

Supporting Information

Theoretical investigation of the reaction mechanism of THP oxidative rearrangement catalysed by BBOX

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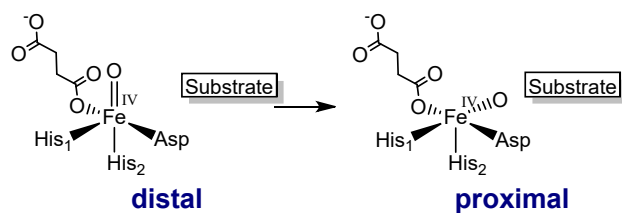
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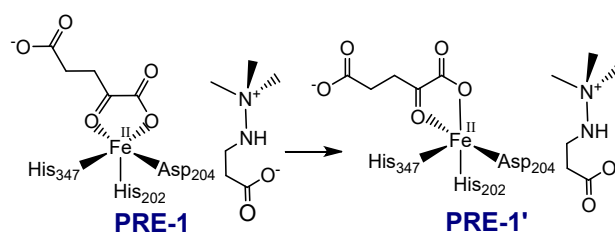
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Part I Supplementary Schemes



Scheme S1. $\text{Fe}^{\text{IV}}=\text{O}$ species transition from distal to proximal type conformation.



Scheme S2. A possible pathway of $\text{Fe}^{\text{IV}}=\text{O}$ group isomerization in BBOX. 2OG rotates before O_2 binding.

Part II Supplementary Tables

Table S1. Spin populations on the key atoms of the stationary point structures along the reaction process of the $\text{Fe}^{\text{IV}}=\text{O}$ group isomerization in the BBOX catalysed THP process.

Compound	Fe	O _P	O _{W1}	O _{W2}
⁵ 1	3.12	0.65	—	—
⁵ TS ₁₋₂	3.20	0.64	—	—
⁵ 1 _W	3.19	0.60	0	0
⁵ TS _{1W}	3.40	0.28	0	0
⁵ INT _{12W1}	3.50	0	0	0
⁵ TS _{2W}	3.52	0	0	0
⁵ INT _{12W2}	3.44	0.19	0.12	0
⁵ TS _{3W}	3.38	0	0.33	0
⁵ 2 _W	3.20	0	0.58	0
⁵ 2	3.12	—	0.66	—

Table S2. Spin populations on the key atoms in the stationary point structures along the BBOX-catalysed THP process.

Compound	Fe	O	C3	N4	N5	C6	C7
⁵ 2	3.12	0.66	0	0	0	0	0
⁵ TS ₂₋₃	3.91	0.12	-0.19	-0.10	0	0	0
⁵ 3	4.21	0.31	-0.83	-0.11	0	0	0
⁵ TS ₃₋₄	4.19	0.37	-0.71	-0.12	-0.14	0	0
⁵ 4	4.21	0.35	0	0	-0.79	0	0
⁵ 4 ₂	4.23	0.29	0	0	-0.78	0	0
⁵ TS ₄₋₅	3.88	0.37	0	0	-0.11	0	0
⁵ 5	3.16	0.62	0	0	0	0	0
⁵ TS ₅₋₆	4.03	0	0	0	0	0	-0.54
⁵ 6	4.21	0.34	0	0	0	0	-1.07
⁵ TS ₆₋₇	4.17	0.29	0	0	0	0	-0.91
⁵ 7	3.82	0	0	0	0	0	0
⁵ TS ₆₋₈	4.23	0.24	0.19	-0.45	0	0	-0.76
⁵ 8	4.23	0.28	0	-0.95	0	0	0
⁵ TS ₈₋₉	4.23	0.24	0	-0.49	0	-0.56	0
⁵ 9	4.23	0.25	0	0	0	-1.07	0
⁵ TS ₉₋₁₀	4.13	0.32	0	0	0	-0.86	0
⁵ TS ₁₀₋	3.76	0	0	0	0	0	0
¹¹ (dehydrogenation)	3.82	0	0	0	0	0	0
⁵ 10 _(dehydrogenation)	3.82	0	0	0	0	0	0
⁵ 10							

Table S3. Spin populations on the key atoms in the stationary point structures along the reaction process of other possible pathways to proceed the first hydrogen atom abstraction from THP catalysed by BBOX.

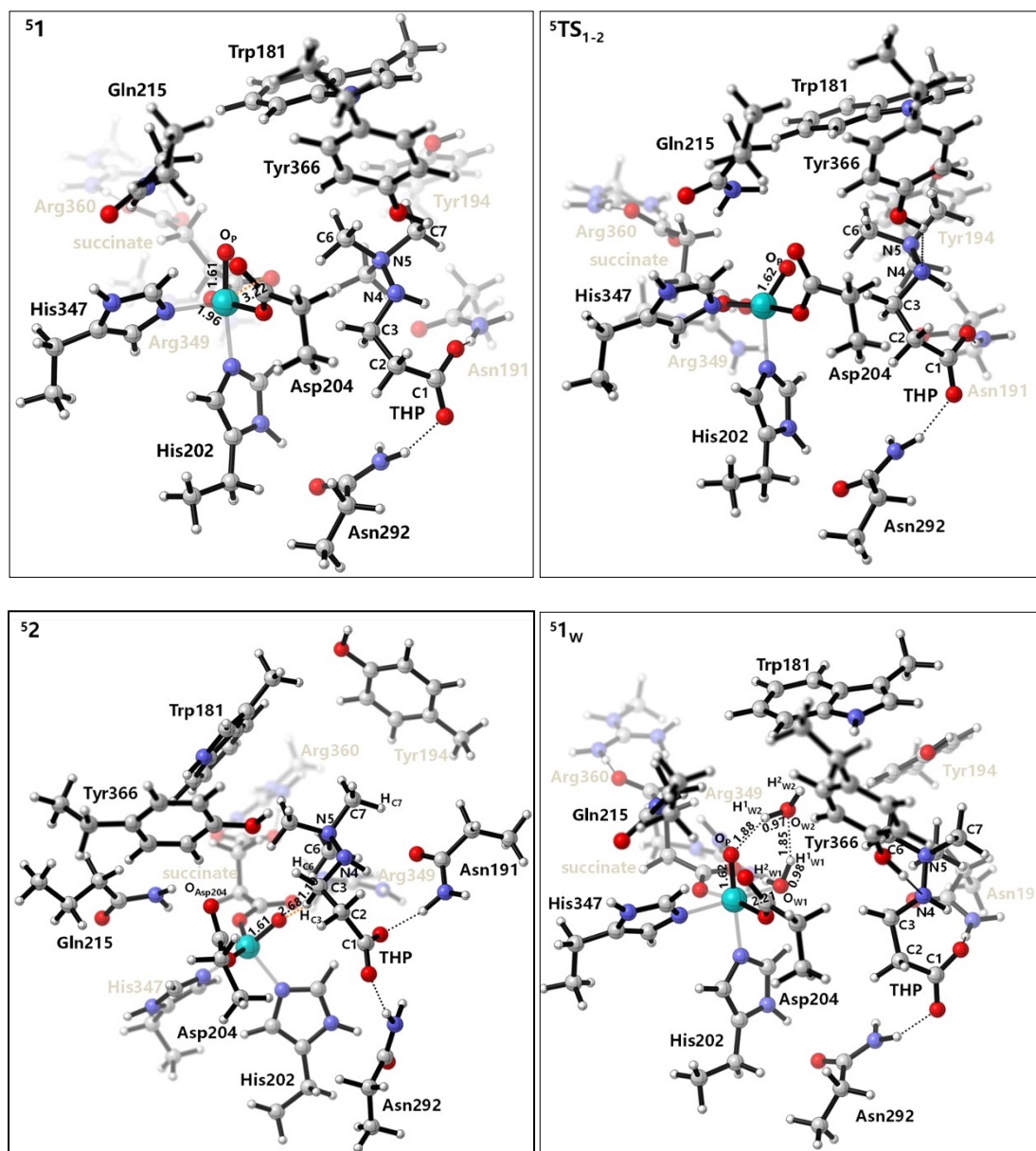
Compound	Fe	O	C3	N4	N5	C6	C7
⁵ TS _{2-3(C3,π)}	3.01	0.23	0.38	0.17	0	0	0
⁵ TS _{2-3(C6,σ)}	4.03	0	0	0	0	-0.57	0
⁵ TS _{2-3(C6,π)}	3.05	0.36	0	0	0	0.53	0
⁵ 3 _(C3,π)	3.19	-0.11	0.69	0	0	0	0
⁵ 3 _(C6,σ)	4.12	0.36	0	0	0	-1.04	0

${}^5\mathbf{3}_{(C6,\pi)}$	2.86	0	0	0	0	1.04	0
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Table S4. Spin populations on the key atoms in the stationary point structures along the reaction process of other possible pathways to generate the C7 methylene radical species in the BBOX catalysed THP process.

Compound	Fe	O	C3	N4	N5	C6	C7
${}^5\mathbf{TS}_{4-6}$	4.20	0.36	0	0	-0.32	0	-0.73
${}^5\mathbf{TS}_{5-6(C7,\pi)}$	3.52	0.30	0	0	0	0	0
${}^5\mathbf{6}_{(C7,\pi)}$	2.88	0	0	0	0	0	1.07

Part III Supplementary Figures



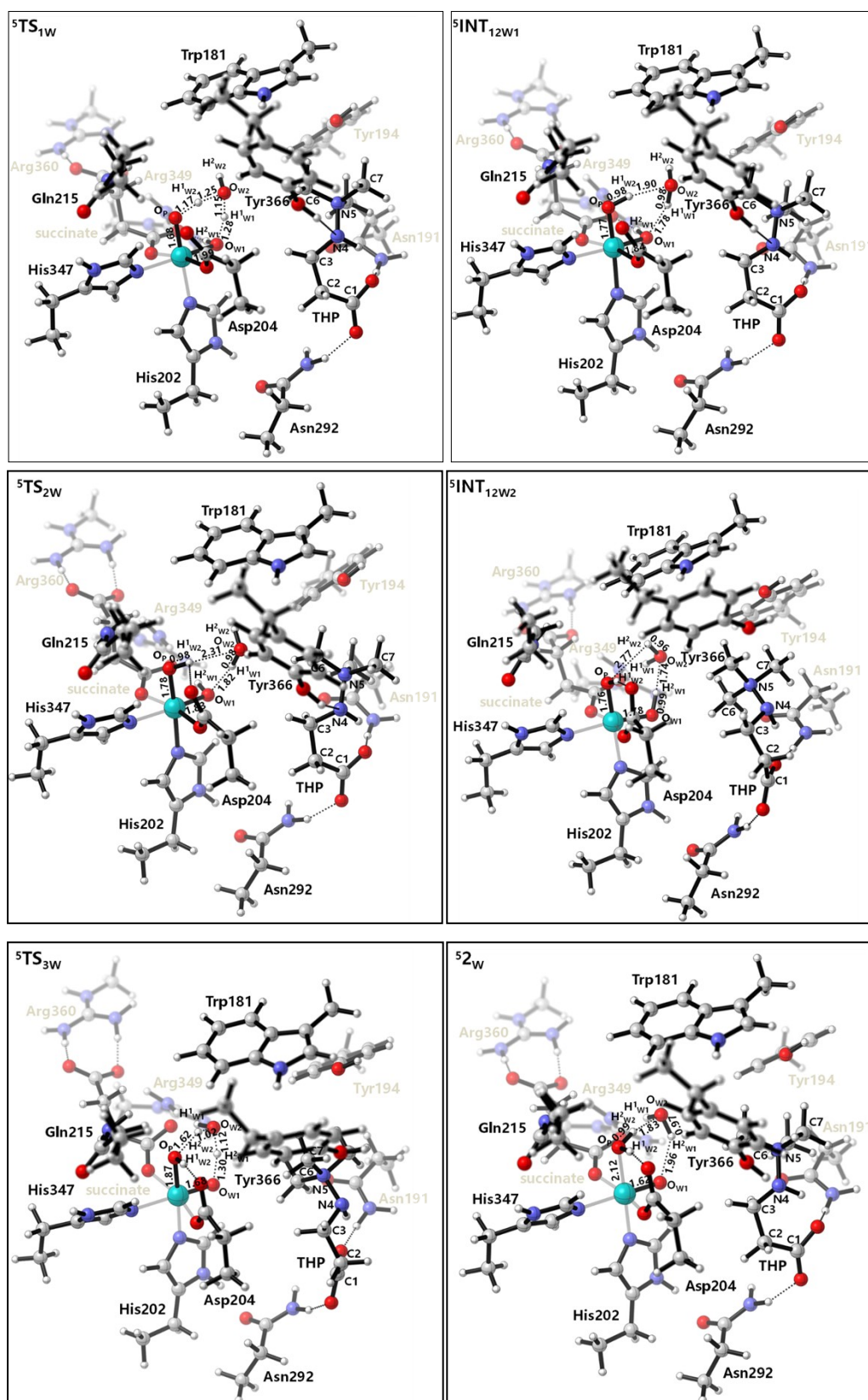
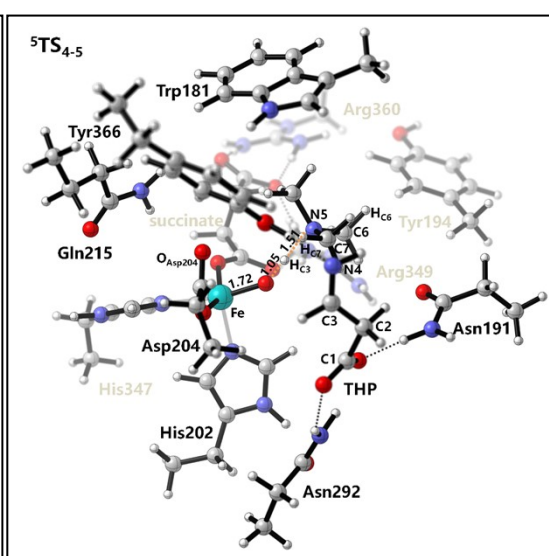
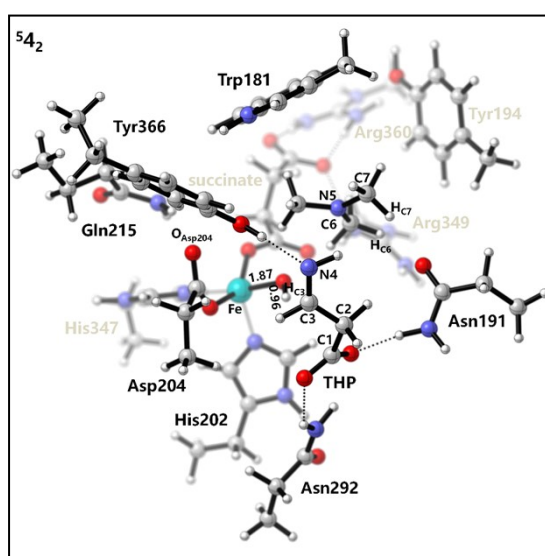
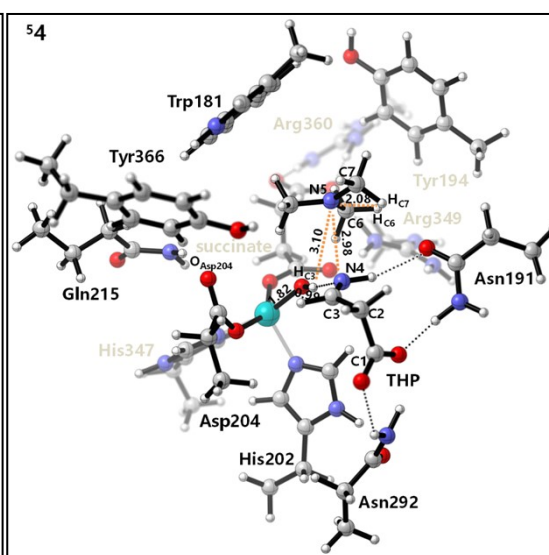
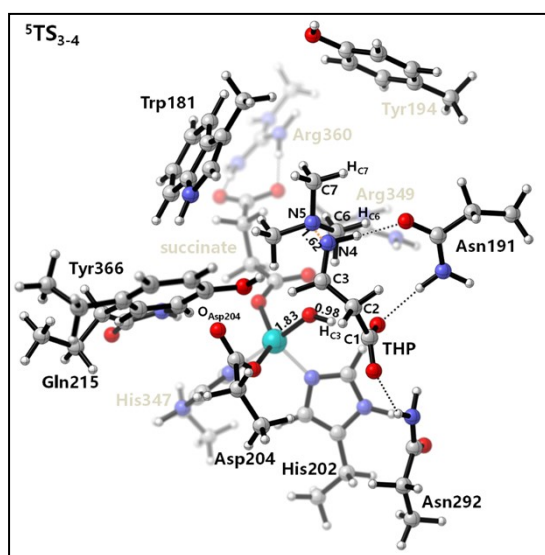
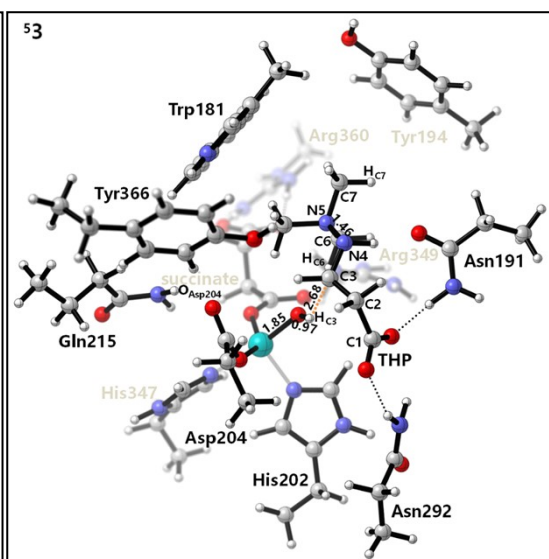
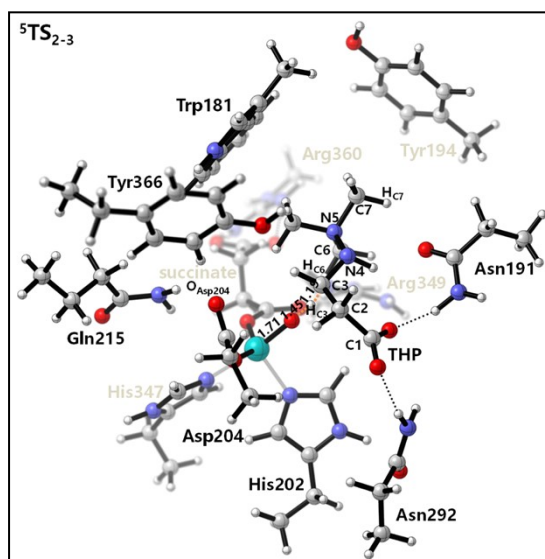
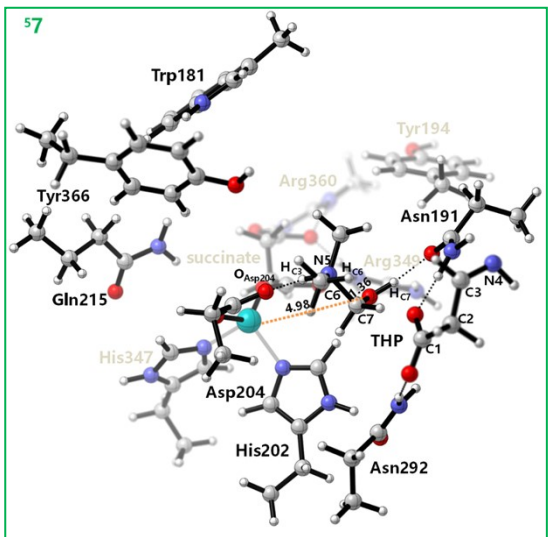
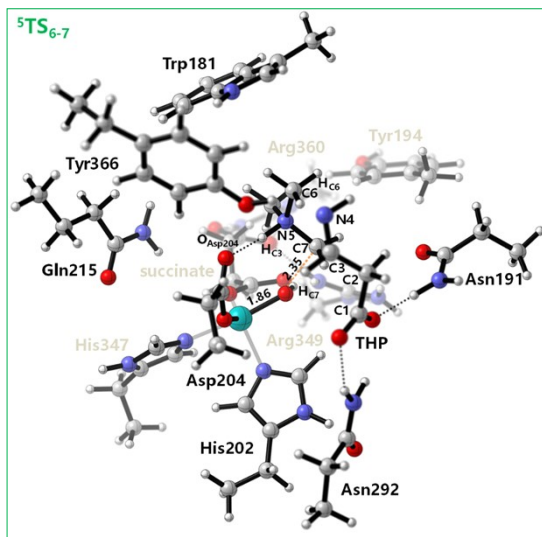
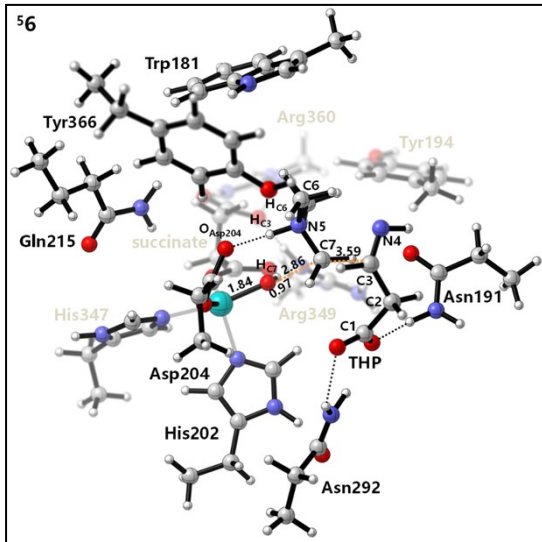
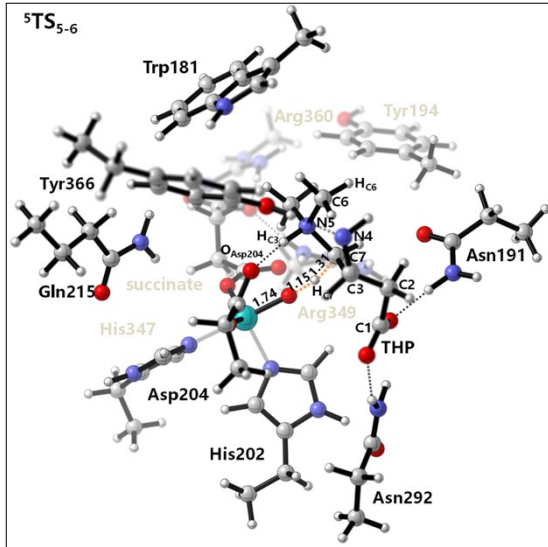
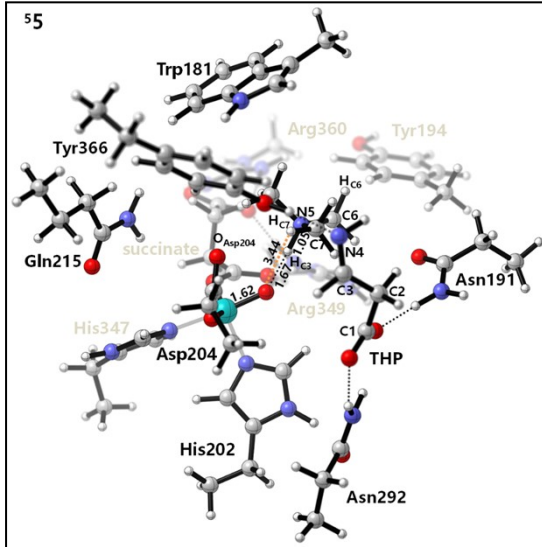
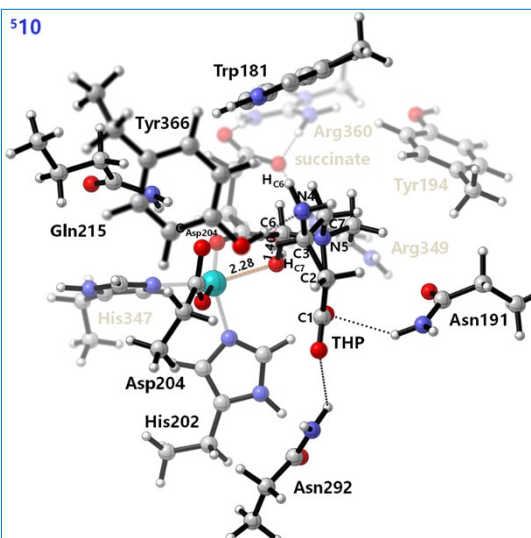
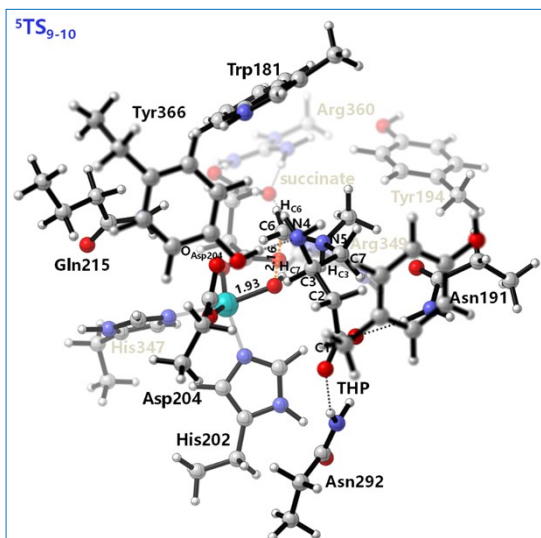
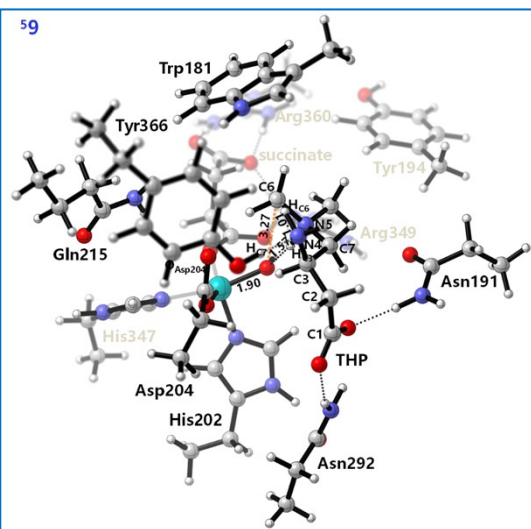
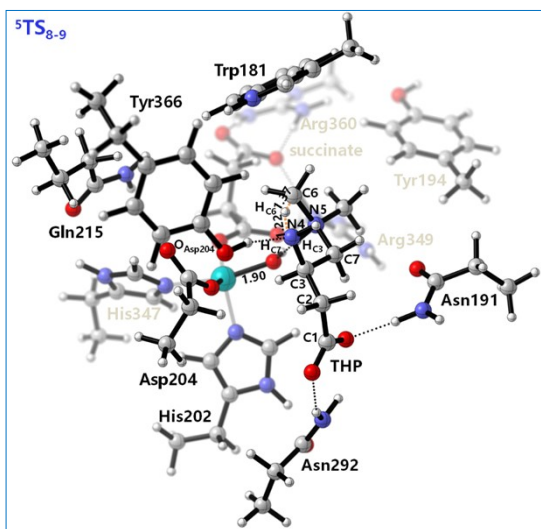
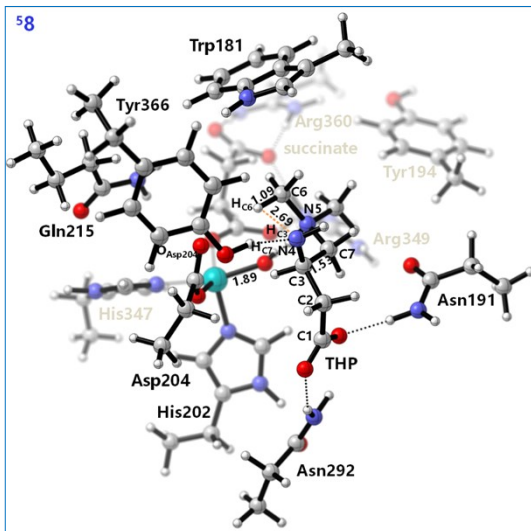
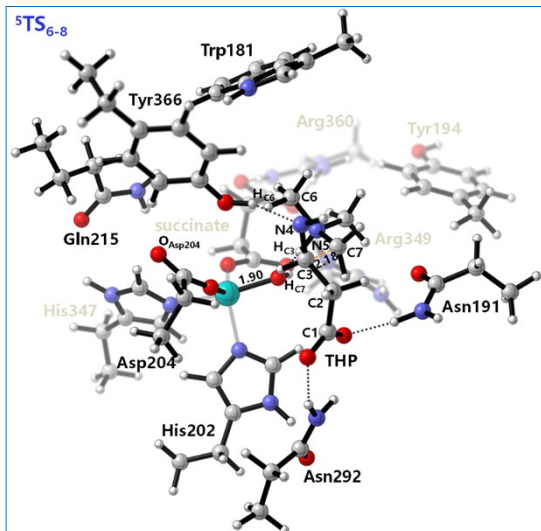


Figure S1. The optimized structures of the stationary points along the $\text{Fe}^{\text{IV}}=\text{O}$ group isomerization process in the quintet spin state of BBOX. Bond lengths are given in Å.







