.387998
C	-0.946010	-0.694116	-2.391477
H	-0.894510	-1.616008	-1.815143
H	-1.533926	-0.884237	-3.303799
C	-2.847520	-0.278201	-0.902975
H	-2.595467	-1.297729	-0.608181
H	-3.643841	-0.331715	-1.661336
C	-3.382676	0.475595	0.327719
H	-3.514933	1.541433	0.110965
H	-4.395024	0.090905	0.503916
C	-2.616016	0.274260	1.647302
H	-2.380478	-0.785019	1.757676
H	-3.270269	0.552079	2.487645

=== Model-1, 3Int ===

Fe	-0.089705	0.102829	0.099799
N	-1.304679	0.688571	1.708583
N	1.514228	0.492734	1.428429
N	1.183219	-0.254491	-1.584574
N	-1.644524	-0.060935	-1.298166
C	-0.519174	0.191667	2.876765
H	-0.973204	0.536155	3.817884
H	-0.552971	-0.896652	2.849084
C	0.920199	0.669372	2.803279
H	1.527720	0.137054	3.544157
H	0.977519	1.729335	3.056885
C	2.376516	-0.735642	1.388744
H	3.184190	-0.611598	2.125443
H	1.749740	-1.567123	1.708913
C	3.018249	-1.051530	0.027599
H	3.616177	-1.957872	0.187551
H	3.749174	-0.281346	-0.238977
C	2.101228	-1.367352	-1.164654
H	1.461702	-2.213067	-0.913457
H	2.732620	-1.637254	-2.023928
C	0.291357	-0.711927	-2.711374
H	0.231676	0.098652	-3.439930
H	0.749555	-1.562996	-3.228204
C	-1.102459	-1.086714	-2.238320
H	-1.078447	-2.027892	-1.690308
H	-1.767038	-1.199819	-3.107665
C	-2.927015	-0.589068	-0.737601
H	-2.733138	-1.619578	-0.434848
H	-3.675182	-0.602432	-1.543002
C	-3.476557	0.180076	0.463321
H	-3.662830	1.231989	0.223775
H	-4.463853	-0.244608	0.682022
C	-2.645972	0.029035	1.737750

H	-2.475580	-1.033820	1.919190	H	-4.621836	1.354449	0.282362
H	-3.206680	0.426321	2.595902	C	-2.901537	1.562321	1.501367
C	-1.482413	2.163725	1.792461	H	-2.905517	0.575851	1.967695
H	-1.971341	2.437063	2.737459	H	-3.505551	2.230738	2.129445
H	-0.520737	2.671138	1.727572	C	-1.484151	3.536467	1.323713
H	-2.098832	2.512273	0.963869	H	-2.046953	4.023430	2.130460
C	2.349777	1.705214	1.189191	H	-0.465018	3.920570	1.322286
H	3.030251	1.864827	2.035650	H	-1.944288	3.787708	0.368376
H	1.708021	2.579592	1.068521	C	2.494603	2.171709	1.238368
H	2.952044	1.600184	0.293694	H	3.180222	2.310368	2.084212
C	1.982236	0.878096	-2.134244	H	2.099191	3.141281	0.938207
H	2.784097	1.159727	-1.460237	H	3.055588	1.756279	0.404953
H	1.339923	1.747788	-2.286569	C	2.158996	0.286421	-1.963042
H	2.435335	0.588354	-3.091050	H	2.869244	0.772412	-1.298361
C	-1.910590	1.213660	-2.019586	H	1.723598	1.044782	-2.612902
H	-0.982227	1.643243	-2.395738	H	2.700251	-0.444210	-2.577776
H	-2.362929	1.938364	-1.342278	C	-1.877122	1.230609	-2.580321
H	-2.594428	1.041544	-2.861954	H	-0.902922	1.343368	-3.054638
N	0.448554	4.222658	-0.833904	H	-2.225707	2.218671	-2.280251
C	0.524489	5.358304	-1.062774	H	-2.580871	0.810425	-3.310218
C	0.619872	6.786385	-1.350444	N	0.318151	2.633541	-0.954554
H	1.662356	7.062780	-1.533354	C	0.591156	3.584856	-1.554752
H	0.243095	7.365173	-0.502094	C	0.934130	4.779913	-2.306884
H	0.027410	7.030183	-2.237098	H	2.000903	4.767888	-2.548792
O	-0.372121	-1.975707	0.387906	H	0.707536	5.667040	-1.708196
O	-0.230746	-2.706063	1.677039	O	0.352089	4.809225	-3.232699
H	0.603778	-4.177936	1.311493	H	-0.845055	-0.686925	1.016091
H	-1.148942	-2.990216	1.837314	O	-0.938630	-1.682922	3.589078
N	1.113052	-5.069002	1.091527	H	-0.850122	-1.085988	1.919583
C	2.097669	-5.465789	1.938704	H	-1.091955	-2.705584	3.660718
C	2.773463	-6.644355	1.648852	N	-1.350601	-4.332723	3.878570
C	2.430577	-7.371993	0.507708	C	-0.773321	-5.243983	3.069796
C	1.410969	-6.924673	-0.329825	C	-0.934839	-6.613608	3.292490
C	0.735139	-5.748195	-0.019452	C	-1.704566	-7.035904	4.375526
C	2.400261	-4.589783	3.117647	C	-2.294410	-6.084840	5.204731
H	2.946044	-3.694054	2.797900	C	-2.100012	-4.728120	4.926427
H	1.482826	-4.261641	3.615642	C	0.053249	-4.710685	1.927774
H	3.020667	-5.125999	3.837956	H	-0.545014	-4.043839	1.296379
H	3.561615	-6.981424	2.311459	H	0.903886	-4.129661	2.303900
H	2.959303	-8.290592	0.274237	H	0.440812	-5.521245	1.305657
H	1.129216	-7.479511	-1.216939	H	-0.461274	-7.330206	2.629645
C	-0.407067	-5.195836	-0.817026	H	-1.840818	-8.095549	4.571624
H	-0.489993	-4.111996	-0.687797	H	-2.897599	-6.381711	6.056412
H	-0.280415	-5.432990	-1.876300	C	-2.731478	-3.644272	5.762714
H	-1.347326	-5.653510	-0.483896	H	-2.033376	-2.816096	5.917287
				H	-3.615541	-3.235991	5.256321
				H	-3.050365	-4.028272	6.735177

=== Model-1, 5Int-ho-oh ===

Fe	-0.274095	0.800475	0.158298
N	-1.487046	2.064723	1.523772
N	1.378377	1.268651	1.632581
N	1.082867	-0.392631	-1.192627
N	-1.786463	0.340408	-1.394683
C	-0.840818	1.723908	2.830889
H	-1.251441	2.360571	3.626627
H	-1.092535	0.693417	3.072994
C	0.677600	1.915456	2.802305
H	1.097549	1.533716	3.740302
H	0.910652	2.981167	2.767956
C	1.940989	-0.074170	2.009102
H	2.718848	0.091164	2.767898
H	1.144391	-0.648476	2.481931
C	2.569955	-0.886812	0.861889
H	2.987030	-1.780376	1.342952
H	3.439467	-0.361238	0.455886
C	1.687248	-1.424457	-0.279744
H	0.864262	-2.008495	0.130822
H	2.308097	-2.091512	-0.894512
C	0.157557	-1.039044	-2.194555
H	0.290681	-0.514393	-3.142124
H	0.466810	-2.077080	-2.365033
C	-1.320489	-1.024595	-1.801326
H	-1.496460	-1.689689	-0.958026
H	-1.911209	-1.381641	-2.655856
C	-3.133530	0.245584	-0.738889
H	-3.123329	-0.643392	-0.106448
H	-3.881000	0.088386	-1.527984
C	-3.544281	1.459567	0.109241
H	-3.433682	2.394560	-0.450351

=== Model-1, 3Int-ho-oh ===

Fe	-0.129610	0.798332	0.155105
N	-1.419551	1.898176	1.464247
N	1.382507	1.187362	1.667608
N	1.249807	-0.240874	-1.161886
N	-1.557144	0.440295	-1.415938
C	-0.848686	1.537092	2.803357
H	-1.336654	2.135840	3.583641
H	-1.078700	0.491486	2.994635
C	0.648198	1.778218	2.850394
H	1.058160	1.365535	3.778429
H	0.856755	2.848787	2.863189
C	1.956716	-0.157050	2.026429
H	2.688121	0.005978	2.829233
H	1.150673	-0.764109	2.434470
C	2.660170	-0.904035	0.885379
H	3.041961	-1.829050	1.334471
H	3.553699	-0.361207	0.563457
C	1.826628	-1.350129	-0.323245
H	0.990477	-1.963270	0.007283
H	2.471290	-1.952120	-0.977635
C	0.408050	-0.816452	-2.278785
H	0.568503	-0.196108	-3.161563
H	0.772209	-1.819404	-2.526967
C	-1.068023	-0.877974	-1.939724
H	-1.254018	-1.616464	-1.163775
H	-1.637674	-1.151370	-2.837669
C	-2.942085	0.245554	-0.877511
H	-2.933672	-0.682687	-0.306103
H	-3.613795	0.117034	-1.736113

