

Supporting Information

Computational Insights into the Hydroxylation Mechanism of Toluene Catalyzed by Non-Heme Diiron Toluene 4-Monooxygenase T4moH

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Table S1 Calculated Mulliken spin population of key atoms in the R_I and R_{II} at nonet spin states

	Fe1	Fe2	Op	Od
¹¹ R/ ^{0S} R _I	3.72/-3.61	3.73/3.91	0.94/-0.14	0.99/-0.34
⁹ R _I / ⁹ R _{II}	4.19/2.82	3.69/4.02	-0.10/0.32	-0.53/0.08
⁷ R _I / ⁷ R _{II}	1.04/1.03	3.71/4.05	0.37/0.17	0.61/0.15
⁵ R _I / ⁵ R _{II}	1.05/-1.02	1.91/4.05	0.35/0.21	0.60/0.18
³ R _I / ³ R _{II}	-1.0/-1.03	1.92/2.85	0.36/0.05	0.65/-1.11

Table S2 Calculated Mulliken spin population of key atoms and groups in transition states and intermediates in T4moH-catalysed hydroxylation reactions at nonet spin states

	Fe1	Fe2	Op	Od	MBN
⁹ TS1 _I / ⁹ IM1 _{I-a}	4.18/4.17	3.71/3.72	0.21/0.19	-0.26/-0.03	-0.68/-0.82
⁹ TS2 _I / ⁹ IM2 _I	4.22/4.21	3.67/2.82	-0.10/0.37	-0.26/0.00	—
⁹ TS3 _I / ⁹ IM3 _I	4.19/4.20	2.94/2.85	0.22/0.33	0.02/0.08	—
⁹ IM4 _I / ⁹ TS5 _I	4.13/4.18	2.91/2.83	0.37/0.35	0.03/0.07	—
⁹ IM1 _{I-b} / ⁹ IM1 _{I-c}	4.01/3.29	3.65/3.66	0.22/-0.01	-0.02/-0.01	-0.73/0.71
⁹ P _I / ⁹ TS1 _{II}	4.12/2.77	3.02/4.09	0.26/0.27	0.01/0.33	—
⁹ IM1 _{II} / ⁹ IM1 _{II} '	2.82/3.14	4.04/3.18	0.03/0.58	0.40/0.57	—

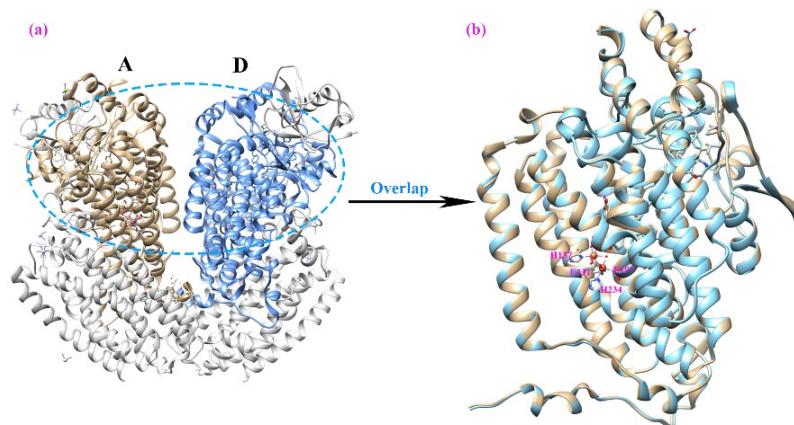


Figure S1 (a) Crystal structure of T4moH (PDB ID: 5TDS); (b) Overlap of chain A (gold) and chain D (blue) in the T4moH-toluene complex.

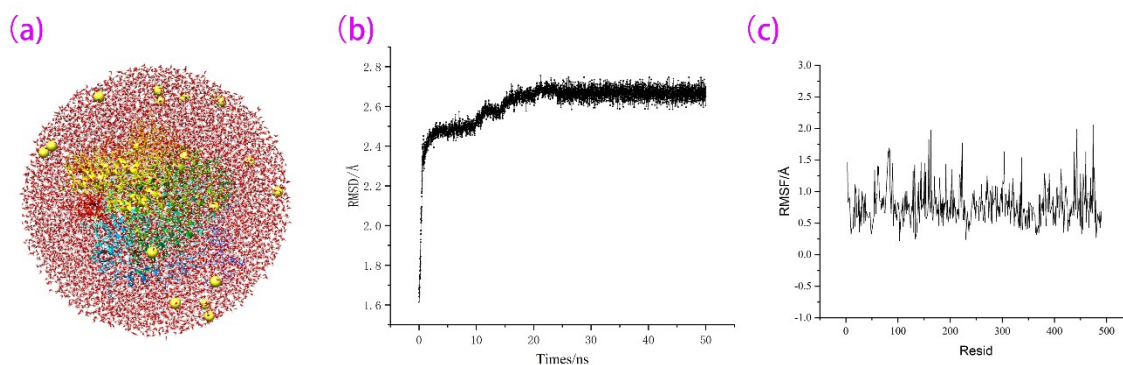


Figure S2 (a) Constructed T4moH-toluene complex solvation model. (b) RMSDs of 50 ns MD simulations for the backbone atoms of T4moH. (c) RMSFs of the system derived from the 50 ns MD simulations.

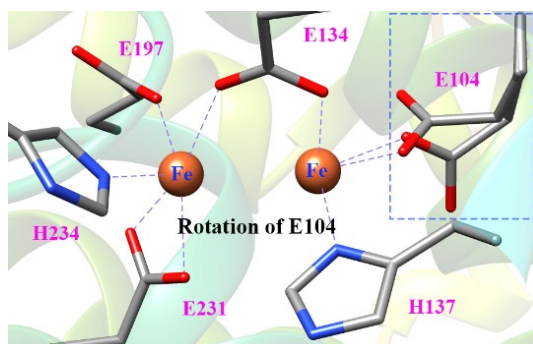


Figure S3. Two conformations of residue Glu104 in the crystal structure of T4moH (PDB ID 4P1B).

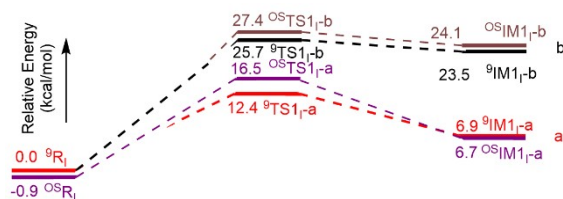


Figure S4. Comparison of potential energy profiles for the nucleophilic attack of FeI^{III}-Op-Od⁻ on C4 of toluene using ⁹R_I and ^{os}R_I as reactants.

Cartesian coordinates of QM regions of optimized species

^{os} R					
C	-5.430	-6.986	5.799	C	-7.948 -12.677 3.101
H	-5.034	-7.599	6.617	H	-7.721 -13.600 3.611
H	-6.413	-7.372	5.517	C	-9.203 -3.016 -3.267
C	-4.487	-7.061	4.582	H	10.075 -2.545 -3.731
H	-4.326	-6.084	4.104	H	-9.330 -4.102 -3.306
H	-3.498	-7.430	4.862	C	-9.082 -2.573 -1.795
C	-5.037	-7.939	3.465	H	-8.099 -2.798 -1.377
O	-6.298	-7.870	3.263	H	-9.264 -1.497 -1.684
O	-4.226	-8.634	2.797	C	10.133 -3.326 -0.995
C	10.263	-7.120	5.548	O	11.339 -3.150 -1.207
H	10.991	-6.740	6.274	O	-9.659 -4.158 -0.112
H	-9.274	-6.780	5.867	C	-9.447 -8.958 -4.285
C	10.622	-6.528	4.167	H	-8.619 -9.553 -3.888
H	11.654	-6.781	3.887	H	-9.549 -9.245 -5.334
H	10.628	-5.437	4.262	C	-9.085 -7.457 -4.153
C	-9.790	-6.848	2.916	H	-8.286 -7.243 -4.872
O	-9.223	-7.957	2.760	H	-9.925 -6.803 -4.390
O	-9.805	-5.932	2.020	C	-8.544 -7.162 -2.751
C	-6.634	-10.792	4.360	O	-7.501 -7.757 -2.402
H	-7.041	-9.830	4.682	O	-9.235 -6.394 -1.983
H	-5.617	-10.613	3.995	C	14.948 -6.504 -0.106
N	-8.793	-12.645	2.025	H	15.010 -5.507 0.337
H	-9.296	-13.461	1.604	H	15.598 -7.174 0.468
C	-7.514	-11.383	3.296	N	13.151 -8.312 0.111
C	-8.848	-11.379	1.584	H	13.771 -9.118 0.335
H	-9.440	-11.069	0.738	C	13.540 -6.993 -0.082
N	-8.077	-10.588	2.320	C	11.800 -8.351 0.091
				H	11.218 -9.249 0.222