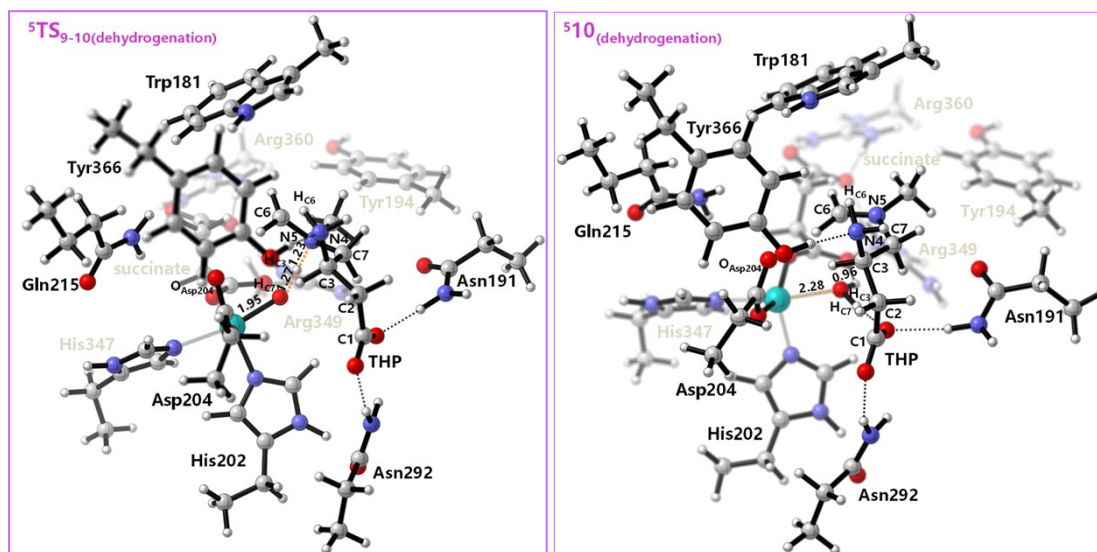
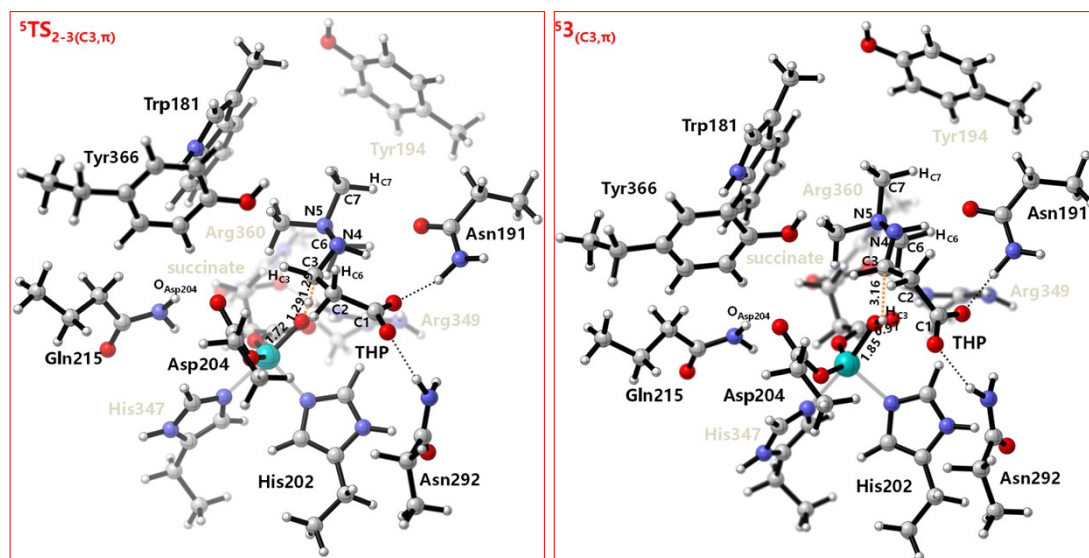


Figure S2. The optimized structures of the stationary points along the reaction process of the THP hydroxylation and rearrangement catalysed by BBOX. Bond lengths are given in Å.



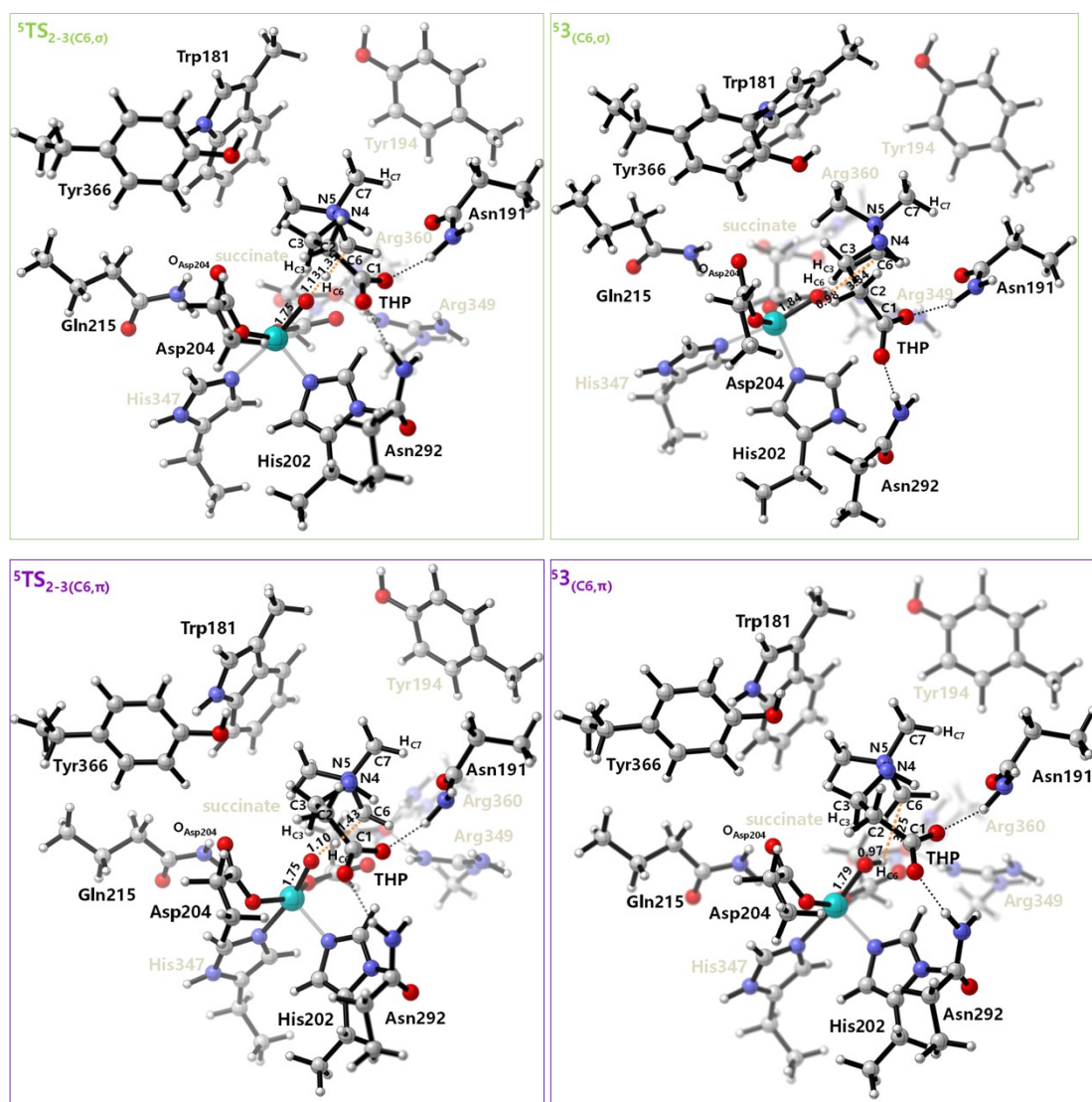


Figure S3. The optimized structures of the stationary points along the reaction process of other possible pathways to proceed the first hydrogen atom abstraction from THP catalysed by BBOX. Bond lengths are given in Å.

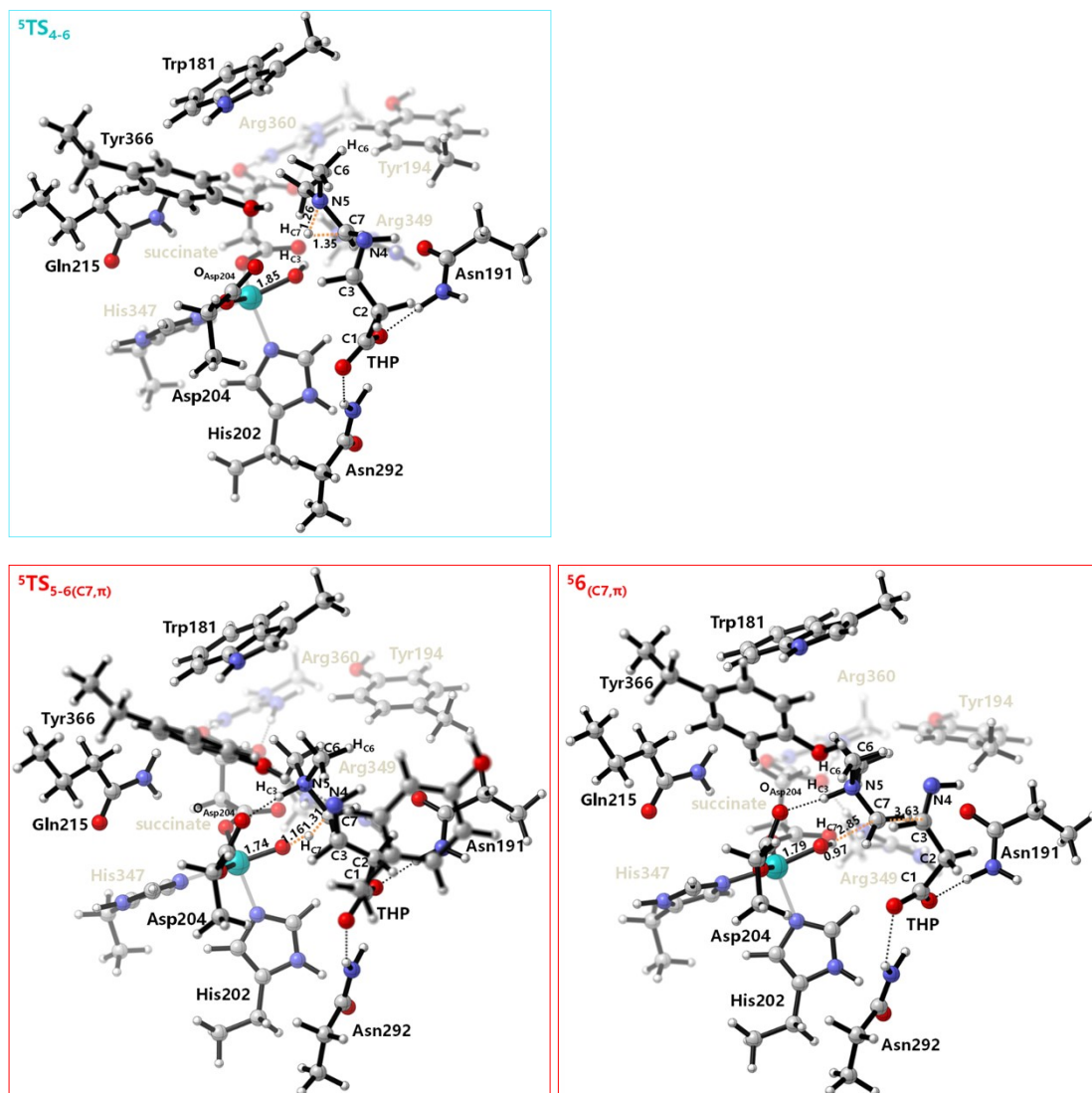


Figure S4. The optimized structures of the stationary points along the reaction process of other possible pathways to generate the C7 methylene radical species in BBOX. Bond lengths are given in Å.

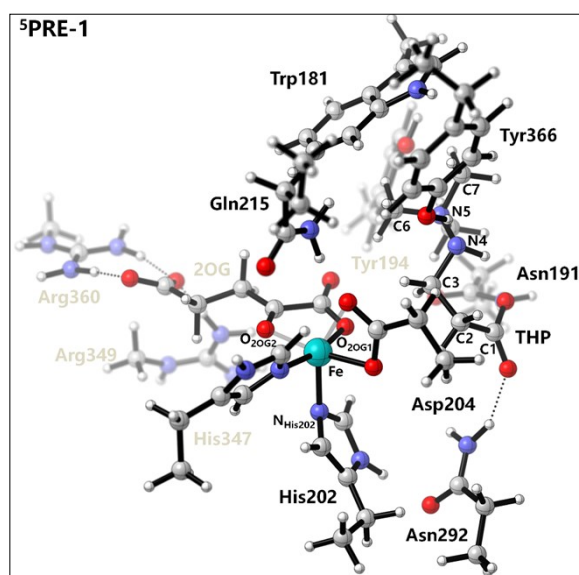


Figure S5. The optimized geometry of $^5\text{PRE-1}$ in the quintet spin state of BBOX.

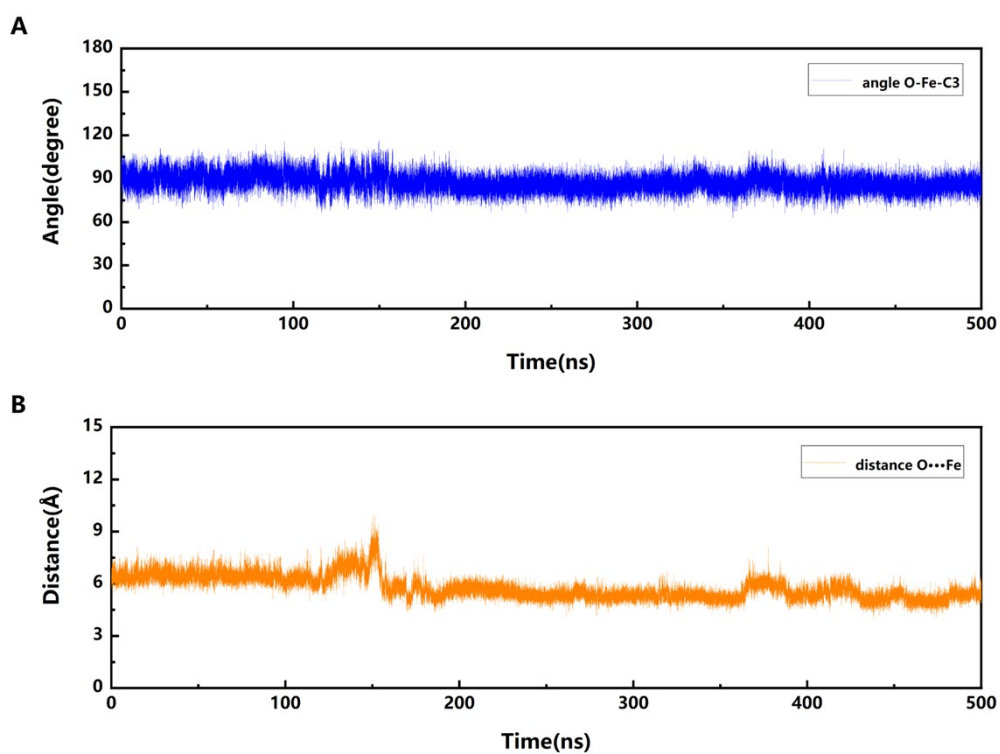


Figure S6. (A) Angle variations of O-Fe-C3 and (B) distance variations of O...C3 in 500 ns MD simulations of the BBOX-THP ferryl-oxo complex.

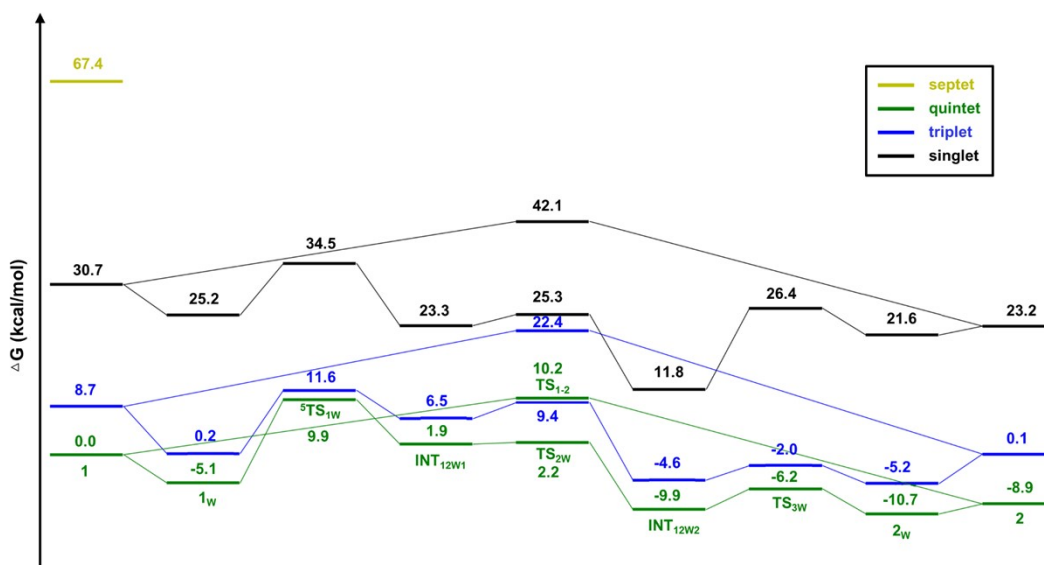


Figure S7. Free energy profile of the Fe^{IV}=O group isomerization processes in BBOX in different spin states.

Part IV DFT calculations of the BBOX-catalysed γ -BB hydroxylation

DFT calculations were performed to investigate the hydroxylation mechanism of γ -BB in BBOX. Similar to that of THP, in the first reaction step, the hydrogen atom at C3 position of γ -BB is abstracted by Fe^{IV}=O moiety through the σ -channel with an energy barrier of 12.2 kcal/mol. After crossing over the transition state ⁵TS_{2-3(γ -BB)}, it generates the intermediate ⁵3_(γ -BB), which is an exothermic process of 3.9 kcal/mol. In the intermediate ⁵3_(γ -BB), Fe^{III}-OH moiety is in complexed with the substrate based C3 radical. In this step, an α electron is completely transferred from γ -BB to Fe^{IV}=O along with the hydrogen transfer, so that in ⁵3_(γ -BB), the spin population on the C3 site is -1.00. From ⁵3_(γ -BB), a very low energy barrier of 1.6 kcal/mol is required for the hydroxyl rebound from Fe^{III}-OH to the C3 radical, which forms the hydroxylation product ⁵4_(γ -BB). After crossing over the transition state ⁵TS_{3-4(γ -BB)}, the resulting hydroxylation product ⁵4_(γ -BB) energy dropped dramatically by 30.8 kcal/mol from ⁵3_(γ -BB), in which the iron centre of ⁵4_(γ -BB) is reduced to a ferrous state. These calculation results indicated that it is conventional for γ -BB to proceed hydroxylation reaction in BBOX, which is distinct from the reaction process of THP in BBOX. The

geometry structures of all the intermediates and transition structures are supplied in supporting information.

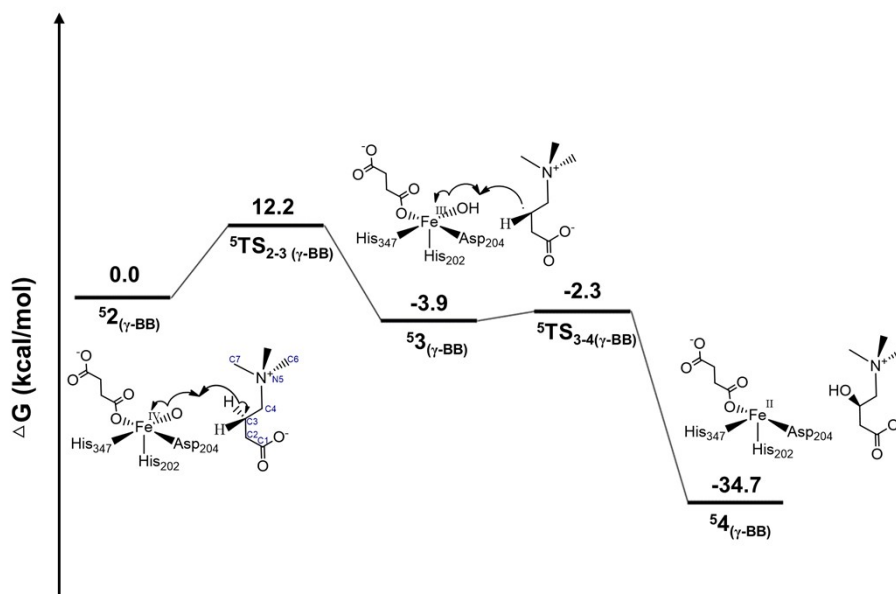


Figure S8. Free energy profile of the BBOX-catalysed γ -BB process in the quintet spin state.

Table S5. Spin populations on the key atoms in the stationary point structures along the BBOX-catalysed γ -BB process.

Compound	Fe	O	C3	N4	N5	C6	C7
$52_{(\gamma\text{-BB})}$	3.12	0.66	0	0	0	0	0
$5\text{TS}_{2-3(\gamma\text{-BB})}$	3.99	0	-0.33	0	0	0	0
$53_{(\gamma\text{-BB})}$	4.20	0.38	-1.00	0	0	0	0
$5\text{TS}_{3-4(\gamma\text{-BB})}$	4.13	0.32	-0.81	0	0	0	0
$54_{(\gamma\text{-BB})}$	3.83	0	0	0	0	0	0

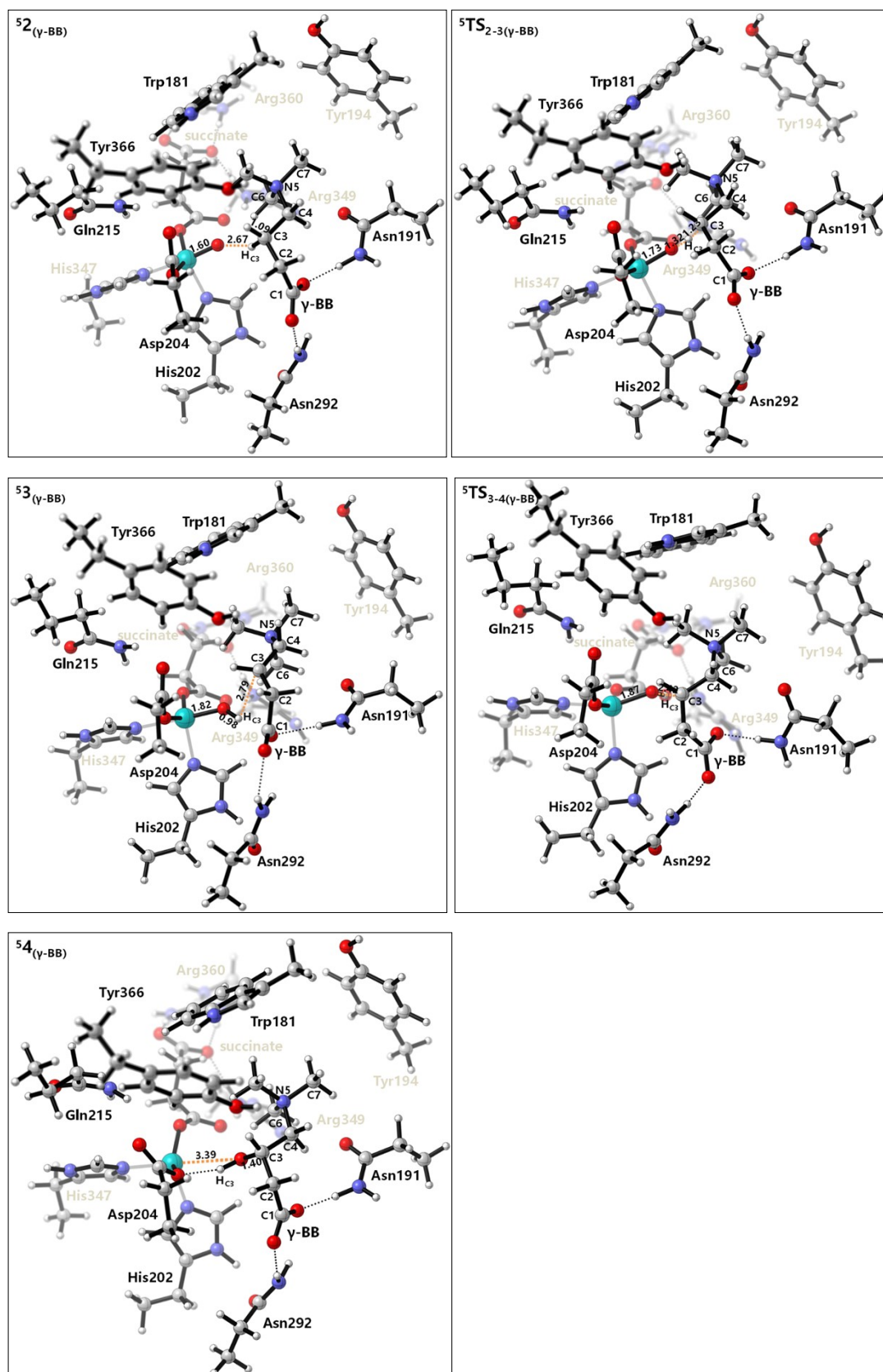


Figure S9. The optimized structures of the stationary points along the reaction process of the γ -BB hydroxylation catalysed by BBOX. Bond lengths are given in Å.