C	-3.458240	1.374266	0.013338	H	-2.621135	-1.269897	-0.615931
H	-3.395738	2.348676	-0.481708	H	-3.632771	-0.289876	-1.689743
H	-4.529231	1.190672	0.158099	C	-3.380644	0.528862	0.295171
C	-2.833042	1.401524	1.406504	H	-3.487244	1.595278	0.067723
H	-2.837008	0.391261	1.816446	H	-4.403427	0.167156	0.458151
H	-3.431815	2.040308	2.068794	C	-2.639198	0.318744	1.627220
C	-1.422450	3.380508	1.302648	H	-2.422750	-0.743596	1.746436
H	-2.015823	3.830856	2.107310	H	-3.299615	0.616461	2.454987
H	-0.409810	3.774440	1.343888	C	-1.619868	2.482641	2.058896
H	-1.858574	3.654542	0.343240	H	-2.157272	2.581101	3.012872
C	2.503875	2.125056	1.365929	H	-0.689562	3.046802	2.115792
H	3.133897	2.230276	2.257405	H	-2.227591	2.917983	1.264741
H	2.109104	3.100542	1.089660	C	2.566687	1.997077	1.420570
H	3.119915	1.755771	0.552319	H	3.285646	1.990346	2.252368
C	2.359794	0.504070	-1.823576	H	2.000899	2.928756	1.447282
H	3.060378	0.901635	-1.096321	H	3.124180	1.965885	0.486655
H	1.956643	1.328577	-2.407869	C	2.255262	1.182602	-2.211779
H	2.903222	-0.177054	-2.489669	H	2.940987	1.536060	-1.444857
C	-1.602620	1.443699	-2.515309	H	1.653215	2.027883	-2.545107
H	-0.612353	1.605415	-2.934959	H	2.847032	0.807770	-3.058915
H	-1.973154	2.395773	-2.138713	C	-1.960736	1.503135	-2.353219
H	-2.272181	1.085853	-3.306898	H	-1.067936	1.946886	-2.793024
N	0.523085	2.824089	-0.893720	H	-2.434811	2.257168	-1.724326
C	0.796587	3.812951	-1.431862	H	-2.654743	1.224459	-3.159124
C	1.135560	5.055488	-2.108044	N	0.107223	2.780668	-0.493575
H	2.220660	5.127399	-2.225802	C	0.180803	3.913851	-0.720677
H	0.778956	5.904313	-1.517310	C	0.271980	5.338017	-1.008532
H	0.662519	5.077719	-3.094196	H	1.316794	5.614741	-1.176674
O	-0.761816	-0.805187	0.876201	H	-0.120538	5.911674	-0.163928
O	-0.910240	-1.828280	3.534865	H	-0.310941	5.571662	-1.904174
H	-0.743867	-1.153488	1.790921	O	-0.314247	-1.227762	0.285665
H	-1.347577	-2.752930	3.411460	O	-0.127471	-2.438974	1.614492
N	-2.104038	-4.253164	3.243079	H	0.604712	-3.813806	1.130068
C	-1.721339	-5.108463	2.273539	H	-1.074588	-2.663111	1.597634
C	-2.311069	-6.368886	2.146810	N	1.086930	-4.739307	0.902605
C	-3.306310	-6.743096	3.048527	C	2.044993	-5.178999	1.756114
C	-3.690394	-5.852334	4.048206	C	2.675752	-6.385600	1.473629
C	-3.067859	-4.601730	4.117423	C	2.317085	-7.096566	0.328053
C	-0.619906	-4.644067	1.355065	C	1.325223	-6.605817	-0.519676
H	-0.821345	-3.632621	0.986160	C	0.695727	-5.403536	-0.211580
H	0.337622	-4.611409	1.890319	C	2.376626	-4.317049	2.938633
H	-0.505886	-5.316055	0.500434	H	3.160070	-3.596712	2.672262
H	-1.989280	-7.041335	1.358406	H	1.502989	-3.752048	3.273286
H	-3.776010	-7.719650	2.972998	H	2.751387	-4.929116	3.762013
H	-4.461013	-6.114483	4.765888	H	3.440339	-6.756272	2.146303
C	-3.457887	-3.574251	5.149683	H	2.809561	-8.036171	0.098735
H	-2.580905	-3.019198	5.495542	H	1.029657	-7.147584	-1.410590
H	-4.158193	-2.846088	4.720101	C	-0.420281	-4.811834	-1.021253
H	-3.947819	-4.039958	6.008980	H	-0.519587	-3.739702	-0.835561
				H	-0.251104	-4.981568	-2.087699
				H	-1.369549	-5.293032	-0.754948

=== Model-1, 5TSoo ===

Fe	-0.040639	0.532794	0.045183
N	-1.345599	1.057272	1.767671
N	1.641224	0.842792	1.525256
N	1.372067	0.113180	-1.681996
N	-1.608126	0.312720	-1.545531
C	-0.513805	0.448880	2.851202
H	-0.951407	0.675010	3.835457
H	-0.521983	-0.631068	2.705723
C	0.932636	0.956218	2.846151
H	1.493159	0.411355	3.617694
H	0.954176	2.009410	3.134469
C	2.410986	-0.438567	1.426674
H	3.208069	-0.418998	2.186971
H	1.724752	-1.245834	1.677273
C	3.077292	-0.721315	0.063948
H	3.671618	-1.630747	0.221501
H	3.815930	0.052681	-0.167925
C	2.209464	-1.023443	-1.175235
H	1.529185	-1.842846	-0.949921
H	2.883124	-1.340582	-1.986293
C	0.477701	-0.323512	-2.810282
H	0.437275	0.500168	-3.526025
H	0.932816	-1.171088	-3.339132
C	-0.948512	-0.714076	-2.405553
H	-0.935590	-1.643080	-1.839404
H	-1.530804	-0.873028	-3.326151
C	-2.846601	-0.247366	-0.921487

=== Model-1, 3TSoo ===

Fe	-0.043178	0.045044	0.134385
N	-1.301097	0.774504	1.670445
N	1.518805	0.509993	1.477474
N	1.293878	-0.321050	-1.517505
N	-1.523566	-0.081569	-1.307227
C	-0.561495	0.280596	2.871142
H	-1.039222	0.648103	3.790762
H	-0.608829	-0.808006	2.854213
C	0.887292	0.729676	2.832338
H	1.461621	0.197746	3.598402
H	0.961290	1.792880	3.066813
C	2.395654	-0.710705	1.505980
H	3.185308	-0.542690	2.252702
H	1.767775	-1.534046	1.843881
C	3.073725	-1.070063	0.174002
H	3.666108	-1.970544	0.379985
H	3.813105	-0.310250	-0.098441
C	2.193938	-1.423592	-1.035036
H	1.547899	-2.264246	-0.785868
H	2.851138	-1.715659	-1.866589
C	0.431585	-0.805500	-2.658071
H	0.417147	-0.023929	-3.419262
H	0.889026	-1.686015	-3.122565
C	-0.988756	-1.131685	-2.227562
H	-1.018340	-2.071798	-1.679697

H	-1.630931	-1.218663	-3.115124	C	-1.059435	-1.445484	-1.214554
C	-2.845222	-0.558132	-0.789617	H	-0.976330	-2.052697	-0.314564
H	-2.694137	-1.584824	-0.451791	H	-1.702951	-1.974265	-1.930541
H	-3.551840	-0.573608	-1.630628	C	-2.876160	-0.403120	0.070500
C	-3.429853	0.259879	0.360176	H	-2.601368	-1.210092	0.751213
H	-3.589995	1.305320	0.078293	H	-3.699306	-0.763300	-0.560885
H	-4.431647	-0.143815	0.549938	C	-3.357812	0.804964	0.887877
C	-2.654256	0.137827	1.670150	H	-3.504173	1.684479	0.251907
H	-2.506766	-0.920465	1.892717	H	-4.358925	0.543562	1.250600
H	-3.238807	0.576483	2.490835	C	-2.531753	1.148272	2.136174
C	-1.451184	2.253543	1.708018	H	-2.283566	0.226209	2.663735
H	-1.963252	2.560852	2.629767	H	-3.138649	1.766845	2.810750
H	-0.479656	2.743076	1.660150	C	-1.536605	3.307537	1.601105
H	-2.035497	2.591467	0.852348	H	-2.026854	3.765550	2.469781
C	2.342788	1.725500	1.208894	H	-0.618642	3.852905	1.385182
H	2.988212	1.934496	2.071167	H	-2.195221	3.394386	0.736827
H	1.694014	2.582609	1.022703	C	2.573866	2.592349	0.914037
H	2.980308	1.587243	0.343251	H	3.339009	2.924151	1.627710
C	2.116573	0.793091	-2.074911	H	1.977200	3.451033	0.608364
H	2.906169	1.081876	-1.390415	H	3.074453	2.190957	0.036044
H	1.488195	1.664898	-2.264433	C	2.082805	0.385486	-2.042613
H	2.587498	0.472334	-3.012470	H	2.783046	1.042949	-1.533667
C	-1.710313	1.202542	-2.042628	H	1.438161	0.994085	-2.675943
H	-0.754249	1.593444	-2.387242	H	2.651182	-0.308119	-2.675133
H	-2.156312	1.948058	-1.385882	C	-2.142424	0.596043	-2.027152
H	-2.369425	1.047786	-2.906554	H	-1.296365	0.830266	-2.671665
N	0.447654	0.478376	-0.964496	H	-2.618791	1.531636	-1.734659
C	0.351132	5.220890	-1.147052	H	-2.863141	-0.009344	-2.591471
C	0.229903	6.657566	-1.376209	N	0.016983	2.483217	-0.906681
H	0.841769	6.953030	-2.233498	C	0.021777	3.400529	-1.612303
H	0.567962	7.207296	-0.492922	C	0.027400	4.548491	-2.502221
H	-0.813203	6.917898	-1.578249	H	0.933541	5.138046	-2.334774
O	-0.316260	-1.682058	0.511631	H	-0.851712	5.168992	-2.304985
O	-0.063516	-2.782643	1.912503	H	0.004090	4.204975	-3.540696
H	0.588316	-4.142646	1.386152	O	-0.210251	-0.679402	1.437799
H	-1.012020	-2.980356	2.002373	O	-0.015653	-1.843187	3.417343
N	1.056030	-5.063932	1.085842	H	0.111214	-1.320657	2.266175
C	2.117211	-5.501112	1.806332	H	-0.653647	-2.638210	3.313608
C	2.731050	-6.690207	1.425255	N	-1.583082	-4.063053	3.278188
C	2.247589	-7.387790	0.318627	C	-1.053860	-5.183832	2.748906
C	1.150562	-6.901219	-0.391854	C	-1.726511	-6.407193	2.822367
C	0.543836	-5.716931	0.014512	C	-2.967021	-6.458762	3.455233
C	2.574874	-4.658037	2.960758	C	-3.504189	-5.293382	3.998408
H	3.392327	-3.997807	2.645557	C	-2.781962	-4.100886	3.892747
H	1.762164	-4.033344	3.338659	C	0.285313	-5.049334	2.069168
H	2.952808	-5.290840	3.767656	H	0.177776	-4.535720	1.105164
H	3.578918	-7.056221	1.992558	H	0.972660	-4.455272	2.679826
H	2.724464	-8.313143	0.011488	H	0.735589	-6.027339	1.880514
H	0.758192	-7.432276	-1.251322	H	-1.279174	-7.298356	2.394452
C	-0.670732	-5.128941	-0.641500	H	-3.506761	-7.398512	3.529318
H	-0.723479	-4.049886	-0.475038	H	-4.465296	-5.302534	4.502018
H	-0.662865	-5.333838	-1.714941	C	-3.306027	-2.799450	4.444711
H	-1.577915	-5.582753	-0.222913	H	-2.520306	-2.263913	4.987001
				H	-3.645695	-2.145433	3.631363
				H	-4.150956	-2.964506	5.118250