N	11.306	-7.135	-0.114	H	-9.307	-6.767	5.938
C	12.383	-6.283	-0.230	C	10.671	-6.501	4.256
H	12.252	-5.223	-0.388	H	11.701	-6.763	3.977
Fe	-7.482	-8.603	1.720	H	10.691	-5.411	4.372
Fe	-9.495	-6.077	-0.014	C	-9.846	-6.760	2.984
C	-3.331	-3.077	2.992	O	-9.129	-7.807	2.867
C	-4.645	-2.601	3.099	O	10.012	-5.903	2.073
C	-5.568	-2.809	2.070	C	-6.694	-10.747	4.363
C	-5.188	-3.495	0.914	H	-7.099	-9.801	4.728
C	-3.883	-3.983	0.801	H	-5.683	-10.555	3.993
C	-2.966	-3.776	1.831	N	-8.873	-12.534	1.986
C	-2.333	-2.854	4.100	H	-9.362	-13.357	1.563
H	-2.299	-3.712	4.785	C	-7.582	-11.297	3.281
H	-2.581	-1.970	4.695	C	-8.902	-11.264	1.548
H	-1.315	-2.733	3.718	H	-9.477	-10.940	0.697
H	-4.942	-2.044	3.984	N	-8.123	-10.485	2.296
H	-6.580	-2.425	2.169	C	-8.039	-12.579	3.072
H	-5.890	-3.645	0.100	H	-7.836	-13.507	3.583
H	-3.578	-4.506	-0.099	C	-9.214	-2.996	-3.266
H	-1.948	-4.143	1.726	H	10.082	-2.525	-3.739
O	-7.601	-6.636	0.625	H	-9.347	-4.082	-3.289
O	-6.650	-6.102	-0.034	C	-9.090	-2.532	-1.800
O	-8.328	-9.203	-0.338	H	-8.099	-2.735	-1.386
H	-7.925	-8.607	-1.027	H	-9.288	-1.458	-1.702
H	-7.976	-10.076	-0.567	C	10.117	-3.298	-0.980
O	-4.701	-8.818	-1.529	O	11.332	-3.131	-1.178
H	-3.774	-9.094	-1.601	O	-9.622	-4.124	-0.115
H	-5.102	-9.021	-2.399	C	-9.447	-8.990	-4.317
O	-5.745	-9.081	0.837	H	-8.626	-9.583	-3.904
H	-5.010	-8.959	1.529	H	-9.556	-9.306	-5.357
H	-5.399	-8.949	-0.085	C	-9.068	-7.493	-4.222
				H	-8.216	-7.323	-4.891
				H	-9.875	-6.835	-4.549
⁹ R-B				C	-8.645	-7.141	-2.790
C	-5.475	-6.937	5.751	O	-7.675	-7.805	-2.315
H	-5.064	-7.587	6.531	O	-9.336	-6.299	-2.144
H	-6.468	-7.304	5.478	C	14.947	-6.502	-0.117
C	-4.562	-6.955	4.511	H	14.980	-5.502	0.325
H	-4.570	-5.996	3.972	H	15.607	-7.154	0.467
H	-3.522	-7.167	4.767	N	13.194	-8.351	0.086
C	-5.029	-7.959	3.476	H	13.822	-9.145	0.324
O	-6.312	-8.005	3.300	C	13.553	-7.026	-0.110
O	-4.206	-8.648	2.838	C	11.843	-8.420	0.038
C	10.292	-7.114	5.616	H	11.286	-9.334	0.167
H	11.023	-6.769	6.355				

N	11.321	-7.222	-0.188	H	-9.392	-6.719	6.048
C	12.381	-6.348	-0.292	C	-10.698	-6.449	4.328
H	12.232	-5.290	-0.463	H	-11.706	-6.725	3.993
Fe	-7.501	-8.435	1.789	H	-10.740	-5.361	4.456
Fe	-9.556	-6.063	-0.040	C	-9.792	-6.679	3.108
C	-3.281	-3.136	2.881	O	-8.875	-7.568	3.190
C	-4.646	-2.812	2.912	O	-10.043	-5.969	2.107
C	-5.473	-3.091	1.821	C	-6.773	-10.642	4.418
C	-4.948	-3.697	0.676	H	-7.200	-9.730	4.845
C	-3.591	-4.026	0.636	H	-5.773	-10.409	4.042
C	-2.769	-3.747	1.728	N	-8.879	-12.358	1.919
C	-2.387	-2.850	4.062	H	-9.353	-13.173	1.482
H	-2.364	-3.699	4.758	C	-7.654	-11.160	3.314
H	-2.726	-1.974	4.624	C	-8.873	-11.072	1.506
H	-1.349	-2.682	3.759	H	-9.283	-10.723	0.570
H	-5.058	-2.316	3.789	N	-8.141	-10.318	2.326
H	-6.529	-2.838	1.867	C	-8.108	-12.433	3.053
H	-5.578	-3.898	-0.184	H	-7.947	-13.373	3.557
H	-3.171	-4.483	-0.255	C	-9.154	-3.100	-3.253
H	-1.710	-3.984	1.674	H	-10.014	-2.508	-3.582
O	-7.604	-6.699	0.627	H	-9.359	-4.157	-3.449
O	-7.095	-5.796	1.410	C	-8.925	-2.943	-1.741
O	-8.329	-9.046	-0.192	H	-8.004	-3.436	-1.421
H	-8.021	-8.455	-0.970	H	-8.859	-1.885	-1.453
H	-7.948	-9.908	-0.414	C	-10.104	-3.546	-0.990
O	-4.716	-8.802	-1.394	O	-11.254	-3.135	-1.199
H	-3.790	-9.074	-1.491	O	-9.838	-4.465	-0.104
H	-5.134	-8.975	-2.266	C	-9.458	-8.979	-4.329
O	-5.805	-9.069	0.904	H	-8.634	-9.578	-3.932
H	-5.049	-9.017	1.567	H	-9.569	-9.271	-5.376
H	-5.448	-8.943	-0.028	C	-9.078	-7.483	-4.217
⁹ TS1-B				H	-8.290	-7.287	-4.953
C	-5.346	-7.036	5.851	H	-9.918	-6.827	-4.453
H	-4.892	-7.587	6.682	C	-8.502	-7.151	-2.830
H	-6.317	-7.482	5.627	O	-7.422	-7.666	-2.500
C	-4.426	-7.122	4.609	O	-9.225	-6.384	-2.077
H	-4.208	-6.140	4.163	C	-14.891	-6.532	-0.110
H	-3.458	-7.563	4.856	H	-14.948	-5.542	0.352
C	-5.030	-7.923	3.470	H	-15.520	-7.216	0.472
O	-6.313	-7.738	3.321	N	-13.076	-8.329	0.029
O	-4.326	-8.666	2.762	H	-13.688	-9.138	0.250
C	-10.358	-7.081	5.687	C	-13.480	-7.009	-0.127
H	-11.124	-6.774	6.408	C	-11.724	-8.355	-0.021
				H	-11.125	-9.249	0.044