Part V Supplementary coordinates

51

C	-1.814061	4.858490	-4.443049	C	-6.746560	-8.979388	-7.206325
C	-3.225867	4.350845	-4.376972	C	-5.850022	-8.253871	-8.215902
C	-3.845549	3.725587	-3.318795	O	-6.216355	-8.076977	-9.387925
C	-4.228774	4.464521	-5.411506	N	-4.665588	-7.809287	-7.771956
N	-5.162931	3.447461	-3.627354	C	-13.818883	-3.246498	-11.396974
C	-5.429413	3.887970	-4.902384	C	-13.768816	-1.873268	-10.711053
C	-4.230342	5.000150	-6.715846	C	-12.553052	-1.669733	-9.855494
C	-6.610476	3.837824	-5.659286	N	-12.577237	-1.083100	-8.602005
C	-5.399966	4.949887	-7.468601	C	-11.229597	-1.975309	-10.074274
C	-6.579285	4.374788	-6.943745	C	-11.325105	-1.053150	-8.108828
C	1.831980	-3.590540	-9.242891	N	-10.487998	-1.590641	-8.979187
C	0.979203	-2.875070	-8.187546	C	-6.562851	0.537435	-16.697928
C	-0.284385	-3.645365	-7.806597	N	-5.331752	-0.217010	-16.943759
O	-1.236506	-3.719503	-8.580498	C	-4.351657	-0.456883	-16.055887
N	-0.272919	-4.211618	-6.579844	N	-4.287337	0.163623	-14.889176
C	1.905864	1.096413	-11.405783	N	-3.385295	-1.339685	-16.403400
C	1.266596	1.355731	-10.064777	C	-5.291868	5.777453	-18.230937
C	-0.108889	1.583142	-9.906884	N	-6.503306	5.277888	-17.585936
C	2.067867	1.394309	-8.911652	C	-6.582927	4.535408	-16.455540
C	-0.671703	1.824676	-8.651817	N	-5.486178	4.158166	-15.791257
C	1.522898	1.628053	-7.649851	N	-7.767138	4.128143	-16.007188
C	0.143307	1.834173	-7.512448	C	-9.479514	3.657314	0.535551
O	-0.450234	2.031816	-6.304177	C	-8.792281	2.364712	1.018644
C	-10.829837	-7.503467	-9.603019	C	-7.865344	1.623397	0.075961
C	-9.315549	-7.318417	-9.557620	C	-8.129422	1.472612	-1.295253
C	-8.803781	-5.907069	-9.545172	C	-6.725083	0.980240	0.585251
N	-7.476808	-5.648939	-9.822542	C	-7.309737	0.699416	-2.120248
C	-9.343308	-4.685115	-9.211841	C	-5.891633	0.205280	-0.223776
C	-7.252414	-4.330954	-9.660377	C	-6.187930	0.051978	-1.583745
N	-8.365472	-3.712581	-9.293419	O	-5.420280	-0.697545	-2.423668
C	-8.604137	-4.296451	-4.577034	C	-6.541409	-0.830134	-10.695383
C	-8.434059	-2.779206	-4.481561	C	-7.121982	1.281960	-12.041760
C	-8.807476	-1.997240	-5.747027	C	-6.984437	2.108085	-13.325349
O	-8.266204	-2.450755	-6.852787	O	-7.732160	-1.265571	-10.445406
O	-9.562701	-1.038535	-5.670541	O	-5.868507	2.083181	-13.969470
C	-12.518629	2.821325	-2.817942	O	-7.947608	2.811831	-13.678655
C	-12.381688	1.896784	-4.043634	C	-3.509834	-5.749545	-5.289501
C	-11.566528	2.514906	-5.185765	N	-4.146538	-2.800626	-5.356199
C	-11.905658	1.969836	-6.574666	O	-2.536521	-4.941899	-5.169986
O	-12.962589	1.410374	-6.835357	C	-4.914793	-5.088754	-5.240357
N	-10.971228	2.234337	-7.534037	N	-3.876746	-1.564348	-6.075682
C	-7.557068	-10.112212	-7.849796	O	-3.438535	-6.980229	-5.433614

C	-4.996303	-3.779936	-6.039440	H	0.217241	2.079439	-5.613622
C	-2.732416	-0.927031	-5.351066	H	2.171547	1.640938	-6.770202
C	-3.513219	-1.740765	-7.526875	H	-1.740842	2.005211	-8.542160
C	-5.083622	-0.681580	-5.967598	H	3.144032	1.229584	-8.996521
O	-8.248825	-0.160649	-8.160584	H	-0.764277	1.570170	-10.780646
Fe	-8.417108	-1.688907	-8.647879	H	2.577490	0.226368	-11.356273
C	-6.408202	-0.078627	-12.033238	H	2.530455	1.952228	-11.710070
H	-6.822379	-0.721356	-12.825767	H	-8.221340	2.603993	1.928760
H	-5.336006	0.056818	-12.213977	H	-9.574795	1.660195	1.352396
H	-9.888724	4.084888	1.427676	H	-6.482012	1.076445	1.645625
H	-8.783497	4.342423	0.099195	H	-9.007689	1.944544	-1.734867
H	-10.291946	3.471825	-0.174944	H	-7.554785	0.561939	-3.172368
H	-12.813459	3.777543	-3.197589	H	-5.014228	-0.283391	0.207027
H	-13.292212	2.434608	-2.187761	H	-4.825458	-1.262349	-1.921557
H	-11.588797	2.929959	-2.250925	H	-7.482611	4.355050	-7.555925
H	2.831309	-3.210873	-9.194323	H	-5.413136	5.366558	-8.477449
H	1.465170	-3.501199	-10.244141	H	-7.519993	3.395708	-5.253238
H	1.902017	-4.665571	-9.017960	H	-3.327322	5.451127	-7.130337
H	-14.007776	-4.045820	-10.711194	H	-3.444074	3.459804	-2.344151
H	-12.927153	-3.454700	-11.950497	H	-5.815557	2.979313	-3.014918
H	-14.647056	-3.256576	-12.121178	H	-1.286275	4.456622	-5.316911
H	-11.305692	-6.917644	-8.844533	H	-1.247878	4.575066	-3.545267
H	-11.242015	-7.253120	-10.558175	H	-7.413849	-8.217666	-6.768926
H	-11.075258	-8.556457	-9.410129	H	-6.137454	-9.357888	-6.373424
H	-6.872641	-10.810967	-8.284578	H	-4.092306	-7.300074	-8.434355
H	-8.191070	-10.620667	-7.153940	H	-4.347439	-7.755540	-6.788536
H	-8.180203	-9.736916	-8.667399	H	-8.926916	-7.801905	-8.651999
H	-8.372860	-4.770397	-3.645895	H	-8.841037	-7.853552	-10.391826
H	-9.595881	-4.563209	-4.876553	H	-10.356506	-4.448619	-8.909528
H	-7.928766	-4.713763	-5.332858	H	-6.785483	-6.405908	-9.935305
H	-2.642892	-1.571839	-15.759189	H	-6.287705	-3.857489	-9.807315
H	-3.477534	-1.932253	-17.215576	H	-13.805366	-1.081321	-11.477590
H	-3.554610	-0.099761	-14.244201	H	-14.670387	-1.732720	-10.096657
H	-4.978656	0.882120	-14.517070	H	-13.357157	-0.625597	-8.140425
H	-5.303833	-0.761221	-17.795652	H	-10.766604	-2.440316	-10.937139
H	-6.365936	1.382212	-16.034280	H	-11.032661	-0.683767	-7.129347
H	-6.933133	0.913509	-17.656724	H	-5.662284	-5.791335	-5.624329
H	-7.851024	3.629378	-15.066196	H	-5.166165	-4.891574	-4.186483
H	-8.603653	4.307457	-16.543731	H	-4.661204	-3.986709	-7.069684
H	-4.601301	4.616227	-15.944215	H	-6.032560	-3.422670	-6.096095
H	-5.579563	3.453692	-15.021835	H	-3.247367	-3.308854	-5.225936
H	-7.375204	5.669252	-17.917968	H	-2.781595	-2.548091	-7.633492
H	-5.475707	5.862855	-19.308055	H	-4.414223	-1.947713	-8.105474
H	-4.465159	5.070663	-18.095992	H	-3.091902	-0.800490	-7.890678

H	-5.933127	-1.188594	-6.427515	C	2.744171	6.162914	0.703102
H	-5.276516	-0.499236	-4.909530	C	1.945000	8.345242	1.305664
H	-4.890112	0.251336	-6.503961	C	1.538782	5.891684	0.051447
H	-2.566409	0.076221	-5.748321	C	0.732327	8.089213	0.666445
H	-2.987699	-0.881380	-4.290238	C	0.519476	6.851544	0.044127
H	-1.841816	-1.543991	-5.500643	O	-0.659534	6.530703	-0.560542
H	-9.050174	-2.368541	-3.671730	C	-0.423695	-6.796501	4.786275
H	-7.389728	-2.540385	-4.236162	C	-0.305128	-5.338967	5.226873
H	-11.950112	0.922972	-3.767622	C	0.088688	-4.333522	4.185861
H	-13.387088	1.684312	-4.434207	N	0.527168	-3.076563	4.552843
H	-11.764109	3.599376	-5.248698	C	0.023973	-4.302775	2.812992
H	-10.486243	2.416598	-5.005794	C	0.704901	-2.341025	3.438274
H	-11.111546	1.831879	-8.451336	N	0.412481	-3.056325	2.362400
H	-10.012316	2.422370	-7.279577	C	-4.399729	-2.842506	1.776793
H	-8.191266	1.160562	-11.832784	C	-4.113026	-2.193136	0.422427
H	-6.716690	1.911036	-11.231447	C	-2.703344	-2.373731	-0.168038
O	-5.561873	-0.994473	-9.977046	O	-1.735180	-2.491909	0.704803
H	-5.023500	6.740182	-17.848791	O	-2.547791	-2.386018	-1.381367
H	-7.302972	-0.089683	-16.246516	C	-4.776566	-3.701392	-6.481685
H	-1.800330	5.926205	-4.511525	C	-3.795813	-4.052921	-5.348771
H	1.218941	0.915354	-12.205932	C	-2.527829	-3.189422	-5.347965
H	1.593474	-2.688633	-7.293902	C	-1.326420	-3.844383	-4.664044
H	0.659254	-1.893699	-8.560557	O	-1.170647	-5.056253	-4.621463
H	0.544344	-4.138645	-5.992583	N	-0.385919	-2.974864	-4.186665
H	-1.100744	-4.686647	-6.173943	C	-2.473439	-4.412508	8.058196
				C	-2.776644	-3.162185	7.222597
				C	-1.563744	-2.232004	7.114084
				O	-0.409130	-2.685762	7.108557
				N	-1.804510	-0.917547	7.003777
				C	2.064024	-8.348719	0.130356
				C	1.682331	-7.705415	-1.214459
				C	0.913676	-6.420300	-1.085492
				N	-0.270570	-6.148511	-1.748852
				C	1.171362	-5.283163	-0.358648
				C	-0.682784	-4.907420	-1.418484
				N	0.172727	-4.356396	-0.573941
				C	8.624279	-1.140026	0.388368
				N	8.253483	-0.075093	1.338578
				C	6.967890	0.234927	1.635791
				N	6.013740	0.079427	0.745702
				N	6.696395	0.734614	2.864845
				C	11.406483	1.628467	-3.613864
				N	10.750624	0.342592	-3.837031
				C	9.451045	0.051605	-3.581490
⁵TS₁₋₂							
C	-1.922001	6.652263	-4.024128				
C	-2.226121	5.184562	-4.114128				
C	-3.459379	4.576412	-4.048336				
C	-1.272657	4.123992	-4.349457				
N	-3.332846	3.211946	-4.226114				
C	-2.005555	2.903617	-4.415466				
C	0.127499	4.087650	-4.515547				
C	-1.377056	1.669010	-4.639861				
C	0.752709	2.864069	-4.735167				
C	0.006281	1.665732	-4.797875				
C	1.081719	6.327760	5.905001				
C	0.176388	5.927694	4.733022				
C	-0.452927	4.542029	4.898300				
O	0.180002	3.516884	4.667658				
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C	4.258089	7.699412	2.073052				
C	2.971377	7.387068	1.350004				

N	8.634159	0.947766	-3.031063	H	-1.061989	-6.914321	3.935566
N	8.973196	-1.164621	-3.846331	H	0.529306	-7.237507	4.580877
C	-7.609787	-0.082550	-6.722895	H	-0.870954	-7.378778	5.603813
C	-8.328029	0.171693	-5.386210	H	-2.159394	-4.091268	9.029689
C	-7.512359	0.479458	-4.146149	H	-3.313152	-5.068549	8.154163
C	-6.167345	0.110270	-3.995964	H	-1.640274	-4.980436	7.634931
C	-8.137711	1.101559	-3.051250	H	-5.394240	-2.650442	2.122028
C	-5.476344	0.330670	-2.801380	H	-4.245215	-3.898487	1.703221
C	-7.461791	1.338748	-1.853967	H	-3.706131	-2.474157	2.541179
C	-6.124706	0.943783	-1.723895	H	5.764962	1.074421	3.065629
O	-5.404284	1.149564	-0.581707	H	7.287338	0.520842	3.655979
C	3.136419	-1.760580	0.107054	H	5.010881	-0.030201	0.985539
C	4.368576	-1.284029	-2.105396	H	6.227280	-0.019814	-0.281930
C	5.816353	-1.043752	-2.557382	H	8.962981	0.264105	1.973669
O	2.092061	-2.510061	0.067266	H	8.486449	-0.826596	-0.649736
O	6.476670	-0.169340	-1.882312	H	9.668483	-1.413680	0.566611
O	6.293708	-1.668006	-3.517845	H	7.938347	-1.372215	-3.749203
C	-3.701075	1.333921	5.107652	H	9.591922	-1.901133	-4.152503
N	-3.457310	1.919412	2.152721	H	8.886619	1.921576	-2.975492
O	-3.656514	2.554575	4.755843	H	7.721801	0.602454	-2.625585
C	-3.674134	0.306210	3.942667	H	11.244841	-0.311423	-4.429920
N	-2.621709	2.717878	1.261687	H	12.477804	1.455428	-3.460943
O	-3.772330	0.898179	6.266169	H	11.020876	2.105824	-2.705848
C	-2.813226	0.741713	2.750016	H	-1.239005	7.297917	-0.571941
C	-3.534116	3.763678	0.695187	H	-0.051253	8.851008	0.659637
C	-1.482737	3.390578	1.970896	H	1.379804	4.939615	-0.454868
C	-2.106335	1.863229	0.142876	H	2.088567	9.313481	1.789899
O	0.051965	-0.973962	-0.439091	H	3.521961	5.396551	0.706793
Fe	0.162309	-2.389029	0.333769	H	4.056859	8.023402	3.105259
C	4.262553	-2.199626	-0.850493	H	4.789868	8.530570	1.583269
H	4.107268	-3.239200	-1.160649	H	-9.042414	0.997219	-5.534290
H	5.197206	-2.169506	-0.274340	H	-8.957045	-0.707990	-5.161461
H	-8.408976	-0.173454	-7.429463	H	-9.184122	1.404281	-3.130676
H	-6.976919	0.732656	-7.004206	H	-5.644467	-0.381534	-4.815595
H	-7.030857	-1.012386	-6.728629	H	-4.447526	-0.004085	-2.681273
H	-4.211985	-3.698477	-7.390685	H	-7.975907	1.825989	-1.021909
H	-5.535425	-4.453998	-6.536167	H	-5.982847	1.321673	0.167099
H	-5.244542	-2.720049	-6.351018	H	0.522866	0.721718	-4.978123
H	1.197101	7.391420	5.925328	H	1.835292	2.824751	-4.868329
H	2.046041	5.865224	5.871583	H	-1.952635	0.746002	-4.695500
H	0.618401	6.050977	6.863964	H	0.713376	5.007195	-4.475419
H	1.201279	-8.696457	0.659257	H	-4.440286	5.020674	-3.897691
H	2.621176	-7.682804	0.755744	H	-4.096091	2.551316	-4.214015
H	2.701470	-9.225570	-0.054868	H	-1.118170	6.851612	-3.304697

H	-2.806807	7.225015	-3.714166	H	-0.612504	6.685200	4.609888
H	-3.064754	-3.431089	6.192012	H	0.750548	5.914752	3.798441
H	-3.632188	-2.610706	7.637795	H	-2.220822	5.423065	5.478665
H	-0.998298	-0.311255	6.909771	H	-2.336440	3.700430	5.320896
H	-2.718716	-0.453952	6.867921				
H	-1.273348	-5.012991	5.628601	52			
H	0.396090	-5.260852	6.069458	C	1.55018600	7.69905900	-0.06100900
H	-0.291566	-5.080470	2.127906	C	0.63749600	6.72348300	-0.74866600
H	0.499914	-2.749098	5.531712	C	-0.73270400	6.79948800	-0.85528900
H	1.042822	-1.309542	3.438633	C	1.03033800	5.56184300	-1.51466600
H	2.595716	-7.514419	-1.801057	N	-1.21356300	5.76637100	-1.63347600
H	1.092403	-8.418348	-1.809138	C	-0.16018900	4.98784800	-2.05092700
H	-0.700457	-6.706791	-2.476613	C	2.26940400	4.94963600	-1.79865600
H	2.006253	-5.067077	0.296919	C	-0.13857000	3.83144400	-2.84568300
H	-1.576636	-4.427602	-1.802561	C	2.29161800	3.79937500	-2.58352900
H	-3.301314	-0.653307	4.317352	C	1.09830800	3.24567100	-3.10159500
H	-4.710187	0.137250	3.608953	C	3.25643600	1.40356400	8.01089200
H	-1.793610	0.950742	3.118301	C	2.40646900	2.09695300	6.93854800
H	-2.741192	-0.069762	2.017305	C	1.58577600	1.14476500	6.07286000
H	-3.658215	2.514807	2.987848	O	1.93577100	0.90178100	4.91398900
H	-1.901890	4.031151	2.750287	N	0.49219900	0.59340600	6.62936800
H	-0.836488	2.645803	2.437515	C	6.96295700	2.72245500	4.66861400
H	-0.912055	3.981973	1.252553	C	6.64991400	3.74739700	3.60016800
H	-1.383890	1.142736	0.529769	C	6.50898300	3.38270300	2.25062100
H	-2.959035	1.350233	-0.304900	C	6.48826800	5.10603300	3.91797300
H	-1.618063	2.509524	-0.591345	C	6.22460400	4.32167300	1.25763400
H	-2.956686	4.425317	0.044334	C	6.20117100	6.05948100	2.93828400
H	-4.319309	3.253724	0.134139	C	6.06912000	5.67313000	1.59559200
H	-3.966377	4.330843	1.525308	O	5.79144900	6.55063100	0.59489800
H	-4.808447	-2.560715	-0.344235	C	-4.50425600	-7.18423400	1.54680200
H	-4.280033	-1.107618	0.469804	C	-3.68897000	-6.37365900	2.54584400
H	-4.286231	-3.986785	-4.365120	C	-2.77661300	-5.33607000	1.97171900
H	-3.483019	-5.100177	-5.467903	N	-1.89386100	-4.64605500	2.78040700
H	-2.197474	-3.009003	-6.385914	C	-2.67569800	-4.74386200	0.73851600
H	-2.718582	-2.198378	-4.914239	C	-1.32296900	-3.66826600	2.06189500
H	0.391691	-3.373125	-3.675958	N	-1.76719100	-3.70284500	0.80892300
H	-0.647366	-2.036161	-3.920611	C	-5.74805800	-0.94675400	1.33410500
H	3.801198	-1.723095	-2.934697	C	-5.15391200	0.13011000	0.41134700
H	3.934315	-0.298684	-1.885478	C	-3.83393600	-0.13218800	-0.32850200
O	3.296047	-0.777037	0.836358	O	-3.42711700	-1.36732900	-0.35498400
H	11.275994	2.271949	-4.458727	O	-3.25441700	0.79468300	-0.88795900
H	7.986613	-1.973349	0.597729	C	-5.89840800	2.44456600	-6.25253200
H	-1.610046	7.026771	-4.976742	C	-5.32987400	1.20975700	-5.53312900
H	4.940990	6.877594	2.129131	C	-3.87674500	1.36946900	-5.06330600

C	-3.15920200	0.03757900	-4.82310100	N	0.39018200	2.24120600	2.20931900
O	-3.24940700	-0.89378800	-5.60952200	O	-3.60893000	-0.41285200	5.38547700
N	-2.34842000	-0.00911900	-3.72636400	C	-1.94007800	1.63262100	2.86721200
C	-5.32559000	-5.96250500	5.83909300	C	1.43815600	3.16503200	2.75830700
C	-4.92496900	-4.48915000	5.68591900	C	1.02415400	0.92764000	1.84026400
C	-3.40890700	-4.26841300	5.65128600	C	-0.22282300	2.87073400	0.99705200
O	-2.63497400	-5.19425700	5.34837600	Fe	-1.64330100	-2.11232600	-0.52012800
N	-2.95796100	-3.03877700	5.92786700	C	2.04602800	-2.74443700	-2.72723500
C	-2.78888300	-7.34386200	-3.67879100	H	1.38034300	-3.00044200	-3.55903900
C	-2.68341900	-6.04631900	-4.49605800	H	2.64295000	-3.64145500	-2.50309200
C	-2.79053700	-4.82837600	-3.63208500	H	-7.20801700	7.23914800	-4.89598700
N	-3.91086000	-4.02143000	-3.55761500	H	-5.55042800	7.04350400	-4.37960700
C	-1.93475100	-4.32533400	-2.68539800	H	-6.46285800	5.63842800	-4.89581600
C	-3.71211300	-3.08479400	-2.60867300	H	-5.34241500	2.60563900	-7.15263100
N	-2.52110200	-3.24948500	-2.05741100	H	-6.92489700	2.26505800	-6.49478100
C	6.45246000	-5.16218500	-1.46363700	H	-5.83747000	3.34888200	-5.63555700
N	6.49720500	-4.49694800	-0.14721400	H	3.88490300	2.13560000	8.47386900
C	5.42730800	-3.85017900	0.38014500	H	3.86137700	0.61869800	7.60711000
N	4.54742500	-3.27258400	-0.40768000	H	2.62902100	0.96024000	8.79734100
N	5.30014300	-3.80650300	1.72671800	H	-3.74612000	-7.44436500	-3.21131700
C	10.52821600	-2.53292300	-4.27399800	H	-2.02133500	-7.40001700	-2.93534600
N	9.33399500	-3.06710000	-4.92416000	H	-2.66343800	-8.21218200	-4.34266700
C	8.05470300	-2.72646400	-4.62793000	H	-5.05222600	-6.57432200	0.85933600
N	7.76810900	-1.96443600	-3.57467700	H	-3.88587200	-7.86747000	1.00309700
N	7.04718300	-3.18504600	-5.37074800	H	-5.23982000	-7.79144200	2.09226600
C	-6.52415200	6.60038400	-4.37609600	H	-4.96516400	-6.32385400	6.77990700
C	-7.10750500	6.46499700	-2.94676600	H	-6.38500400	-6.10242400	5.78598400
C	-6.15725400	6.13193800	-1.81335900	H	-4.86061000	-6.58431900	5.06853500
C	-5.51747500	4.88383900	-1.70625200	H	-6.53648400	-0.49545900	1.89969600
C	-5.92988600	7.05855800	-0.78416400	H	-6.13553400	-1.77520700	0.77948200
C	-4.70282800	4.56371200	-0.61862000	H	-5.00162300	-1.32102300	2.04489000
C	-5.12186800	6.75606700	0.31568100	H	4.57910700	-3.22945500	2.13967100
C	-4.51151300	5.49941800	0.41030600	H	5.71128100	-4.51882000	2.31363500
O	-3.72755500	5.14032800	1.46477400	H	3.60408800	-2.96938300	-0.11045100
C	1.22276800	-2.46571500	-1.45233100	H	4.82601800	-2.93412500	-1.36963600
C	2.97492900	-1.56710500	-3.13651300	H	7.25076100	-4.73024800	0.48488400
C	4.33457400	-2.03764200	-3.67047100	H	6.61425300	-4.45990100	-2.28595200
O	-0.04166400	-2.30888900	-1.66362000	H	7.20631500	-5.95498000	-1.48342400
O	5.23481700	-2.27272700	-2.77973500	H	6.06527100	-2.81924900	-5.21887300
O	4.52865000	-2.17740400	-4.88726500	H	7.22087000	-3.82060200	-6.13537800
C	-2.59970100	0.08788700	4.85326900	H	8.49366000	-1.49785000	-3.05493000
N	-0.60489500	2.09236700	3.27929300	H	6.77039400	-1.96804900	-3.22609700
O	-1.41905100	-0.37654500	4.85712200	H	9.48045300	-3.48383500	-5.83449800
C	-2.80892700	1.43117800	4.11501000	H	11.35063200	-3.24411200	-4.41017700

H	10.37050400	-2.42199800	-3.19538900	H	1.77911500	1.10636900	1.06741000
H	5.75112800	7.44583000	0.94441700	H	-0.90803100	2.16703100	0.52344800
H	6.08393900	7.10911600	3.21986000	H	-0.74850900	3.77875200	1.29809400
H	6.12597800	4.02338700	0.21355000	H	0.58016100	3.12204900	0.29978900
H	6.59244500	5.43578400	4.95410200	H	2.19825400	3.33684300	1.98965500
H	6.62999900	2.33590000	1.96184500	H	0.94997700	4.10251600	3.03601300
H	6.13545200	2.62281000	5.38582100	H	1.88227000	2.68015500	3.63179400
H	7.85766300	3.00484500	5.24333200	H	-5.88191300	0.40694100	-0.36960100
H	-7.60232300	7.41329400	-2.69130100	H	-4.98667500	1.05835900	0.97364400
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H	-3.75017500	5.82904200	2.13567300	H	-2.51197200	0.56616100	-2.90328700
H	1.14314800	2.34610600	-3.71746800	H	2.47983900	-0.95540200	-3.90045900
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H	-1.05523000	3.40414700	-3.24940600	O	1.78973200	-2.44705000	-0.35711100
H	3.19760600	5.37382200	-1.41433100	H	10.79815200	-1.59548700	-4.71354300
H	-1.41693200	7.53244300	-0.43758000	H	5.47100800	-5.58303700	-1.53048300
H	-2.19076900	5.58697500	-1.81450300	H	2.07428900	8.27655000	-0.79372900
H	2.29531200	7.19135900	0.56702000	H	7.14099800	1.75972100	4.23672800
H	0.98617000	8.39240700	0.57688200	H	1.73597800	2.82893500	7.41674800
H	-5.32462500	-4.06345300	4.74920000	H	3.05689400	2.65449200	6.25396800
H	-5.36161600	-3.87805200	6.48964500	H	0.18703700	0.87890300	7.54875000
H	-1.96577100	-2.87393500	5.79716100	H	-0.18552300	0.08397100	6.02883400
H	-3.49052200	-2.15011300	5.89432500	O	-0.97721400	-1.10617600	0.54082500
H	-4.37280600	-5.84499600	3.22194100				
H	-3.10717500	-7.04587600	3.19252000				
H	-3.20645300	-4.97775900	-0.17526400				
H	-1.84752000	-4.80841700	3.80496500				
H	-0.63224800	-2.93465700	2.46200600				
H	-1.72228600	-6.01898100	-5.03007100				
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H	-0.94472800	-4.67070600	-2.41511400				
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H	-3.86618500	1.51135700	3.83453500				
H	-2.61530700	2.25085300	4.82651200				
H	-1.90857600	0.70058900	2.28197000				
H	-2.40361500	2.41047900	2.25316600				
H	-0.21660500	1.38063800	3.90823400				
H	1.47999700	0.51946200	2.74655600				
H	0.25565100	0.25374700	1.45281400				
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				C	-1.81307200	4.85847600	-4.44308700
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				C	-4.31974700	4.50874600	-5.15512600
				N	-5.08443900	3.50173000	-3.28644100
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				C	-6.73406300	3.96325800	-5.14289700
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				C	-6.82796600	4.52458600	-6.41403800
				C	1.83200100	-3.59051400	-9.24292100
				C	0.94783700	-2.87015400	-8.21425900
				C	-0.29467300	-3.65547300	-7.78072000
				O	-1.40016300	-3.43189600	-8.26554000
				N	-0.08214400	-4.57849800	-6.81005700

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C	1.22235300	1.28705800	-10.07176000	C	-6.97016300	4.76711500	-16.66507800
C	-0.15649500	1.08606800	-9.89987100	N	-6.04202100	4.42307300	-15.77492000
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C	1.37245500	1.79673300	-7.68662200	C	-8.80281500	2.37825200	1.06270400
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O	-0.62918200	1.66400000	-6.32470600	C	-8.14781300	1.48317400	-1.26137800
C	-10.82986500	-7.50366900	-9.60299200	C	-7.11021900	0.55551900	0.69318000
C	-9.31270800	-7.34156500	-9.56680800	C	-7.45215800	0.57680700	-2.06826300
C	-8.76495400	-5.94411900	-9.55703600	C	-6.40345000	-0.35187000	-0.09502300
N	-7.41763400	-5.73324500	-9.76796400	C	-6.58096100	-0.34876000	-1.48430700
C	-9.27819900	-4.70290000	-9.26048700	O	-5.91119400	-1.21083200	-2.30750700
C	-7.15296200	-4.42667500	-9.59028600	C	-7.71072800	-0.72115900	-11.61495300
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C	-8.73872100	-1.95378900	-5.75002700	O	-6.82166300	2.47058000	-14.11989100
O	-8.26180700	-2.45588400	-6.85642500	O	-8.89958200	3.26661400	-14.04204400
O	-9.35951100	-0.90196000	-5.65160700	C	-3.15730500	-5.88848100	-5.15880800
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O	-12.99659600	1.28994200	-6.79905100	O	-3.25561300	-7.09662500	-5.41718700
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O	-6.14383000	-8.14192400	-9.36824100	O	-8.26073300	-0.17235900	-8.27485600
N	-4.64898800	-7.81135400	-7.71500100	Fe	-8.32122000	-1.73598800	-8.69239600
C	-13.81906400	-3.24656400	-11.39713000	C	-8.38296400	0.15497700	-12.68172600
C	-13.73514200	-1.89551800	-10.66517300	H	-9.44548900	-0.10482900	-12.75172500
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N	-12.53600600	-1.18896500	-8.52086600	H	-9.88853900	4.08495300	1.42772900
C	-11.21485100	-2.11935500	-9.99155400	H	-8.78344100	4.34239700	0.09924400
C	-11.28246000	-1.21364600	-8.02315600	H	-10.29288900	3.45707700	-0.16995800
N	-10.46110000	-1.77489900	-8.89192700	H	-12.81326500	3.77758800	-3.19762700
C	-6.56285500	0.53748100	-16.69789400	H	-13.29215300	2.43461100	-2.18768800
N	-5.24352000	-0.01941500	-16.35076300	H	-11.58638900	2.92619600	-2.25471900
C	-4.91612000	-0.41555000	-15.09722100	H	2.83131500	-3.21089300	-9.19429300
N	-5.43240500	0.17071500	-14.04112300	H	1.46514100	-3.50120500	-10.24413100
N	-4.00932500	-1.41344400	-14.95802200	H	1.90197600	-4.66532900	-9.01810100
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H	-12.92709400	-3.45465000	-11.95041900	H	-5.68922500	3.07088400	-2.60249900
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H	-11.08470100	-8.55492400	-9.41125800	H	-6.14545600	-9.39195700	-6.34848700
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H	-8.19109900	-10.62062900	-7.15394100	H	-4.32097500	-7.77879400	-6.73590400
H	-8.17386100	-9.72520600	-8.66541100	H	-8.92911400	-7.83096300	-8.66211700
H	-8.37278700	-4.77036900	-3.64589800	H	-8.85614100	-7.88881000	-10.40397300
H	-9.59587300	-4.56325000	-4.87654400	H	-10.29562000	-4.43215500	-9.00819900
H	-7.92282200	-4.70146000	-5.33456700	H	-6.74343000	-6.50870700	-9.86256700
H	-3.68820800	-1.65740900	-14.03028300	H	-6.16301300	-3.99091900	-9.65614900
H	-3.89707800	-2.11423400	-15.67727300	H	-13.73086100	-1.07658000	-11.40405900
H	-5.55033800	-0.30482900	-13.12288000	H	-14.64288900	-1.74574900	-10.06178400
H	-5.95584500	1.08069000	-14.11048800	H	-13.29357000	-0.68907300	-8.06438500
H	-4.66174400	-0.36247100	-17.10294500	H	-10.76414600	-2.58108400	-10.86150300
H	-6.68104500	1.56034700	-16.33133500	H	-10.98018400	-0.83037300	-7.05188800
H	-6.67137100	0.51302100	-17.78643100	H	-5.16704200	-5.45226500	-5.86757900
H	-8.52124000	4.02014000	-15.49005800	H	-4.93861900	-5.18558100	-4.14224400
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H	-6.30103500	3.71475900	-15.03276700	H	-2.68050900	-3.71131600	-4.23998700
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H	-4.56500100	5.02365600	-17.90718900	H	-1.32101000	-0.77004800	-5.68489500
H	-0.01474800	2.01447400	-5.67345100	H	-4.26310900	-0.95862200	-5.89997000
H	1.98223500	2.07536900	-6.82305100	H	-4.66685800	-0.74466300	-4.16301200
H	-1.84426500	1.06820100	-8.54014000	H	-3.40080300	0.27370200	-4.94442100
H	3.04288000	1.82851600	-9.03358400	H	-1.72025600	-0.36874000	-3.32529400
H	-0.77251800	0.80406000	-10.75630200	H	-3.03509200	-1.25753900	-2.47921400
H	2.60292100	0.24497200	-11.37082900	H	-1.51886800	-2.10399600	-2.91342800
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H	-9.58407000	1.74955600	1.52532100	H	-11.94838000	0.91840100	-3.75376200
H	-6.96894500	0.52861600	1.77589700	H	-13.40673900	1.65383300	-4.40186200
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H	-7.61149300	0.55388500	-3.14526200	H	-10.52857700	2.43390800	-5.03417100
H	-5.71920500	-1.06476700	0.37151500	H	-11.15120300	1.64980800	-8.43534700
H	-5.59982600	-1.97874300	-1.81892400	H	-10.05855500	2.29796500	-7.29284800
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H	-5.80678700	5.50269600	-8.05609700	H	-7.36166000	1.82244600	-11.69770300
H	-7.61074700	3.55300900	-4.64286700	O	-6.45688500	-0.86323800	-11.65149500
H	-3.58161200	5.49300100	-6.95200100	H	-5.02345500	6.74015500	-17.84875400
H	-3.24451700	3.48376400	-2.18258200	H	-7.30296300	-0.08972200	-16.24655400