=== Model-1, 5TShat ===

Fe	-0.059969	0.728931	0.389086
N	-1.245629	1.878433	1.880477
N	1.699549	1.566621	1.546258
N	1.259924	-0.378339	-1.065007
N	-1.695856	-0.147679	-0.820905
C	-0.346032	1.752083	3.071732
H	-0.730926	2.369038	3.895269
H	-0.366091	0.711848	3.392961
C	1.085200	2.198194	2.769569
H	1.711813	1.988609	3.644375
H	1.108090	3.278883	2.620739
C	2.527589	0.367627	1.916567
H	3.374816	0.722700	2.520114
H	1.919206	-0.270280	2.556331
C	3.101080	-0.445588	0.741474
H	3.730622	-1.213474	1.207850
H	3.798010	0.166496	0.161459
C	2.159114	-1.217449	-0.199057
H	1.520782	-1.889024	0.374176
H	2.781283	-1.832151	-0.864463
C	0.313863	-1.245734	-1.857056
H	0.196522	-0.782664	-2.838271
H	0.770709	-2.227912	-2.026294

=== Model-1, 3TShat ===

Fe	-0.121676	0.814778	0.278037
N	-1.299372	1.926646	1.676294
N	1.524562	1.271224	1.656553
N	1.128189	-0.292021	-1.091643
N	-1.687203	0.338644	-1.121660
C	-0.610123	1.596167	2.968575
H	-1.044574	2.200093	3.776068
H	-0.803102	0.547266	3.185438
C	0.878957	1.872500	2.884641
H	1.374573	1.487722	3.782286
H	1.063805	2.947118	2.861250
C	2.171117	-0.042118	2.004324
H	2.984229	0.174250	2.710077
H	1.438041	-0.649228	2.533005
C	2.764870	-0.822807	0.825352
H	3.220699	-1.717297	1.266924
H	3.600882	-0.274767	0.380787
C	1.820621	-1.343801	-0.265048
H	1.043213	-1.969365	0.170231
H	2.410506	-1.958754	-0.957194
C	0.201395	-0.951450	-2.089931

H	0.272891	-0.391548	-3.023048	H	2.436448	-0.657957	-2.330427
H	0.557849	-1.965059	-2.300931	C	0.047689	0.429401	-3.072802
C	-1.236200	-1.003881	-1.614005	H	-0.003330	1.272199	-3.764725
H	-1.343635	-1.700073	-0.785254	H	0.479649	-0.408970	-3.633350
H	-1.883310	-1.330125	-2.438723	C	-1.365270	0.045457	-2.628051
C	-3.018770	0.172648	-0.455120	H	-1.344456	-0.888498	-2.068922
H	-2.964416	-0.732535	0.149857	H	-1.983353	-0.099193	-3.525724
H	-3.761971	0.009304	-1.246025	C	-3.212566	0.519006	-1.089028
C	-3.455646	1.338385	0.429291	H	-2.988258	-0.510778	-0.806269
H	-3.439920	2.291454	-0.109105	H	-4.013250	0.494079	-1.841459
H	-4.508797	1.162184	0.676630	C	-3.709524	1.279107	0.151034
C	-2.707658	1.418721	1.758758	H	-3.806337	2.351268	-0.052193
H	-2.664454	0.424037	2.202665	H	-4.733278	0.927806	0.328509
H	-3.250091	2.078000	2.448450	C	-2.939531	1.024992	1.456918
C	-1.327609	3.402551	1.473244	H	-2.730231	-0.041903	1.544732
H	-1.864290	3.872482	2.305784	H	-3.572715	1.312160	2.308629
H	-0.318374	3.805445	1.429092	C	-1.878589	3.163325	1.927513
H	-1.834508	3.643326	0.539984	H	-2.392926	3.236420	2.895751
C	2.584450	2.230219	1.227416	H	-0.939484	3.712713	1.983304
H	3.290900	2.379669	2.052818	H	-2.497964	3.633283	1.162617
H	2.137653	3.186981	0.965386	C	2.297570	2.593237	1.156190
H	3.134030	1.854502	0.369788	H	3.033003	2.536654	1.970686
C	2.145496	0.452426	-1.891126	H	1.766946	3.543259	1.223252
H	2.870983	0.944383	-1.250976	H	2.832840	2.568688	0.209472
H	1.655394	1.203823	-2.506552	C	1.872775	1.884347	-2.480676
H	2.675039	-0.253232	-2.542097	H	2.584474	2.200812	-1.721743
C	-1.832410	1.285025	-2.264041	H	1.285766	2.751658	-2.782722
H	-0.878623	1.441224	-2.762725	H	2.433871	1.511803	-3.348617
H	-2.196585	2.247776	-1.908074	C	-2.342852	2.284677	-2.522341
H	-2.549679	0.875568	-2.985334	H	-1.456318	2.726835	-2.976025
N	0.382826	2.726223	-0.849945	H	-2.796927	3.031167	-1.870438
C	0.601221	3.701886	-1.434238	H	-3.056404	2.022235	-3.315149
C	0.876500	4.927959	-2.164676	N	-0.197955	3.457835	-0.641375
H	1.950784	5.009031	-2.354330	C	-0.109030	4.591338	-0.858293
H	0.546476	5.787888	-1.574435	C	0.002384	6.015274	-1.133111
H	0.339912	4.915532	-3.117933	H	1.051663	6.277952	-1.295998
O	-0.636444	-0.685949	1.149813	H	-0.385380	6.585656	-0.284096
O	-0.591376	-1.879077	3.184502	H	-0.575382	6.262763	-2.028428
H	-0.345630	-1.244674	1.978629	O	-0.610858	-0.400137	0.130906
H	-1.156947	-2.690132	2.975411	O	-0.673958	-2.057422	1.531876
N	-2.069874	-4.202259	2.788112	H	0.115046	-3.213745	1.077853
C	-1.463958	-5.292340	2.279757	H	-1.569424	-2.151764	1.164448
C	-2.090706	-6.543007	2.286031	N	0.735776	-4.106650	0.833494
C	-3.368935	-6.653990	2.828971	C	1.617168	-4.538781	1.766334
C	-3.987515	-5.519771	3.352375	C	2.399976	-5.654255	1.482299
C	-3.306316	-4.299276	3.315630	C	2.264918	-6.289035	0.247902
C	-0.089416	-5.096245	1.690347	C	1.344987	-5.812575	-0.684947
H	-0.162663	-4.793667	0.637284	C	0.565089	-4.703169	-0.368786
H	0.446977	-4.306222	2.223248	C	1.707808	-3.764038	3.049811
H	0.497251	-6.018503	1.728472	H	2.455038	-2.965885	2.957530
H	-1.579192	-7.408707	1.877352	H	0.750345	-3.297034	3.292970
H	-3.874925	-7.615063	2.851043	H	2.016457	-4.417067	3.869620
H	-4.979707	-5.574909	3.788666	H	3.105316	-6.013111	2.223036
C	-3.920623	-3.028390	3.847051	H	2.873976	-7.156746	0.014631
H	-3.164078	-2.412913	4.342624	H	1.221489	-6.294957	-1.647781
H	-4.340662	-2.432441	3.026138	C	-0.491141	-4.144137	-1.278604
H	-4.728979	-3.240112	4.552352	H	-0.692955	-3.095146	-1.048729

=== Model-1, 5Int-oh ===

Fe	-0.395084	1.254737	-0.206422
N	-1.632421	1.743533	1.583802
N	1.333470	1.468731	1.252236
N	0.973443	0.824661	-1.955084
N	-1.983892	1.076624	-1.739492
C	-0.786847	1.083058	2.628481
H	-1.194915	1.296572	3.627599
H	-0.828139	0.007309	2.452524
C	0.664212	1.568139	2.594988
H	1.239784	0.999837	3.337381
H	0.710903	2.615288	2.902051
C	2.055585	0.161026	1.109305
H	2.862016	0.136773	1.858571
H	1.339465	-0.626250	1.342782
C	2.691630	-0.105830	-0.268675
H	3.259124	-1.037367	-0.146775
H	3.449948	0.650272	-0.495541
C	1.791002	-0.347910	-1.494939
H	1.094626	-1.157264	-1.280427