N	-11.250	-7.126	-0.202	H	-9.305	-6.791	5.879
C	-12.332	-6.283	-0.280	C	10.625	-6.609	4.144
H	-12.211	-5.221	-0.415	H	11.628	-6.930	3.831
Fe	-7.528	-8.188	1.942	H	10.694	-5.520	4.216
Fe	-9.316	-6.328	-0.058	C	-9.721	-6.880	2.930
C	-3.366	-3.185	3.025	O	-9.247	-8.053	2.730
C	-4.725	-2.888	3.207	O	-9.580	-5.914	2.140
C	-5.674	-3.267	2.255	C	-6.641	-10.769	4.376
C	-5.278	-3.943	1.096	H	-7.063	-9.822	4.719
C	-3.926	-4.235	0.900	H	-5.625	-10.576	4.020
C	-2.981	-3.860	1.857	N	-8.835	-12.602	2.057
C	-2.340	-2.808	4.065	H	-9.330	-13.420	1.630
H	-2.218	-3.602	4.812	C	-7.518	-11.344	3.303
H	-2.622	-1.896	4.601	C	-8.911	-11.331	1.633
H	-1.351	-2.658	3.624	H	-9.552	-11.018	0.827
H	-5.039	-2.340	4.093	N	-8.109	-10.542	2.347
H	-6.722	-3.027	2.413	C	-7.953	-12.638	3.102
H	-6.010	-4.236	0.350	H	-7.707	-13.562	3.601
H	-3.605	-4.740	-0.005	C	-9.195	-3.015	-3.265
H	-1.930	-4.080	1.688	H	10.065	-2.521	-3.709
O	-7.628	-6.275	0.573	H	-9.339	-4.099	-3.315
O	-8.593	-7.936	0.409	C	-9.040	-2.602	-1.791
O	-8.745	-9.961	-1.178	H	-8.067	-2.889	-1.385
H	-8.144	-9.209	-1.301	H	-9.153	-1.518	-1.664
H	-8.390	-10.692	-1.723	C	10.126	-3.287	-0.976
O	-4.837	-8.763	-1.344	O	11.322	-3.068	-1.222
H	-3.922	-9.081	-1.356	O	-9.711	-4.086	-0.043
H	-5.182	-8.922	-2.248	C	-9.444	-8.980	-4.307
O	-6.063	-8.842	0.902	H	-8.640	-9.617	-3.928
H	-5.257	-8.902	1.497	H	-9.565	-9.233	-5.363
H	-5.764	-8.696	-0.048	C	-9.025	-7.502	-4.131
				H	-8.160	-7.315	-4.780
⁷ R				H	-9.806	-6.802	-4.436
C	-5.613	-6.865	5.643	C	-8.617	-7.218	-2.679
H	-5.139	-7.566	6.339	O	-7.821	-8.064	-2.154
H	-6.639	-7.198	5.460	O	-9.133	-6.246	-2.067
C	-4.852	-6.832	4.305	C	14.888	-6.497	-0.116
H	-5.009	-5.888	3.766	H	14.951	-5.497	0.322
H	-3.776	-6.960	4.444	H	15.524	-7.166	0.476
C	-5.352	-7.912	3.359	N	13.091	-8.296	0.096
O	-6.633	-7.911	3.173	H	13.712	-9.098	0.309
O	-4.544	-8.708	2.827	C	13.476	-6.977	-0.101
C	10.280	-7.156	5.545	C	11.736	-8.326	0.096
H	11.032	-6.783	6.250	H	11.155	-9.223	0.234

N	11.233	-7.112	-0.097	H	-9.307	-6.788	5.862
C	12.314	-6.267	-0.229	C	-10.626	-6.619	4.122
H	12.186	-5.205	-0.378	H	-11.626	-6.948	3.810
Fe	-7.653	-8.612	1.686	H	-10.698	-5.530	4.187
Fe	-9.356	-5.994	0.035	C	-9.709	-6.899	2.920
C	-3.314	-3.099	2.944	O	-9.307	-8.089	2.682
C	-4.650	-2.681	3.025	O	-9.476	-5.919	2.166
C	-5.542	-2.926	1.976	C	-6.614	-10.790	4.368
C	-5.109	-3.588	0.825	H	-7.024	-9.834	4.698
C	-3.781	-4.013	0.736	H	-5.594	-10.613	4.014
C	-2.894	-3.770	1.786	N	-8.845	-12.616	2.082
C	-2.351	-2.846	4.078	H	-9.340	-13.432	1.651
H	-2.319	-3.697	4.771	C	-7.498	-11.365	3.302
H	-2.632	-1.961	4.657	C	-8.938	-11.343	1.672
H	-1.326	-2.709	3.722	H	-9.603	-11.024	0.888
H	-4.989	-2.140	3.906	N	-8.117	-10.558	2.368
H	-6.573	-2.588	2.056	C	-7.935	-12.658	3.104
H	-5.789	-3.776	0.001	H	-7.677	-13.585	3.592
H	-3.436	-4.521	-0.160	C	-9.190	-3.025	-3.258
H	-1.859	-4.088	1.698	H	-10.063	-2.528	-3.695
O	-7.566	-6.952	0.754	H	-9.333	-4.109	-3.316
O	-6.406	-6.371	0.612	C	-9.031	-2.625	-1.780
O	-8.515	-9.166	-0.049	H	-8.060	-2.923	-1.378
H	-8.206	-8.577	-0.864	H	-9.135	-1.541	-1.646
H	-8.122	-10.024	-0.276	C	-10.124	-3.304	-0.968
O	-4.724	-8.672	-1.150	O	-11.317	-3.070	-1.214
H	-3.797	-8.951	-1.182	O	-9.721	-4.108	-0.034
H	-5.096	-8.919	-2.028	C	-9.444	-8.977	-4.301
O	-6.049	-9.302	0.941	H	-8.641	-9.617	-3.925
H	-5.339	-9.210	1.675	H	-9.565	-9.221	-5.359
H	-5.621	-8.959	0.090	C	-9.024	-7.501	-4.111
				H	-8.168	-7.302	-4.768
⁵ R				H	-9.808	-6.797	-4.396
C	-5.636	-6.844	5.629	C	-8.595	-7.236	-2.661
H	-5.144	-7.552	6.305	O	-7.809	-8.096	-2.148
H	-6.665	-7.179	5.465	O	-9.084	-6.256	-2.038
C	-4.910	-6.788	4.275	C	-14.887	-6.494	-0.116
H	-5.117	-5.854	3.736	H	-14.957	-5.494	0.323
H	-3.827	-6.875	4.388	H	-15.519	-7.167	0.475
C	-5.392	-7.893	3.352	N	-13.081	-8.281	0.110
O	-6.678	-7.931	3.183	H	-13.700	-9.085	0.318
O	-4.569	-8.680	2.833	C	-13.472	-6.965	-0.097
C	-10.282	-7.156	5.530	C	-11.726	-8.304	0.120
H	-11.034	-6.778	6.230	H	-11.139	-9.195	0.266

N	-11.228	-7.088	-0.076	H	-9.274	-6.793	5.807
C	-12.312	-6.249	-0.219	C	-10.633	-6.600	4.100
H	-12.187	-5.188	-0.373	H	-11.657	-6.887	3.826
Fe	-7.672	-8.628	1.689	H	-10.666	-5.509	4.165
Fe	-9.326	-6.011	0.055	C	-9.791	-6.915	2.851
C	-3.325	-3.107	2.926	O	-9.307	-8.078	2.678
C	-4.667	-2.703	2.991	O	-9.716	-5.972	2.009
C	-5.540	-2.950	1.927	C	-6.616	-10.789	4.369
C	-5.083	-3.600	0.777	H	-7.028	-9.834	4.700
C	-3.750	-4.013	0.706	H	-5.596	-10.609	4.014
C	-2.882	-3.768	1.771	N	-8.839	-12.617	2.077
C	-2.380	-2.848	4.073	H	-9.335	-13.433	1.647
H	-2.345	-3.702	4.762	C	-7.499	-11.365	3.301
H	-2.680	-1.970	4.654	C	-8.929	-11.344	1.665
H	-1.352	-2.696	3.731	H	-9.587	-11.027	0.874
H	-5.024	-2.170	3.869	N	-8.111	-10.557	2.363
H	-6.575	-2.621	1.993	C	-7.935	-12.658	3.104
H	-5.747	-3.782	-0.061	H	-7.680	-13.584	3.595
H	-3.387	-4.511	-0.187	C	-9.175	-3.027	-3.237
H	-1.843	-4.075	1.696	H	-10.053	-2.530	-3.661
O	-7.498	-7.026	0.734	H	-9.322	-4.110	-3.299
O	-6.368	-6.391	0.680	C	-8.994	-2.633	-1.758
O	-8.592	-9.210	-0.055	H	-8.004	-2.901	-1.383
H	-8.253	-8.637	-0.855	H	-9.131	-1.553	-1.617
H	-8.204	-10.072	-0.271	C	-10.042	-3.366	-0.926
O	-4.743	-8.679	-1.146	O	-11.250	-3.148	-1.142
H	-3.816	-8.959	-1.177	O	-9.583	-4.176	-0.034
H	-5.110	-8.924	-2.026	C	-9.448	-8.943	-4.265
O	-6.062	-9.339	0.950	H	-8.638	-9.570	-3.880
H	-5.355	-9.215	1.674	H	-9.548	-9.183	-5.326
H	-5.641	-9.005	0.093	C	-9.066	-7.456	-4.062
				H	-8.198	-7.237	-4.696
3R				H	-9.861	-6.773	-4.364
C	-5.633	-6.846	5.633	C	-8.678	-7.197	-2.602
H	-5.143	-7.551	6.313	O	-7.819	-7.985	-2.104
H	-6.661	-7.182	5.466	O	-9.287	-6.291	-1.956
C	-4.902	-6.794	4.281	C	-14.893	-6.500	-0.114
H	-5.100	-5.857	3.744	H	-14.939	-5.497	0.319
H	-3.820	-6.889	4.398	H	-15.540	-7.155	0.481
C	-5.389	-7.893	3.354	N	-13.126	-8.330	0.098
O	-6.676	-7.926	3.185	H	-13.757	-9.127	0.310
O	-4.569	-8.681	2.832	C	-13.489	-7.004	-0.093
C	-10.262	-7.147	5.498	C	-11.773	-8.384	0.111
H	-10.990	-6.751	6.214	H	-11.207	-9.290	0.250