H	-1.80102500	5.92621700	-4.51149000	C	-4.04867400	-3.00869900	2.21165000
H	1.21891500	0.91523700	-12.20588500	C	-3.79511600	-2.61369900	0.75586200
H	1.54837100	-2.64353700	-7.31925500	C	-2.34849800	-2.73711500	0.24635500
H	0.59891500	-1.91288100	-8.61613900	O	-1.42488700	-2.36759800	1.09060500
H	0.83928600	-4.70003100	-6.41566200	O	-2.15122500	-3.15078700	-0.89052100
H	-0.86014300	-5.01486000	-6.29120400	C	-3.83735700	-5.63793500	-5.67018800
O	-6.14979500	-1.72508100	-9.10237300	C	-2.88629900	-5.65855100	-4.45555300
H	-6.11442200	-1.48143900	-10.06424600	C	-1.64388300	-4.77786300	-4.62401000
H	-5.77029300	-0.94005700	-8.66017900	C	-0.46211900	-5.17465000	-3.73691400
O	-5.66927800	0.85201200	-8.20612000	O	-0.34751900	-6.28296300	-3.22953900
H	-5.43282100	1.41404600	-7.46392300	N	0.50965700	-4.22276500	-3.62355600
H	-6.64137000	0.78588200	-8.16979200	C	-2.29914800	-2.93300800	8.73582800
				C	-2.72677400	-1.94489900	7.64181400
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				O	-0.44372400	-1.17715600	7.45029300
				N	-2.05587100	0.31672900	6.95431200
				C	3.15610100	-7.78873900	1.98330900
				C	2.74786100	-7.46571300	0.53369500
				C	1.86470700	-6.25400200	0.41098400
				N	0.78521900	-6.15691200	-0.45378100
				C	1.92044800	-5.03138700	1.03763000
				C	0.23543600	-4.93348700	-0.32858200
				N	0.90127500	-4.23007200	0.57099400
				C	8.70397800	0.14946200	0.85393100
				N	8.13116100	1.34381200	1.49915600
				C	6.79702700	1.56233100	1.59131700
				N	5.96931000	1.12800800	0.66821300
				N	6.33736100	2.27685800	2.64755800
				C	11.33000000	2.36750900	-3.57409700
				N	10.96701100	0.95582300	-3.54510500
				C	9.73269600	0.46156800	-3.28217900
				N	8.70445300	1.27270400	-3.04456400
				N	9.53587700	-0.85543600	-3.22609400
				C	-7.09596600	-2.57996700	-6.77164900
				C	-7.94093500	-2.15265000	-5.55757200
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				C	-5.91912800	-1.62339800	-4.05210200
				C	-8.09078700	-0.80844700	-3.43781100
				C	-5.37858400	-1.08792900	-2.87841800
				C	-7.56957900	-0.26225100	-2.26544800
				C	-6.20685400	-0.40962600	-1.97740700
				O	-5.63964000	0.10629700	-0.84681200
				C	3.60857300	-1.34538700	0.60296900
				C	4.94475800	-1.50254900	-1.58086200
⁵TS_{1w}							
C	-2.49004200	5.29545500	-5.44093100				
C	-2.61780000	3.81530600	-5.22061600				
C	-3.77052100	3.09466100	-5.00324900				
C	-1.54556200	2.84652700	-5.25547200				
N	-3.48320600	1.74748200	-4.89886800				
C	-2.12931000	1.56175800	-5.05530000				
C	-0.15137700	2.93978500	-5.44549800				
C	-1.36119800	0.38705600	-5.04846000				
C	0.61278900	1.77647600	-5.43817600				
C	0.01159000	0.51190900	-5.24509100				
C	-0.04415600	7.49597400	4.40220000				
C	-0.81120100	6.73239300	3.31216700				
C	-1.33207200	5.35685800	3.74261500				
O	-0.73970500	4.32298100	3.44732700				
N	-2.49700000	5.37461000	4.43654400				
C	3.14273300	8.45321700	0.45521000				
C	1.92135200	7.81808200	-0.16517900				
C	1.75791100	6.42866200	-0.27596900				
C	0.87700700	8.63269700	-0.63440800				
C	0.59776300	5.86706700	-0.81541800				
C	-0.29032500	8.08963100	-1.17064600				
C	-0.43878000	6.69860500	-1.25425200				
O	-1.57578700	6.11337400	-1.73505900				
C	0.22564300	-5.64731300	6.11902400				
C	0.12759500	-4.12896500	6.21457200				
C	0.41837400	-3.34509700	4.96998800				
N	0.60348300	-1.97877700	5.04388100				
C	0.44726900	-3.64017200	3.62801600				
C	0.72254100	-1.48925700	3.79958400				
N	0.64540600	-2.47334000	2.91298500				

C	6.32990800	-1.06794600	-2.07361400	H	8.72325300	1.87347400	2.12426300
O	2.72943200	-2.21164100	0.83996000	H	8.61120000	0.19404700	-0.23441100
O	6.71002500	0.10609400	-1.71062600	H	9.75815800	0.07561100	1.13751400
O	7.01527000	-1.82104700	-2.78382600	H	8.56116200	-1.25082900	-3.09228600
C	-4.18373800	2.06974900	4.72838900	H	10.32052400	-1.48994500	-3.25539000
N	-4.37283500	2.29880900	1.72547000	H	8.75760800	2.25611200	-3.25776200
O	-4.36938200	3.23487600	4.25411300	H	7.83961100	0.86266600	-2.59207900
C	-3.94136800	0.94631600	3.68130800	H	11.64500400	0.30453200	-3.91800100
N	-3.89315400	3.17374000	0.65701200	H	12.39372700	2.46359100	-3.32703300
O	-4.19202700	1.74985800	5.92652400	H	10.76893300	2.92419000	-2.81437000
C	-3.35435800	1.43897400	2.35310800	H	-2.15608400	6.78893100	-2.09785200
C	-5.12571600	3.79259000	0.07466400	H	-1.08842600	8.75129100	-1.51718000
C	-2.98026600	4.25817300	1.14909500	H	0.48348600	4.78607600	-0.89384000
C	-3.20151100	2.36598200	-0.40056400	H	0.96995900	9.71897000	-0.57162100
O	0.48832300	-1.83170500	-0.78545500	H	2.54835600	5.76097400	0.07295600
Fe	0.54814600	-2.15285400	0.86748600	H	2.87304600	8.98532000	1.38095400
C	4.90230200	-1.84545400	-0.06233600	H	3.57869500	9.20442000	-0.22080600
H	4.98913900	-2.92877700	0.07885900	H	-8.72613300	-1.46861400	-5.91780600
H	5.74849000	-1.38069000	0.45858300	H	-8.48682800	-3.04188000	-5.19573000
H	-7.83476400	-2.92774100	-7.46375300	H	-9.15832200	-0.69420400	-3.63827500
H	-6.55851100	-1.76281900	-7.20514500	H	-5.25750300	-2.16516900	-4.72771800
H	-6.40417400	-3.39900200	-6.54869300	H	-4.32583100	-1.22624300	-2.63607500
H	-3.22657700	-5.74848700	-6.54200100	H	-8.22423000	0.27354100	-1.57378500
H	-4.48817400	-6.48242600	-5.58149200	H	-6.30847800	0.29458500	-0.18178900
H	-4.41977900	-4.71493400	-5.75042600	H	0.63568800	-0.38364000	-5.25688200
H	-0.06857200	8.54534800	4.19417000	H	1.69135400	1.83720700	-5.59478000
H	0.97215500	7.17493800	4.49714500	H	-1.82413100	-0.58791600	-4.89871200
H	-0.52080400	7.36490900	5.38505100	H	0.32337800	3.90939300	-5.60350400
H	2.31653100	-8.13279300	2.55051000	H	-4.79769000	3.44311500	-4.92587000
H	3.58560800	-6.93489100	2.46444100	H	-4.16315200	1.01909700	-4.73824900
H	3.90986300	-8.58829900	1.98911800	H	-1.74861100	5.73925300	-4.76369300
H	-0.34209100	-6.02948700	5.29639300	H	-3.44839600	5.80784400	-5.28097400
H	1.23792000	-5.98532300	6.04106500	H	-2.92748700	-2.46675100	6.69053100
H	-0.18900400	-6.09405000	7.03307900	H	-3.66762500	-1.44409300	7.91144200
H	-2.08541800	-2.37335700	9.62279200	H	-1.33017800	0.99073500	6.74126100
H	-3.05114400	-3.66379700	8.94829100	H	-3.01554800	0.62615600	6.72404600
H	-1.37663900	-3.45412600	8.46479700	H	-0.89140300	-3.86031100	6.52183200
H	-5.07791900	-2.88763000	2.47877300	H	0.77775300	-3.75926600	7.02003900
H	-3.75519300	-4.02452800	2.37362600	H	0.31477900	-4.59537000	3.13719000
H	-3.45138400	-2.38985100	2.89113500	H	0.46864300	-1.45165000	5.92236100
H	5.35595300	2.51920200	2.68392600	H	0.82957500	-0.43988700	3.55128500
H	6.84058900	2.28603400	3.52380400	H	3.65327700	-7.31176900	-0.07730800
H	4.96909800	0.89417700	0.85401300	H	2.23467200	-8.33222200	0.09065900
H	6.30992900	0.75476000	-0.25296800	H	0.49520100	-6.80486700	-1.18276000

H	2.63068700	-4.67010600	1.77070300	C	-3.22648200	4.36470300	-4.32309600
H	-0.62864000	-4.56469000	-0.87848600	C	-3.81798400	3.75706400	-3.23857900
H	-3.26326700	0.19904600	4.10900700	C	-4.26635700	4.49924300	-5.31813300
H	-4.89936200	0.43307700	3.50106500	N	-5.15107500	3.50383400	-3.49730200
H	-2.41456000	1.97481900	2.56770700	C	-5.45837600	3.95174400	-4.76094600
H	-3.11990100	0.58757400	1.70548800	C	-4.30890300	5.04190200	-6.61913300
H	-4.63421300	2.93079500	2.51460400	C	-6.67274700	3.93997000	-5.46422700
H	-3.51865800	4.84790800	1.89552100	C	-5.51222900	5.03256500	-7.31826700
H	-2.10051800	3.81290100	1.61915400	C	-6.68346600	4.48833400	-6.74382400
H	-2.67451200	4.87927600	0.30308300	C	1.83201400	-3.59049800	-9.24293100
H	-2.26540400	1.96982000	-0.00521600	C	0.95053100	-2.85597500	-8.22130400
H	-3.86606400	1.54972100	-0.69292600	C	-0.30610300	-3.61886700	-7.78793000
H	-2.98589800	3.01982300	-1.24932000	O	-1.41306900	-3.35178700	-8.24694700
H	-4.83642700	4.49696200	-0.71187400	N	-0.10226800	-4.57284600	-6.84595300
H	-5.74969400	2.99522100	-0.33233700	C	1.90589900	1.09646900	-11.40583900
H	-5.66243100	4.31675100	0.87151300	C	1.24991300	1.29684600	-10.06048500
H	-4.40770600	-3.22096000	0.07676600	C	-0.11523900	1.05689800	-9.83971600
H	-4.09690000	-1.57194900	0.58422300	C	2.02111700	1.70783900	-8.96033600
H	-3.41363400	-5.37913700	-3.53103300	C	-0.69186800	1.20266000	-8.57556000
H	-2.53841800	-6.69027500	-4.30368500	C	1.46342200	1.85345300	-7.69002600
H	-1.26532000	-4.85241800	-5.65872900	C	0.10145900	1.59095100	-7.48997700
H	-1.87953800	-3.71543800	-4.46470300	O	-0.48649100	1.68198000	-6.26034000
H	1.26680000	-4.39689100	-2.97565300	C	-10.82985900	-7.50374900	-9.60298300
H	0.29209800	-3.25125200	-3.79068200	C	-9.31412800	-7.35645200	-9.56847700
H	4.60511900	-2.36348400	-2.16846900	C	-8.77473000	-5.95960100	-9.57214600
H	4.26433600	-0.66431300	-1.78890800	N	-7.43041700	-5.73149300	-9.79066300
O	3.49238900	-0.11108300	0.84294400	C	-9.31081300	-4.72782800	-9.28585300
H	11.16612200	2.79342700	-4.54188600	C	-7.18216400	-4.42340400	-9.62878500
H	8.16847300	-0.70091400	1.22129200	N	-8.30545000	-3.78122400	-9.33368200
H	-2.17549600	5.49864500	-6.44317600	C	-8.60413100	-4.29641000	-4.57714900
H	3.92187300	7.76438600	0.70685500	C	-8.47039200	-2.77496300	-4.48420900
H	-1.66662700	7.34216500	2.98120300	C	-8.79008200	-1.97172200	-5.75662400
H	-0.17304700	6.57549200	2.43597100	O	-8.35427000	-2.48117000	-6.87482100
H	-2.96743900	6.24953300	4.61710200	O	-9.40620900	-0.91550000	-5.65323000
H	-3.05372000	4.51898700	4.58909600	C	-12.51901800	2.82125300	-2.81805300
O	0.72285200	-0.20578400	1.25163200	C	-12.40664800	1.87969800	-4.03647100
H	1.69259200	-0.03560000	1.24022600	C	-11.67124300	2.49796100	-5.22956800
H	0.27800900	0.34506100	0.18693600	C	-11.97650000	1.83802900	-6.57551100
O	-0.11010500	0.48651600	-0.88481100	O	-12.97051500	1.15052900	-6.77495400
H	0.55332700	0.96526200	-1.39262000	N	-11.09845300	2.14741800	-7.57242800
H	0.12993800	-0.73603900	-1.00022700	C	-7.55704100	-10.11229400	-7.84978400
				C	-6.74171900	-8.99300300	-7.18746700
				C	-5.83585000	-8.25947400	-8.17966200
⁵INT_{12w1}				O	-6.17103500	-8.11832900	-9.36685400
C	-1.81312500	4.85855900	-4.44308400				

N	-4.68641600	-7.75475500	-7.71145600	Fe	-8.30769900	-1.79689900	-8.77375600
C	-13.81908500	-3.24653400	-11.39713800	C	-8.49438600	0.21259400	-12.78933400
C	-13.70848500	-1.90296700	-10.64995900	H	-9.53655500	-0.10646900	-12.90537100
C	-12.47328100	-1.78344200	-9.79810900	H	-7.98429200	0.00364700	-13.73790100
N	-12.43617200	-1.17875300	-8.54918700	H	-9.88864700	4.08493200	1.42769000
C	-11.17550600	-2.16488800	-10.04010200	H	-8.78346000	4.34234500	0.09913400
C	-11.17430900	-1.21289500	-8.08358100	H	-10.29252700	3.45614200	-0.16982100
N	-10.38810300	-1.80792800	-8.96597900	H	-12.81325400	3.77758400	-3.19764700
C	-6.56286900	0.53748300	-16.69791600	H	-13.29210600	2.43458500	-2.18764600
N	-5.24215800	0.02837200	-16.28887500	H	-11.58380300	2.92344000	-2.25928900
C	-4.94065500	-0.30325200	-15.00983300	H	2.83131600	-3.21089500	-9.19428400
N	-5.49614200	0.31634200	-13.99413400	H	1.46512700	-3.50121900	-10.24412600
N	-4.01429200	-1.27213700	-14.80396100	H	1.89678200	-4.66423100	-9.01276500
C	-5.29190200	5.77748300	-18.23095100	H	-14.00770300	-4.04580300	-10.71115400
N	-6.66067800	5.42691800	-17.87350000	H	-12.92706900	-3.45466000	-11.95037500
C	-7.04300900	4.82125500	-16.72270100	H	-14.65512500	-3.21222300	-12.10908000
N	-6.15204800	4.50049200	-15.78762000	H	-11.30567500	-6.91754100	-8.84460100
N	-8.32313600	4.50999800	-16.52137500	H	-11.24203300	-7.25300600	-10.55813700
C	-9.47970100	3.65737600	0.53565100	H	-11.09374800	-8.55297600	-9.41129700
C	-8.80231300	2.37926100	1.06345100	H	-6.87263800	-10.81095900	-8.28458800
C	-8.00937100	1.48232400	0.13386300	H	-8.19109700	-10.62062800	-7.15393800
C	-8.14073200	1.48778000	-1.26265100	H	-8.17528500	-9.72842100	-8.66588600
C	-7.14091100	0.53046300	0.69717500	H	-8.37287000	-4.77039400	-3.64589000
C	-7.45279600	0.57407800	-2.06805700	H	-9.59589500	-4.56326100	-4.87646200
C	-6.44286900	-0.38522800	-0.08875800	H	-7.92178800	-4.69942500	-5.33490400
C	-6.60541400	-0.37166300	-1.47993500	H	-3.71987100	-1.47271100	-13.85722100
O	-5.94792000	-1.24361100	-2.29936400	H	-3.86963100	-2.00135400	-15.48837500
C	-7.82346100	-0.63966200	-11.69869400	H	-5.63594700	-0.12167600	-13.05715900
C	-8.43629600	1.73398300	-12.46680800	H	-6.05619100	1.19827600	-14.11647300
C	-8.16760100	2.61160400	-13.69370800	H	-4.63348000	-0.33726500	-17.00838800
O	-8.58387500	-1.28418900	-10.93754700	H	-6.71692500	1.57091400	-16.37663000
O	-6.97738400	2.54731300	-14.17850100	H	-6.63580400	0.46875900	-17.78755500
O	-9.05864100	3.33756000	-14.16277400	H	-8.63725100	4.09048900	-15.59957000
C	-3.16939200	-5.83671100	-5.15609800	H	-8.99516000	4.60709100	-17.26837600
N	-3.36942600	-2.98053400	-4.21993600	H	-5.21253600	4.86307700	-15.81959400
O	-2.07286600	-5.24410000	-4.90630500	H	-6.43529200	3.79041900	-15.05466800
C	-4.44599400	-4.95005000	-5.10781600	H	-7.39559000	5.83200400	-18.43819100
N	-2.70819900	-1.69219100	-4.41388300	H	-5.20725700	5.80014900	-19.32374800
O	-3.31625000	-7.04049000	-5.41686900	H	-4.59173700	5.01573200	-17.86857300
C	-4.19100600	-3.45702500	-5.34577200	H	0.13844500	2.05645800	-5.63282800
C	-2.07703900	-1.37624900	-3.09355300	H	2.09312500	2.16547300	-6.85271300
C	-1.64684400	-1.72624300	-5.47403800	H	-1.75280200	1.00896000	-8.41935700
C	-3.72271400	-0.63594800	-4.73816400	H	3.08589500	1.91090300	-9.09259500
O	-8.38035300	-0.07398500	-8.36606600	H	-0.74951700	0.73909800	-10.66984600

C	1.81808600	7.83474600	-0.08738400	C	9.80374000	0.66395000	-3.19625600
C	1.58897600	6.45180700	-0.00555300	N	8.74934700	1.44566400	-2.97732500
C	0.86635000	8.60892300	-0.77082800	N	9.63707600	-0.65822300	-3.16997300
C	0.45160600	5.86096100	-0.56000200	C	-6.93216400	-2.64620800	-6.90112200
C	-0.27907800	8.03691100	-1.32610200	C	-7.82196900	-2.24710100	-5.70807300
C	-0.49819500	6.65770800	-1.21045900	C	-7.22962800	-1.61713600	-4.46288400
O	-1.62095200	6.05319400	-1.69845900	C	-5.87370400	-1.68876400	-4.11161800
C	0.28442100	-5.71519200	6.04814800	C	-8.09865700	-0.98415000	-3.55627900
C	0.14999600	-4.20463200	6.18328100	C	-5.40000800	-1.17129200	-2.90101300
C	0.46328800	-3.39435200	4.96517600	C	-7.64580300	-0.45881000	-2.34694000
N	0.64530300	-2.02848400	5.05787200	C	-6.29000100	-0.56037000	-2.00976400
C	0.51946200	-3.67900200	3.62374800	O	-5.79125900	-0.06804500	-0.83854900
C	0.78923400	-1.52649500	3.82296800	C	3.68170500	-1.32794700	0.57416600
N	0.73084600	-2.50492600	2.92700400	C	5.04421300	-1.42274400	-1.59974000
C	-3.99015200	-3.11539400	2.11519700	C	6.42661700	-0.96010700	-2.07094600
C	-3.72318400	-2.70039100	0.66690400	O	2.84991800	-2.23114700	0.84717000
C	-2.26628200	-2.66338000	0.17401200	O	6.79230900	0.20614800	-1.66849000
O	-1.34993100	-2.41758000	1.06468400	O	7.12519400	-1.68172000	-2.80046100
O	-2.04518200	-2.83178500	-1.02451000	C	-4.29241600	1.94061900	4.72342000
C	-3.62974100	-5.65370000	-5.79117800	N	-4.60196900	2.30275600	1.75033500
C	-2.69958700	-5.67789500	-4.55966400	O	-4.47927200	3.12819700	4.31233900
C	-1.45247300	-4.79980000	-4.70004000	C	-4.09253400	0.86222900	3.62047900
C	-0.29961000	-5.18640100	-3.77162900	N	-4.17153900	3.21695600	0.69555100
O	-0.24008400	-6.26122600	-3.18606700	O	-4.27071500	1.56385200	5.90556300
N	0.70575500	-4.26869600	-3.70159400	C	-3.56373500	1.40722400	2.28813400
C	-2.32434400	-3.07807800	8.66153800	C	-5.42499300	3.89615300	0.23900100
C	-2.74986800	-2.08688100	7.57033200	C	-3.19463200	4.25068300	1.17363400
C	-1.68223800	-1.02275100	7.30093000	C	-3.58159100	2.44809900	-0.45037100
O	-0.47445700	-1.28385500	7.42806600	O	0.66257600	-1.90819300	-0.85811800
N	-2.10028300	0.18370000	6.89755400	Fe	0.65509000	-2.14389000	0.90622500
C	3.30674600	-7.75531400	1.92749600	C	4.99367900	-1.78224000	-0.08672900
C	2.88166400	-7.40379900	0.48671500	H	5.11068900	-2.86376300	0.04684200
C	1.97436000	-6.20456300	0.39834900	H	5.82060800	-1.29867200	0.44817100
N	0.89956100	-6.09451300	-0.47258800	H	-7.65546700	-3.00024500	-7.60628400
C	2.01083700	-5.00001600	1.06010600	H	-6.40501000	-1.81429200	-7.31895900
C	0.33621700	-4.88147500	-0.31939800	H	-6.23031300	-3.45346800	-6.66812600
N	0.98690400	-4.19714600	0.60593000	H	-3.00619800	-5.74336500	-6.65608200
C	8.71596600	0.29837900	0.95403800	H	-4.26567800	-6.51121500	-5.71959000
N	8.09119100	1.47873600	1.57618800	H	-4.22649600	-4.73967900	-5.86710200
C	6.75033300	1.66912400	1.62405100	H	-0.25637700	8.48951800	4.27190400
N	5.96088800	1.21260800	0.67875800	H	0.80641700	7.13582300	4.57342200
N	6.24302900	2.38033300	2.66077600	H	-0.69981000	7.28821900	5.44486900
C	11.35447300	2.61413100	-3.41615400	H	2.46692200	-8.12147500	2.48026500
N	11.03301400	1.19248500	-3.41226400	H	3.71392200	-6.89889200	2.42321700

H	4.07448100	-8.54034400	1.91451300	H	-1.76722500	5.75042100	-4.73934900
H	-0.26560800	-6.09912200	5.21442400	H	-3.46271100	5.79640600	-5.27436700
H	1.30382500	-6.03317400	5.97961200	H	-2.93035200	-2.60261100	6.61162500
H	-0.13108400	-6.19218100	6.94689500	H	-3.70094200	-1.60046900	7.82997300
H	-2.13246800	-2.52421700	9.55712300	H	-1.38233600	0.87162300	6.70370900
H	-3.06487200	-3.82524900	8.85660200	H	-3.06359200	0.48070400	6.66029700
H	-1.38888400	-3.58103100	8.40109600	H	-0.88363200	-3.96536100	6.46441300
H	-5.02479400	-3.01687400	2.37044000	H	0.76818700	-3.84211900	7.01638400
H	-3.67939300	-4.12724600	2.26998500	H	0.39444800	-4.62972300	3.12349400
H	-3.41509800	-2.49138100	2.80924800	H	0.48092300	-1.51216400	5.93994300
H	5.25690500	2.60550700	2.66340600	H	0.90418700	-0.47583900	3.58345300
H	6.71793700	2.40572400	3.55233900	H	3.77843600	-7.21601100	-0.12759500
H	4.96004800	0.96700100	0.83442700	H	2.38093900	-8.26824300	0.02572600
H	6.33439000	0.84231600	-0.23232100	H	0.62020200	-6.71816500	-1.22890600
H	8.65094300	2.02801400	2.21398800	H	2.71495500	-4.64895900	1.80359500
H	8.65938600	0.33806800	-0.13705500	H	-0.51292300	-4.50954900	-0.88701100
H	9.76148400	0.25344000	1.27374500	H	-3.39562300	0.10187100	3.99145100
H	8.66885300	-1.07708500	-3.06604900	H	-5.05655800	0.35276700	3.46217700
H	10.43727600	-1.27347600	-3.18356600	H	-2.60885900	1.92420300	2.47946000
H	8.78829300	2.43576400	-3.16009000	H	-3.36990500	0.58666300	1.58973700
H	7.89165000	1.00841700	-2.53641400	H	-4.81791100	2.90293400	2.57645700
H	11.73656700	0.56620300	-3.78073000	H	-3.66139200	4.81648700	1.98412600
H	12.41085600	2.73718200	-3.15041700	H	-2.29882900	3.75786200	1.55642600
H	10.76607800	3.14461000	-2.65845600	H	-2.92598400	4.90325200	0.33911300
H	-2.14694100	6.69586800	-2.18268500	H	-2.61142200	2.02643800	-0.17279000
H	-1.00546900	8.66841700	-1.84419600	H	-4.27592400	1.64750600	-0.71501600
H	0.28598000	4.78699100	-0.47985400	H	-3.43916500	3.13845500	-1.28567800
H	1.01316700	9.68674000	-0.86694800	H	-5.17659700	4.62438200	-0.53989500
H	2.30658100	5.81437300	0.51505400	H	-6.10772100	3.13558200	-0.14575800
H	2.69400200	8.99939400	1.50558300	H	-5.88142400	4.40250300	1.09530100
H	3.43173200	9.27757100	-0.07381700	H	-4.26046000	-3.35636000	-0.03164500
H	-8.60073300	-1.56556900	-6.08716000	H	-4.11959200	-1.69347500	0.47803400
H	-8.37230100	-3.14895000	-5.38612800	H	-3.24506700	-5.40016900	-3.64493400
H	-9.16200800	-0.90701500	-3.79370000	H	-2.35761800	-6.71066900	-4.40193800
H	-5.16434000	-2.17759300	-4.77979800	H	-1.04522900	-4.88033500	-5.72320200
H	-4.35180200	-1.27223900	-2.62355200	H	-1.69130900	-3.73593200	-4.55297000
H	-8.34936200	0.02222300	-1.66274400	H	1.45295600	-4.42212500	-3.03777400
H	-6.50205800	0.12890500	-0.22128900	H	0.55300400	-3.31237500	-3.98572300
H	0.73608400	-0.31470600	-5.12913700	H	4.72488000	-2.28247200	-2.20041900
H	1.75336100	1.92060400	-5.47659400	H	4.35090900	-0.59430600	-1.80410800
H	-1.72885700	-0.56469200	-4.82310100	O	3.50351400	-0.09599600	0.78163500
H	0.34650100	3.96464900	-5.54136200	H	11.19470000	3.04742900	-4.38134800
H	-4.77749800	3.40642100	-4.95613100	H	8.19219200	-0.56595400	1.30539500
H	-4.10024100	0.99755300	-4.73334600	H	-2.17097700	5.52004000	-6.42339200