=== Model-1, 5P ===

Fe	0.207092	0.681059	-0.299977
N	-0.373046	0.506302	1.813529
N	2.200816	1.277167	0.545080
N	0.975833	0.788368	-2.418595
N	-1.652520	-0.006150	-1.260557
C	0.937157	0.142900	2.443119
H	0.838241	0.180556	3.536109
H	1.178626	-0.883447	2.163138
C	2.054763	1.096078	2.031251
H	3.000903	0.731624	2.448171
H	1.881816	2.083663	2.461765
C	3.186150	0.289309	-0.018218
H	4.164811	0.512758	0.428483
H	2.886274	-0.702596	0.319782
C	3.352699	0.304794	-1.547415
H	4.146374	-0.423191	-1.755872
H	3.764434	1.263309	-1.877719

C	2.178097	-0.113937	-2.447323	H	3.813671	-1.065426	-1.520150
H	1.841035	-1.115209	-2.178817	H	3.629784	0.618761	-1.895532
H	2.540519	-0.147818	-3.483921	C	1.864212	-0.614895	-2.189826
C	-0.140870	0.217994	-3.249049	H	1.437938	-1.528919	-1.778020
H	-0.685532	1.058810	-3.681386	H	2.152260	-0.810966	-3.230585
H	0.280321	-0.350494	-4.086548	C	-0.429090	-0.137066	-2.954619
C	-1.103688	-0.679772	-2.479068	H	-0.892088	0.686294	-3.499887
H	-0.604092	-1.591611	-2.153322	H	-0.093953	-0.864047	-3.702342
H	-1.926941	-0.963350	-3.147394	C	-1.430302	-0.781779	-2.023754
C	-2.321433	-1.026698	-0.384861	H	-1.023722	-1.692617	-1.586196
H	-1.695882	-1.921031	-0.389614	H	-2.339509	-1.041762	-2.579387
H	-3.277277	-1.288289	-0.856520	C	-2.576871	-0.658677	0.096968
C	-2.566126	-0.593776	1.064286	H	-2.073725	-1.619672	0.213893
H	-3.075697	0.373968	1.115679	H	-3.558041	-0.847307	-0.354993
H	-3.278174	-1.315799	1.480384	C	-2.744616	-0.019970	1.469530
C	-1.336496	-0.633578	1.978473	H	-3.178554	0.983125	1.410180
H	-0.780734	-1.555749	1.799239	H	-3.482822	-0.625381	2.007852
H	-1.660938	-0.640687	3.027119	C	-1.466574	-0.048506	2.298625
C	-0.937231	1.728054	2.446626	H	-1.031411	-1.048689	2.259756
H	-1.105703	1.543783	3.514692	H	-1.693641	0.176421	3.347815
H	-0.254577	2.569455	2.338330	C	-0.805512	2.290668	2.274866
H	-1.885397	1.990200	1.977698	H	-0.974443	2.306147	3.357358
C	2.697886	2.663852	0.324688	H	-0.029835	3.011811	2.029165
H	3.652209	2.802254	0.848531	H	-1.724583	2.581931	1.769095
H	1.976612	3.383658	0.709988	C	2.761176	2.449243	0.043801
H	2.854718	2.861354	-0.731930	H	3.734064	2.553001	0.538046
C	1.326393	2.106603	-3.016776	H	2.136570	3.298631	0.312745
H	2.171394	2.557339	-2.503975	H	2.921902	2.455549	-1.028560
H	0.476361	2.784714	-2.951960	C	1.223404	1.590653	-3.020747
H	1.594901	1.972780	-4.072246	H	2.136164	2.017048	-2.618804
C	-2.639225	1.041057	-1.637518	H	0.450544	2.356488	-3.032412
H	-2.180433	1.795540	-2.274172	H	1.418958	1.266417	-4.049364
H	-3.022271	1.530963	-0.742630	C	-2.632968	1.257584	-1.397177
H	-3.475176	0.581191	-2.178702	H	-2.107087	1.838450	-2.151302
N	-0.372568	2.643406	-0.390000	H	-2.907483	1.919118	-0.576910
C	-0.704904	3.749563	-0.444859	H	-3.545236	0.842863	-1.840559
C	-1.121210	5.137654	-0.510007	N	-0.215094	2.703848	-0.565098
H	-0.429786	5.696017	-1.148015	C	-0.412857	3.822841	-0.779753
H	-1.116280	5.566522	0.496608	C	-0.663514	5.227150	-1.047426
H	-2.131105	5.196056	-0.926815	H	0.138679	5.629390	-1.673196
O	0.621948	-0.876776	-0.232983	H	-0.699554	5.777811	-0.102678
O	1.881904	-2.944641	1.355370	H	-1.620182	5.333978	-1.567572
H	1.458463	-3.819293	1.552126	O	0.373969	-0.871178	0.124397
H	1.341231	-2.560380	0.646345	O	1.233570	-2.818554	2.030736
N	0.789317	-5.543053	1.811934	H	1.125631	-3.793878	1.893977
C	0.101016	-5.883377	2.920282	H	0.869243	-2.412261	1.226219
C	-0.258492	-7.208498	3.179079	N	0.948954	-5.630999	1.610990
C	0.107841	-8.197911	2.266083	C	-0.153229	-6.278217	2.037730
C	0.819370	-7.838594	1.125340	C	-0.249560	-7.672112	1.980828
C	1.144810	-6.490571	0.925532	C	0.820818	-8.401335	1.464835
C	-0.263162	-4.761162	3.859849	C	1.954560	-7.724095	1.022411
H	-0.692997	-5.142258	4.790065	C	1.986400	-6.327282	1.109831
H	0.618876	-4.158434	4.101637	C	-1.284309	-5.425897	2.558699
H	-0.996489	-4.090743	3.394757	H	-1.821979	-5.925327	3.370607
H	-0.809579	-7.456578	4.080543	H	-0.903502	-4.465061	2.914646
H	-0.154914	-9.236518	2.446763	H	-2.011512	-5.221260	1.761633
H	1.124373	-8.584153	0.397524	H	-1.145389	-8.170730	2.337914
C	1.893629	-6.035225	-0.303269	H	0.772908	-9.485530	1.413393
H	2.375332	-5.071970	-0.118440	H	2.806557	-8.263200	0.619428
H	2.649074	-6.767828	-0.604406	C	3.180409	-5.534398	0.635944
H	1.205305	-5.910447	-1.149800	H	3.110711	-4.501485	0.985340

=== Model-1, 3P ===

Fe	0.130649	0.696681	-0.173995
N	-0.400738	0.914943	1.860377
N	2.119803	1.177142	0.494856
N	0.765972	0.416287	-2.218389
N	-1.779312	0.140948	-0.893239
C	0.864473	0.523562	2.568820
H	0.767670	0.754657	3.637068
H	0.988359	-0.553610	2.466510
C	2.049478	1.269159	1.998825
H	2.977409	0.880546	2.431925
H	1.997942	2.326374	2.262226
C	3.001521	0.020706	0.097984
H	4.004406	0.229883	0.492142
H	2.621169	-0.868831	0.599577
C	3.122857	-0.220779	-1.410241

=== Model-2, 5RC ===

Fe	0.091258	1.033656	0.048759
N	-1.337195	1.157082	1.763896
N	1.653975	1.305384	1.664207
N	1.617235	0.195127	-1.362372
N	-1.377310	0.048270	-1.350278
C	-0.467868	0.819870	2.930660
H	-0.989693	1.051193	3.870437
H	-0.295950	-0.258805	2.905202
C	0.856568	1.568379	2.903107
H	1.443859	1.292638	3.789895
H	0.685422	2.645530	2.961785
C	2.397280	0.012361	1.814323

H	-3.353147	0.798855	0.033043
H	-3.982012	-0.664316	0.737544
C	-2.394435	0.149057	1.886454
H	-1.983047	-0.784289	2.273509
H	-3.168589	0.481547	2.593956
C	-1.880619	2.518372	1.780476
H	-2.527915	2.717831	2.646686
H	-1.094945	3.272530	1.744457
H	-2.472420	2.608550	0.869092
C	2.404582	2.796015	1.479036
H	3.023302	3.136416	2.322093
H	1.677834	3.571295	1.234641
H	3.051689	2.654970	0.615881
C	2.597316	1.120191	-1.842874
H	3.146090	1.767156	-1.161504
H	1.884702	1.733618	-2.395073
H	3.313247	0.677313	-2.550135
C	-1.619222	0.480683	-2.225827
H	-0.801929	1.006895	-2.718561
H	-2.306179	1.229537	-1.829595
H	-2.150979	-0.129879	-2.970585
N	0.014980	2.647135	-0.688656
C	-0.116055	3.668822	-1.218421
C	-0.279309	4.952402	-1.886429
H	0.694489	5.439233	-1.993082
H	-0.939119	5.595374	-1.296713
H	-0.716286	4.801337	-2.877770
O	0.278470	-1.400973	1.134609
O	0.554384	-1.869305	2.527634
H	0.880382	-3.047830	1.373750
H	-0.339191	-2.111645	2.835600
N	1.152091	-4.013855	1.027871
C	1.427242	-5.067854	0.667791
C	1.771873	-6.395715	0.212052
H	0.859707	-6.996297	0.142181
H	2.462279	-6.853965	0.926617
H	2.246134	-6.327977	-0.771654