N	-11.254	-7.177	-0.069	H	-9.342	-6.752	6.003
C	-12.316	-6.309	-0.205	C	10.677	-6.485	4.303
H	-12.164	-5.249	-0.347	H	11.697	-6.753	3.999
Fe	-7.672	-8.614	1.686	H	10.707	-5.396	4.423
Fe	-9.431	-6.156	0.027	C	-9.812	-6.738	3.057
C	-3.323	-3.104	2.935	O	-9.061	-7.766	2.984
C	-4.662	-2.694	3.012	O	-9.969	-5.900	2.133
C	-5.547	-2.941	1.957	C	-6.683	-10.746	4.366
C	-5.105	-3.596	0.806	H	-7.076	-9.793	4.726
C	-3.774	-4.013	0.722	H	-5.669	-10.570	3.992
C	-2.894	-3.769	1.776	N	-8.871	-12.504	1.978
C	-2.366	-2.849	4.074	H	-9.361	-13.322	1.550
H	-2.332	-3.702	4.765	C	-7.579	-11.286	3.286
H	-2.656	-1.968	4.655	C	-8.905	-11.220	1.570
H	-1.341	-2.705	3.723	H	-9.491	-10.882	0.730
H	-5.008	-2.158	3.892	N	-8.125	-10.453	2.327
H	-6.580	-2.609	2.033	C	-8.032	-12.567	3.059
H	-5.781	-3.781	-0.023	H	-7.823	-13.503	3.553
H	-3.421	-4.514	-0.175	C	-9.193	-3.045	-3.266
H	-1.856	-4.081	1.693	H	10.053	-2.496	-3.662
O	-7.536	-6.990	0.769	H	-9.371	-4.118	-3.386
O	-6.398	-6.385	0.658	C	-9.017	-2.758	-1.767
O	-8.585	-9.211	-0.057	H	-8.080	-3.174	-1.387
H	-8.254	-8.611	-0.832	H	-9.012	-1.679	-1.563
H	-8.172	-10.060	-0.283	C	10.178	-3.372	-0.984
O	-4.729	-8.674	-1.155	O	11.343	-3.050	-1.284
H	-3.803	-8.957	-1.192	O	-9.878	-4.178	-0.029
H	-5.105	-8.910	-2.034	C	-9.441	-8.977	-4.301
O	-6.060	-9.310	0.937	H	-8.624	-9.582	-3.896
H	-5.354	-9.201	1.665	H	-9.553	-9.273	-5.346
H	-5.633	-8.974	0.085	C	-9.050	-7.485	-4.179
				H	-8.232	-7.298	-4.886
				H	-9.867	-6.812	-4.447
IM1				C	-8.544	-7.161	-2.765
C	-5.342	-7.093	5.963	O	-7.596	-7.888	-2.334
H	-4.948	-7.599	6.851	O	-9.121	-6.263	-2.091
H	-6.306	-7.542	5.707	C	14.891	-6.505	-0.122
C	-4.358	-7.287	4.794	H	14.934	-5.507	0.322
H	-3.958	-6.345	4.395	H	15.529	-7.168	0.474
H	-3.478	-7.853	5.109	N	13.110	-8.323	0.076
C	-4.943	-7.991	3.576	H	13.733	-9.118	0.310
O	-6.207	-7.902	3.394	C	13.487	-7.004	-0.133
O	-4.135	-8.584	2.817	C	11.756	-8.368	0.037
C	10.318	-7.106	5.662	H	11.186	-9.272	0.177
H	11.065	-6.782	6.395				

N	11.249	-7.164	-0.194	H	-9.309	-6.761	5.944
C	12.322	-6.309	-0.311	C	10.673	-6.492	4.263
H	12.186	-5.251	-0.481	H	11.702	-6.757	3.983
Fe	-7.473	-8.309	1.818	H	10.698	-5.403	4.384
Fe	-9.363	-6.126	0.055	C	-9.843	-6.745	2.991
C	-3.812	-3.632	2.555	O	-9.099	-7.771	2.888
C	-5.036	-2.914	2.471	O	10.033	-5.899	2.073
C	-6.094	-3.397	1.754	C	-6.695	-10.736	4.364
C	-6.039	-4.712	1.052	H	-7.094	-9.789	4.729
C	-4.729	-5.422	1.176	H	-5.682	-10.549	3.994
C	-3.690	-4.887	1.880	N	-8.870	-12.510	1.975
C	-2.667	-3.098	3.362	H	-9.359	-13.331	1.552
H	-2.438	-3.766	4.203	C	-7.583	-11.277	3.277
H	-2.881	-2.108	3.770	C	-8.893	-11.235	1.544
H	-1.753	-3.039	2.758	H	-9.462	-10.908	0.689
H	-5.124	-1.967	2.998	N	-8.116	-10.458	2.295
H	-7.037	-2.863	1.708	C	-8.040	-12.559	3.064
H	-6.281	-4.577	-0.017	H	-7.840	-13.489	3.574
H	-4.643	-6.387	0.687	C	-9.210	-2.997	-3.265
H	-2.752	-5.430	1.957	H	10.082	-2.533	-3.739
O	-7.465	-6.586	0.746	H	-9.339	-4.084	-3.279
O	-7.139	-5.472	1.637	C	-9.083	-2.520	-1.804
O	-8.297	-8.936	-0.135	H	-8.084	-2.702	-1.400
H	-7.950	-8.421	-0.953	H	-9.298	-1.449	-1.712
H	-7.945	-9.827	-0.277	C	10.086	-3.299	-0.962
O	-4.677	-8.742	-1.328	O	11.306	-3.138	-1.147
H	-3.771	-9.076	-1.421	O	-9.566	-4.113	-0.104
H	-5.098	-8.923	-2.198	C	-9.452	-8.991	-4.325
O	-5.787	-9.105	0.981	H	-8.627	-9.577	-3.909
H	-5.020	-8.983	1.627	H	-9.564	-9.316	-5.362
H	-5.449	-8.969	0.052	C	-9.079	-7.492	-4.243
				H	-8.236	-7.321	-4.924
TS2				H	-9.893	-6.839	-4.563
C	-5.442	-7.005	5.833	C	-8.634	-7.131	-2.818
H	-5.067	-7.616	6.662	O	-7.659	-7.796	-2.357
H	-6.426	-7.380	5.541	O	-9.307	-6.277	-2.168
C	-4.482	-7.104	4.634	C	14.919	-6.508	-0.118
H	-4.333	-6.139	4.132	H	14.953	-5.510	0.327
H	-3.490	-7.452	4.929	H	15.569	-7.165	0.471
C	-5.004	-7.995	3.518	N	13.158	-8.350	0.074
O	-6.273	-7.973	3.330	H	13.787	-9.143	0.314
O	-4.181	-8.647	2.829	C	13.521	-7.025	-0.123
C	10.294	-7.108	5.621	C	11.808	-8.416	0.021
H	11.025	-6.766	6.363	H	11.247	-9.328	0.148