H	3.79173900	7.82256200	0.82743300	C	-8.46143100	-2.77847800	-4.44639200
H	-1.82202300	7.26874400	3.03357100	C	-8.39213300	-1.96881800	-5.74662400
H	-0.30759100	6.54628100	2.48674300	O	-8.61959300	-2.58086300	-6.83918500
H	-3.07462400	6.13098100	4.69925900	O	-8.12088000	-0.74917100	-5.65651300
H	-3.14286000	4.40207500	4.63057400	C	-12.51898200	2.82128500	-2.81801700
O	0.76761000	-0.35006000	1.26673900	C	-12.40163800	1.87416300	-4.02929300
H	1.71253900	-0.09309100	1.11810200	C	-11.69135200	2.49498700	-5.23548500
H	-0.23344400	0.52714100	0.02138500	C	-11.98602100	1.79161000	-6.56125300
O	-0.74068200	0.79945100	-0.76991900	O	-12.87805500	0.96210700	-6.69255700
H	-0.08251100	1.18525500	-1.35485000	N	-11.21456400	2.19583300	-7.60716200
H	-0.13470000	-1.40214900	-1.10545700	C	-7.55700800	-10.11238300	-7.84976700
				C	-6.75262500	-8.98855300	-7.18519100
				C	-5.83574100	-8.24696000	-8.16249300
				O	-6.15433600	-8.09937200	-9.35524000
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				C	-13.81888400	-3.24655900	-11.39705200
				C	-13.68921100	-1.90053700	-10.66019400
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				N	-12.42706700	-1.27447600	-8.53250800
				C	-11.13649500	-2.11836700	-10.08104600
				C	-11.16267500	-1.30408800	-8.07255700
				N	-10.35734900	-1.81175300	-8.98708500
				C	-6.56288500	0.53748900	-16.69796600
				N	-5.24109100	0.10375500	-16.21975500
				C	-4.95206300	-0.08454500	-14.90943800
				N	-5.57840700	0.58686500	-13.97286300
				N	-3.96589200	-0.95941700	-14.59068800
				C	-5.29195000	5.77749400	-18.23092500
				N	-6.68596700	5.46184200	-17.94511700
				C	-7.13999600	4.90177800	-16.79773100
				N	-6.30781400	4.61445400	-15.80042500
				N	-8.43235200	4.60486500	-16.65843200
				C	-9.47984700	3.65726900	0.53561800
				C	-8.86096700	2.30706500	0.99197200
				C	-7.58186900	1.83233200	0.33443800
				C	-7.57379200	1.16021500	-0.89999400
				C	-6.35011400	1.98666000	0.99035700
				C	-6.39892500	0.63481300	-1.44242700
				C	-5.16498700	1.46823400	0.46406500
				C	-5.18662700	0.76984900	-0.74925900
				O	-4.06486300	0.21406800	-1.29089900
				C	-7.80738100	-0.28026800	-11.57195700
				C	-8.69936700	1.95155700	-12.52204200
				C	-8.42156800	2.75695700	-13.79686600

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C	-1.81314700	4.85859800	-4.44321900
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N	-5.11975000	3.45553400	-3.47285700
C	-5.40203600	3.74578300	-4.78670700
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C	-6.56930700	3.96091100	-6.86182000
C	1.83205100	-3.59051300	-9.24294300
C	0.93369600	-2.91096800	-8.20470500
C	-0.42297000	-3.60189100	-8.04464100
O	-1.37311100	-3.32901000	-8.76762900
N	-0.49947900	-4.51530900	-7.03980300
C	1.90578400	1.09637100	-11.40571700
C	1.19309400	1.33336700	-10.09562000
C	-0.20059300	1.20749400	-9.98004100
C	1.91203100	1.67025200	-8.93752600
C	-0.85872100	1.38987100	-8.76312400
C	1.27282600	1.85102300	-7.70977100
C	-0.11766000	1.69929200	-7.61667300
O	-0.79204600	1.82206300	-6.43705900
C	-10.82993900	-7.50372800	-9.60298500
C	-9.31341300	-7.35635200	-9.57597000
C	-8.77219500	-5.96066000	-9.61992200
N	-7.42939400	-5.73996000	-9.85882700
C	-9.30176200	-4.72206000	-9.35339500
C	-7.17750000	-4.43012000	-9.72460900
N	-8.29479700	-3.77660600	-9.42628600
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O	-8.45047600	-1.05628500	-10.82026400	H	-6.76671000	1.58026300	-16.43924000
O	-7.23552500	2.65057200	-14.28373700	H	-6.59141900	0.41454500	-17.78498800
O	-9.29501300	3.48746500	-14.28983800	H	-8.79678700	4.20985800	-15.74710900
C	-3.66417500	-6.01282200	-4.88570500	H	-9.05667100	4.66032800	-17.44979800
N	-3.01522900	-3.11488600	-4.38410000	H	-5.36236900	4.96252700	-15.79426600
O	-2.84804300	-5.46266700	-5.68903800	H	-6.63107700	3.90160600	-15.08761100
C	-4.03502200	-5.17974700	-3.62795300	H	-7.38033900	5.85589000	-18.56603200
N	-3.10064100	-1.93292000	-5.23554700	H	-5.14793500	5.78165200	-19.31760000
O	-4.19483900	-7.12841300	-5.00635300	H	-4.63012500	5.00619800	-17.81969000
C	-4.28893400	-3.69739700	-3.94439700	H	-0.18472000	2.08487700	-5.73989600
C	-1.68812700	-1.44956800	-5.34461600	H	1.85910900	2.10446500	-6.82250500
C	-3.64728000	-2.22116900	-6.60997300	H	-1.94104800	1.28613600	-8.69314300
C	-3.92835400	-0.87479100	-4.57912400	H	2.99662700	1.78809900	-8.98822000
O	-8.25007700	-0.15903900	-8.16881900	H	-0.79388700	0.95143200	-10.86046400
Fe	-8.26085100	-1.79564000	-8.80271100	H	2.57779200	0.22685800	-11.34056300
C	-8.60958400	0.40832200	-12.69503100	H	2.52757600	1.95992700	-11.68639700
H	-9.61454700	-0.02611200	-12.74339100	H	-8.66090900	2.37333300	2.07104700
H	-8.10950100	0.16239000	-13.64136200	H	-9.62321700	1.51859100	0.89352800
H	-9.88854600	4.08502000	1.42769300	H	-6.31156900	2.50309000	1.95169500
H	-8.78344300	4.34234900	0.09916700	H	-8.51037600	1.01078700	-1.44141000
H	-10.28952100	3.51083300	-0.18743800	H	-6.42525700	0.09574600	-2.38750100
H	-12.81325300	3.77759100	-3.19763100	H	-4.22689500	1.59077200	1.01148300
H	-13.29211200	2.43457400	-2.18766000	H	-3.33239100	0.29706700	-0.67297900
H	-11.58333800	2.92768000	-2.25929400	H	-7.46848200	3.83315000	-7.46693300
H	2.83131300	-3.21088600	-9.19428600	H	-5.44619100	4.83423300	-8.49709700
H	1.46511500	-3.50121600	-10.24412100	H	-7.46344700	3.11012400	-5.07737700
H	1.90894400	-4.66866700	-9.03182900	H	-3.36436200	5.14111900	-7.17949500
H	-14.00782900	-4.04578000	-10.71116200	H	-3.39799500	3.65415100	-2.21131200
H	-12.92712100	-3.45468500	-11.95044900	H	-5.74897500	3.01858700	-2.81460400
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H	-11.30564300	-6.91753800	-8.84458400	H	-1.20843300	4.57644000	-3.57020900
H	-11.24200000	-7.25305200	-10.55816300	H	-7.42091200	-8.22864700	-6.74513000
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H	-8.37288000	-4.77034700	-3.64586500	H	-8.86399900	-7.93208100	-10.39742900
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H	-3.74638400	-1.73343400	-15.20198700	H	-13.69234800	-1.07872800	-11.39542400
H	-5.67929700	0.26296700	-12.98889500	H	-14.57099200	-1.73437200	-10.02383000
H	-6.22061700	1.39467800	-14.17365000	H	-13.16875400	-0.79291600	-8.02944900
H	-4.60548900	-0.30435000	-16.89118900	H	-10.70097100	-2.53553300	-10.98047100

H	-10.87165600	-0.94256600	-7.09511800	C	-4.10491200	4.39400300	-3.65746600
H	-4.92947500	-5.61090500	-3.16313000	C	-1.87401700	4.27889500	-3.94920600
H	-3.21590100	-5.25929600	-2.89479600	N	-3.79152600	3.08982300	-3.98380700
H	-5.07615700	-3.63914400	-4.71407400	C	-2.43269900	2.98602100	-4.16877500
H	-4.65558900	-3.17428600	-3.04926000	C	-0.48113200	4.45129800	-4.08301600
H	-2.61284100	-3.86035400	-4.99266000	C	-1.64038400	1.87866800	-4.50904100
H	-2.98783300	-2.92269800	-7.12725600	C	0.30640400	3.35669700	-4.42553700
H	-4.64741200	-2.64506100	-6.51344600	C	-0.26921200	2.08351400	-4.63661300
H	-3.70287400	-1.28461900	-7.16864200	C	-0.59779600	5.55253900	6.73716700
H	-4.98134200	-1.15368100	-4.63373200	C	-1.32051200	5.12897900	5.45298200
H	-3.61577300	-0.77069000	-3.53844100	C	-1.44571700	3.61099100	5.29885900
H	-3.78080000	0.06530800	-5.11746400	O	-0.58032300	2.94895700	4.73677100
H	-1.64864800	-0.56803700	-5.98792100	N	-2.58038900	3.06294900	5.80609900
H	-1.33625400	-1.21494900	-4.33669800	C	2.52284800	7.98035300	3.41777400
H	-1.08935000	-2.26155500	-5.76300500	C	1.43111900	7.45322600	2.51519300
H	-9.29414000	-2.35415200	-3.86169900	C	1.54617600	6.19921100	1.89307200
H	-7.56048500	-2.51564100	-3.87568700	C	0.25811600	8.18764700	2.27914100
H	-11.90537500	0.93169700	-3.74987800	C	0.53536200	5.68127200	1.08333200
H	-13.41360400	1.59149200	-4.35161800	C	-0.76717600	7.68411200	1.47589200
H	-12.01737500	3.54100600	-5.36994700	C	-0.63610500	6.42040000	0.88313500
H	-10.60162000	2.54004500	-5.08270200	O	-1.61884100	5.85748400	0.12473800
H	-11.31063100	1.73158500	-8.50009100	C	0.56240800	-7.35842200	3.95727500
H	-10.39550500	2.76904800	-7.47118000	C	0.36709400	-5.97850500	4.57112400
H	-9.68428100	2.23456900	-12.13203400	C	0.66327700	-4.80581000	3.68957800
H	-7.94413400	2.28152600	-11.79302700	N	0.74939800	-3.53509300	4.22352000
O	-6.57839000	-0.01430300	-11.49281100	C	0.77925800	-4.63798600	2.33177800
H	-5.02341300	6.74016800	-17.84881700	C	0.89269400	-2.65688800	3.22091500
H	-7.30296300	-0.08970600	-16.24653200	N	0.92588500	-3.29143100	2.05417000
H	-1.80098700	5.92622700	-4.51132800	C	-3.87531500	-3.83776100	1.05701100
H	1.21897300	0.91536400	-12.20596300	C	-3.67832200	-2.96024700	-0.17956700
H	1.45809100	-2.88271700	-7.23692200	C	-2.24271900	-2.55089200	-0.54374700
H	0.73284000	-1.87361000	-8.49543500	O	-1.31279000	-2.86070900	0.27323300
H	0.30872100	-4.74155600	-6.47908600	O	-2.07865800	-1.92444300	-1.61111100
H	-1.36901500	-5.01387600	-6.81554400	C	-3.47296000	-3.64750800	-7.24265100
O	-6.49518100	-1.97293900	-8.76281100	C	-2.53887900	-4.02363400	-6.07545300
H	-6.03754800	-1.09532500	-8.75812000	C	-1.36342700	-3.06342500	-5.87493200
H	-5.66451700	0.30981700	-10.01149400	C	-0.19927000	-3.66563800	-5.08495500
O	-5.25109200	0.40941800	-9.12521800	O	-0.08283000	-4.86797400	-4.87997600
H	-5.81336600	1.05287300	-8.68210900	N	0.74014400	-2.76684700	-4.67808000
H	-8.15119600	-0.23607000	-7.15648600	C	-2.14521100	-5.84706600	7.26994800
				C	-2.64548500	-4.58518200	6.55539800
				C	-1.66229600	-3.41531700	6.65168100
⁵TS_{3W}				O	-0.43462000	-3.61018600	6.67647600
C	-2.87280500	6.63572800	-3.33074200	N	-2.18935100	-2.18562200	6.68843600
C	-2.96638400	5.16609600	-3.61978200				

C	3.63827000	-7.79542500	-0.58425300	C	5.11920900	-1.58734000	-0.88904800
C	3.19405800	-6.99936900	-1.82933000	H	5.15347500	-2.68240000	-0.90384600
C	2.23429400	-5.87712600	-1.52800300	H	5.87806500	-1.25836400	-0.16530400
N	1.09256500	-5.61102100	-2.26622700	H	-7.64268900	-0.75202800	-8.12118300
C	2.25406500	-4.89997400	-0.55829700	H	-6.44901300	0.33692900	-7.45627200
C	0.47890100	-4.53177800	-1.74336100	H	-6.16065100	-1.38624600	-7.40617900
N	1.15744600	-4.07815600	-0.70549100	H	-2.85486200	-3.41970700	-8.08593500
C	8.63527000	0.39625100	1.14662600	H	-4.06520500	-4.51216700	-7.45775400
N	7.85622400	1.34564800	1.95317100	H	-4.11606800	-2.78874300	-7.02259500
C	6.52204900	1.52183400	1.81573000	H	-0.69320900	6.60699200	6.89224600
N	5.91623500	1.24952400	0.68463200	H	0.43782200	5.28347800	6.74379800
N	5.83284300	2.02788400	2.86951700	H	-1.05775400	5.07043300	7.61350000
C	11.11140800	4.13490600	-2.21705400	H	2.82312700	-8.36259300	-0.18571100
N	11.03070600	2.76841200	-2.71774700	H	4.00794800	-7.12735900	0.16544900
C	9.90145400	2.02267000	-2.77600400	H	4.44207700	-8.49507300	-0.84955700
N	8.72241200	2.54338000	-2.44464400	H	0.02327100	-7.47729300	3.04060100
N	9.95704000	0.74198100	-3.14132300	H	1.59544200	-7.58558300	3.79524800
C	-6.93039000	-0.61065600	-7.33474900	H	0.17889900	-8.11780800	4.65303300
C	-7.77537900	-0.74382000	-6.03840100	H	-1.97154800	-5.60551200	8.29812100
C	-7.39973500	0.06963900	-4.81731700	H	-2.84619000	-6.65294600	7.20697700
C	-6.31585000	-0.26789700	-3.98814500	H	-1.18945300	-6.18871700	6.86237000
C	-8.19756700	1.15563900	-4.42338000	H	-4.91075900	-3.87904800	1.32411000
C	-6.05936400	0.42038000	-2.80012400	H	-3.51356000	-4.82809700	0.87634300
C	-7.95682600	1.85590100	-3.23918300	H	-3.32339500	-3.43700700	1.91610500
C	-6.89639700	1.47618900	-2.40842400	H	4.84454800	2.21494500	2.76422600
O	-6.64148100	2.10205500	-1.22251100	H	6.16584400	1.89268400	3.81398600
C	3.75600800	-1.13992700	-0.33017300	H	4.90455600	1.05710000	0.59665000
C	5.43838900	-1.01752700	-2.29966700	H	6.41837200	1.01097000	-0.21218100
C	6.79740900	-0.32293700	-2.43878200	H	8.28870400	1.73481800	2.77941000
O	2.93689800	-2.02954900	-0.02114800	H	8.70492100	0.71056000	0.10155400
O	7.01235300	0.67493500	-1.65528000	H	9.63838100	0.32490800	1.57812100
O	7.61015700	-0.69276400	-3.29990100	H	9.06921100	0.17556600	-3.24581200
C	-4.58199600	-0.40635000	4.98629800	H	10.84795200	0.27432200	-3.22435300
N	-4.47915300	1.55758000	2.70185800	H	8.59703600	3.53957600	-2.36024300
O	-3.74996700	0.54950000	5.08817300	H	7.94439100	1.87023800	-2.20202200
C	-5.57514400	-0.30818400	3.79576000	H	11.84861800	2.39937300	-3.18445300
N	-3.37354200	2.02565900	1.87109400	H	12.12023400	4.30745100	-1.82419400
O	-4.67471800	-1.39790300	5.72616100	H	10.40979800	4.27964800	-1.38717000
C	-4.90947000	0.16857500	2.49532900	H	-2.33800800	6.48307700	0.00124300
C	-3.31270100	3.49903800	2.12874700	H	-1.67394400	8.27344400	1.31715700
C	-2.05231200	1.39281300	2.22251300	H	0.64018100	4.70673600	0.60579400
C	-3.66856800	1.79621900	0.42311400	H	0.13212500	9.17088300	2.73744800
O	0.51880700	-1.40814700	-1.39055100	H	2.44850900	5.60380000	2.04835500
Fe	0.72460500	-2.25378100	0.26192200	H	2.16139200	8.11647500	4.44806500

H	2.89818200	8.95570800	3.07358200	H	-4.10358800	-3.43701500	-1.07626200
H	-8.81505300	-0.48470000	-6.28519300	H	-4.23652900	-2.01877700	-0.07639500
H	-7.81109300	-1.80751800	-5.75359200	H	-3.10291100	-4.11728600	-5.13416600
H	-9.04747000	1.45234100	-5.04149700	H	-2.11979200	-5.02097400	-6.27013900
H	-5.67057100	-1.10842400	-4.25171300	H	-0.94243200	-2.76796300	-6.85168000
H	-5.23171000	0.11883100	-2.16096800	H	-1.68590800	-2.12919000	-5.39081800
H	-8.61198200	2.68293700	-2.95354500	H	1.48180900	-3.08335900	-4.06769800
H	-7.34624700	2.72778400	-1.02958100	H	0.53544100	-1.77917200	-4.65141300
H	0.37676700	1.24723900	-4.90855500	H	5.37477400	-1.80910200	-3.05558300
H	1.38498300	3.48009900	-4.53711100	H	4.69278500	-0.25116300	-2.56011700
H	-2.08495100	0.89609300	-4.66698600	O	3.57491800	0.11523700	-0.21788900
H	-0.02507700	5.42947100	-3.92338600	H	10.92049600	4.84986100	-2.98988100
H	-5.13783300	4.67965400	-3.47960000	H	8.15825300	-0.56030500	1.19470000
H	-4.45884900	2.33557900	-4.06245300	H	-2.57113000	7.18331600	-4.19900200
H	-2.13047100	6.84126600	-2.54826400	H	3.34663800	7.29799900	3.44305700
H	-3.83881000	7.04195700	-3.00068600	H	-2.32049200	5.58984600	5.43413200
H	-2.80541400	-4.77307000	5.47992700	H	-0.77794700	5.49489300	4.57414900
H	-3.62455600	-4.27690300	6.94716400	H	-3.26873500	3.63351800	6.27473400
H	-1.54102700	-1.40770100	6.67822600	H	-2.79216900	2.06084400	5.72220100
H	-3.18121100	-1.95223500	6.48438600	O	0.55953800	-0.83806200	1.14940700
H	-0.67727500	-5.87498700	4.89323000	H	0.82323800	0.20170400	0.41312100
H	0.96288300	-5.88764300	5.49042400	H	2.13740300	0.68299100	-0.37277300
H	0.73608300	-5.38367400	1.54910400	O	1.13706200	0.86145900	-0.44010800
H	0.52524700	-3.33807700	5.21631800	H	0.86131400	0.14672200	-1.10718200
H	0.94280000	-1.58075300	3.34076800	H	-0.44637300	-1.53133700	-1.62009400
H	4.08196400	-6.57993200	-2.33095600				
H	2.73205800	-7.67792100	-2.56166900				
H	0.80690500	-6.01246600	-3.15644500				
H	2.98669400	-4.72442000	0.21971600				
H	-0.43033500	-4.10060700	-2.14418200				
H	-6.03614300	-1.28912100	3.63058600				
H	-6.38369800	0.38992900	4.06735700				
H	-4.07256300	-0.51222600	2.26801800				
H	-5.62258500	0.11467000	1.66030700				
H	-4.09825500	1.54154100	3.67275900				
H	-1.78570600	1.64756200	3.25211800				
H	-2.13344000	0.31155900	2.10531900				
H	-1.29367300	1.77715000	1.53732300				
H	-3.56792700	0.73357600	0.19977800				
H	-4.68386900	2.13333100	0.20616000				
H	-2.94335500	2.35750700	-0.17261500				
H	-2.48560000	3.93881000	1.56747300				
H	-4.26765900	3.93176900	1.82017000				
H	-3.17187800	3.64606200	3.20151300				
				5_{2w}			
				C	-1.81316700	4.85853000	-4.44310200
				C	-3.21583700	4.36380100	-4.23422900
				C	-3.73109600	3.72704500	-3.12749200
				C	-4.32100600	4.52003300	-5.15286600
				N	-5.07869900	3.47538200	-3.30232600
				C	-5.47117000	3.95432000	-4.53111700
				C	-4.45087700	5.09341200	-6.43455900
				C	-6.72941500	3.95318300	-5.15306500
				C	-5.69683800	5.09502700	-7.05263700
				C	-6.82507500	4.53141600	-6.41564900
				C	1.83202800	-3.59044500	-9.24294700
				C	0.94940800	-2.86843500	-8.21382500
				C	-0.30023900	-3.65232200	-7.79914600
				O	-1.37935600	-3.49102800	-8.36127500
				N	-0.12069100	-4.50795500	-6.76228600
				C	1.90586300	1.09645600	-11.40578300
				C	1.20791700	1.29046700	-10.07923300

C	-0.18318700	1.15707000	-9.94054600	N	-6.28003000	4.57979500	-15.80161800
C	1.94630900	1.59910300	-8.92507400	N	-8.41450700	4.58612600	-16.63450000
C	-0.82008800	1.30572600	-8.70631800	C	-9.47973000	3.65734700	0.53556200
C	1.32945600	1.74500500	-7.68193100	C	-8.80227600	2.37981900	1.06856900
C	-0.05858700	1.58770900	-7.56625500	C	-7.98598100	1.49035400	0.15194500
O	-0.70598800	1.67978800	-6.36638600	C	-8.16336700	1.42728700	-1.23841600
C	-10.82982300	-7.50329900	-9.60304800	C	-7.05175400	0.60833000	0.72368200
C	-9.31245000	-7.39329700	-9.58533800	C	-7.45854300	0.51341600	-2.02849700
C	-8.75015000	-6.01105900	-9.66266100	C	-6.33423300	-0.30603400	-0.04724500
N	-7.40687500	-5.80469300	-9.90581300	C	-6.54520700	-0.36200500	-1.43046800
C	-9.27227500	-4.76562800	-9.41781900	O	-5.86999500	-1.23438300	-2.23854900
C	-7.14799900	-4.49334600	-9.78863900	C	-7.76220200	-0.26327600	-11.51093100
N	-8.26138200	-3.82956800	-9.50289300	C	-8.66092600	1.95504500	-12.47952000
C	-8.60429300	-4.29647000	-4.57697100	C	-8.38860700	2.74346900	-13.76657300
C	-8.47027500	-2.77537200	-4.46128100	O	-8.42184200	-0.98031500	-10.70545700
C	-8.46635600	-1.93824800	-5.74858200	O	-7.20766900	2.62472400	-14.26312700
O	-8.52153300	-2.54409800	-6.86961400	O	-9.26150300	3.47472900	-14.25901800
O	-8.39921400	-0.69514000	-5.62093900	C	-3.23781000	-5.84655200	-5.18768100
C	-12.51902900	2.82123200	-2.81809300	N	-3.63290800	-2.94345300	-4.43606800
C	-12.40284400	1.86672700	-4.02433200	O	-2.19192100	-5.17153200	-4.93259200
C	-11.69416400	2.47358400	-5.23868500	C	-4.57399700	-5.05443700	-5.15124500
C	-11.99153200	1.75463300	-6.55597800	N	-3.07411200	-1.63044700	-4.75210500
O	-12.91916700	0.96548700	-6.69052700	O	-3.29335200	-7.05862900	-5.44643300
N	-11.18472100	2.10635000	-7.59521900	C	-4.43315200	-3.56897900	-5.50101600
C	-7.55707800	-10.11222900	-7.84985100	C	-2.47993700	-1.13666900	-3.46925200
C	-6.73466500	-8.99301900	-7.19691600	C	-2.00556900	-1.68466400	-5.80511600
C	-5.81498100	-8.29090600	-8.19963100	C	-4.16718600	-0.69412200	-5.17353000
O	-6.14764700	-8.16651300	-9.38928900	O	-8.25618500	0.12484500	-8.07458000
N	-4.65644800	-7.79976900	-7.73966500	Fe	-8.22369600	-1.85961200	-8.82460300
C	-13.81896800	-3.24655400	-11.39705700	C	-8.57939200	0.40829700	-12.63274600
C	-13.67008500	-1.90384800	-10.65013100	H	-9.58721400	-0.02094200	-12.65885400
C	-12.42854400	-1.80387300	-9.79968400	H	-8.09387800	0.14608100	-13.58210900
N	-12.41687300	-1.31297700	-8.50460700	H	-9.88861200	4.08493100	1.42770600
C	-11.11152100	-2.10828600	-10.06355100	H	-8.78346000	4.34237100	0.09917400
C	-11.15218500	-1.34286100	-8.03987700	H	-10.29176300	3.45534600	-0.17047400
N	-10.33473800	-1.82011600	-8.96072800	H	-12.81330300	3.77756800	-3.19765100
C	-6.56285800	0.53747700	-16.69787100	H	-13.29208600	2.43459200	-2.18761700
N	-5.24041600	0.09558800	-16.22974100	H	-11.58578700	2.92827100	-2.25716900
C	-4.94262000	-0.10635400	-14.92378300	H	2.83132600	-3.21092100	-9.19428000
N	-5.56773400	0.54871600	-13.97508500	H	1.46512400	-3.50124000	-10.24412700
N	-3.94888000	-0.97970000	-14.62305800	H	1.90062100	-4.66484800	-9.01545500
C	-5.29192100	5.77747600	-18.23089400	H	-14.00775100	-4.04579600	-10.71115900
N	-6.68198100	5.45626500	-17.93072200	H	-12.92709900	-3.45464200	-11.95043000
C	-7.12350300	4.88283400	-16.78501700	H	-14.65826700	-3.19647900	-12.10348100

H	-11.30569300	-6.91770100	-8.84448900	H	-1.15560200	4.56737600	-3.61262000
H	-11.24204100	-7.25320200	-10.55818500	H	-7.38933400	-8.21606400	-6.76638700
H	-11.11099000	-8.54864000	-9.41053300	H	-6.14106700	-9.38163100	-6.35713500
H	-6.87262500	-10.81098600	-8.28452400	H	-4.06752700	-7.32058100	-8.41058800
H	-8.19107000	-10.62065400	-7.15393100	H	-4.32724800	-7.75060800	-6.75957000
H	-8.17542100	-9.73051800	-8.66646500	H	-8.93164600	-7.84058200	-8.65807300
H	-8.37275700	-4.77041000	-3.64592600	H	-8.88330000	-7.99774300	-10.39698700
H	-9.59587100	-4.56322600	-4.87657600	H	-10.28702100	-4.49097500	-9.16053500
H	-7.91769400	-4.69345400	-5.33320500	H	-6.73040300	-6.58566100	-9.96221800
H	-3.67157100	-1.08938400	-13.65643200	H	-6.16501700	-4.04615600	-9.88788000
H	-3.72919900	-1.74436000	-15.24595200	H	-13.66363900	-1.07942800	-11.38231900
H	-5.64834300	0.22196700	-12.99103800	H	-14.55117500	-1.72953000	-10.01503700
H	-6.20825500	1.36286700	-14.16106200	H	-13.16369700	-0.83989700	-8.00081700
H	-4.60326900	-0.29539700	-16.90979000	H	-10.67133100	-2.50306200	-10.97121600
H	-6.76166800	1.57923700	-16.43156700	H	-10.87061600	-1.00132700	-7.05164500
H	-6.59779300	0.42080700	-17.78538900	H	-5.28175100	-5.51365400	-5.85088100
H	-8.77193500	4.19040500	-15.72044700	H	-5.01104600	-5.16198500	-4.14567200
H	-9.04957700	4.65881900	-17.41586000	H	-3.96031500	-3.48918500	-6.49448600
H	-5.33703300	4.93448500	-15.79540500	H	-5.42194900	-3.10323900	-5.55837600
H	-6.60067000	3.87156500	-15.08420000	H	-2.82119200	-3.59559900	-4.36111100
H	-7.38393500	5.85751600	-18.53843000	H	-1.21803000	-2.35688800	-5.45459000
H	-5.15921100	5.78463100	-19.31901100	H	-2.41810900	-2.08463300	-6.73382700
H	-4.62320600	5.00779000	-17.82801800	H	-1.61448200	-0.67798000	-5.97342900
H	-0.09089500	1.98140700	-5.69177600	H	-4.56446500	-1.01850500	-6.13546500
H	1.93214600	1.97521500	-6.79938900	H	-4.94646600	-0.71876500	-4.40932300
H	-1.90191300	1.20221900	-8.61873100	H	-3.74546000	0.30937200	-5.27486300
H	3.02941500	1.72167300	-8.99196200	H	-2.00989300	-0.16375200	-3.64294500
H	-0.79228300	0.92581100	-10.81711700	H	-3.28392400	-1.05191200	-2.73620400
H	2.60102200	0.24399600	-11.36518400	H	-1.73409000	-1.86207100	-3.12994300
H	2.50286300	1.98130500	-11.67409500	H	-9.26965700	-2.35939100	-3.82872900
H	-8.15549900	2.67244000	1.91105600	H	-7.54164500	-2.50524800	-3.94114000
H	-9.58661800	1.74915200	1.52382600	H	-11.90720800	0.92643700	-3.73726900
H	-6.88397900	0.62809100	1.80280400	H	-13.41578500	1.58364900	-4.34328100
H	-8.88189600	2.08691600	-1.72471600	H	-12.02320800	3.51683500	-5.38715700
H	-7.63735000	0.44395800	-3.10067100	H	-10.60482700	2.52203500	-5.08790100
H	-5.61571100	-0.97764400	0.42901200	H	-11.27679900	1.60847700	-8.47055100
H	-5.50938900	-1.96496100	-1.72735600	H	-10.30829200	2.58264700	-7.44109300
H	-7.79050900	4.55449700	-6.92393000	H	-9.64210600	2.24677000	-12.08701400
H	-5.80975300	5.53954600	-8.04281000	H	-7.90154200	2.29457100	-11.75930700
H	-7.60083300	3.51996700	-4.66298200	O	-6.52864400	-0.04442200	-11.46882400
H	-3.58696000	5.53367000	-6.93465200	H	-5.02344800	6.74018500	-17.84883400
H	-3.23635000	3.44154000	-2.20217800	H	-7.30299500	-0.08970000	-16.24657800
H	-5.67955200	3.02310200	-2.62940500	H	-1.80094800	5.92621500	-4.51149500
H	-1.38356100	4.46429900	-5.37357600	H	1.21891700	0.91528300	-12.20589600