=== Model-2, 3TS1 ===

Fe	0.258622	0.563038	0.384423
N	-1.232241	1.090482	1.809102
N	1.617550	1.454071	1.767281
N	1.799638	0.044580	-1.042430
N	-1.052676	-0.341298	-1.018866
C	-0.467944	0.997712	3.089481
H	-1.073746	1.378696	3.924815
H	-0.255586	-0.053673	3.272529
C	0.828796	1.779772	3.007263
H	1.436417	1.586379	3.899725
H	0.622068	2.851321	2.996632
C	2.634600	0.391142	2.075286
H	3.310925	0.784442	2.848744
H	2.096109	-0.455829	2.498330
C	3.491579	-0.069033	0.886574
H	4.198083	-0.800566	1.299260
H	4.120116	0.749765	0.522733
C	2.795451	-0.782331	-0.281093
H	2.256187	-1.648092	0.098197
H	3.565760	-1.126985	-0.986345
C	1.136426	-0.797371	-2.098475
H	0.971039	-0.162901	-2.971104
H	1.812112	-1.599968	-2.419285
C	-0.179456	-1.389018	-1.628612
H	-0.007489	-2.142398	-0.860776
H	-0.690664	-1.866299	-2.477788
C	-2.235080	-1.026671	-0.405307
H	-1.850556	-1.882598	0.150323
H	-2.872419	-1.400658	-1.219120
C	-3.062613	-0.159261	0.541691
H	-3.409012	0.759494	0.057012
H	-3.972853	-0.725971	0.772911
C	-2.377498	0.130160	1.876778
H	-1.991725	-0.808390	2.276567
H	-3.110932	0.521004	2.596073
C	-1.780046	2.464953	1.650486
H	-2.424985	2.713214	2.504368
H	-0.974729	3.193170	1.584406
H	-2.364206	2.532007	0.733137

C	2.319283	2.713501	1.392050
H	2.918176	3.072183	2.239622
H	1.587329	3.472123	1.118501
H	2.982748	2.559594	0.547155
C	2.522002	1.122969	-1.774771
H	3.118125	1.727876	-1.098228
H	1.805888	1.773021	-2.276258
H	3.195510	0.679748	-2.520327
C	-1.541414	0.584130	-2.076516
H	-0.710060	1.103837	-2.547494
H	-2.197714	1.337260	-1.641458
H	-2.096982	0.021819	-2.839156
N	0.026474	2.950379	-0.839624
C	-0.104533	3.979603	-1.358362
C	-0.268674	5.273397	-2.010749
H	0.705870	5.755381	-2.131234
H	-0.912785	5.916822	-1.404399
H	-0.724666	5.138222	-2.995794
O	0.272848	-1.532339	1.198513
O	0.518550	-1.995129	2.602239
H	0.886058	-3.158059	1.490843
H	-0.381866	-2.225444	2.898078
N	1.190016	-4.112752	1.124793
C	1.504646	-5.145688	0.736496
C	1.901000	-6.446240	0.243622
H	1.051357	-7.131688	0.319343
H	2.733072	-6.821795	0.846713
H	2.211119	-6.356784	-0.801858

=== Model-2, 5TShooh ===

Fe	0.072928	0.603114	0.271574
N	-1.186173	1.287539	1.945084
N	1.769455	1.269738	1.561819
N	1.413368	-0.048722	-1.408075
N	-1.556409	-0.051812	-1.123181
C	-0.266153	0.990048	3.090952
H	-0.685831	1.397560	4.021242
H	-0.197508	-0.092227	3.190870
C	1.130977	1.582380	2.893622
H	1.778708	1.227754	3.704424
H	1.089372	2.669346	2.980475
C	2.668106	0.066147	1.652560
H	3.490459	0.311115	2.340218
H	2.092749	-0.741628	2.102388
C	3.298689	-0.400589	0.324547
H	3.978874	-1.215153	0.602667
H	3.951372	0.377873	-0.081532
C	2.414748	-0.988786	-0.794169
H	1.879036	-1.862808	-0.428049
H	3.080690	-1.339562	-1.595128
C	0.512620	-0.754667	-2.394812
H	0.389403	-0.085174	-3.247623
H	1.013597	-1.652859	-2.773868
C	-0.871391	-1.153970	-1.866321
H	-0.802437	-2.018746	-1.209549
H	-1.480229	-1.462725	-2.727926
C	-2.712503	-0.594086	-0.333234
H	-2.388978	-1.529145	0.126646
H	-3.521748	-0.832970	-1.036406
C	-3.256171	0.337778	0.760498
H	-3.492309	1.328795	0.358561
H	-4.221690	-0.085683	1.062139
C	-2.421920	0.442364	2.046354
H	-2.111642	-0.556684	2.354576
H	-3.048143	0.853621	2.849422
C	-1.574683	2.721895	1.959436
H	-2.105723	2.954067	2.891645
H	-0.694425	3.359162	1.887033
H	-2.225915	2.944819	1.114516
C	2.575798	2.461930	1.182772
H	3.329792	2.665551	1.954192
H	1.927157	3.331543	1.081343
H	3.087008	2.303729	0.236861
C	2.150402	0.997859	-2.172244
H	2.831277	1.544053	-1.525101
H	1.446304	1.705359	-2.606718
H	2.733426	0.531029	-2.976251
C	-2.062862	0.954643	-2.092573

H	-1.244926	1.357434	-2.688659	O	-0.112315	-1.279811	1.036638
H	-2.540930	1.780784	-1.567072	O	0.020267	-2.098760	2.594690
H	-2.795304	0.487550	-2.763841	H	0.134788	-2.121805	0.589310
N	-0.009355	2.637946	-0.672397	H	-0.880020	-2.475871	2.562002
C	-0.046233	3.715329	-1.094581	N	0.379166	-3.892314	-0.033459
C	-0.093351	5.066866	-1.627951	C	0.516373	-5.022632	-0.249021
H	0.825916	5.274248	-2.183576	C	0.687944	-6.444453	-0.518077
H	-0.189433	5.782969	-0.806552	H	1.602263	-6.805308	-0.038186
H	-0.951832	5.167223	-2.298529	H	0.759263	-6.612881	-1.596496
O	-0.062754	-1.204268	1.006239	H	-0.166581	-7.002371	-0.124428
O	0.344971	-2.008069	2.559719				
H	0.133875	-2.061681	0.555953				
H	-0.537831	-2.417439	2.654168				
N	0.345982	-3.817424	-0.006426				
C	0.523548	-4.946441	-0.196750				
C	0.747909	-6.366407	-0.432955				
H	1.415468	-6.768540	0.334582				
H	1.204170	-6.511696	-1.416395				
H	-0.204093	-6.903829	-0.396810				

=== Model-2, 3TShooh ===

Fe	0.081138	0.579858	0.270188
N	-1.267170	1.225819	1.777069
N	1.598076	1.209408	1.647124
N	1.487049	-0.037017	-1.241117
N	-1.390377	-0.020939	-1.147524
C	-0.488005	0.951234	3.029577
H	-1.018171	1.370803	3.895005
H	-0.424991	-0.130256	3.149554
C	0.899195	1.553260	2.942948
H	1.505680	1.211688	3.789038
H	0.850014	2.640934	3.009758
C	2.488174	0.008669	1.843129
H	3.232762	0.273652	2.605771
H	1.870642	-0.794369	2.242255
C	3.244441	-0.461807	0.592093
H	3.874262	-1.295644	0.925406
H	3.950181	0.304868	0.258979
C	2.444351	-1.006794	-0.599311
H	1.882169	-1.889925	-0.304267
H	3.157283	-1.326129	-1.371144
C	0.690391	-0.721479	-2.330697
H	0.626063	-0.028990	-3.170809
H	1.235939	-1.601067	-2.688214
C	-0.705543	-1.127710	-1.891492
H	-0.675660	-2.002808	-1.245778
H	-1.294795	-1.401181	-2.777058
C	-2.635436	-0.581782	-0.524143
H	-2.367134	-1.529602	-0.056404
H	-3.344495	-0.797311	-1.333404
C	-3.299351	0.314764	0.518371
H	-3.545876	1.300665	0.111529
H	-4.263318	-0.149498	0.757204
C	-2.529942	0.417247	1.833585
H	-2.257816	-0.583620	2.168648
H	-3.172415	0.861784	2.604520
C	-1.635596	2.669168	1.714621
H	-2.235889	2.928989	2.595063
H	-0.745889	3.293599	1.692334
H	-2.215481	2.872051	0.815291
C	2.445278	2.395725	1.323484
H	3.119517	2.598184	2.164430
H	1.812940	3.264606	1.153428
H	3.047843	2.226939	0.437731
C	2.289783	1.017255	-1.934302
H	2.962541	1.516011	-1.245122
H	1.627994	1.758736	-2.375719
H	2.889262	0.549451	-2.724024
C	-1.787290	1.042881	-2.115993
H	-0.912856	1.446119	-2.620713
H	-2.286136	1.859101	-1.596449
H	-2.470483	0.619786	-2.862383
N	0.113284	2.842874	-0.727786
C	0.125168	3.928765	-1.132945
C	0.138698	5.292270	-1.643044
H	1.107199	5.504165	-2.105225
H	-0.029919	5.995510	-0.822330
H	-0.651152	5.414664	-2.389874