N	11.290	-7.217	-0.210	H	-9.328	-6.750	5.936
C	12.351	-6.345	-0.310	C	-10.613	-6.524	4.188
H	12.204	-5.286	-0.480	H	-11.610	-6.829	3.840
Fe	-7.486	-8.342	1.741	H	-10.677	-5.434	4.280
Fe	-9.495	-6.098	-0.032	C	-9.671	-6.782	2.998
C	-3.968	-3.650	2.615	O	-8.879	-7.778	3.058
C	-5.207	-3.008	2.384	O	-9.776	-5.992	2.024
C	-6.090	-3.482	1.437	C	-6.711	-10.714	4.394
C	-5.818	-4.701	0.712	H	-7.128	-9.780	4.777
C	-4.540	-5.334	0.946	H	-5.701	-10.506	4.027
C	-3.660	-4.821	1.873	N	-8.834	-12.474	1.945
C	-2.978	-3.095	3.603	H	-9.327	-13.289	1.520
H	-2.674	-3.853	4.336	C	-7.583	-11.258	3.297
H	-3.384	-2.237	4.147	C	-8.800	-11.208	1.487
H	-2.058	-2.772	3.097	H	-9.226	-10.874	0.549
H	-5.446	-2.109	2.946	N	-8.049	-10.444	2.277
H	-7.027	-2.971	1.246	C	-8.065	-12.528	3.081
H	-6.240	-4.790	-0.285	H	-7.918	-13.455	3.612
H	-4.296	-6.232	0.388	C	-9.157	-3.086	-3.248
H	-2.704	-5.312	2.036	H	-10.026	-2.525	-3.609
O	-7.550	-6.732	0.495	H	-9.339	-4.153	-3.404
O	-7.095	-5.796	1.410	C	-8.945	-2.850	-1.741
O	-8.328	-9.070	-0.229	H	-7.983	-3.246	-1.403
H	-8.019	-8.482	-0.997	H	-8.980	-1.781	-1.496
H	-7.896	-9.918	-0.410	C	-10.061	-3.546	-0.970
O	-4.670	-8.752	-1.367	O	-11.240	-3.192	-1.137
H	-3.765	-9.087	-1.471	O	-9.699	-4.480	-0.144
H	-5.105	-8.916	-2.233	C	-9.450	-8.993	-4.328
O	-5.791	-9.096	0.927	H	-8.624	-9.565	-3.896
H	-5.040	-9.024	1.599	H	-9.548	-9.339	-5.360
H	-5.431	-8.946	0.007	C	-9.090	-7.490	-4.300
IM2				H	-8.345	-7.317	-5.083
C	-5.390	-6.998	5.806	H	-9.956	-6.862	-4.523
H	-4.951	-7.591	6.616	C	-8.446	-7.050	-2.975
H	-6.369	-7.415	5.559	O	-7.254	-7.284	-2.768
C	-4.477	-7.047	4.560	O	-9.238	-6.435	-2.135
H	-4.392	-6.073	4.056	C	-14.912	-6.530	-0.101
H	-3.462	-7.364	4.809	H	-14.946	-5.535	0.349
C	-5.016	-7.945	3.464	H	-15.565	-7.190	0.482
O	-6.307	-7.913	3.340	N	-13.149	-8.384	0.014
O	-4.244	-8.614	2.745	H	-13.775	-9.182	0.243
C	-10.299	-7.105	5.582	C	-13.514	-7.047	-0.106
H	-11.062	-6.745	6.281	C	-11.801	-8.452	-0.049
				H	-11.231	-9.368	-0.023

N	-11.291	-7.235	-0.203	H	-9.298	-6.755	5.947
C	-12.346	-6.353	-0.247	C	-10.503	-6.509	4.148
H	-12.191	-5.291	-0.364	H	-11.501	-6.776	3.771
Fe	-7.459	-8.348	1.866	H	-10.528	-5.418	4.230
Fe	-9.373	-6.426	-0.178	C	-9.536	-6.846	3.004
C	-3.630	-3.219	2.978	O	-8.914	-7.941	3.008
C	-4.977	-3.044	2.963	O	-9.452	-6.004	2.049
C	-5.816	-3.665	1.927	C	-6.688	-10.765	4.356
C	-5.119	-4.333	0.764	H	-7.117	-9.820	4.699
C	-3.648	-4.315	0.771	H	-5.672	-10.560	4.002
C	-2.969	-3.874	1.853	N	-8.737	-12.598	1.901
C	-2.757	-2.640	4.060	H	-9.255	-13.410	1.493
H	-2.259	-3.430	4.637	C	-7.529	-11.349	3.255
H	-3.328	-2.011	4.748	C	-8.660	-11.352	1.401
H	-1.955	-2.032	3.630	H	-9.105	-11.074	0.456
H	-5.456	-2.403	3.700	N	-7.938	-10.568	2.190
H	-6.818	-3.265	1.780	C	-8.020	-12.621	3.067
H	-5.621	-4.392	-0.200	H	-7.905	-13.532	3.632
H	-3.123	-4.633	-0.124	C	-9.216	-3.021	-3.274
H	-1.882	-3.892	1.849	H	-10.084	-2.545	-3.741
O	-8.239	-7.723	0.359	H	-9.346	-4.107	-3.321
O	-5.762	-5.103	1.801	C	-9.110	-2.595	-1.796
O	-8.880	-9.897	-1.096	H	-8.125	-2.818	-1.378
H	-8.323	-9.147	-0.815	H	-9.298	-1.521	-1.677
H	-8.347	-10.514	-1.631	C	-10.157	-3.368	-0.997
O	-4.864	-8.811	-1.445	O	-11.366	-3.154	-1.199
H	-3.952	-9.135	-1.496	O	-9.685	-4.222	-0.155
H	-5.227	-8.899	-2.352	C	-9.434	-9.002	-4.317
O	-5.935	-8.904	0.880	H	-8.616	-9.608	-3.913
H	-5.130	-8.886	1.491	H	-9.549	-9.309	-5.358
H	-5.675	-8.780	-0.083	C	-9.035	-7.510	-4.220
				H	-8.198	-7.346	-4.908
¹¹ R				H	-9.842	-6.839	-4.518
C	-5.211	-7.150	6.053	C	-8.572	-7.175	-2.800
H	-4.782	-7.567	6.972	O	-7.557	-7.804	-2.368
H	-6.144	-7.677	5.837	O	-9.273	-6.382	-2.099
C	-4.211	-7.371	4.898	C	-14.992	-6.466	-0.112
H	-3.720	-6.451	4.555	H	-15.031	-5.456	0.307
H	-3.388	-8.014	5.222	H	-15.673	-7.101	0.467
C	-4.806	-7.999	3.647	N	-13.273	-8.331	0.153
O	-6.065	-7.852	3.467	H	-13.912	-9.123	0.379
O	-4.030	-8.610	2.869	C	-13.603	-7.000	-0.053
C	-10.260	-7.096	5.558	C	-11.926	-8.421	0.161
H	-11.041	-6.715	6.225	H	-11.405	-9.352	0.325

N	-11.371	-7.231	-0.041	H	-9.440	-6.675	6.088
C	-12.412	-6.339	-0.180	C	-10.742	-6.382	4.371
H	-12.233	-5.286	-0.343	H	-11.746	-6.662	4.029
Fe	-7.260	-8.527	1.956	H	-10.788	-5.296	4.521
Fe	-9.493	-6.208	-0.014	C	-9.820	-6.597	3.162
C	-3.256	-2.992	3.108	O	-8.857	-7.418	3.288
C	-4.518	-2.428	3.339	O	-10.101	-5.941	2.125
C	-5.534	-2.537	2.389	C	-6.694	-10.700	4.422
C	-5.302	-3.210	1.189	H	-7.079	-9.759	4.822
C	-4.053	-3.792	0.952	H	-5.686	-10.520	4.035
C	-3.041	-3.686	1.908	N	-8.904	-12.374	1.999
C	-2.159	-2.855	4.130	H	-9.380	-13.177	1.544
H	-2.160	-3.693	4.839	C	-7.614	-11.206	3.351
H	-2.265	-1.937	4.717	C	-8.952	-11.069	1.647
H	-1.167	-2.847	3.670	H	-9.442	-10.714	0.752
H	-4.699	-1.878	4.258	N	-8.177	-10.332	2.441
H	-6.504	-2.087	2.581	C	-8.056	-12.480	3.074
H	-6.080	-3.270	0.436	H	-7.843	-13.434	3.531
H	-3.863	-4.299	0.011	C	-9.167	-3.093	-3.248
H	-2.065	-4.123	1.710	H	-10.037	-2.537	-3.611
O	-6.848	-5.641	-0.250	H	-9.341	-4.162	-3.408
O	-6.147	-6.077	0.647	C	-8.968	-2.867	-1.740
O	-8.342	-8.207	-0.023	H	-8.014	-3.282	-1.407
H	-7.834	-8.052	-0.923	H	-8.977	-1.796	-1.496
H	-8.957	-8.923	-0.228	C	-10.105	-3.534	-0.958
O	-4.687	-8.778	-1.490	O	-11.274	-3.154	-1.177
H	-3.762	-9.056	-1.584	O	-9.779	-4.428	-0.096
H	-5.114	-9.022	-2.338	C	-9.425	-8.946	-4.230
O	-5.608	-8.956	0.919	H	-8.623	-9.568	-3.823
H	-4.838	-8.853	1.570	H	-9.500	-9.196	-5.292
H	-5.312	-8.905	-0.030	C	-9.043	-7.454	-4.054
TS3				H	-8.333	-7.202	-4.850
C	-5.243	-7.179	6.068	H	-9.908	-6.799	-4.170
H	-4.765	-7.565	6.976	C	-8.321	-7.134	-2.729
H	-6.191	-7.706	5.930	O	-7.170	-7.545	-2.549
C	-4.318	-7.476	4.872	O	-8.967	-6.386	-1.883
H	-3.693	-6.622	4.580	C	-14.906	-6.514	-0.114
H	-3.597	-8.250	5.149	H	-14.957	-5.519	0.335
C	-4.995	-7.968	3.591	H	-15.542	-7.186	0.473
O	-6.256	-7.755	3.481	N	-13.113	-8.332	0.024
O	-4.269	-8.540	2.742	H	-13.729	-9.135	0.253
C	-10.399	-7.043	5.719	C	-13.498	-7.004	-0.127
H	-11.172	-6.763	6.443	C	-11.762	-8.374	-0.029
				H	-11.173	-9.276	0.026