H	1.54792100	-2.64907800	-7.31603800	C	-3.87800800	-0.11472200	-0.35607800
H	0.60944100	-1.90679600	-8.61390500	O	-3.44107900	-1.33049000	-0.35971400
H	0.78145800	-4.58446400	-6.31585600	O	-3.32558500	0.82008000	-0.94236500
H	-0.91194400	-4.94952400	-6.26836900	C	-5.89842000	2.44030000	-6.25826600
O	-6.61149900	-1.91427200	-8.74185800	C	-5.31455800	1.21370500	-5.53820100
H	-5.55986800	-0.26324700	-8.69794900	C	-3.85454100	1.39288300	-5.09329300
H	-5.85456400	0.62905600	-9.84224700	C	-3.12242100	0.06995100	-4.84962700
O	-5.65025500	0.68279500	-8.88935200	O	-3.15178900	-0.83739300	-5.66825400
H	-7.36419500	0.49299000	-8.27945000	N	-2.37566800	0.00360300	-3.70932900
H	-8.27949900	-0.03839900	-7.07989400	C	-5.32711700	-5.96689100	5.83337100

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C	1.55117200	7.69346800	-0.06674300	C	-3.37326500	-4.33144700	5.66784200
C	0.70566400	6.66330100	-0.76252900	O	-2.62033300	-5.28691300	5.42272900
C	-0.66546500	6.65655100	-0.88500200	N	-2.88469400	-3.10590100	5.92163400
C	1.17651500	5.53341400	-1.53245900	C	-2.79063900	-7.34868300	-3.68452500
N	-1.07400000	5.60298200	-1.67644600	C	-2.66677500	-6.04597100	-4.49205500
C	0.02879400	4.89455100	-2.08952800	C	-2.75312200	-4.82783000	-3.62412100
C	2.45325000	5.00117700	-1.80995800	N	-3.86372800	-4.00843400	-3.55544600
C	0.12850900	3.75397400	-2.90140900	C	-1.89443900	-4.32658300	-2.67558100
C	2.55413900	3.86741300	-2.61316500	C	-3.65320100	-3.07040900	-2.60750100
C	1.40230900	3.25092900	-3.15427400	N	-2.46710800	-3.24141000	-2.05125900
C	3.25625500	1.39767100	8.00517200	C	6.45109500	-5.16866100	-1.46937200
C	2.42313800	2.10278400	6.92473100	N	6.51614600	-4.54394300	-0.13440400
C	1.63357100	1.17426100	6.00716100	C	5.45356900	-3.90023000	0.41173100
O	1.93962500	1.07493400	4.81330200	N	4.59511300	-3.26762400	-0.35486200
N	0.61724100	0.48149600	6.54661500	N	5.31346700	-3.91602100	1.75861800
C	6.96300500	2.71588100	4.66288800	C	10.52732300	-2.54012400	-4.27973600
C	6.65840600	3.75032500	3.60129200	N	9.33030100	-3.07424900	-4.92304100
C	6.84557600	3.48155700	2.23485700	C	8.05327300	-2.73311100	-4.61807300
C	6.19978900	5.03218000	3.94660500	N	7.77637500	-1.96147300	-3.56928200
C	6.59325500	4.44093700	1.25259900	N	7.03982600	-3.20029100	-5.34690500
C	5.94116500	6.00457500	2.97761200	C	-6.52346500	6.59623500	-4.38184800
C	6.14000400	5.71602900	1.61880800	C	-7.07298400	6.45187700	-2.94235600
O	5.90626300	6.61625700	0.62738200	C	-6.10585700	5.97985100	-1.87261500
C	-4.50598300	-7.18875200	1.54106700	C	-5.55118300	4.68674700	-1.88056700
C	-3.69703200	-6.39174200	2.55542500	C	-5.76007300	6.81619700	-0.80020200
C	-2.76020200	-5.36410800	2.00468900	C	-4.69891800	4.23976300	-0.86961900
N	-1.84786200	-4.72775600	2.82546100	C	-4.91448300	6.38626900	0.22770200
C	-2.65922700	-4.72954600	0.79304300	C	-4.38298800	5.09063200	0.20142400
C	-1.26087700	-3.73806300	2.13491300	O	-3.55891200	4.61275700	1.17628300
N	-1.72321200	-3.71563400	0.88924800	C	1.29787000	-2.45664500	-1.33652800
C	-5.74867500	-0.95104100	1.32837200	C	2.98424900	-1.57830600	-3.09293400
C	-5.19037300	0.13658100	0.39477200	C	4.34612900	-2.04084100	-3.62616900
				O	0.05100800	-2.20714700	-1.50955400

O	5.25534700	-2.24535500	-2.73752700	H	6.05788100	-2.83548900	-5.18716700
O	4.53178800	-2.20231900	-4.84191700	H	7.20749400	-3.84430900	-6.10578200
C	-2.25169100	-0.10195500	4.43597400	H	8.50734700	-1.48923800	-3.06241600
N	-0.22491700	1.69172000	2.73960600	H	6.78155300	-1.95985800	-3.20993800
O	-1.05644100	-0.49252400	4.58125900	H	9.47083000	-3.49690200	-5.83152800
C	-2.48472200	1.01959100	3.38760700	H	11.34897000	-3.25154500	-4.41980500
N	0.86111800	1.83586300	1.77822900	H	10.37506000	-2.42988800	-3.20020400
O	-3.26396700	-0.48476200	5.04645400	H	5.65612900	7.46460000	1.00539300
C	-1.46870700	1.15950200	2.26773700	H	5.58714000	6.99301500	3.28188000
C	1.75297700	2.91999100	2.31596800	H	6.75088300	4.22043500	0.19639300
C	1.63659200	0.54873700	1.64666000	H	6.04182500	5.28491300	4.99742400
C	0.34052500	2.24929000	0.43323800	H	7.20485500	2.49735700	1.92453000
Fe	-1.59342000	-2.06323900	-0.37082300	H	6.13711700	2.61841400	5.38054400
C	2.08660600	-2.76014300	-2.62584600	H	7.86030400	2.99294400	5.23844500
H	1.39624700	-3.03867900	-3.42961700	H	-7.47089000	7.42769400	-2.62684900
H	2.70269400	-3.64436400	-2.40585100	H	-7.94442400	5.77618500	-2.96131400
H	-7.20714000	7.23513300	-4.90173500	H	-6.17078900	7.82701400	-0.74945600
H	-5.54959900	7.03915000	-4.38532100	H	-5.80648200	3.99620200	-2.68519600
H	-6.46478000	5.63518400	-4.90405500	H	-4.29146400	3.22851700	-0.88605200
H	-5.34238900	2.60127500	-7.15836400	H	-4.67871700	7.06221200	1.05407900
H	-6.92493300	2.26097700	-6.50052000	H	-3.48342500	5.26216300	1.88144700
H	-5.83846900	3.34721700	-5.64535000	H	1.50989100	2.36918600	-3.78786500
H	3.88484200	2.12958800	8.46813100	H	3.53806600	3.45276000	-2.84084300
H	3.86104700	0.61269400	7.60136700	H	-0.75605000	3.27697200	-3.32167300
H	2.62291900	0.95727700	8.78806100	H	3.35082100	5.47292600	-1.40870300
H	-3.74789300	-7.44901600	-3.21705200	H	-1.39674100	7.34657000	-0.47406900
H	-2.02310000	-7.40497500	-2.94108100	H	-2.03621800	5.37032300	-1.87613300
H	-2.66567900	-8.21447700	-4.35178600	H	2.29413300	7.23365700	0.60041000
H	-5.05384600	-6.57873900	0.85360300	H	0.93676900	8.37817000	0.53237500
H	-3.88772000	-7.87209200	0.99736000	H	-5.26819900	-4.07628600	4.72425300
H	-5.24577600	-7.79894700	2.07814400	H	-5.32896500	-3.87394100	6.46302800
H	-4.96674100	-6.32828900	6.77417200	H	-1.88234200	-2.99369400	5.82132600
H	-6.38653500	-6.10661300	5.78024300	H	-3.37731700	-2.20962200	5.80063300
H	-4.86782900	-6.59981100	5.06828500	H	-4.38738300	-5.85861800	3.22166300
H	-6.53701500	-0.49961200	1.89396200	H	-3.13552900	-7.07621000	3.20708000
H	-6.13629300	-1.77943000	0.77374600	H	-3.20644300	-4.91191900	-0.12289900
H	-4.99095500	-1.31818500	2.02942700	H	-1.78818200	-4.92252600	3.83905200
H	4.58786600	-3.35582100	2.18623800	H	-0.55122500	-3.03265200	2.55146600
H	5.69437700	-4.67120400	2.31154400	H	-1.70547700	-6.03383900	-5.02667500
H	3.63701800	-2.98360800	-0.06835000	H	-3.44271000	-6.00143700	-5.27026800
H	4.87502900	-2.92116800	-1.31092000	H	-4.66323700	-4.04089000	-4.17455300
H	7.25467600	-4.82863300	0.49440300	H	-0.91020300	-4.68627400	-2.39944800
H	6.60063700	-4.44103600	-2.27171600	H	-4.36332000	-2.29624500	-2.34653300
H	7.20615200	-5.95856200	-1.52568300	H	-3.47503900	0.87876200	2.94521200

H	-2.53144600	1.97111200	3.94410200	C	1.07405700	3.41538700	-3.34432100
H	-1.31194500	0.10790600	1.72287200	C	3.25597000	1.39833100	8.00521100
H	-1.88412600	1.77923700	1.46625700	C	2.47202500	2.17082000	6.93494600
H	0.14009700	1.14664100	3.53418200	C	1.63213700	1.41097900	5.91725100
H	2.02609600	0.30113600	2.63764200	O	1.71590800	1.73967100	4.72384900
H	0.95508300	-0.22581800	1.28071900	N	0.79873600	0.45332100	6.34053600
H	2.45046500	0.70912700	0.93253700	C	6.96251000	2.71718200	4.66290200
H	-0.22867700	1.42519400	-0.00005000	C	6.61649700	3.73714200	3.59935100
H	-0.28345100	3.13776300	0.55127400	C	6.79566100	3.46351000	2.23268200
H	1.19877000	2.48473800	-0.20181300	C	6.12860900	5.00910800	3.94074800
H	2.58975400	3.05876600	1.62511900	C	6.50842200	4.40891400	1.24661700
H	1.16317200	3.83707800	2.39119300	C	5.83493600	5.96766800	2.96779500
H	2.10671100	2.59987600	3.30009800	C	6.02653100	5.67450200	1.60894100
H	-5.93546800	0.38830400	-0.37858500	O	5.75756300	6.56071200	0.61347700
H	-5.04310700	1.07637100	0.94454200	C	-4.50471200	-7.18950200	1.54106700
H	-5.93113000	0.95305300	-4.66162300	C	-3.69776100	-6.40080200	2.56308900
H	-5.35978100	0.34936000	-6.21726600	C	-2.73441600	-5.39760300	2.01597200
H	-3.28513800	1.88462300	-5.90005200	N	-1.81972300	-4.76784900	2.83897900
H	-3.78675600	2.05267900	-4.21767900	C	-2.60781600	-4.78530300	0.79582500
H	-1.90532700	-0.87707000	-3.54008500	C	-1.20662900	-3.80199600	2.14028600
H	-2.60354000	0.54405800	-2.87504600	N	-1.65469000	-3.78776300	0.88732600
H	2.46625700	-1.00726000	-3.87277700	C	-5.74847400	-0.95201900	1.32839900
H	3.18248300	-0.89975300	-2.25204400	C	-5.14541700	0.12887500	0.42105600
O	1.88908000	-2.48621700	-0.24764400	C	-3.83569400	-0.15666700	-0.32132300
H	10.79742800	-1.60273700	-4.71927700	O	-3.34332000	-1.34795100	-0.19335900
H	5.46956600	-5.58933300	-1.53621900	O	-3.31667100	0.72983000	-1.00242300
H	2.07529800	8.27087800	-0.79946900	C	-5.89887600	2.43930600	-6.25826100
H	7.14086800	1.75312600	4.23098700	C	-5.31974000	1.20293600	-5.55004400
H	1.72667400	2.81202000	7.40110900	C	-3.85436200	1.36298800	-5.11615900
H	3.08014600	2.68991800	6.27231800	C	-3.12832300	0.03035000	-4.90677600
H	0.33188200	0.64463400	7.50136000	O	-3.17246900	-0.86115000	-5.74161200
H	-0.02362900	-0.03504300	5.91165300	N	-2.36928100	-0.06062500	-3.77642200
O	-1.00667300	-0.96320000	0.79665700	C	-5.32603200	-5.96780000	5.83334500
				C	-4.93785600	-4.49591600	5.66191900
				C	-3.42601600	-4.25528900	5.58885600
53				O	-2.63132700	-5.19433000	5.40957200
C	1.54978400	7.69380900	-0.06673700	N	-3.01261900	-2.98665800	5.69554300
C	0.62973500	6.73087500	-0.76360700	C	-2.78933800	-7.34911200	-3.68451200
C	-0.74581400	6.77187400	-0.80437100	C	-2.67393600	-6.03620200	-4.47940400
C	1.01779500	5.62612500	-1.61224400	C	-2.76266300	-4.82725600	-3.59807300
N	-1.23387500	5.77227900	-1.62032700	N	-3.89494700	-4.04454900	-3.46989000
C	-0.18043300	5.05119500	-2.12997100	C	-1.87833700	-4.30703200	-2.68437000
C	2.25823400	5.06841600	-1.98821900	C	-3.67081900	-3.10811100	-2.52238600
C	-0.16502100	3.94736300	-2.99656400	N	-2.45541900	-3.24593700	-2.02342700
C	2.27510700	3.97013100	-2.84468400				

C	6.45200800	-5.16745100	-1.46937500	H	-5.83549100	3.34204900	-5.63998300
N	6.51982800	-4.53902500	-0.13708100	H	3.88449400	2.13032500	8.46809100
C	5.45701000	-3.88443400	0.39590600	H	3.86091100	0.61343000	7.60135700
N	4.61737200	-3.24034400	-0.37995600	H	2.60742600	0.96769900	8.78092000
N	5.29710500	-3.90202600	1.74116300	H	-3.74657400	-7.44963800	-3.21706400
C	10.52777100	-2.53818800	-4.27973900	H	-2.02178000	-7.40528700	-2.94109000
N	9.33732000	-3.07777400	-4.92904100	H	-2.66372700	-8.20862900	-4.35913600
C	8.06043000	-2.72322900	-4.63903000	H	-5.05267600	-6.57958800	0.85359600
N	7.78301600	-1.93543200	-3.60286200	H	-3.88632400	-7.87273200	0.99735600
N	7.04903700	-3.19144200	-5.36977700	H	-5.24708000	-7.80111000	2.07335100
C	-6.52464800	6.59510200	-4.38185700	H	-4.96563900	-6.32911100	6.77418100
C	-7.08369600	6.46396200	-2.94543700	H	-6.38545400	-6.10769500	5.78025000
C	-6.13986600	5.96905700	-1.86627000	H	-4.86470100	-6.59475100	5.06477100
C	-5.56470100	4.68568100	-1.90523700	H	-6.53695500	-0.50072800	1.89393300
C	-5.84492000	6.76812600	-0.75116400	H	-6.13599600	-1.78046200	0.77373900
C	-4.74217600	4.21257200	-0.88223400	H	-5.00628800	-1.32655400	2.04218800
C	-5.02960500	6.31092300	0.28938300	H	4.56362300	-3.34149800	2.15488200
C	-4.47896300	5.02431000	0.23269600	H	5.65209300	-4.66961800	2.29439100
O	-3.68464200	4.51755500	1.21558100	H	3.64844600	-2.96246300	-0.11367800
C	1.33720700	-2.46737100	-1.37132800	H	4.90496100	-2.90224600	-1.33496800
C	3.00051500	-1.55375100	-3.12974600	H	7.24340400	-4.84064900	0.50112200
C	4.36370200	-2.01206800	-3.66089500	H	6.60215800	-4.44207300	-2.27380200
O	0.08724600	-2.20927400	-1.51798300	H	7.20724000	-5.95722100	-1.52572200
O	5.27075100	-2.21802900	-2.77100300	H	6.06858200	-2.81881100	-5.21798400
O	4.55027300	-2.17339000	-4.87679600	H	7.21700500	-3.84760400	-6.11804600
C	-2.30095000	-0.00203300	4.58592100	H	8.51556800	-1.46800700	-3.09388400
N	-0.19527200	2.22380900	2.75443700	H	6.78749100	-1.93218900	-3.24302400
O	-1.22209400	-0.63892300	4.77070200	H	9.48452200	-3.50842100	-5.83268100
C	-2.16247600	1.45021800	4.00313900	H	11.35300200	-3.24659900	-4.41387500
N	0.73884000	2.16822200	1.63440500	H	10.36916000	-2.42726900	-3.20113300
O	-3.45787200	-0.38357000	4.82962900	H	5.50207400	7.40880100	0.98832300
C	-1.43150400	1.56545700	2.69744300	H	5.45785200	6.94840200	3.26914900
C	1.64809100	3.34671400	1.83134600	H	6.66050000	4.18494700	0.19027000
C	1.54752400	0.89320500	1.63683400	H	5.97485400	5.26538500	4.99127300
C	0.01307500	2.30033300	0.33048100	H	7.17720900	2.48689800	1.92508000
Fe	-1.52361800	-2.10642200	-0.33259800	H	6.15798500	2.61585400	5.40365600
C	2.10919700	-2.74526000	-2.67387300	H	7.87216200	3.00979100	5.21063400
H	1.40960200	-3.00942500	-3.47458600	H	-7.46131200	7.44904600	-2.63369600
H	2.72969600	-3.63225800	-2.47869200	H	-7.97134200	5.80930300	-2.97040800
H	-7.20844000	7.23390800	-4.90173300	H	-6.27279800	7.77030300	-0.67670900
H	-5.55087200	7.03822400	-4.38532700	H	-5.77970100	4.02394900	-2.74483400
H	-6.46872700	5.63209900	-4.90045100	H	-4.31858900	3.20925000	-0.92256600
H	-5.34286400	2.60037800	-7.15836700	H	-4.83359300	6.95673600	1.14945000
H	-6.92534500	2.25979400	-6.50053100	H	-3.64200200	5.13422300	1.95221300

H	1.11488100	2.55965600	-4.02030100	H	2.48225500	-0.98006000	-3.90758800
H	3.22962500	3.53581200	-3.14809900	H	3.19311300	-0.88004000	-2.28363000
H	-1.08779500	3.51919100	-3.38559100	O	1.93761000	-2.51936300	-0.28927100
H	3.19241200	5.49362100	-1.61844400	H	10.79770100	-1.60075000	-4.71927900
H	-1.42878400	7.46135400	-0.31620300	H	5.47055600	-5.58830000	-1.53622300
H	-2.21304900	5.57767700	-1.77453900	H	2.07380900	8.27129600	-0.79947900
H	2.29391400	7.17537000	0.55383300	H	7.14054300	1.75446300	4.23097400
H	0.99201100	8.38484700	0.57863900	H	1.79414700	2.88681400	7.43024600
H	-5.36981000	-4.07715200	4.73670500	H	3.16251700	2.77564600	6.33537200
H	-5.35586400	-3.88364900	6.47550700	H	0.70334600	0.26109700	7.32754000
H	-2.03190000	-2.76913500	5.53984300	H	0.10123400	0.02279100	5.68833600
H	-3.58420800	-2.14189600	5.56268900	O	-0.79425800	-0.97717800	0.93155000
H	-4.38709100	-5.84998100	3.21600500				
H	-3.15785100	-7.09165600	3.22631800				
H	-3.14784200	-4.97319800	-0.12318900				
H	-1.79442700	-4.92969800	3.86470200				
H	-0.48498700	-3.10520800	2.55109300				
H	-1.71371400	-6.01123800	-5.01497400				
H	-3.45150600	-5.98708100	-5.25579200				
H	-4.72283700	-4.10166000	-4.04882000				
H	-0.87124000	-4.63628300	-2.45783100				
H	-4.39406800	-2.35969200	-2.22340900				
H	-3.17452700	1.86078100	3.89106800				
H	-1.65667300	2.05136700	4.77739900				
H	-1.30273400	-0.57351500	1.65195700				
H	-2.01920900	1.73573900	1.79707700				
H	0.36357200	1.99931100	3.59533200				
H	2.04706000	0.82078300	2.60591000				
H	0.86099800	0.05524000	1.46904700				
H	2.27626600	0.95053900	0.82175500				
H	-0.54305200	1.37929400	0.14427100				
H	-0.65365100	3.16308900	0.38468300				
H	0.75708400	2.45254600	-0.45631200				
H	2.39883300	3.35084400	1.03699400				
H	1.04345900	4.25532400	1.79098800				
H	2.12378900	3.24542800	2.81059000				
H	-5.86998000	0.44203800	-0.34806100				
H	-4.95288100	1.04022100	1.00539500				
H	-5.93167500	0.94115300	-4.67056900				
H	-5.37922300	0.34474300	-6.23582400				
H	-3.28900600	1.86740200	-5.91790600				
H	-3.77392200	2.00317100	-4.22749400				
H	-1.90041600	-0.94509600	-3.62505800				
H	-2.58280800	0.47153900	-2.93407500				
				⁵TS₃₋₄			
				C	1.33547600	7.67773600	0.14048000
				C	0.45428100	6.69617400	-0.57956800
				C	-0.91211800	6.56514300	-0.47731100
				C	0.86906200	5.74571100	-1.58759700
				N	-1.37062500	5.60176600	-1.35163700
				C	-0.30563900	5.08119500	-2.04863100
				C	2.11425600	5.39827900	-2.15276700
				C	-0.26148500	4.09195300	-3.04347300
				C	2.15985000	4.41711100	-3.13958600
				C	0.98231000	3.77057000	-3.58059100
				C	3.21523300	1.23135700	8.05320200
				C	2.41972900	2.04171200	7.01360600
				C	1.68382100	1.39013300	5.84805600
				O	1.62249300	2.01987800	4.78733200
				N	1.09446200	0.19013200	6.00684700
				C	6.88090700	2.72471800	4.73936100
				C	6.52345500	3.76393200	3.69807000
				C	6.73037100	3.53127900	2.32772700
				C	5.99453200	5.01227200	4.06454100
				C	6.42958100	4.49304900	1.36175400
				C	5.68601800	5.98633900	3.11188000
				C	5.90326400	5.73351700	1.74868800
				O	5.61901700	6.63551100	0.77243100
				C	-4.33942500	-7.38837900	1.39050700
				C	-3.56320300	-6.62774600	2.45410400
				C	-2.58277300	-5.62058400	1.95299100
				N	-1.60505900	-5.09297900	2.77470700
				C	-2.49059600	-4.91816000	0.78064100
				C	-0.99041900	-4.09453700	2.12098200
				N	-1.49868100	-3.96440900	0.90042800

C	-5.74017200	-1.18088900	1.33265400	C	4.39884500	-1.77911200	-3.61641700
C	-5.13716400	-0.06760300	0.46593700	O	0.13983200	-2.10379300	-1.44291100
C	-3.79182100	-0.30175500	-0.23309600	O	5.32045200	-2.00404600	-2.74616000
O	-3.25707900	-1.47150900	-0.09035900	O	4.56848100	-1.90540200	-4.83895900
O	-3.28917600	0.60703400	-0.89700400	C	-1.99213200	-0.17784200	4.26064300
C	-5.99061400	2.39045400	-6.16827300	N	-0.16895600	2.46342400	2.60033500
C	-5.38498300	1.15199700	-5.48551400	O	-0.92789600	-0.83153500	4.01066500
C	-3.92724000	1.33334600	-5.03577300	C	-1.92485500	1.36768800	3.98742300
C	-3.17672900	0.01191100	-4.83968400	N	0.92281900	2.05799400	1.46927400
O	-3.22068300	-0.88018600	-5.67435600	O	-3.05293700	-0.60796000	4.72835200
N	-2.39477900	-0.06657300	-3.72429200	C	-1.34684800	1.79515700	2.67692600
C	-5.18288600	-6.29331300	5.71256400	C	1.83522900	3.22903100	1.44716300
C	-4.79497800	-4.81942400	5.55920900	C	1.64370400	0.80637400	1.82778100
C	-3.28012800	-4.59874200	5.47075000	C	0.20028600	1.90514100	0.18288100
O	-2.49234300	-5.54828600	5.35225500	Fe	-1.41633600	-2.17256200	-0.18167200
N	-2.84281700	-3.32828200	5.50332900	C	2.13375600	-2.55705500	-2.68124100
C	-2.63073700	-7.37660500	-3.83968500	H	1.41366000	-2.74199800	-3.48598900
C	-2.53529200	-6.01417200	-4.55495300	H	2.74058000	-3.46841500	-2.57405100
C	-2.62217100	-4.85538300	-3.60297600	H	-7.41778100	7.11584400	-4.69273300
N	-3.73038000	-4.03837000	-3.48709300	H	-5.75481300	6.94940700	-4.18348300
C	-1.76137200	-4.40442800	-2.62797800	H	-6.63943600	5.53212900	-4.72920600
C	-3.51455400	-3.15229900	-2.48892600	H	-5.44058200	2.58749800	-7.06489000
N	-2.32870300	-3.35204400	-1.94367800	H	-7.01270900	2.19111800	-6.41351500
C	6.55706800	-5.01764200	-1.58391800	H	-5.94967900	3.27991900	-5.52914600
N	6.61878600	-4.43860500	-0.22925000	H	3.82603600	1.96739800	8.53307600
C	5.53983400	-3.83360000	0.32999000	H	3.83894900	0.47208500	7.62940200
N	4.68724000	-3.17596900	-0.41865400	H	2.57255000	0.76448900	8.81253100
N	5.37745700	-3.91660600	1.67286700	H	-3.58423000	-7.51265100	-3.37357600
C	10.55990500	-2.21840700	-4.33430000	H	-1.86056500	-7.43161600	-3.09888400
N	9.36632800	-2.75903700	-4.97768000	H	-2.48284800	-8.19720900	-4.55567000
C	8.08967600	-2.42582700	-4.66104500	H	-4.90389900	-6.77580800	0.71894100
N	7.81790900	-1.67213700	-3.59861600	H	-3.70509700	-8.04227700	0.82937000
N	7.07326100	-2.88256000	-5.39240800	H	-5.07295300	-8.03658100	1.89244200
C	-6.71712100	6.48192900	-4.18960000	H	-4.81168700	-6.66837100	6.64377000
C	-7.27663400	6.30897800	-2.75810800	H	-6.23855300	-6.45852300	5.65745600
C	-6.33440000	5.79643200	-1.68612800	H	-4.71605400	-6.90436600	4.93436100
C	-5.72667100	4.53039600	-1.76628600	H	-6.53865900	-0.76360900	1.91014000
C	-6.07886400	6.55735100	-0.53524400	H	-6.10780000	-2.00499600	0.75834100
C	-4.91114700	4.03631100	-0.74762400	H	-4.99522100	-1.56527700	2.03974000
C	-5.27205700	6.07824800	0.50161000	H	4.62869400	-3.39375600	2.10774200
C	-4.69016000	4.80780000	0.40465600	H	5.74806300	-4.70118400	2.19084800
O	-3.90479800	4.27917100	1.38160400	H	3.70733200	-2.93564800	-0.14815600
C	1.38901000	-2.38074700	-1.34512500	H	4.97238600	-2.78392900	-1.35304200
C	3.03989300	-1.34651300	-3.05286200	H	7.34841600	-4.75275500	0.39587900