=== Model-2, 5Int ===

Fe	0.121860	0.630477	0.350984
N	-1.357289	1.295194	1.860003
N	1.641352	1.391573	1.840425
N	1.679981	-0.130288	-1.087782
N	-1.306123	-0.267187	-1.154428
C	-0.562047	1.081820	3.106251
H	-1.098482	1.491491	3.974892
H	-0.465553	0.009283	3.260234
C	0.825275	1.732553	3.053841
H	1.372027	1.456439	3.965415
H	0.716647	2.818649	3.078144
C	2.552057	0.234526	2.105287
H	3.292155	0.541009	2.861107
H	1.953422	-0.558833	2.550078
C	3.329694	-0.309124	0.889256
H	3.996417	-1.078871	1.298582
H	4.003978	0.459096	0.498291
C	2.581151	-1.002919	-0.266809
H	1.969569	-1.816159	0.121555
H	3.336843	-1.441007	-0.936545
C	0.924738	-0.939924	-2.108262
H	0.850288	-0.329372	-3.010198
H	1.508388	-1.828206	-2.382997
C	-0.478103	-1.390253	-1.683008
H	-0.410911	-2.141354	-0.897583
H	-0.964166	-1.849599	-2.557984
C	-2.536938	-0.785689	-0.481349
H	-2.252913	-1.677210	0.079122
H	-3.257371	-1.090805	-1.254929
C	-3.224062	0.205675	0.474182
H	-3.406891	1.166536	-0.019253
H	-4.220046	-0.207454	0.675844
C	-2.564378	0.409285	1.849388
H	-2.262777	-0.563334	2.239923
H	-3.305238	0.827226	2.546089
C	-1.791995	2.710783	1.771558
H	-2.406268	2.975175	2.643722
H	-0.929239	3.374893	1.729899
H	-2.378687	2.865865	0.865762
C	2.447886	2.589532	1.498532
H	3.097935	2.871631	2.339064
H	1.786453	3.423497	1.263184
H	3.075123	2.398827	0.629815
C	2.494953	0.865032	-1.831559
H	3.074689	1.480920	-1.147273
H	1.840811	1.520564	-2.406650
H	3.188496	0.357472	-2.516341
C	-1.703191	0.633984	-2.260845
H	-0.824475	1.062771	-2.742146
H	-2.307551	1.456542	-1.876906
H	-2.287767	0.083229	-3.012243
N	0.082286	2.633494	-0.704005
C	0.048340	3.665472	-1.228437
C	0.003841	4.962416	-1.887667
H	1.021763	5.324812	-2.058178
H	-0.531221	5.678243	-1.256853
H	-0.512436	4.872336	-2.847767
O	-0.113685	-1.357062	1.099531
O	0.246726	-2.003447	2.422345
H	0.830763	-2.827908	2.145284
H	-0.610901	-2.367917	2.728817
N	1.677753	-4.054346	1.749957
C	2.289409	-4.998454	1.483693
C	3.059397	-6.186064	1.147755
H	2.380583	-7.019756	0.946632
H	3.715461	-6.447879	1.982778

H 3.666318 -5.992076 0.258715

=== Model-2, 3Int ===

Fe	0.106106	0.595823	0.297192
N	-1.302012	1.191230	1.777307
N	1.572896	1.239408	1.724313
N	1.564191	-0.090362	-1.134863
N	-1.309420	-0.141016	-1.111000
C	-0.544665	0.953396	3.042831
H	-1.100131	1.356044	3.902044
H	-0.455744	-0.122891	3.177779
C	0.828258	1.595009	2.983304
H	1.414885	1.301725	3.862341
H	0.736461	2.681734	3.018517
C	2.458711	0.053780	1.981680
H	3.180708	0.333975	2.762179
H	1.828894	-0.736247	2.386547
C	3.245172	-0.467028	0.770341
H	3.864075	-1.288480	1.152546
H	3.961424	0.285910	0.426764
C	2.462565	-1.054463	-0.411656
H	1.833337	-1.872157	-0.062812
H	3.184975	-1.454913	-1.137431
C	0.810058	-0.816210	-2.218049
H	0.725380	-0.140321	-3.070916
H	1.389049	-1.682243	-2.560652
C	-0.568359	-1.263682	-1.768422
H	-0.489886	-2.067004	-1.036167
H	-1.134061	-1.635966	-2.634788
C	-2.561748	-0.705800	-0.511584
H	-2.283632	-1.627890	-0.000568
H	-3.244534	-0.964965	-1.332463
C	-3.273304	0.211441	0.481613
H	-3.513483	1.183893	0.039157
H	-4.241546	-0.254526	0.701218
C	-2.548653	0.362654	1.818322
H	-2.269465	-0.628598	2.177178
H	-3.226419	0.803750	2.562085
C	-1.699526	2.624051	1.693863
H	-2.306785	2.895774	2.567526
H	-0.821984	3.265323	1.652874
H	-2.281786	2.797823	0.789322
C	2.426125	2.420982	1.409885
H	3.065291	2.656846	2.270737
H	1.795137	3.278854	1.183615
H	3.065876	2.230278	0.553663
C	2.403939	0.924730	-1.831246
H	3.041287	1.454219	-1.129991
H	1.763891	1.650940	-2.329777
H	3.043061	0.431333	-2.575084
C	-1.698314	0.864385	-2.138002
H	-0.816845	1.296934	-2.606044
H	-2.262225	1.673541	-1.675413
H	-2.320153	0.389853	-2.908661
N	0.149222	2.856232	-0.747608
C	0.133587	3.913003	-1.224027
C	0.113299	5.240778	-1.824104
H	1.136165	5.573655	-2.022870
H	-0.367790	5.948621	-1.142921
H	-0.443852	5.213834	-2.765070
O	-0.107105	-1.558034	1.016907
O	0.022380	-2.220139	2.369513
H	0.705455	-2.987702	2.206325
H	-0.850231	-2.647175	2.499131
N	1.737027	-4.138337	1.974533
C	2.483467	-5.011612	1.844427
C	3.423016	-6.110668	1.681493
H	2.876555	-7.033680	1.467443
H	4.002104	-6.239466	2.600391
H	4.103756	-5.894363	0.853218

=== Model-2, 5Int-ho-oh1 ===

Fe	0.058026	0.589885	0.226011
N	-1.299793	1.273974	1.832408
N	1.666181	1.213223	1.668484
N	1.534701	0.004634	-1.377991
N	-1.433219	0.022430	-1.322053
C	-0.479051	0.905360	3.033592

H	-0.961923	1.293300	3.941044
H	-0.446963	-0.181391	3.098559
C	0.937040	1.478579	2.964101
H	1.519898	1.075130	3.800298
H	0.906512	2.561134	3.098354
C	2.541115	-0.007373	1.780739
H	3.306702	0.202124	2.540993
H	1.915144	-0.821995	2.143560
C	3.269742	-0.426994	0.490034
H	3.923693	-1.255848	0.788176
H	3.954750	0.361319	0.163667
C	2.469246	-0.967966	-0.709424
H	1.887643	-1.838901	-0.411483
H	3.190598	-1.307361	-1.465951
C	0.710063	-0.676561	-2.443881
H	0.640445	0.012735	-3.286819
H	1.240018	-1.564045	-2.807636
C	-0.696124	-1.089729	-2.003699
H	-0.655151	-1.936664	-1.321381
H	-1.252415	-1.414376	-2.893288
C	-2.655738	-0.515889	-0.634920
H	-2.379349	-1.465706	-0.174720
H	-3.408552	-0.725142	-1.406390
C	-3.272039	0.397261	0.436363
H	-3.453503	1.404744	0.046526
H	-4.267769	-0.013580	0.640797
C	-2.548539	0.440936	1.791504
H	-2.270524	-0.572465	2.082888
H	-3.236393	0.832425	2.552720
C	-1.668471	2.712227	1.884109
H	-2.264164	2.908901	2.784457
H	-0.776482	3.336630	1.908148
H	-2.252794	2.983735	1.005283
C	2.508989	2.408604	1.392081
H	3.217190	2.565678	2.215788
H	1.878415	3.291493	1.293792
H	3.074281	2.285856	0.471876
C	2.337647	1.061567	-2.054673
H	2.969980	1.585359	-1.342332
H	1.676322	1.785559	-2.528568
H	2.978323	0.607801	-2.821150
C	-1.837388	1.043456	-2.324130
H	-0.960756	1.470306	-2.808929
H	-2.388966	1.849979	-1.842128
H	-2.476906	0.581769	-3.086933
N	0.083414	2.652549	-0.602164
C	0.062436	3.738118	-1.003475
C	0.033629	5.101072	-1.505415
H	1.053379	5.436712	-1.715574
H	-0.417462	5.756991	-0.754905
H	-0.558609	5.140336	-2.424380
O	-0.085585	-1.086237	0.949571
O	0.092255	-2.314191	2.989502
H	0.120806	-1.984687	0.616009
H	-0.721324	-2.717265	2.620920
N	0.309369	-3.823117	0.094408
C	0.454354	-4.963364	-0.054975
C	0.637592	-6.397235	-0.240528
H	1.460320	-6.750490	0.387798
H	0.870633	-6.609879	-1.287892
H	-0.277628	-6.928074	0.037072

=== Model-2, 3Int-ho-oh1 ===

Fe	0.058160	0.575013	0.264692
N	-1.280272	1.277447	1.790248
N	1.608476	1.203618	1.648660
N	1.465903	-0.059019	-1.263259
N	-1.425716	-0.007712	-1.173730
C	-0.490702	0.963040	3.029817
H	-1.007212	1.384354	3.902671
H	-0.445005	-0.120628	3.134402
C	0.905164	1.545685	2.944034
H	1.505288	1.185781	3.786813
H	0.875019	2.633386	3.019997
C	2.474384	-0.015000	1.833457
H	3.225473	0.235588	2.594564
H	1.834587	-0.805345	2.222818
C	3.217194	-0.490205	0.577779