N	-11.270	-7.154	-0.211	H	-9.517	-6.622	6.162
C	-12.340	-6.296	-0.284	C	-10.834	-6.294	4.462
H	-12.202	-5.234	-0.421	H	-11.843	-6.559	4.126
Fe	-7.565	-8.111	2.010	H	-10.878	-5.213	4.647
Fe	-9.285	-6.406	0.076	C	-9.934	-6.478	3.235
C	-4.711	-3.847	2.402	O	-8.951	-7.276	3.348
C	-6.002	-3.376	2.165	O	-10.245	-5.829	2.200
C	-6.782	-3.965	1.174	C	-6.758	-10.670	4.409
C	-6.377	-5.202	0.469	H	-7.141	-9.733	4.819
C	-5.001	-5.686	0.829	H	-5.763	-10.471	3.997
C	-4.226	-5.025	1.719	N	-8.980	-12.370	2.009
C	-3.799	-3.158	3.368	H	-9.433	-13.185	1.548
H	-3.423	-3.869	4.114	C	-7.705	-11.184	3.360
H	-4.283	-2.322	3.878	C	-9.132	-11.052	1.737
H	-2.911	-2.787	2.838	H	-9.711	-10.673	0.912
H	-6.383	-2.532	2.733	N	-8.375	-10.307	2.533
H	-7.769	-3.589	0.933	C	-8.072	-12.472	3.035
H	-6.494	-5.179	-0.624	H	-7.779	-13.432	3.432
H	-4.646	-6.583	0.333	C	-9.174	-3.094	-3.257
H	-3.227	-5.384	1.953	H	-10.020	-2.476	-3.572
O	-8.700	-8.076	0.637	H	-9.404	-4.141	-3.483
O	-7.417	-5.942	1.111	C	-8.957	-2.994	-1.740
O	-9.017	-10.046	-1.049	H	-8.079	-3.563	-1.423
H	-8.514	-9.326	-0.627	H	-8.811	-1.952	-1.424
H	-8.420	-10.620	-1.563	C	-10.183	-3.520	-0.996
O	-4.797	-8.765	-1.325	O	-11.312	-3.085	-1.297
H	-3.926	-9.188	-1.358	O	-9.985	-4.362	-0.040
H	-5.166	-8.872	-2.226	C	-9.443	-8.923	-4.223
O	-6.066	-8.779	0.949	H	-8.625	-9.532	-3.827
H	-5.247	-8.787	1.537	H	-9.525	-9.174	-5.283
H	-5.793	-8.754	-0.007	C	-9.086	-7.429	-4.028
				H	-8.278	-7.185	-4.727
TS4				H	-9.926	-6.774	-4.260
C	-5.303	-7.175	6.023	C	-8.558	-7.151	-2.607
H	-4.797	-7.593	6.901	O	-7.544	-7.785	-2.241
H	-6.265	-7.684	5.908	O	-9.211	-6.327	-1.877
C	-4.440	-7.469	4.784	C	-15.023	-6.460	-0.124
H	-3.530	-6.868	4.741	H	-15.103	-5.462	0.316
H	-4.108	-8.514	4.862	H	-15.669	-7.138	0.444
C	-5.148	-7.349	3.434	N	-13.210	-8.233	0.174
O	-6.369	-7.681	3.379	H	-13.817	-9.040	0.414
O	-4.441	-6.933	2.466	C	-13.612	-6.931	-0.095
C	-10.467	-7.002	5.780	C	-11.857	-8.250	0.155
H	-11.245	-6.766	6.516	H	-11.254	-9.119	0.359

N	-11.382	-7.044	-0.126	H	-9.513	-6.648	6.182
C	-12.463	-6.219	-0.297	C	-10.798	-6.330	4.459
H	-12.337	-5.170	-0.510	H	-11.790	-6.623	4.093
Fe	-7.782	-8.055	2.006	H	-10.873	-5.250	4.641
Fe	-9.412	-6.251	0.185	C	-9.847	-6.502	3.266
C	-4.822	-3.262	2.761	O	-8.893	-7.331	3.372
C	-6.179	-3.373	3.186	O	-10.102	-5.802	2.243
C	-7.113	-4.180	2.567	C	-6.743	-10.657	4.425
C	-6.742	-4.966	1.439	H	-7.150	-9.733	4.845
C	-5.353	-4.923	1.029	H	-5.744	-10.444	4.030
C	-4.458	-3.978	1.645	N	-8.922	-12.354	1.981
C	-3.846	-2.410	3.535	H	-9.384	-13.165	1.526
H	-3.444	-2.957	4.398	C	-7.659	-11.173	3.352
H	-4.318	-1.502	3.920	C	-9.000	-11.051	1.640
H	-2.988	-2.124	2.918	H	-9.473	-10.686	0.740
H	-6.491	-2.780	4.045	N	-8.247	-10.306	2.449
H	-8.139	-4.213	2.911	C	-8.073	-12.451	3.059
H	-5.142	-5.250	0.015	H	-7.844	-13.405	3.508
H	-4.964	-5.999	1.679	C	-9.135	-3.078	-3.181
H	-3.443	-3.914	1.261	H	-10.043	-2.632	-3.600
O	-8.990	-8.000	0.775	H	-9.227	-4.169	-3.220
O	-7.541	-5.796	0.851	C	-8.951	-2.645	-1.706
O	-8.222	-10.029	-0.876	H	-7.918	-2.783	-1.376
H	-8.075	-9.186	-1.355	H	-9.217	-1.590	-1.570
H	-8.022	-10.744	-1.515	C	-9.861	-3.508	-0.823
O	-4.651	-8.534	-0.850	O	-11.088	-3.270	-0.812
H	-3.732	-8.837	-0.847	O	-9.253	-4.431	-0.169
H	-5.001	-8.828	-1.720	C	-9.438	-8.996	-4.303
O	-6.508	-9.056	0.907	H	-8.642	-9.649	-3.933
H	-7.086	-9.573	0.275	H	-9.557	-9.227	-5.364
H	-5.779	-8.671	0.347	C	-8.992	-7.531	-4.100
				H	-8.188	-7.326	-4.817
				H	-9.798	-6.822	-4.304
IM3				C	-8.426	-7.299	-2.684
C	-5.271	-7.149	6.025	O	-7.418	-7.949	-2.340
H	-4.819	-7.573	6.930	O	-9.067	-6.473	-1.943
H	-6.224	-7.654	5.848	C	-14.891	-6.490	-0.126
C	-4.324	-7.411	4.836	H	-14.982	-5.501	0.330
H	-3.722	-6.535	4.556	H	-15.499	-7.190	0.458
H	-3.584	-8.168	5.111	N	-13.041	-8.237	0.031
C	-4.996	-7.904	3.551	H	-13.640	-9.053	0.236
O	-6.216	-7.574	3.357	C	-13.465	-6.922	-0.133
O	-4.289	-8.600	2.776	C	-11.689	-8.237	0.017
C	-10.459	-7.026	5.788	H	-11.066	-9.111	0.107
H	-11.248	-6.791	6.511				