H	6.68232400	-4.25890800	-2.36148500	H	-4.22670100	-2.39361800	-2.18969800
H	7.33201600	-5.78476300	-1.67593100	H	-2.94794700	1.76010700	4.07073000
H	6.09100500	-2.52524300	-5.21698700	H	-1.34852400	1.80123300	4.82022800
H	7.23836200	-3.51090800	-6.16481700	H	-0.92560300	-1.08974700	2.14789100
H	8.55301200	-1.21728000	-3.08196800	H	-1.97943500	1.78644900	1.79145700
H	6.82654900	-1.69042900	-3.22640800	H	0.38719600	2.38812500	3.46578400
H	9.50503800	-3.16220200	-5.89524800	H	2.10839100	0.94446900	2.80653700
H	11.39401200	-2.90824600	-4.50489300	H	0.92248000	-0.01609500	1.83607800
H	10.41999500	-2.14188100	-3.25008300	H	2.40223100	0.61099400	1.06017700
H	5.31977000	7.46108900	1.16472100	H	-0.43293500	1.01705600	0.24390100
H	5.27435900	6.94673900	3.43256000	H	-0.39306600	2.80335700	-0.00143800
H	6.60065500	4.30001400	0.30222200	H	0.93601100	1.77783100	-0.61727500
H	5.81850400	5.23712100	5.11873800	H	2.61139000	3.06509000	0.69259100
H	7.14419700	2.57428500	2.00069000	H	1.25648300	4.12148400	1.19805900
H	6.07197300	2.58809400	5.46970800	H	2.29432600	3.33947800	2.43384600
H	7.77965500	3.02095300	5.30306900	H	-5.84292800	0.24382900	-0.32083400
H	-7.66596400	7.28203200	-2.42352900	H	-4.98717800	0.83517400	1.07588200
H	-8.15760100	5.64610500	-2.80272000	H	-5.99735700	0.85623200	-4.61717800
H	-6.53149800	7.54580400	-0.43003300	H	-5.42007700	0.30833400	-6.19055200
H	-5.90835700	3.90011600	-2.63720000	H	-3.36394400	1.86182300	-5.82356200
H	-4.45928400	3.04709000	-0.81902300	H	-3.86591600	1.96086200	-4.13638400
H	-5.10791700	6.69243500	1.39096700	H	-1.90317800	-0.94025400	-3.58297300
H	-3.86449000	4.87908500	2.13187400	H	-2.60133000	0.45661400	-2.87520800
H	1.04563700	3.00877300	-4.35958500	H	2.52803800	-0.71411300	-3.78850600
H	3.11702900	4.14757600	-3.58992400	H	3.23930300	-0.73568800	-2.16216000
H	-1.16715000	3.59338800	-3.38695200	O	2.01032800	-2.52757100	-0.28205200
H	3.03023700	5.89202600	-1.82426400	H	10.80530400	-1.26397400	-4.75105500
H	-1.60910200	7.10731400	0.15496300	H	5.58638900	-5.46133000	-1.65977500
H	-2.33581700	5.31803800	-1.44461800	H	1.84337700	8.28603000	-0.57856000
H	2.09780100	7.17519100	0.75371700	H	7.08227100	1.77766600	4.28369700
H	0.75168700	8.33467500	0.79803300	H	1.66415900	2.65333500	7.53560900
H	-5.23872800	-4.37985200	4.64980400	H	3.08557500	2.76522500	6.52724900
H	-5.19090300	-4.21753100	6.39193300	H	1.07688300	-0.26430300	6.90850400
H	-1.85469500	-3.16601300	5.35114200	H	0.48215200	-0.18412200	5.26324200
H	-3.38910500	-2.47491900	5.36325800	O	-0.71888700	-1.19442600	1.19377200
H	-4.27231200	-6.09312300	3.09970600				
H	-3.04353600	-7.33796700	3.11257200	54			
H	-3.08336400	-5.01204600	-0.11957100	C	1.54974400	7.69383900	-0.06674900
H	-1.55206000	-5.31560200	3.78187400	C	0.59267300	6.76744100	-0.76330900
H	-0.22289000	-3.45984900	2.54762500	C	-0.78316000	6.82296000	-0.75540700
H	-1.58112500	-5.95174600	-5.09911200	C	0.93917100	5.69369500	-1.66748000
H	-3.32111400	-5.92170400	-5.31914900	N	-1.30947500	5.86163800	-1.59377200
H	-4.52847300	-4.03171700	-4.10896000	C	-0.28205500	5.15297700	-2.16863700
H	-0.77755000	-4.78290500	-2.37448500	C	2.15877500	5.13573800	-2.10460600

C	-0.30618700	4.08305500	-3.07743900	N	9.35993800	-3.09911800	-4.94920100
C	2.13848600	4.07264300	-3.00417100	C	8.07197100	-2.77534800	-4.67517800
C	0.91562500	3.55153200	-3.48579700	N	7.76518500	-1.97242000	-3.65940400
C	3.25597100	1.39837300	8.00521800	N	7.08029400	-3.29265200	-5.39986600
C	2.46326700	2.09125600	6.88568200	C	-6.52464800	6.59510500	-4.38185800
C	1.52227900	1.21564600	6.05700100	C	-7.08197500	6.46920800	-2.94396200
O	1.49385200	1.31529500	4.82380600	C	-6.15804700	5.94971200	-1.85656900
N	0.72202700	0.37547200	6.73173900	C	-5.54443200	4.68545200	-1.92880000
C	-4.50471100	-7.18949600	1.54106100	C	-5.93844300	6.69822400	-0.68948100
C	-3.69697200	-6.37775100	2.55285200	C	-4.76159100	4.18068900	-0.88859200
C	-2.76233600	-5.33314800	2.02050300	C	-5.16302900	6.20951100	0.36739000
N	-1.95519500	-4.61717100	2.88552300	C	-4.57698000	4.94029400	0.27763400
C	-2.56140300	-4.76630000	0.78661800	O	-3.82160100	4.40535200	1.27910500
C	-1.32792200	-3.65735400	2.19383200	C	1.36118400	-2.60227000	-1.42178300
N	-1.66536200	-3.71784500	0.90806700	C	2.95448500	-1.72610200	-3.25691500
C	-5.74845700	-0.95202700	1.32839600	C	4.34622900	-2.13616200	-3.74897000
C	-5.14803200	0.11902700	0.40486300	O	0.11359500	-2.36548000	-1.59151200
C	-3.83105300	-0.16686800	-0.33205200	O	5.24775500	-2.25988100	-2.83873600
O	-3.30443800	-1.33226800	-0.14857400	O	4.55715000	-2.33829900	-4.95494600
O	-3.34859600	0.70505300	-1.05893100	C	-2.62415000	0.08880500	5.66206700
C	-5.89888000	2.43930600	-6.25825600	N	-0.93946000	0.71732200	2.95903700
C	-5.31980300	1.19898600	-5.55649300	O	-1.63725700	-0.69023400	5.81264900
C	-3.85000400	1.35080500	-5.13359600	C	-2.27751000	1.43881800	4.91611300
C	-3.12710400	0.01290600	-4.94524600	N	0.93796300	2.15660600	1.13612300
O	-3.16178900	-0.85825000	-5.80136300	O	-3.80183300	-0.09134500	5.98772800
N	-2.38440400	-0.10534900	-3.80652900	C	-2.03486600	1.12185700	3.47794700
C	-5.32601200	-5.96778900	5.83333200	C	1.23346800	3.14929400	2.14049500
C	-5.02928900	-4.47103500	5.72689900	C	1.80940900	1.01894700	0.97973700
C	-3.55120800	-4.11232700	5.84575300	C	-0.13483400	2.32395600	0.18854700
O	-2.66986400	-4.90158500	5.46271800	Fe	-1.46929100	-2.07862000	-0.36452100
N	-3.28012600	-2.90854600	6.35260000	C	2.14622400	-2.93551700	-2.70313400
C	-2.78934100	-7.34910300	-3.68451000	H	1.46171400	-3.30099600	-3.47680500
C	-2.68629300	-6.02901700	-4.47126900	H	2.82414000	-3.76302600	-2.44992300
C	-2.78718600	-4.82279700	-3.58668800	H	-7.20844100	7.23390700	-4.90173300
N	-3.94603100	-4.09194000	-3.39591800	H	-5.55087100	7.03822200	-4.38532700
C	-1.87794700	-4.25587600	-2.72786100	H	-6.47099800	5.63162500	-4.89968400
C	-3.71000700	-3.13875700	-2.46674700	H	-5.34286500	2.60037800	-7.15836700
N	-2.46248400	-3.21583300	-2.03928500	H	-6.92534400	2.25979300	-6.50053400
C	6.45200800	-5.16745200	-1.46937600	H	-5.83404900	3.34023200	-5.63762800
N	6.52032200	-4.53420600	-0.14016100	H	3.88451900	2.13031200	8.46807700
C	5.45795600	-3.87137900	0.38121300	H	3.86087700	0.61339400	7.60137400
N	4.62652700	-3.22798000	-0.40368400	H	2.61179400	0.97572500	8.78840500
N	5.28999500	-3.87513700	1.72637800	H	-3.74657400	-7.44963900	-3.21706500
C	10.52777500	-2.53818900	-4.27973900	H	-2.02177900	-7.40528600	-2.94109100

H	-2.66313400	-8.20417400	-4.36429600	H	-3.12932700	-7.05909100	3.20419900
H	-5.05268200	-6.57958900	0.85359900	H	-3.00940100	-5.02507100	-0.16416500
H	-3.88632200	-7.87272900	0.99735500	H	-1.99378500	-4.72336200	3.92205000
H	-5.24066700	-7.79792300	2.08469100	H	-0.66506000	-2.91982500	2.63282400
H	-4.96564400	-6.32910300	6.77418500	H	-1.72563400	-5.98877300	-5.00457000
H	-6.38545500	-6.10769000	5.78026300	H	-3.46296200	-5.98501300	-5.24914600
H	-4.84052400	-6.55112200	5.04784800	H	-4.80550700	-4.19654400	-3.91956100
H	-6.53696000	-0.50072400	1.89392400	H	-0.84413700	-4.53042100	-2.56076200
H	-6.13599900	-1.78046000	0.77373800	H	-4.44984700	-2.42222600	-2.13202300
H	-5.00220800	-1.33247000	2.03707700	H	-3.10979100	2.14027000	5.02328100
H	4.54175800	-3.32283100	2.12497100	H	-1.37492100	1.86571300	5.37269200
H	5.63043100	-4.64580400	2.28484400	H	-0.88991700	-0.32931400	1.49448300
H	3.64417100	-2.96741600	-0.15575100	H	-2.90831400	1.18188400	2.81541800
H	4.90983800	-2.91624800	-1.36677800	H	-0.18411800	0.68061600	3.65772400
H	7.23896000	-4.83737000	0.50291900	H	2.50831400	0.95908100	1.81643100
H	6.60451700	-4.44601000	-2.27685200	H	1.18170800	0.11063900	0.90382900
H	7.20663700	-5.95805800	-1.52247000	H	2.35852400	1.12266600	0.03095500
H	6.08882700	-2.94133500	-5.26766000	H	-0.55666800	1.34037300	-0.04763200
H	7.27219300	-3.97346300	-6.11980000	H	-0.90154400	2.98890200	0.58845200
H	8.47376700	-1.44229000	-3.17814300	H	0.27382900	2.76582700	-0.73800400
H	6.76494000	-1.97688600	-3.31347200	H	2.18954800	3.63592500	1.88539300
H	9.52890000	-3.53902300	-5.84444100	H	0.44104700	3.89961700	2.17813200
H	11.36540700	-3.23651400	-4.38870000	H	1.35478600	2.65460500	3.11896900
H	10.34249900	-2.42000700	-3.20613600	H	-5.87427000	0.40826000	-0.37162200
H	-7.44013400	7.46088600	-2.62985300	H	-4.96916800	1.04669500	0.96708500
H	-7.98401400	5.83393900	-2.97133500	H	-5.92610100	0.93687200	-4.67328600
H	-6.39619900	7.68461800	-0.58675100	H	-5.38817300	0.34361700	-6.24502100
H	-5.69789000	4.06175300	-2.80962200	H	-3.29060200	1.86181700	-5.93517600
H	-4.31438500	3.18894900	-0.95653000	H	-3.76076400	1.97990900	-4.23818000
H	-5.02688100	6.81577900	1.26689100	H	-1.92862500	-0.99878300	-3.66661500
H	-3.87032700	4.96930100	2.05722100	H	-2.61099800	0.40970600	-2.95608200
H	0.92446400	2.72086900	-4.19336600	H	2.40273900	-1.25224700	-4.07753500
H	3.07812100	3.63814200	-3.34827800	H	3.09867900	-0.97513900	-2.46847000
H	-1.24564300	3.67879600	-3.45187300	O	1.95765600	-2.58865800	-0.33408500
H	3.10920400	5.53405400	-1.74552300	H	10.79770100	-1.60075000	-4.71927900
H	-1.44171400	7.49834700	-0.21635100	H	5.47055600	-5.58830100	-1.53622300
H	-2.29534900	5.68409300	-1.72496200	H	2.07384200	8.27125800	-0.79948500
H	2.29459800	7.14772500	0.53142300	H	1.85166400	2.90648900	7.30822100
H	1.02415100	8.38678000	0.60274700	H	3.15457800	2.56108000	6.17378500
H	-5.36822200	-4.07165700	4.75487400	H	0.71622400	0.38818500	7.74143800
H	-5.60348100	-3.91836400	6.48530000	H	-0.08891000	-0.09288700	6.26918700
H	-2.35782800	-2.47428600	6.24749700	O	-0.62587800	-0.87539700	0.70886900
H	-3.99291900	-2.19074600	6.47083200	C	6.79906900	1.26115600	3.06727600
H	-4.39166500	-5.85191700	3.22044700	C	6.70981100	1.84471100	1.67385100

C	6.39450200	1.05191600	0.55780300	C	-1.17410900	-3.83220300	2.15951000
C	6.93877400	3.21197100	1.44451400	N	-1.58255400	-3.84450400	0.89214600
C	6.30821200	1.58695100	-0.72936900	C	-5.74845700	-0.95202500	1.32838500
C	6.85839700	3.76500200	0.16425800	C	-5.10737900	0.08569200	0.39858100
C	6.54179800	2.95352900	-0.93684800	C	-3.83142600	-0.30984800	-0.35026500
O	6.44731500	3.42815100	-2.20631600	O	-3.31019200	-1.45698700	-0.02951500
H	6.63166900	4.37216600	-2.22029900	O	-3.34116300	0.43738100	-1.19521000
H	7.04608600	4.83231900	0.02195700	C	-5.89887900	2.43930400	-6.25826000
H	6.05327900	0.95642400	-1.58108500	C	-5.31713700	1.18866200	-5.57581400
H	7.19037200	3.86700000	2.28163400	C	-3.81932200	1.30063700	-5.24834300
H	6.20640400	-0.01499900	0.69234400	C	-3.11937300	-0.05195400	-5.08913300
H	6.04429300	1.69949800	3.73800900	O	-3.20941300	-0.92587600	-5.93813700
H	7.78335100	1.44996500	3.52122500	N	-2.32282600	-0.18049700	-3.98573300
H	6.64093200	0.17451800	3.05954800	C	-5.32601100	-5.96779500	5.83331600
				C	-5.02064500	-4.47466100	5.66808000
				C	-3.53984300	-4.11473300	5.52819400
				O	-2.66650800	-4.99296000	5.42104000
				N	-3.25692400	-2.80856700	5.48637200
				C	-2.78934200	-7.34911700	-3.68452200
				C	-2.67332600	-6.03358000	-4.47599300
				C	-2.75029600	-4.82473200	-3.59190400
				N	-3.85649700	-4.00101800	-3.49919800
				C	-1.87641600	-4.33447400	-2.65148300
				C	-3.63074200	-3.07388400	-2.54325200
				N	-2.43667000	-3.25378300	-2.00669500
				C	6.45198700	-5.16742500	-1.46938500
				N	6.53298800	-4.55135400	-0.13410700
				C	5.48928300	-3.87914600	0.40802600
				N	4.63140900	-3.25438000	-0.36491600
				N	5.36482800	-3.85719400	1.75713800
				C	10.52791100	-2.53823100	-4.27971100
				N	9.35309200	-3.09107600	-4.94598100
				C	8.06636000	-2.78803200	-4.64618800
				N	7.76746100	-1.97778000	-3.63417700
				N	7.06764600	-3.33934200	-5.33696700
				C	-6.52464900	6.59510500	-4.38185900
				C	-7.01756100	6.43951800	-2.92541600
				C	-6.05048700	5.79552300	-1.94224400
				C	-5.35408700	4.61505600	-2.25476100
				C	-5.85219100	6.32202500	-0.65431300
				C	-4.50837500	3.99277300	-1.33812800
				C	-5.00765800	5.71155000	0.28353900
				C	-4.32298500	4.53041800	-0.05002900
				O	-3.47457300	3.87414500	0.76411000

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C	1.35243900	-2.49880600	-1.35092700	H	4.89442000	-2.94702100	-1.33868200
C	2.97529300	-1.67358600	-3.19075900	H	7.28279500	-4.82777700	0.48477100
C	4.34392700	-2.14421000	-3.69948600	H	6.59691500	-4.43643100	-2.26976200
O	0.10454500	-2.22312800	-1.49980800	H	7.20543000	-5.95817700	-1.53719800
O	5.24401200	-2.32344500	-2.79834400	H	6.07979000	-2.98099000	-5.21180500
O	4.53995800	-2.33535200	-4.90954400	H	7.25237000	-4.05220400	-6.02727500
C	-2.60876600	0.33075800	4.97844200	H	8.44403100	-1.34211900	-3.24195200
N	-2.89300700	3.75255300	3.46292200	H	6.77427100	-1.98184100	-3.28339400
O	-1.56647900	-0.38125300	5.00738800	H	9.51236400	-3.52897100	-5.84402100
C	-2.41553000	1.88266200	5.05009900	H	11.36222500	-3.23969400	-4.39335800
N	1.00630600	2.04003000	1.30591000	H	10.34139500	-2.41848200	-3.20661500
O	-3.79051000	-0.05426500	4.91829500	H	-3.70660500	8.72768800	7.74267100
C	-3.17086200	2.61620000	3.97778000	H	-5.10761200	7.91862700	6.08202500
C	1.40395200	3.19852400	2.06908000	H	-3.52520500	5.60224300	9.35167800
C	1.76430200	0.81769200	1.43988800	H	-6.32764100	5.93949200	5.26386900
C	-0.05256000	2.10537200	0.33462100	H	-4.75757800	3.61199600	8.53068000
Fe	-1.49134600	-2.15393100	-0.30647400	H	-5.70065600	2.70959900	5.77730600
C	2.10934800	-2.84581200	-2.64389600	H	-7.18109700	3.66648400	5.62901100
H	1.40073900	-3.16842800	-3.41474900	H	-7.28516100	7.43541700	-2.54060100
H	2.74610500	-3.70974700	-2.40489300	H	-7.96132600	5.86609500	-2.92490300
H	-7.20844100	7.23390700	-4.90173300	H	-6.37404500	7.23710500	-0.36304200
H	-5.55087100	7.03822300	-4.38532600	H	-5.48687500	4.15271200	-3.23217100
H	-6.47495300	5.63786600	-4.91291600	H	-4.01241700	3.05348900	-1.57732000
H	-5.34286300	2.60037800	-7.15836600	H	-4.88425900	6.15175400	1.27511600
H	-6.92534500	2.25979400	-6.50053000	H	-3.47565800	4.12617200	1.71767600
H	-5.82865400	3.33531400	-5.63251300	H	1.35082600	2.36830900	-3.78484500
H	3.88451500	2.13030700	8.46809100	H	3.41550800	3.42126200	-2.88207400
H	3.86087600	0.61339000	7.60138100	H	-0.89019500	3.31904900	-3.27995200
H	2.58978300	0.97203400	8.76697800	H	3.28862800	5.45419300	-1.46027900
H	-3.74657100	-7.44963300	-3.21705900	H	-1.41437200	7.37742400	-0.39845500
H	-2.02178100	-7.40527500	-2.94108800	H	-2.11062600	5.40666100	-1.77848000
H	-2.66325500	-8.20654700	-4.36129400	H	2.29660600	7.21951200	0.58719400
H	-5.05269600	-6.57959700	0.85360300	H	0.95633200	8.38273000	0.54819900
H	-3.88632600	-7.87273600	0.99735900	H	-5.52812900	-4.07347300	4.77439400
H	-5.24745800	-7.80078400	2.07293700	H	-5.43928600	-3.90402800	6.51197500
H	-4.96564800	-6.32910100	6.77418700	H	-2.30946100	-2.45978200	5.35050300
H	-6.38545600	-6.10768900	5.78027600	H	-3.93374700	-2.04519700	5.42779800
H	-4.85576500	-6.57299200	5.05398500	H	-4.39270300	-5.83465200	3.20445600
H	-6.53695800	-0.50072800	1.89393000	H	-3.17803400	-7.09291100	3.24263200
H	-6.13600900	-1.78045900	0.77374400	H	-3.06009200	-5.04015500	-0.13142200
H	-5.01453000	-1.33612200	2.04590000	H	-1.83870700	-4.87944000	3.90050000
H	4.64371500	-3.28450800	2.17526700	H	-0.45157500	-3.13725000	2.57309100
H	5.74141000	-4.60403600	2.32423100	H	-1.71690400	-6.01229000	-5.01884900
H	3.67294400	-2.96635300	-0.08240900	H	-3.45599000	-5.97828100	-5.24658700

H	-4.66624100	-4.02649200	-4.10581200	O	7.57865000	1.58016400	-2.13043700
H	-0.88952500	-4.70021200	-2.39340400	H	7.81996600	2.37152600	-2.62162500
H	-4.33867000	-2.29917100	-2.27686300	H	7.79130900	4.01689100	-0.98881400
H	-2.83528900	2.18905100	6.02246800	H	6.66891800	-0.09907100	-0.39128800
H	-1.35639400	2.17329800	5.04448600	H	7.24527200	4.51174700	1.36110400
H	-1.36868900	-0.70715700	1.66493800	H	6.14053300	0.39514200	1.98251700
H	-4.06187800	2.09872400	3.59998000	H	5.45123800	2.25687800	3.66126900
H	-2.06133600	4.16765600	3.89503700	H	6.19719500	3.85805400	3.49259200
H	2.24687500	0.79721500	2.42100800	H	7.18380000	2.46677700	3.96763900
H	1.08013000	-0.03448400	1.30624000				
H	2.51991800	0.78392500	0.63695600				
H	-0.49805700	1.11010100	0.22342700				
H	-0.80162200	2.84607800	0.62347400				
H	0.37419300	2.41304900	-0.64063500				
H	2.38335600	3.54512600	1.70133100				
H	0.67103700	3.99988900	1.95636700				
H	1.52998100	2.89624200	3.12076000				
H	-5.82074400	0.43605800	-0.36296800				
H	-4.83543500	0.99052000	0.95955700				
H	-5.87564000	0.95299500	-4.65495100				
H	-5.45205100	0.33073800	-6.25137600				
H	-3.29790200	1.78389500	-6.09155600				
H	-3.65300400	1.93921900	-4.37176200				
H	-1.87480500	-1.08062100	-3.86728100				
H	-2.53686400	0.31059200	-3.11991600				
H	2.44182800	-1.16424900	-4.00220300				
H	3.16434000	-0.93842600	-2.39648400				
O	1.95563500	-2.50942700	-0.27017200				
H	10.79758600	-1.60072700	-4.71930100				
H	5.47056700	-5.58832700	-1.53622300				
H	2.07382700	8.27123700	-0.79951200				
H	-6.79966700	2.82851200	7.12211300				
H	1.80421700	2.87631000	7.35471400				
H	3.21150100	2.73767900	6.30266500				
H	0.49621900	0.57721800	7.34552800				
H	-0.01351300	0.14507500	5.73879000				
O	-0.76284600	-0.98774700	0.96854800				
C	6.35165800	2.78499000	3.31963100				
C	6.65302700	2.49355300	1.86600100				
C	6.50504800	1.19805100	1.33738100				
C	7.11666900	3.49106800	0.99482900				
C	6.80751600	0.90517600	0.00744000				
C	7.42889800	3.21510600	-0.34036600				
C	7.28030700	1.91578500	-0.84252800				
				⁵ TS ₄₋₅			
				C	1.68174200	-2.36191100	-7.27178400
				C	1.90163400	-1.04270500	-6.58631600
				C	3.06388300	-0.55686900	-6.01406300
				C	0.93521100	0.02517300	-6.47856500
				N	2.87871500	0.73080700	-5.57401700
				C	1.58521100	1.12128900	-5.84131700
				C	-0.41148400	0.16725700	-6.87235600
				C	0.93391800	2.33789300	-5.60296800
				C	-1.06579800	1.37392500	-6.63043000
				C	-0.39845500	2.44861200	-6.00542800
				C	0.45957000	-8.40242500	1.08019200
				C	0.99466500	-7.23690300	0.23074200
				C	0.92419000	-5.87911900	0.93617400
				O	-0.08940200	-5.18831000	0.88194600
				N	2.03682100	-5.53107300	1.62121300
				C	0.50445500	2.94435500	7.93461400
				C	0.57650700	1.50488000	7.42710600
				C	0.05766300	1.24326300	6.04588500
				N	0.02528500	-0.04301300	5.53644100
				C	-0.32386300	2.05308200	5.00635900
				C	-0.32704700	0.01446100	4.24596400
				N	-0.55847200	1.27460900	3.88600300
				C	4.31721900	1.85570300	2.44209400
				C	3.77119000	2.53283500	1.17861400
				C	2.25229400	2.47792000	0.94169300
				O	1.52659900	2.36680500	2.01780000
				O	1.78094300	2.57564900	-0.18419800
				C	3.07520800	7.80520300	-3.25731600

C	2.31519100	7.22513400	-2.05253200	O	2.95030300	-3.11433500	2.75190500
C	1.12342300	6.34813300	-2.44566600	C	4.70701600	-3.13725600	1.09221900
C	0.19798600	6.00159500	-1.27698900	N	-0.16367400	-1.14005000	-0.92611800
O	0.22780600	6.59356600	-0.20979700	O	4.85435000	-2.00327600	3.17951300
N	-0.72298900	5.02645500	-1.54224400	C	5.13175300	-1.96509300	0.26070300
C	3.31329900	-0.47817600	8.93042800	C	-0.50736000	-0.27856400	-2.06082300
C	3.72539400	-0.84663900	7.49995100	C	1.21754700	-1.63284500	-0.97737800
C	2.68738700	-1.60244600	6.67174700	C	-1.13976800	-2.21015600	-0.69707400
O	1.51048800	-1.71472800	7.05596400	Fe	-0.37542100	1.87990200	1.90233900
N	3.11753400	-2.08444500	5.50212700	C	-4.53945900	2.09056600	0.60016600
C	-2.89875500	6.42914100	5.37547300	H	-4.45862400	3.17385500	0.74541800
C	-2.68571000	6.71990900	3.87923200	H	-5.35571200	1.73457700	1.24420200
C	-1.73299900	5.75584100	3.24033900	H	6.79798700	6.20669400	-6.43934100
N	-0.39673100	6.02067600	2.99946100	H	5.55471600	4.98260400	-6.52245000
C	-1.89636500	4.44156000	2.88419200	H	5.48563400	6.22387200	-5.27303800
C	0.18756200	4.90988900	2.51036200	H	2.36184200	8.22801300	-3.93385600
N	-0.69685300	3.92945700	2.43696100	H	3.73846400	8.57139800	-2.91428900
C	-8.60637900	-0.62988200	1.81667700	H	3.65238900	7.04637100	-3.79641600
N	-7.88204700	-1.91074800	1.80877900	H	0.44514400	-9.27958100	0.46490600
C	-6.52961100	-1.97300400	1.78302000	H	-0.53804300	-8.18970400	1.40970800
N	-5.83948700	-1.00871800	1.21214600	H	1.08753000	-8.59350600	1.96079000
N	-5.91491700	-3.02865300	2.35651800	H	-1.99304800	6.55434200	5.93119300
C	-11.77862300	-1.00954200	-2.78978900	H	-3.27237200	5.43708100	5.52107800
N	-11.31138600	0.26782900	-2.26304700	H	-3.63759700	7.12880000	5.79266800
C	-10.01353500	0.60655400	-2.06052200	H	0.96896200	3.64630100	7.27389000
N	-9.03678200	-0.28746500	-2.17934100	H	-0.50695800	3.24189700	8.11717200
N	-9.69860600	1.85210200	-1.70155800	H	1.03229600	3.01051300	8.89585300
C	6.14816800	5.58017700	-5.86260200	H	3.20631400	-1.35310500	9.53764000
C	7.03568000	4.67424000	-4.98223400	H	4.09064500	0.13944000	9.32924400
C	6.35032400	3.53809800	-4.24286000	H	2.36726600	0.06752900	8.96666400
C	5.07013000	3.67951100	-3.67603000	H	5.36443800	1.66045000	2.33874000
C	7.00069200	2.30261100	-4.04575700	H	4.14753000	2.42242800	3.33393800
C	4.46878500	2.65447300	-2.95191900	H	3.84091300	0.87960700	2.59122300
C	6.41856500	1.25965500	-3.32226400	H	-4.93091300	-3.19345700	2.19271200
C	5.13417000	1.42190600	-2.75883900	H	-6.38169100	-3.60864300	3.03834300
O	4.48232600	0.48662700	-2.07141600	H	-4.83829900	-0.81408800	1.38989400
C	-3.26147700	1.38982800	1.09991800	H	-6.26717500	-0.42222900	0.45256400
C	-4.85490700	1.78574300	-0.89058600	H	-8.38816000	-2.76237900	2.00903600
C	-6.35645900	1.59935100	-1.14193600	H	-8.71446900	-0.20506200	0.81453000
O	-2.21813000	2.14392200	1.12923500	H	-9.59017900	-0.78447000	2.27107200
O	-6.82930800	0.44492400	-0.83800100	H	-8.68518700	2.15199600	-1.65897800
O	-7.03894600	2.52643500	-1.60535200	H	-10.42107900	2.53952500	-1.54781500
C	4.10683200	-2.70937400	2.47327800	H	-9.20544000	-1.22074500	-2.52153200
N	5.16724300	-1.88566200	-1.01526100	H	-8.10930100	-0.05093800	-1.73874800