H	-2.501927	-0.369719	1.955120
H	-3.266357	1.121181	2.533489
C	-1.540300	2.832226	1.822240
H	-2.105248	3.066436	2.732514
H	-0.588991	3.358478	1.849910
H	-2.099632	3.180563	0.955304
C	2.463969	2.209317	1.324125
H	3.171965	2.287392	2.157964
H	1.897189	3.134775	1.248670
H	3.027934	2.070662	0.406978
C	2.174655	1.045336	-2.070100
H	2.877157	1.458580	-1.353531
H	1.590323	1.859022	-2.494249
H	2.743143	0.555228	-2.869641
C	-1.895274	1.471014	-2.243389
H	-0.982256	1.828155	-2.714013
H	-2.342055	2.297960	-1.693120
H	-2.593599	1.140123	-3.021761
N	0.174924	2.900272	-0.615145
C	0.281414	3.989447	-0.995164
C	0.418568	5.357073	-1.471631
H	1.458449	5.544468	-1.755237
H	0.128426	6.053352	-0.679246
H	-0.226965	5.510348	-2.341547
O	-0.411975	-1.088519	0.673460
O	0.257061	-2.708183	2.943567
H	-0.103874	-1.590729	1.452759
H	0.506786	-3.545235	2.456684
N	0.951268	-4.991708	1.425164
C	1.207465	-5.935235	0.803650
C	1.527808	-7.122879	0.021562
H	2.261471	-7.733630	0.555573
H	1.943628	-6.829221	-0.946609
H	0.622714	-7.714766	-0.142761

=== Model-2, 5TSoo ===

Fe	0.120528	0.601519	0.377357
N	-1.363265	1.313526	1.862303
N	1.632932	1.403623	1.847911
N	1.679904	-0.149565	-1.069194
N	-1.298217	-0.288981	-1.140217
C	-0.574219	1.107784	3.114471
H	-1.112079	1.529429	3.976233
H	-0.484064	0.036196	3.279061
C	0.816892	1.751336	3.060808
H	1.361897	1.474170	3.972806
H	0.713923	2.837991	3.082745
C	2.552347	0.254291	2.121334
H	3.290357	0.572857	2.873871
H	1.958895	-0.539506	2.572049
C	3.333816	-0.292816	0.908976
H	4.007614	-1.052899	1.324643
H	4.001061	0.477974	0.511113
C	2.593165	-1.004005	-0.242005
H	1.994284	-1.824354	0.150564
H	3.354659	-1.435490	-0.909291
C	0.932353	-0.978380	-2.081052
H	0.867626	-0.385757	-2.995400
H	1.517098	-1.872421	-2.332648
C	-0.476410	-1.419585	-1.663356
H	-0.420851	-2.171692	-0.878509
H	-0.960962	-1.873097	-2.541859
C	-2.535579	-0.793263	-0.467589
H	-2.260587	-1.682130	0.101576
H	-3.253454	-1.100293	-1.242454
C	-3.222465	0.211745	0.474027
H	-3.398700	1.167523	-0.031544
H	-4.221348	-0.195156	0.673736
C	-2.572124	0.429408	1.851759
H	-2.275971	-0.538825	2.257181
H	-3.317584	0.857256	2.537240
C	-1.793713	2.729175	1.759297
H	-2.413146	3.001898	2.625099
H	-0.929060	3.390834	1.718981
H	-2.373846	2.878345	0.848356
C	2.431675	2.603298	1.492770
H	3.083635	2.894597	2.328472
H	1.765379	3.432442	1.254582

H	3.056053	2.409273	0.622813
C	2.482711	0.847769	-1.824085
H	3.055406	1.477921	-1.146903
H	1.820907	1.488987	-2.406271
H	3.181763	0.340664	-2.503353
C	-1.684717	0.609711	-2.253410
H	-0.800972	1.024963	-2.737006
H	-2.281250	1.440994	-1.876777
H	-2.273442	0.058202	-3.000594
N	0.074001	2.593012	-0.705872
C	0.050627	3.628074	-1.224536
C	0.019534	4.928593	-1.877146
H	1.041144	5.281834	-2.044780
H	-0.509369	5.646221	-1.243184
H	-0.496597	4.848040	-2.838169
O	-0.101444	-1.248478	1.093615
O	0.252448	-1.988483	2.463228
H	0.821540	-2.788549	2.143333
H	-0.621544	-2.362649	2.700635
N	1.686371	-4.055864	1.699374
C	2.291632	-4.999137	1.413868
C	3.054309	-6.185593	1.055362
H	2.371693	-7.017019	0.857808
H	3.723311	-6.456024	1.877296
H	3.647617	-5.985635	0.158481

=== Model-2, 3TSoo ===

Fe	0.103124	0.551549	0.329043
N	-1.312952	1.208576	1.783530
N	1.562560	1.236241	1.740999
N	1.571262	-0.129893	-1.106732
N	-1.301570	-0.166786	-1.096579
C	-0.566057	0.979280	3.057168
H	-1.121103	1.402106	3.906780
H	-0.491566	-0.095653	3.208536
C	0.816619	1.601910	2.998341
H	1.396691	1.301378	3.878976
H	0.739208	2.689740	3.033429
C	2.466025	0.066120	2.010517
H	3.189336	0.369523	2.780960
H	1.850457	-0.724843	2.433993
C	3.255712	-0.461873	0.803435
H	3.884140	-1.271249	1.195855
H	3.964077	0.295123	0.452580
C	2.487146	-1.072203	-0.377349
H	1.877397	-1.904837	-0.031158
H	3.221167	-1.457937	-1.099370
C	0.821159	-0.871657	-2.183800
H	0.752615	-0.212300	-3.050864
H	1.396208	-1.749108	-2.502454
C	-0.568844	-1.299897	-1.747325
H	-0.508791	-2.103325	-1.014839
H	-1.130621	-1.662058	-2.620251
C	-2.561885	-0.713959	-0.497662
H	-2.295516	-1.632267	0.026429
H	-3.240871	-0.979127	-1.319632
C	-3.275027	0.222672	0.476863
H	-3.503542	1.190263	0.017927
H	-4.249010	-0.232968	0.692577
C	-2.565400	0.389163	1.820239
H	-2.298512	-0.598288	2.198447
H	-3.250190	0.845372	2.548209
C	-1.696933	2.642900	1.677991
H	-2.315382	2.929330	2.538999
H	-0.813435	3.276414	1.644868
H	-2.262869	2.811516	0.762294
C	2.400902	2.423503	1.406881
H	3.047241	2.672046	2.258628
H	1.759916	3.273683	1.181053
H	3.032179	2.232083	0.544674
C	2.397168	0.889915	-1.813958
H	3.033904	1.428689	-1.119364
H	1.748611	1.607457	-2.313535
H	3.036519	0.397466	-2.558081
C	-1.676057	0.835734	-2.132341
H	-0.788358	1.248260	-2.606458
H	-2.225802	1.658654	-1.677766
H	-2.306176	0.362687	-2.896905

N	0.146039	2.817800	-0.753628
C	0.134134	3.877274	-1.224147
C	0.117602	5.209210	-1.814972
H	1.141550	5.543084	-2.006245
H	-0.366586	5.912238	-1.130957
H	-0.435024	5.189380	-2.758762
O	-0.078482	-1.406974	1.011186
O	0.027296	-2.168085	2.392211
H	0.697313	-2.922373	2.184111
H	-0.851763	-2.594825	2.453892
N	1.740407	-4.108806	1.907432
C	2.482191	-4.982788	1.753857
C	3.416109	-6.082823	1.563569
H	2.863709	-7.005476	1.363653
H	4.020488	-6.213362	2.465775
H	4.074267	-5.866774	0.717150

=== Model-2, 5TShat ===

Fe	-0.127357	0.000253	0.018060
N	0.020290	0.025584	2.239453
N	2.119105	-0.204766	0.144135
N	-0.140115	-0.034662	-2.238729
N	-2.314620	0.199049	-0.228601
C	1.198338	-0.876683	2.437223
H	1.492812	-0.880084	3.495235
H	0.888820	-1.887966	2.179147
C	2.408317	-0.449405	1.604708
H	3.188596	-1.212987	1.701745
H	2.823929	0.474059	2.011068
C	2.454520	-1.416967	-0.680789
H	3.539807	-1.574659	-0.611324
H	1.972228	-2.278152	-0.220020
C	2.087052	-1.339385	-2.173783
H	2.477126	-2.267096	-2.610325
H	2.655616	-0.543031	-2.663390
C	0.609552	-1.286891	-2.602979
H	0.064866	-2.127710	-2.175801
H	0.576892	-1.385135	-3.696987
C	-1.596408	-0.154272	-2.611378
H	-1.919531	0.822922	-2.973769
H	-1.703792	-0.851008	-3.450933
C	-2.508818	-0.611891	-1.473593
H	-2.308751	-1.650774	-1.218147
H	-3.551113	-0.531592	-1.809865
C	-3.004317	-0.467636	0.926788
H	-2.842310	-1.541737	0.825817
H	-4.081231	-0.280374	0.824006
C	-2.544586	-0.019937	2.322447
H	-2.558530	1.070904	2.419441
H	-3.309593	-0.380124	3.020252
C	-1.213776	-0.608067	2.813178
H	-1.180660	-1.670624	2.566928
H	-1.158115	-0.516620	3.905913
C	0.257656	1.333744	2.903301
H	0.405756	1.182825	3.980074
H	1.140228	1.820310	2.490084
H	-0.598583	1.990626	2.752131
C	2.972928	0.935673	-0.289749
H	4.031658	0.685212	-0.146690
H	2.735573	1.820993	0.298594
H	2.811165	1.165878	-1.340151
C	0.416798	1.117280	-2.999355
H	1.473553	1.253569	-2.782755
H	-0.111426	2.030872	-2.728641
H	0.302114	0.944504	-4.077139
C	-2.864355	1.567802	-0.410799
H	-2.355024	2.081759	-1.224821
H	-2.727842	2.150610	0.500038
H	-3.935548	1.509747	-0.641371
N	0.112539	2.160343	-0.041902
C	0.209657	3.313356	-0.060165
C	0.333771	4.760031	-0.082765
H	0.858415	5.095811	0.816639
H	-0.662171	5.211859	-0.112488
H	0.898543	5.065166	-0.968605
O	-0.391016	-1.739875	0.111336
O	0.005221	-4.011670	0.509407
H	0.003586	-2.706606	0.350404