N	-11.233	-6.998	-0.147	H	-9.447	-6.678	6.092
C	-12.325	-6.175	-0.258	C	-10.675	-6.400	4.318
H	-12.202	-5.111	-0.389	H	-11.651	-6.711	3.922
Fe	-7.715	-8.212	1.932	H	-10.759	-5.315	4.457
Fe	-9.290	-6.408	0.118	C	-9.671	-6.616	3.176
C	-4.591	-3.777	2.573	O	-8.820	-7.545	3.286
C	-5.951	-3.579	2.911	O	-9.784	-5.846	2.173
C	-6.937	-4.344	2.329	C	-6.731	-10.695	4.396
C	-6.632	-5.270	1.220	H	-7.145	-9.762	4.788
C	-5.196	-5.512	0.988	H	-5.726	-10.489	4.015
C	-4.235	-4.747	1.602	N	-8.877	-12.451	1.961
C	-3.518	-2.996	3.274	H	-9.357	-13.269	1.526
H	-3.045	-3.632	4.035	C	-7.622	-11.240	3.315
H	-3.914	-2.110	3.775	C	-8.884	-11.177	1.531
H	-2.722	-2.701	2.582	H	-9.312	-10.832	0.599
H	-6.206	-2.843	3.668	N	-8.132	-10.414	2.326
H	-7.983	-4.230	2.586	C	-8.081	-12.514	3.079
H	-6.796	-4.452	0.424	H	-7.904	-13.449	3.588
H	-4.944	-6.306	0.290	C	-9.152	-3.125	-3.263
H	-3.185	-4.916	1.383	H	-9.981	-2.455	-3.508
O	-9.010	-8.095	0.643	H	-9.426	-4.144	-3.556
O	-7.464	-6.301	0.941	C	-8.890	-3.156	-1.751
O	-8.898	-10.122	-1.062	H	-8.078	-3.842	-1.507
H	-8.342	-9.328	-1.096	H	-8.621	-2.160	-1.371
H	-8.485	-10.773	-1.662	C	-10.155	-3.572	-1.004
O	-4.726	-8.687	-1.220	O	-11.217	-2.963	-1.237
H	-3.849	-9.099	-1.253	O	-10.090	-4.494	-0.108
H	-5.118	-8.878	-2.099	C	-9.444	-8.942	-4.262
O	-6.089	-9.014	0.994	H	-8.630	-9.563	-3.880
H	-5.292	-8.929	1.605	H	-9.542	-9.182	-5.324
H	-5.755	-8.892	0.067	C	-9.060	-7.455	-4.069
				H	-8.294	-7.212	-4.815
IM4				H	-9.905	-6.787	-4.243
C	-5.299	-7.104	5.936	C	-8.434	-7.182	-2.684
H	-4.878	-7.600	6.817	O	-7.385	-7.777	-2.390
H	-6.258	-7.572	5.700	O	-9.070	-6.355	-1.921
C	-4.329	-7.282	4.745	C	-14.837	-6.572	-0.106
H	-3.905	-6.336	4.381	H	-14.898	-5.589	0.369
H	-3.464	-7.882	5.037	H	-15.457	-7.266	0.474
C	-4.943	-7.941	3.513	N	-12.993	-8.348	0.043
O	-6.199	-7.745	3.322	H	-13.597	-9.165	0.234
O	-4.191	-8.609	2.764	C	-13.419	-7.035	-0.123
C	-10.393	-7.047	5.690	C	-11.636	-8.339	0.054
H	-11.191	-6.754	6.381	H	-11.019	-9.220	0.129

N	-11.180	-7.099	-0.096	H	-9.545	-6.639	6.242
C	-12.281	-6.287	-0.222	C	-10.855	-6.289	4.546
H	-12.180	-5.223	-0.344	H	-11.876	-6.517	4.224
Fe	-7.553	-8.399	1.921	H	-10.863	-5.208	4.742
Fe	-9.238	-6.236	0.076	C	-9.977	-6.489	3.309
C	-4.427	-3.395	2.649	O	-8.944	-7.234	3.410
C	-5.814	-3.526	3.082	O	-10.349	-5.891	2.269
C	-6.781	-4.178	2.378	C	-6.755	-10.625	4.440
C	-6.476	-4.767	1.089	H	-7.171	-9.711	4.872
C	-5.052	-4.657	0.587	H	-5.758	-10.382	4.058
C	-4.080	-3.936	1.461	N	-8.952	-12.314	2.009
C	-3.450	-2.679	3.549	H	-9.412	-13.125	1.553
H	-3.212	-3.284	4.432	C	-7.661	-11.132	3.355
H	-3.863	-1.731	3.911	C	-9.045	-11.012	1.675
H	-2.507	-2.477	3.032	H	-9.552	-10.652	0.793
H	-6.082	-3.063	4.031	N	-8.268	-10.263	2.461
H	-7.797	-4.255	2.744	C	-8.077	-12.410	3.065
H	-5.076	-4.203	-0.416	H	-7.836	-13.364	3.509
H	-4.703	-5.686	0.405	C	-9.170	-3.120	-3.259
H	-3.056	-3.859	1.100	H	-9.998	-2.451	-3.512
O	-8.547	-7.814	0.536	H	-9.444	-4.138	-3.553
O	-7.311	-5.350	0.374	C	-8.921	-3.150	-1.745
O	-8.824	-9.993	-1.077	H	-8.099	-3.824	-1.494
H	-8.263	-9.200	-1.085	H	-8.660	-2.153	-1.361
H	-8.406	-10.644	-1.674	C	-10.171	-3.590	-0.983
O	-4.748	-8.813	-1.400	O	-11.269	-3.069	-1.265
H	-3.852	-9.176	-1.465	O	-10.022	-4.420	-0.009
H	-5.157	-8.977	-2.275	C	-9.417	-8.954	-4.210
O	-5.907	-8.908	0.899	H	-8.640	-9.624	-3.830
H	-5.110	-8.872	1.514	H	-9.494	-9.143	-5.285
H	-5.601	-8.859	-0.053	C	-8.982	-7.495	-3.938
				H	-8.135	-7.272	-4.600
TS5				H	-9.771	-6.780	-4.182
C	-5.316	-7.177	6.023	C	-8.510	-7.260	-2.489
H	-4.835	-7.601	6.912	O	-7.584	-8.002	-2.055
H	-6.283	-7.673	5.890	O	-9.095	-6.352	-1.824
C	-4.429	-7.493	4.805	C	-15.030	-6.457	-0.128
H	-3.503	-6.917	4.792	H	-15.121	-5.462	0.318
H	-4.139	-8.549	4.892	H	-15.667	-7.147	0.436
C	-5.104	-7.335	3.439	N	-13.191	-8.219	0.085
O	-6.269	-7.797	3.292	H	-13.786	-9.037	0.315
O	-4.416	-6.751	2.541	C	-13.612	-6.907	-0.107
C	-10.490	-7.019	5.847	C	-11.842	-8.224	0.050
H	-11.275	-6.815	6.584	H	-11.221	-9.096	0.161

N	-11.388	-6.991	-0.161	H	-9.555	-6.633	6.208
C	-12.477	-6.168	-0.277	C	-10.882	-6.297	4.520
H	-12.361	-5.111	-0.442	H	-11.915	-6.502	4.225
Fe	-7.863	-8.147	1.970	H	-10.857	-5.214	4.702
Fe	-9.529	-6.304	0.247	C	-10.042	-6.525	3.261
C	-5.005	-3.255	2.681	O	-9.018	-7.300	3.361
C	-6.335	-3.389	3.165	O	-10.401	-5.939	2.220
C	-7.267	-4.249	2.612	C	-6.784	-10.603	4.430
C	-6.910	-5.073	1.514	H	-7.218	-9.701	4.871
C	-5.549	-4.994	1.041	H	-5.782	-10.345	4.070
C	-4.668	-3.990	1.564	N	-8.897	-12.274	1.910
C	-4.010	-2.387	3.411	H	-9.370	-13.083	1.468
H	-3.647	-2.894	4.314	C	-7.652	-11.102	3.309
H	-4.450	-1.439	3.732	C	-8.883	-10.987	1.507
H	-3.132	-2.180	2.792	H	-9.293	-10.620	0.575
H	-6.628	-2.780	4.018	N	-8.132	-10.243	2.327
H	-8.277	-4.299	2.998	C	-8.119	-12.365	3.040
H	-5.368	-5.393	0.048	H	-7.971	-13.311	3.538
H	-5.057	-5.961	1.724	C	-9.166	-3.119	-3.265
H	-3.674	-3.906	1.129	H	-10.001	-2.466	-3.537
O	-9.155	-7.991	0.694	H	-9.425	-4.147	-3.540
O	-7.691	-5.991	1.011	C	-8.927	-3.111	-1.750
O	-9.070	-10.208	-1.003	H	-8.085	-3.749	-1.475
H	-8.560	-9.388	-1.057	H	-8.706	-2.099	-1.383
H	-8.616	-10.837	-1.598	C	-10.172	-3.578	-0.998
O	-4.483	-8.611	-0.976	O	-11.273	-3.055	-1.267
H	-3.548	-8.854	-1.049	O	-10.027	-4.438	-0.049
H	-4.873	-8.901	-1.831	C	-9.437	-8.950	-4.260
O	-6.603	-8.594	0.417	H	-8.629	-9.576	-3.870
H	-7.013	-8.225	-0.407	H	-9.532	-9.202	-5.320
H	-5.639	-8.638	0.198	C	-9.040	-7.464	-4.089
				H	-8.247	-7.253	-4.818
IM5				H	-9.871	-6.794	-4.315
C	-5.260	-7.118	5.930	C	-8.472	-7.140	-2.691
H	-4.748	-7.575	6.783	O	-7.395	-7.691	-2.351
H	-6.206	-7.643	5.773	O	-9.152	-6.340	-1.962
C	-4.376	-7.269	4.678	C	-14.997	-6.473	-0.125
H	-3.660	-6.456	4.525	H	-15.080	-5.480	0.326
H	-3.751	-8.166	4.790	H	-15.628	-7.164	0.445
C	-5.130	-7.467	3.379	N	-13.155	-8.236	0.067
O	-6.335	-7.758	3.357	H	-13.749	-9.052	0.300
O	-4.388	-7.370	2.307	C	-13.579	-6.924	-0.122
C	-10.502	-7.019	5.824	C	-11.805	-8.239	0.011
H	-11.280	-6.807	6.567	H	-11.182	-9.110	0.124

N	-11.355	-7.007	-0.209	H	-9.497	-6.664	6.142
C	-12.446	-6.185	-0.307	C	-10.799	-6.363	4.427
H	-12.334	-5.126	-0.470	H	-11.799	-6.643	4.077
Fe	-7.927	-8.083	1.917	H	-10.858	-5.281	4.593
Fe	-9.479	-6.314	0.100	C	-9.871	-6.547	3.220
C	-5.115	-3.218	2.633	O	-8.894	-7.377	3.330
C	-6.291	-3.595	3.301	O	-10.128	-5.870	2.203
C	-7.213	-4.467	2.729	C	-6.748	-10.680	4.404
C	-6.986	-4.988	1.442	H	-7.166	-9.756	4.808
C	-5.886	-4.508	0.713	H	-5.742	-10.451	4.038
C	-4.958	-3.655	1.312	N	-8.867	-12.400	1.920
C	-4.054	-2.421	3.354	H	-9.350	-13.217	1.488
H	-3.615	-3.007	4.172	C	-7.617	-11.208	3.299
H	-4.460	-1.508	3.800	C	-8.838	-11.130	1.481
H	-3.230	-2.147	2.689	H	-9.243	-10.774	0.542
H	-6.470	-3.216	4.306	N	-8.086	-10.374	2.290
H	-8.091	-4.776	3.282	C	-8.097	-12.471	3.058
H	-5.744	-4.833	-0.312	H	-7.954	-13.406	3.576
H	-4.978	-7.556	1.493	C	-9.159	-3.128	-3.280
H	-4.085	-3.352	0.740	H	-9.986	-2.457	-3.534
O	-9.066	-8.023	0.545	H	-9.432	-4.146	-3.575
O	-7.712	-6.030	0.949	C	-8.915	-3.158	-1.768
O	-8.691	-10.003	-1.159	H	-8.106	-3.844	-1.507
H	-8.161	-9.205	-1.316	H	-8.644	-2.166	-1.381
H	-8.341	-10.697	-1.753	C	-10.183	-3.572	-1.031
O	-4.779	-8.990	-1.506	O	-11.257	-2.996	-1.291
H	-3.835	-9.188	-1.590	O	-10.101	-4.456	-0.093
H	-5.162	-9.071	-2.406	C	-9.446	-8.968	-4.294
O	-6.062	-8.018	0.470	H	-8.631	-9.578	-3.897
H	-6.512	-7.265	0.031	H	-9.550	-9.245	-5.346
H	-5.634	-8.538	-0.281	C	-9.057	-7.477	-4.154
TS6				H	-8.245	-7.282	-4.864
C	-5.227	-7.155	6.020	H	-9.884	-6.813	-4.415
H	-4.697	-7.553	6.892	C	-8.529	-7.148	-2.743
H	-6.161	-7.710	5.900	O	-7.474	-7.710	-2.372
C	-4.352	-7.363	4.773	O	-9.239	-6.356	-2.030
H	-3.595	-6.591	4.617	C	-14.923	-6.520	-0.115
H	-3.782	-8.294	4.900	H	-15.001	-5.533	0.350
C	-5.118	-7.534	3.477	H	-15.546	-7.217	0.458
O	-6.308	-7.914	3.482	N	-13.065	-8.275	0.060
O	-4.434	-7.318	2.398	H	-13.659	-9.097	0.269
C	-10.448	-7.044	5.762	C	-13.502	-6.967	-0.121
H	-11.229	-6.795	6.490	C	-11.712	-8.261	0.037
				H	-11.083	-9.130	0.134

N	-11.273	-7.020	-0.151	H	-9.368	-6.702	5.990
C	-12.374	-6.212	-0.266	C	-10.585	-6.440	4.201
H	-12.275	-5.151	-0.409	H	-11.580	-6.711	3.823
Fe	-7.805	-8.299	1.953	H	-10.608	-5.349	4.301
Fe	-9.389	-6.259	0.047	C	-9.609	-6.749	3.056
C	-5.016	-3.159	2.642	O	-8.859	-7.755	3.161
C	-6.293	-3.493	3.117	O	-9.658	-5.966	2.049
C	-7.175	-4.274	2.367	C	-6.709	-10.721	4.386
C	-6.796	-4.721	1.094	H	-7.138	-9.787	4.759
C	-5.576	-4.297	0.558	H	-5.700	-10.509	4.017
C	-4.693	-3.553	1.338	N	-8.834	-12.538	1.981
C	-4.018	-2.436	3.517	H	-9.324	-13.358	1.556
H	-3.615	-3.101	4.292	C	-7.580	-11.296	3.305
H	-4.467	-1.578	4.028	C	-8.839	-11.280	1.515
H	-3.162	-2.079	2.935	H	-9.285	-10.957	0.583
H	-6.596	-3.158	4.107	N	-8.085	-10.499	2.289
H	-8.144	-4.548	2.763	C	-8.040	-12.575	3.100
H	-5.311	-4.570	-0.457	H	-7.864	-13.496	3.632
H	-5.110	-7.447	1.577	C	-9.173	-3.115	-3.270
H	-3.722	-3.300	0.920	H	-10.007	-2.463	-3.546
O	-8.894	-7.902	0.581	H	-9.433	-4.141	-3.552
O	-7.500	-5.687	0.404	C	-8.933	-3.109	-1.754
O	-8.697	-9.979	-1.121	H	-8.065	-3.711	-1.481
H	-8.193	-9.165	-1.298	H	-8.760	-2.089	-1.383
H	-8.341	-10.663	-1.722	C	-10.158	-3.638	-1.014
O	-4.881	-8.880	-1.225	O	-11.280	-3.165	-1.267
H	-3.916	-8.909	-1.288	O	-9.976	-4.507	-0.065
H	-5.202	-9.010	-2.143	C	-9.401	-8.935	-4.183
O	-6.194	-7.676	0.717	H	-8.611	-9.560	-3.758
H	-6.796	-6.684	0.412	H	-9.451	-9.193	-5.245
H	-5.857	-8.145	-0.097	C	-9.003	-7.444	-4.036
				H	-8.223	-7.244	-4.778
P-H				H	-9.847	-6.789	-4.267
C	-5.422	-7.005	5.806	C	-8.415	-7.029	-2.669
H	-5.056	-7.621	6.634	O	-7.206	-7.217	-2.428
H	-6.404	-7.377	5.501	O	-9.244	-6.450	-1.865
C	-4.441	-7.095	4.617	C	-14.908	-6.543	-0.101
H	-4.244	-6.119	4.154	H	-14.955	-5.550	0.355
H	-3.470	-7.492	4.921	H	-15.563	-7.209	0.473
C	-4.968	-7.932	3.463	N	-13.129	-8.377	0.071
O	-6.231	-7.812	3.227	H	-13.751	-9.182	0.276
O	-4.178	-8.644	2.802	C	-13.506	-7.049	-0.082
C	-10.324	-7.055	5.597	C	-11.774	-8.417	0.087
H	-11.111	-6.705	6.275	H	-11.195	-9.325	0.152

N	-11.271	-7.195	-0.050
C	-12.341	-6.342	-0.170
H	-12.201	-5.282	-0.295
Fe	-7.492	-8.518	1.843
Fe	-9.280	-6.301	0.092
C	-4.212	-3.739	2.420
C	-5.486	-3.177	2.249
C	-6.428	-3.747	1.393
C	-6.110	-4.913	0.692
C	-4.864	-5.520	0.879
C	-3.926	-4.921	1.721
C	-3.178	-3.090	3.315
H	-2.758	-3.803	4.035
H	-3.607	-2.258	3.881
H	-2.334	-2.698	2.734
H	-5.742	-2.269	2.790
H	-7.406	-3.297	1.261
H	-4.628	-6.449	0.369
H	-5.037	-9.026	1.554
H	-2.951	-5.391	1.836
O	-8.352	-7.830	0.414
O	-7.062	-5.418	-0.175
O	-8.953	-9.987	-1.035
H	-8.473	-9.180	-0.766
H	-8.381	-10.549	-1.589
O	-4.725	-8.751	-1.389
H	-3.818	-9.079	-1.494
H	-5.140	-8.847	-2.274
O	-5.811	-9.119	0.914
H	-6.736	-6.118	-0.784
H	-5.494	-8.999	-0.027