H	-0.045065	-4.390860	-0.408169
N	-0.102130	-5.062334	-2.146407
C	-0.177598	-5.569620	-3.185490
C	-0.271531	-6.209490	-4.492031
H	-0.330137	-7.295001	-4.370509
H	0.610213	-5.964429	-5.091228
H	-1.166996	-5.860063	-5.014072

=== Model-2, 3TShat ===

Fe	-0.154045	-0.020614	0.009226
N	-0.016681	0.007504	2.152789
N	2.011844	-0.252921	0.100429
N	-0.218761	-0.053527	-2.157195
N	-2.285311	0.205136	-0.152882
C	1.153169	-0.901908	2.388167
H	1.425293	-0.881040	3.451458
H	0.839929	-1.915546	2.146568
C	2.350748	-0.484446	1.556539
H	3.134519	-1.245608	1.631407
H	2.774645	0.441923	1.945804
C	2.351755	-1.474676	-0.710554
H	3.439361	-1.611259	-0.647042
H	1.890069	-2.337740	-0.233833
C	1.967327	-1.414734	-2.193802
H	2.315119	-2.362314	-2.622406
H	2.546183	-0.644214	-2.711376
C	0.482727	-1.321691	-2.567320
H	-0.069941	-2.150178	-2.128652
H	0.404180	-1.392807	-3.660049
C	-1.679967	-0.126597	-2.540420
H	-1.979445	0.863743	-2.885178
H	-1.797069	-0.805646	-3.391630
C	-2.565983	-0.582282	-1.398976
H	-2.384509	-1.628313	-1.164043
H	-3.619414	-0.458275	-1.680765
C	-3.015385	-0.440239	0.985793
H	-2.880684	-1.517138	0.884990
H	-4.082049	-0.215662	0.857692
C	-2.563852	-0.007980	2.379272
H	-2.589086	1.079767	2.500493
H	-3.310839	-0.395882	3.081412
C	-1.222087	-0.598912	2.806700
H	-1.212805	-1.664307	2.575217
H	-1.096377	-0.484719	3.890788
C	0.248712	1.339616	2.768200
H	0.420110	1.212440	3.843517
H	1.124923	1.804314	2.321770
H	-0.605188	1.998721	2.620132
C	2.873115	0.878985	-0.353953
H	3.924854	0.621374	-0.182362
H	2.630761	1.779074	0.206495
H	2.738109	1.077836	-1.412656
C	0.357296	1.095733	-2.915126
H	1.421308	1.199867	-2.728088
H	-0.140199	2.019344	-2.625816
H	0.208411	0.929219	-3.988748
C	-2.774826	1.604161	-0.310725
H	-2.266583	2.102613	-1.132639
H	-2.595984	2.171158	0.601198
H	-3.851937	1.587661	-0.515187
N	0.132406	2.236942	-0.068387
C	0.252123	3.388554	-0.091178
C	0.402157	4.833993	-0.117780
H	0.930564	5.164187	0.781456
H	-0.585071	5.304343	-0.150943
H	0.973998	5.127741	-1.002863
O	-0.512561	-1.803976	0.113371
O	0.215739	-4.065758	0.544437
H	0.038842	-2.619708	0.364193
H	0.169940	-4.424211	-0.377598
N	0.148792	-5.059261	-2.181435
C	0.092538	-5.557297	-3.226601
C	0.023208	-6.185503	-4.540710
H	-0.807011	-6.897175	-4.569464
H	0.956184	-6.717217	-4.748902
H	-0.133114	-5.424114	-5.310399

=== Model-2, 5P ===

Fe	0.362108	0.462799	-0.355506	H	3.610327	1.248626	1.954496
N	0.217081	0.193965	1.823628	H	2.282576	2.388761	2.083505
N	2.515182	0.948816	0.105950	C	3.490131	0.611506	-0.435670
N	0.697039	0.656512	-2.575631	H	4.448895	1.068260	-0.159426
N	-1.677506	-0.110981	-0.960901	H	3.444994	-0.379207	0.014668
C	1.605314	-0.265378	2.148862	C	3.432313	0.503315	-1.962300
H	1.731254	-0.305957	3.238832	H	4.303041	-0.098699	-2.248912
H	1.732655	-1.274832	1.756164	H	3.602664	1.479580	-2.426644
C	2.664811	0.671426	1.577164	C	2.223102	-0.193978	-2.592919
H	3.655274	0.242268	1.768459	H	2.135518	-1.210791	-2.211868
H	2.634173	1.631395	2.094836	H	2.381806	-0.247047	-3.677433
C	3.331032	-0.023959	-0.700092	C	-0.203717	-0.346274	-2.988622
H	4.387133	0.148521	-0.450081	H	-0.948786	0.340680	-3.392094
H	3.070969	-1.026968	-0.361310	H	0.198532	-0.910877	-3.836164
C	3.185858	0.079747	-2.227045	C	-0.841183	-1.291765	-1.995801
H	3.900183	-0.647447	-2.632290	H	-0.144995	-2.075936	-1.701944
H	3.548778	1.049458	-2.581303	H	-1.722026	-1.764054	-2.447816
C	1.842134	-0.267353	-2.887507	C	-1.639458	-1.595558	0.265695
H	1.535614	-1.273854	-2.601256	H	-0.885343	-2.383277	0.236796
H	1.986109	-0.256213	-3.976606	H	-2.589721	-2.030297	-0.067059
C	-0.576114	0.151412	-3.197215	C	-1.768861	-1.087193	1.695997
H	-1.163273	1.022767	-3.491505	H	-2.456259	-0.238846	1.774603
H	-0.341364	-0.395839	-4.117663	H	-2.235387	-1.894026	2.272705
C	-1.405656	-0.748887	-2.286949	C	-0.424591	-0.805740	2.354254
H	-0.888432	-1.689354	-2.099777	H	0.242503	-1.653648	2.194247
H	-2.354438	-0.975379	-2.789959	H	-0.555869	-0.686924	3.436768
C	-2.207086	-1.142519	-0.006390	C	-0.373631	1.621738	2.451210
H	-1.636128	-2.058498	-0.168251	H	-0.353156	1.540968	3.543694
H	-3.248374	-1.346057	-0.287083	H	0.139403	2.533883	2.155877
C	-2.139014	-0.765229	1.478009	H	-1.408922	1.682169	2.119685
H	-2.574314	0.222027	1.664033	C	2.597157	2.869688	-0.194394
H	-2.794164	-1.471720	2.000532	H	3.574809	3.209910	0.166257
C	-0.758993	-0.905252	2.130369	H	1.821984	3.488363	0.252920
H	-0.304620	-1.845559	1.814291	H	2.568922	2.994314	-1.271381
H	-0.874842	-0.945704	3.221044	C	0.887082	1.781677	-3.109363
C	-0.131044	1.400943	2.621218	H	1.693069	2.429852	-2.782639
H	-0.075763	1.161293	3.690115	H	-0.061186	2.292990	-2.956846
H	0.557122	2.217524	2.407588	H	1.016000	1.584208	-4.179856
H	-1.142265	1.730941	2.384655	C	-2.435466	0.297334	-1.031570
C	3.004448	2.334942	-0.129418	H	-2.209470	1.031293	-1.801111
H	4.048925	2.419285	0.195722	H	-2.742455	0.822757	-0.128896
H	2.399492	3.043209	0.435738	H	-3.262089	-0.334367	-1.375600
H	2.950443	2.595051	-1.182803	N	-0.397425	2.308177	-0.394398
C	0.962915	2.000498	-3.158691	C	-0.928338	3.331424	-0.485147
H	1.890152	2.417066	-2.775341	C	-1.596313	4.615382	-0.595672
H	0.147696	2.680201	-2.913981	H	-1.228274	5.144727	-1.479596
H	1.044149	1.920225	-4.250027	H	-1.390625	5.212208	0.298063
C	-2.668995	0.988634	-1.104073	H	-2.675102	4.458021	-0.688061
H	-2.304006	1.750483	-1.791071	O	1.240500	-0.984780	-0.128297
H	-2.853360	1.454994	-0.137104	O	2.298023	-3.072949	1.548268
H	-3.612670	0.584747	-1.490796	H	1.560578	-3.685153	1.736563
N	-0.133387	2.443977	-0.236124	H	1.966800	-2.527065	0.814598
C	-0.431723	3.559280	-0.172265	N	-0.070439	-4.783821	2.026443
C	-0.803974	4.958908	-0.091600	C	-0.945294	-5.494703	2.298079
H	-0.016809	5.571909	-0.540693	C	-2.044371	-6.390284	2.640791
H	-0.932871	5.241239	0.957565	H	-2.678004	-5.928593	3.403562
H	-1.742862	5.117998	-0.630435	H	-1.648702	-7.333003	3.029857
O	0.716952	-1.109451	-0.441058	H	-2.648497	-6.597332	1.752699
O	2.180313	-3.366704	0.608899				
H	1.604004	-3.857310	1.227418				
H	1.562420	-2.830789	0.085298				
N	0.328591	-4.756471	2.434016				
C	-0.332320	-5.390871	3.144446				
C	-1.162444	-6.189847	4.038722				
H	-1.974547	-6.658371	3.475339				
H	-1.590616	-5.553706	4.818732				
H	-0.558168	-6.971243	4.508615				

=== Model-2, 3P ===

Fe	0.537229	0.464895	-0.244891
N	0.288217	0.421489	1.859699
N	2.403575	1.440777	0.198184
N	0.895288	0.483106	-2.370440
N	-1.246633	-0.561239	-0.749364
C	1.706519	0.333723	2.343569
H	1.726712	0.458336	3.433478
H	2.073670	-0.665209	2.111582
C	2.556824	1.405235	1.699829