C	-0.39164600	5.42328300	-2.36309900	N	5.39360900	-3.76214700	1.73409400
C	2.03308000	5.61172100	-2.59325900	C	10.52846600	-2.53871200	-4.28019400
C	-0.46804800	4.55973800	-3.46752500	N	9.34829500	-3.08464400	-4.94261400
C	1.96055700	4.74622600	-3.68128000	C	8.06524100	-2.74962300	-4.65857700
C	0.71931900	4.22864500	-4.11692400	N	7.76382000	-2.00003800	-3.60265900
C	3.25301700	1.39756700	8.00711900	N	7.07050400	-3.20173900	-5.42401500
C	2.47791900	2.11546000	6.88517200	C	-6.52454600	6.59480500	-4.38091500
C	1.62199100	1.20654000	5.99699100	C	-7.04337800	6.45466800	-2.93481000
O	2.04983700	0.78461300	4.92325700	C	-6.11109500	5.81667300	-1.91685600
N	0.39606000	0.91021400	6.47843700	C	-5.19846500	4.80688000	-2.26009100
C	-4.50485000	-7.18969500	1.54113200	C	-6.16578200	6.18431200	-0.56032500
C	-3.69408800	-6.39470600	2.55834500	C	-4.38537400	4.19362000	-1.30603600
C	-2.72741800	-5.39720700	2.00454500	C	-5.35618500	5.58606600	0.41125300
N	-1.87184600	-4.69706400	2.83472300	C	-4.44796500	4.57554100	0.04772400
C	-2.54608300	-4.85905500	0.75684800	O	-3.61144200	3.95913400	0.89765500
C	-1.24177700	-3.76385500	2.11064500	C	1.28879900	-2.48009300	-1.43941700
N	-1.61849200	-3.83573400	0.83598200	C	2.96562100	-1.62872800	-3.21257800
C	-5.49246700	-0.48784900	1.53202500	C	4.33466000	-2.08811000	-3.73132800
C	-4.97811200	0.19781100	0.25320700	O	0.02190100	-2.32763000	-1.64288200
C	-3.56952100	-0.18626100	-0.22121800	O	5.21586200	-2.33208400	-2.82849200
O	-3.29574700	-1.46453800	-0.17534700	O	4.54339800	-2.20658400	-4.94806400
O	-2.78403900	0.64572600	-0.65527800	C	-2.95420700	0.42770800	5.23095700
C	-5.89892100	2.43959200	-6.25818400	N	-3.37321500	3.77561800	3.62540500
C	-5.33505400	1.20469200	-5.53814300	O	-1.85026800	-0.17674700	5.18610000
C	-3.81649900	1.24279600	-5.35627600	C	-2.91365500	1.99060300	5.30940600
C	-3.22242400	-0.06843700	-4.83937700	N	0.23522600	1.24542000	1.01953100
O	-3.87669000	-1.09098300	-4.70856700	O	-4.09669400	-0.07040300	5.22351100
N	-1.88266600	-0.02643500	-4.57658600	C	-3.62266200	2.64061200	4.15837900
C	-5.32614100	-5.96706100	5.83363800	C	0.30579100	1.84308500	-0.34410500
C	-5.03784100	-4.46860800	5.67832900	C	-0.72783100	1.97537400	1.89399500
C	-3.56229300	-4.08669600	5.55673600	C	1.57436200	1.10280400	1.65689600
O	-2.68314200	-4.95211600	5.39464600	Fe	-1.52962400	-2.19607100	-0.42878500
N	-3.28850200	-2.77961900	5.58867700	C	2.09444500	-2.81198200	-2.70889800
C	-2.78938600	-7.34884800	-3.68444100	H	1.42296100	-3.14585800	-3.50779500
C	-2.68120800	-6.02315400	-4.45873900	H	2.73286700	-3.66703900	-2.44331200
C	-2.76789600	-4.83481000	-3.54989800	H	-7.20829800	7.23392100	-4.90190400
N	-3.91547000	-4.08669300	-3.35530400	H	-5.55099600	7.03849000	-4.38597200
C	-1.86236200	-4.32116100	-2.65711400	H	-6.47908900	5.63545600	-4.90868600
C	-3.68288400	-3.16596500	-2.40159600	H	-5.34292300	2.60023300	-7.15843000
N	-2.44552900	-3.29041000	-1.94992200	H	-6.92530300	2.25974700	-6.50067000
C	6.45230700	-5.16776700	-1.46953900	H	-5.83236100	3.34565200	-5.64646200
N	6.52753700	-4.52077100	-0.15028400	H	3.88583000	2.12998700	8.46679400
C	5.49140800	-3.83816500	0.39036100	H	3.86196100	0.61457900	7.60070500
N	4.59559200	-3.27167800	-0.39126700	H	2.58686700	0.97007700	8.76818500

H	-3.74656500	-7.44977700	-3.21707500	H	-3.96480900	-2.00724700	5.57054500
H	-2.02173700	-7.40544700	-2.94114700	H	-4.38133200	-5.83605100	3.20674000
H	-2.66330800	-8.20041900	-4.36836800	H	-3.15592300	-7.08322300	3.22630900
H	-5.05265100	-6.57961600	0.85355300	H	-3.03153000	-5.12200200	-0.17380500
H	-3.88626200	-7.87262700	0.99729500	H	-1.89521600	-4.78742200	3.87395900
H	-5.24496500	-7.79992100	2.07758600	H	-0.55438700	-3.03014600	2.51687100
H	-4.96558600	-6.32903600	6.77418800	H	-1.72335500	-5.98426100	-4.99748700
H	-6.38537700	-6.10815500	5.77992400	H	-3.46385700	-5.96067700	-5.22919000
H	-4.85091200	-6.56385800	5.05111400	H	-4.75061700	-4.11864700	-3.92550000
H	-6.21469500	0.11860000	2.03806300	H	-0.84198100	-4.63124700	-2.47141100
H	-5.89591300	-1.46703000	1.37771500	H	-4.40556300	-2.43522200	-2.06516900
H	-4.67272000	-0.60814700	2.25143900	H	-3.45815300	2.26421200	6.22759700
H	4.76601200	-3.09524600	2.16199000	H	-1.89274700	2.38436400	5.40781500
H	5.89479000	-4.39367500	2.34145100	H	-0.15941000	0.27927000	0.89317500
H	3.66808300	-2.95021000	-0.07508100	H	-4.44589100	2.05785000	3.72531600
H	4.84555200	-2.96539000	-1.36744200	H	-2.60408000	4.25446500	4.10362500
H	7.31551000	-4.72534600	0.44853900	H	-1.67587600	2.07750000	1.36298100
H	6.60758100	-4.45858100	-2.28772700	H	-0.86592200	1.40353700	2.81430000
H	7.20170700	-5.96425900	-1.51204800	H	-0.32136300	2.96659400	2.11901000
H	6.08718900	-2.84448800	-5.27831900	H	2.17844900	0.42153400	1.05245700
H	7.26008800	-3.81335400	-6.20393200	H	2.05213300	2.08785900	1.70493300
H	8.47701600	-1.57230600	-3.03304700	H	1.46655100	0.71093600	2.67394400
H	6.76547100	-2.01610400	-3.26785200	H	0.61088500	2.89068200	-0.26980900
H	9.50711400	-3.49413200	-5.85401000	H	1.03318700	1.28500700	-0.93926800
H	11.35837200	-3.24357400	-4.40509100	H	-0.68439900	1.76274000	-0.79863800
H	10.35699500	-2.42477100	-3.20506200	H	-5.65918900	0.01129100	-0.59399800
H	-7.31400700	7.45645000	-2.56649500	H	-4.95267300	1.28436700	0.38544600
H	-7.99236900	5.88949400	-2.95011000	H	-5.81827000	1.07620000	-4.55756700
H	-6.86338500	6.96425500	-0.24504000	H	-5.58869600	0.30229300	-6.11351000
H	-5.11946200	4.47705700	-3.29546600	H	-3.32213800	1.46370800	-6.31810700
H	-3.71024700	3.38506000	-1.58124900	H	-3.52256400	2.05580900	-4.67475500
H	-5.42909500	5.90200200	1.45346000	H	-1.45270100	-0.83079800	-4.14059500
H	-3.74922500	4.12207100	1.86406500	H	-1.38046400	0.84786800	-4.53713200
H	0.69092100	3.56966100	-4.98729900	H	2.43922200	-1.08567600	-4.00728400
H	2.87140400	4.47378400	-4.21771400	H	3.15783900	-0.92681900	-2.38936600
H	-1.42723000	4.17595400	-3.81375000	O	1.86787700	-2.39812500	-0.35461700
H	2.99587300	6.01668300	-2.27662000	H	10.79711700	-1.60037400	-4.71883600
H	-1.43207500	7.26208500	0.12271700	H	5.47038800	-5.58792900	-1.53610100
H	-2.35751900	5.67357200	-1.58237000	H	2.07409500	8.27064700	-0.79978300
H	2.28939700	7.10532100	0.49726200	H	1.84714100	2.90583900	7.32249000
H	1.05740800	8.38111000	0.63382100	H	3.19158800	2.61200900	6.21434100
H	-5.53695200	-4.07200400	4.77756700	H	0.08855100	1.31617900	7.35023300
H	-5.47846700	-3.90688100	6.51660500	H	-0.32543800	0.41385900	5.92203300
H	-2.34064400	-2.43515000	5.46169700	O	-0.80503500	-1.24599200	0.66916300

C	6.44340200	0.97486800	3.98681100	O	-2.10058600	1.14726600	0.48811100
C	7.26650900	0.57901100	2.78094300	C	-2.65086100	5.90618600	6.22269600
C	6.70247200	0.50434000	1.49562300	C	-1.96124100	5.82525700	4.85341700
C	8.64109200	0.31234600	2.89417500	C	-0.91198800	4.71667400	4.75074800
C	7.46541200	0.18350100	0.36996500	C	-0.10728000	4.75776400	3.44990800
C	9.41958900	-0.01298300	1.78021300	O	-0.10222300	5.72579100	2.70578900
C	8.83443300	-0.07650100	0.50839500	N	0.63453500	3.64215500	3.19384600
O	9.55377700	-0.39483800	-0.61310100	C	-3.30940300	3.36380600	-8.27950600
H	10.49148700	-0.38037900	-0.39821500	C	-3.67758600	2.44401400	-7.11055300
H	10.48711500	-0.21242900	1.90575800	C	-2.61340400	1.41486600	-6.72671200
H	7.00534800	0.14161900	-0.61710500	O	-1.47894600	1.43780800	-7.23468100
H	9.12345600	0.36335800	3.87247100	N	-2.96450700	0.52778500	-5.78997500
H	5.63874200	0.71166200	1.36252700	C	3.20404400	7.98580200	-2.35067900
H	6.55030700	2.05139000	4.19374400	C	2.99808900	7.61731300	-0.87006900
H	6.76724400	0.44001400	4.89014000	C	2.03174300	6.48335300	-0.70512500
H	5.37403600	0.77690900	3.84348700	N	0.70076900	6.63471400	-0.36069200
				C	2.17050200	5.14291100	-0.96744000
				C	0.10013800	5.42719400	-0.40501100
				N	0.96453900	4.50258200	-0.78251500
				C	8.64126700	-0.10482300	-2.12664900
				N	7.85920800	-1.26916200	-2.56343000
				C	6.51366400	-1.34044200	-2.42881100
				N	5.90557100	-0.65001600	-1.49105500
				N	5.81897900	-2.12361600	-3.28283100
				C	11.82593600	-2.44996300	1.84638400
				N	11.44391800	-1.04385100	1.91215200
				C	10.16459900	-0.59296500	1.94561500
				N	9.13931200	-1.41194800	1.73684400
				N	9.91575600	0.70030800	2.15807100
				C	-5.79491200	2.91630000	7.75776400
				C	-6.75191100	2.50322400	6.62000100
				C	-6.18273800	1.67295200	5.48228700
				C	-4.85581100	1.79942400	5.04244300
				C	-6.99665300	0.76128000	4.78662700
				C	-4.36279100	1.05154700	3.97177300
				C	-6.52028500	-0.00073800	3.71556000
				C	-5.18454900	0.12971500	3.29626200
				O	-4.61973300	-0.59662000	2.31892300
				C	3.34967100	1.43444800	-0.27929100
				C	5.04553700	1.06645700	1.64064300
				C	6.55824800	0.82025100	1.69865700
				O	2.32017300	2.20086700	-0.15195800
				O	7.01178400	-0.04979900	0.86868600
				O	7.27174400	1.42897000	2.51029300
⁵TS₅₋₆							
C	-1.64837500	-5.05450100	5.68809500				
C	-1.81017900	-3.56236400	5.60388600				
C	-2.97719500	-2.84065600	5.49120600				
C	-0.75566500	-2.58605600	5.76053100				
N	-2.71785100	-1.48835700	5.57596300				
C	-1.36766600	-1.29766100	5.74088200				
C	0.64112200	-2.67458300	5.93474600				
C	-0.62202900	-0.11848600	5.90013900				
C	1.38366900	-1.50591100	6.08087800				
C	0.75602000	-0.23950700	6.06783900				
C	-0.73055700	-7.17647800	-4.43091300				
C	-1.21381800	-6.48966500	-3.13693000				
C	-1.13508600	-4.96030000	-3.10220200				
O	-0.24671300	-4.38739600	-2.47294700				
N	-2.09973500	-4.30820800	-3.78912100				
C	-0.35607800	5.97730500	-6.03391300				
C	-0.49888700	4.47324600	-6.20873100				
C	0.07357200	3.62943600	-5.11892800				
N	0.16897200	2.25773700	-5.25311000				
C	0.46196300	3.90052700	-3.83283100				
C	0.56247900	1.74224900	-4.08257800				
N	0.75722200	2.71169900	-3.19068300				
C	-4.08297900	3.39272200	-1.56953700				
C	-3.62630000	2.86558300	-0.19110300				
C	-2.23345500	2.21994400	-0.11199700				
O	-1.25813600	2.87722500	-0.64425000				

C	-4.09944900	-1.25285300	-3.30212000	H	9.25655200	-2.41073000	1.65370300
N	-5.50394000	-1.98559800	0.09602600	H	8.22769700	-0.96583700	1.45535400
O	-2.92103100	-1.58060000	-3.61274000	H	12.14583400	-0.41375700	2.27816700
C	-4.85923600	-2.18461800	-2.30653700	H	12.84826500	-2.52032800	1.45747100
N	-0.96307900	-1.29700600	0.37050500	H	11.17612600	-2.99897000	1.15763500
O	-4.73908800	-0.26000000	-3.69619900	H	-7.58887700	1.94059900	7.06187900
C	-5.27196800	-1.46958800	-1.05060900	H	-7.21267800	3.41442700	6.19866100
C	0.34772200	-1.29993800	1.08099100	H	-8.03827700	0.63287200	5.09131600
C	-1.91545200	-2.28838700	0.95520700	H	-4.18666900	2.50309100	5.53703400
C	-0.80884900	-1.47873100	-1.08358700	H	-3.34007800	1.18153500	3.62008100
Fe	0.59808600	2.36041100	-1.14976200	H	-7.18152600	-0.70594100	3.20879000
C	4.62201000	1.93685100	0.42553200	H	-5.23004700	-1.04829800	1.68870600
H	4.49121800	2.97862600	0.73859500	H	1.36037300	0.65844900	6.21191800
H	5.41106900	1.92620000	-0.34082100	H	2.46386000	-1.56568800	6.22604100
H	-6.41468100	3.27327200	8.55520700	H	-1.10923200	0.85577900	5.91817800
H	-5.22207900	2.08052200	8.10124700	H	1.13584000	-3.64687200	5.96546900
H	-5.10791000	3.71783600	7.46463400	H	-3.99747100	-3.19389900	5.36808500
H	-1.91624700	5.98937500	6.99653500	H	-3.40490600	-0.75481900	5.45035500
H	-3.28439300	6.76816800	6.23882100	H	-0.99841900	-5.45123100	4.89356600
H	-3.26234500	5.02043100	6.42898800	H	-2.61329000	-5.57372400	5.63085900
H	-0.74772700	-8.22878700	-4.22913800	H	-3.88554400	3.03648000	-6.20335600
H	0.27289500	-6.88209400	-4.66692400	H	-4.61862600	1.91245700	-7.32193800
H	-1.37657200	-6.96297700	-5.29248100	H	-2.30379700	-0.16719500	-5.45799600
H	2.30054100	8.35919900	-2.78549100	H	-3.83298200	0.51515600	-5.24061600
H	3.53571600	7.12844300	-2.89830800	H	-1.56491900	4.22113200	-6.28240400
H	3.96882800	8.76979100	-2.44811200	H	-0.05632400	4.16749200	-7.16794900
H	-0.78701200	6.36217900	-5.13325200	H	0.52700100	4.85470700	-3.32662500
H	0.66544300	6.28834100	-6.10172600	H	-0.22697500	1.74319700	-6.06757900
H	-0.88190200	6.47763200	-6.86017500	H	0.67293800	0.68339000	-3.88214200
H	-3.24232900	2.81178500	-9.19409000	H	3.95981300	7.32751700	-0.42209200
H	-4.06338000	4.11721800	-8.37254300	H	2.65105200	8.49135700	-0.29913000
H	-2.34455100	3.85469600	-8.12907000	H	0.27395900	7.47439200	0.00821100
H	-5.14327600	3.30251100	-1.68401700	H	3.05655400	4.60737200	-1.28757000
H	-3.78930900	4.40368900	-1.76203200	H	-0.93775300	5.24818600	-0.15615500
H	-3.65485100	2.77556700	-2.37100300	H	-5.77633100	-2.50990200	-2.82320300
H	4.85196100	-2.34661600	-3.09170000	H	-4.29081600	-3.09295800	-2.06281400
H	6.20757500	-2.42552200	-4.16393100	H	-1.37915800	-0.32546400	0.48331500
H	4.88645600	-0.47136800	-1.45767900	H	-5.37348700	-0.37975300	-1.13759100
H	6.39974600	-0.37097800	-0.60406800	H	-5.41382600	-3.00607000	0.07377500
H	8.31281500	-1.97969300	-3.12037400	H	-2.01224900	-2.10094800	2.02601200
H	8.81273400	-0.10076000	-1.04583600	H	-2.88996200	-2.15770800	0.48429500
H	9.59895200	-0.10848100	-2.65691800	H	-1.53273500	-3.29821300	0.77207500
H	8.92266200	1.02958200	2.30064000	H	-0.15335200	-0.39582800	-1.44372600
H	10.67250500	1.36048300	2.25625000	H	-0.21832600	-2.35729500	-1.36507500

H	-1.74972700	-1.38157100	-1.63463000	C	0.41830400	6.17275000	-1.88830000
H	0.78124200	-2.30514700	1.03347700	N	-1.74280900	6.48328500	-1.32119300
H	1.00585900	-0.58501500	0.58292000	C	-0.92849100	5.85273500	-2.23118900
H	0.18623700	-1.01458200	2.12399200	C	1.46334900	5.65433300	-2.68122800
H	-3.63916300	3.67656200	0.55573000	C	-1.24572100	5.04729300	-3.33602700
H	-4.32501000	2.10824200	0.17820700	C	1.15211200	4.85114700	-3.77499900
H	-2.71221800	5.68916500	4.05959600	C	-0.19100700	4.55418200	-4.10092400
H	-1.46932000	6.78381000	4.63423300	C	3.25301600	1.39756500	8.00712900
H	-0.18581700	4.79999300	5.57831700	C	2.48432400	2.10427800	6.88147100
H	-1.37625000	3.72462300	4.85697400	C	1.62980200	1.23009900	5.96173300
H	1.18389900	3.60026900	2.34622800	O	1.66395800	1.39505100	4.74314400
H	0.58831100	2.81800900	3.77300500	N	0.83849000	0.31562400	6.56644300
H	4.71819800	1.53903600	2.57474100	C	-4.50484900	-7.18969200	1.54113600
H	4.56878200	0.07827100	1.57382100	C	-3.69514700	-6.38821500	2.55482900
O	3.38265800	0.37749800	-0.91573000	C	-2.74558700	-5.37324600	2.00142500
H	11.79219500	-2.88534100	2.82329900	N	-1.92378300	-4.64344100	2.84019900
H	8.08026700	0.76362700	-2.40270300	C	-2.54995800	-4.84679800	0.74976500
H	-1.19484800	-5.27758300	6.63127400	C	-1.29732500	-3.70752500	2.11799700
H	-2.25063300	-6.79963100	-2.92741100	N	-1.64482100	-3.80390200	0.83513300
H	-0.60130300	-6.83888900	-2.29556800	C	-5.74788200	-0.95186000	1.32885000
H	-2.83294900	-4.83208700	-4.24461800	C	-5.05929600	0.12450300	0.47048700
H	-2.24341500	-3.28624800	-3.71923400	C	-3.60256100	-0.10085500	0.04656400
O	0.32708200	0.65782600	-1.41743600	O	-3.24323500	-1.32121400	-0.18429200
C	3.50102400	-6.17552600	-1.22771600	O	-2.85156700	0.86926200	-0.09593300
C	4.84454400	-5.83800800	-0.62085400	C	-5.89890800	2.43959100	-6.25818500
C	4.98010100	-4.79952200	0.31884400	C	-5.32735100	1.22305400	-5.51700900
C	5.99915700	-6.56955800	-0.93928600	C	-3.82291600	1.31997000	-5.25174500
C	6.20425000	-4.50340100	0.91981000	C	-3.20576000	0.01632200	-4.74107100
C	7.23558400	-6.28415200	-0.35050700	O	-3.74650800	-1.06964400	-4.88308300
C	7.34246200	-5.24910200	0.58630500	N	-1.97994700	0.14602200	-4.15834100
O	8.53062400	-4.92380700	1.18888400	C	-5.32614200	-5.96706000	5.83364300
H	9.16741700	-5.62781900	1.03223000	C	-5.06748600	-4.46621100	5.68330700
H	8.11444800	-6.87531700	-0.62139200	C	-3.60278100	-4.04615800	5.57108100
H	6.28166800	-3.70226500	1.65434600	O	-2.70012800	-4.88589800	5.40330100
H	5.94019100	-7.38758100	-1.66022000	N	-3.37890900	-2.73290300	5.61013900
H	4.10466800	-4.20932500	0.59874900	C	-2.78938700	-7.34884800	-3.68443900
H	2.90001400	-6.78549900	-0.53537200	C	-2.70254700	-6.04869200	-4.50021900
H	3.60953800	-6.75116400	-2.15624700	C	-2.79995900	-4.83348200	-3.63151800
H	2.91077500	-5.27839400	-1.45590800	N	-3.94190900	-4.07064700	-3.46483500
				C	-1.89551700	-4.30258300	-2.74926200
				C	-3.69954300	-3.12562700	-2.53287600
				N	-2.46723000	-3.24829000	-2.07211800
				C	6.45230700	-5.16776600	-1.46953900
				N	6.52376600	-4.44782400	-0.18985500
56							
C	1.54935200	7.69450200	-0.06647800				
C	0.37236400	7.03523600	-0.72880700				
C	-0.96178300	7.18981200	-0.42783500				

C	5.52012300	-3.67856000	0.29191900	H	3.86196000	0.61458400	7.60069400
N	4.64266400	-3.13774400	-0.52612600	H	2.60019500	0.97449900	8.78266200
N	5.43978800	-3.48639700	1.62644500	H	-3.74656500	-7.44977900	-3.21707600
C	10.52846700	-2.53871200	-4.28019600	H	-2.02173700	-7.40544700	-2.94114700
N	9.40065200	-3.12688600	-4.99278200	H	-2.66480600	-8.21631600	-4.34983900
C	8.10031100	-2.81132300	-4.77503000	H	-5.05264900	-6.57961600	0.85355100
N	7.74471300	-2.02675200	-3.76263800	H	-3.88626100	-7.87262800	0.99729700
N	7.14647900	-3.31383600	-5.55992400	H	-5.24314300	-7.79975100	2.08008800
C	-6.52454300	6.59480400	-4.38091900	H	-4.96559200	-6.32903200	6.77419200
C	-7.13967500	6.51756600	-2.96068200	H	-6.38537500	-6.10816300	5.77991200
C	-6.29177700	6.06759400	-1.78731000	H	-4.84686400	-6.55610800	5.04809300
C	-5.68436800	4.79996400	-1.73099100	H	-6.53728400	-0.50098900	1.89368100
C	-6.16500000	6.88695100	-0.65416100	H	-6.13625800	-1.78024400	0.77360000
C	-5.00511500	4.36050800	-0.59516600	H	-5.04263900	-1.35308000	2.06968600
C	-5.49646700	6.46086700	0.49867500	H	4.83450900	-2.76853000	2.00036800
C	-4.92653600	5.18183200	0.54212600	H	5.89907700	-4.10214300	2.28129200
O	-4.29298000	4.68482300	1.63483600	H	3.74161100	-2.74025800	-0.22222000
C	1.34701200	-2.44061000	-1.60060500	H	4.87670800	-2.93161700	-1.53400000
C	2.96589500	-1.76821800	-3.49181300	H	7.29902900	-4.63898500	0.42946800
C	4.34611900	-2.22839300	-3.97322900	H	6.62617300	-4.50825900	-2.32509700
O	0.08293100	-2.38074600	-1.77346600	H	7.19623500	-5.97034600	-1.45795300
O	5.20862100	-2.45292200	-3.04633200	H	6.15113800	-2.97544300	-5.45969900
O	4.58977200	-2.35545700	-5.18210300	H	7.37507900	-3.96854000	-6.29297300
C	-2.61135600	0.32641100	5.65732100	H	8.42744100	-1.55049900	-3.19428000
N	-1.67306400	3.75227300	4.78730400	H	6.73985100	-2.07326900	-3.45062400
O	-1.64385500	-0.49108100	5.61241300	H	9.61374600	-3.55330000	-5.88515000
C	-2.29923100	1.76675800	6.17741400	H	11.38303200	-3.22157700	-4.35041100
N	-0.64133400	1.72196300	1.33856600	H	10.29904400	-2.41425100	-3.21699600
O	-3.78967800	0.10929900	5.32811100	H	-7.52895500	7.51667100	-2.71544300
C	-2.46353000	2.80059700	5.09867200	H	-8.03292200	5.87109200	-3.00955500
C	0.74656900	1.82829100	0.80965600	H	-6.61945200	7.88009700	-0.65451600
C	-1.27923500	3.07520200	1.48393300	H	-5.75859900	4.12562100	-2.58559200
C	-0.70994500	0.94821900	2.56902300	H	-4.54108200	3.37693000	-0.56714700
Fe	-1.49024700	-2.17447300	-0.43932300	H	-5.43770800	7.12016800	1.36829400
C	2.16372800	-2.90927200	-2.81114000	H	-4.28796500	5.32151900	2.35622900
H	1.49899700	-3.38263800	-3.54249100	H	-0.40521700	3.94209200	-4.97917800
H	2.84818200	-3.68632300	-2.44298800	H	1.95342200	4.45526500	-4.40165700
H	-7.20829900	7.23392100	-4.90190300	H	-2.28237800	4.83241300	-3.59379800
H	-5.55099700	7.03849300	-4.38597200	H	2.50419100	5.88671300	-2.44953300
H	-6.47520600	5.62224900	-4.88077200	H	-1.42533200	7.76900100	0.36631400
H	-5.34292400	2.60023600	-7.15843000	H	-2.75027500	6.42510900	-1.29362500
H	-6.92530500	2.25975000	-6.50066500	H	2.25248300	6.95947300	0.35450500
H	-5.83811700	3.35375500	-5.65581400	H	1.23606200	8.36479900	0.74373600
H	3.88583300	2.12998500	8.46679300	H	-5.57201200	-4.08133000	4.78036800

H	-5.52718800	-3.91913700	6.52136600	H	0.00025000	-0.07132200	6.08238100
H	-2.45504400	-2.29370400	5.53324000	O	-0.40404100	-1.15367800	0.64326400
H	-4.10947500	-2.02568000	5.64554100	C	5.71261100	1.78634700	3.14354200
H	-4.38409000	-5.84170500	3.21162800	C	6.67153900	1.24159200	2.10895800
H	-3.14246300	-7.07224900	3.21588700	C	6.25470000	0.99230500	0.78825000
H	-3.00815200	-5.12816200	-0.19007300	C	8.02073100	1.00103700	2.41097500
H	-1.95665700	-4.72363900	3.88176700	C	7.13741700	0.53104600	-0.18921900
H	-0.63874600	-2.94994800	2.52904200	C	8.91881600	0.53466700	1.44530200
H	-1.74906900	-6.01402200	-5.04724300	C	8.48071400	0.29959900	0.13634800
H	-3.49100000	-6.02725100	-5.26680600	O	9.31748100	-0.15959100	-0.84655100
H	-4.77467800	-4.11359300	-4.03742600	H	10.22488700	-0.12122500	-0.52892900
H	-0.87716600	-4.61523900	-2.55583000	H	9.96375200	0.36089000	1.71558100
H	-4.41715800	-2.37752100	-2.22132900	H	6.79172300	0.35735100	-1.20778100
H	-3.04426300	1.97437600	6.96126800	H	8.39014400	1.18391600	3.42214100
H	-1.30065300	1.83618700	6.62616600	H	5.21378800	1.17179100	0.51006200
H	-1.23293700	1.20577300	0.64647800	H	5.55033300	2.86570300	2.99740300
H	-3.38634100	2.70309200	4.50859800	H	6.09799600	1.65006700	4.16205900
H	-0.84939500	3.74338400	5.39846900	H	4.72781400	1.30421000	3.09050600
H	-1.17885200	3.60871400	0.53626900				
H	-2.33459200	2.93600700	1.71264600	⁵ TS ₆₋₇			
H	-0.79938400	3.61861700	2.30229000	C	-1.69658300	7.30210300	-2.02175500
H	0.53134600	-1.39056600	0.49045300	C	-2.05983300	6.05885000	-2.78448900
H	0.10084300	1.04738700	3.29202100	C	-3.29251500	5.45360600	-2.88718200
H	-1.66466400	0.48382700	2.78562500	C	-1.17435300	5.29551000	-3.63457000
H	1.35993000	2.37789500	1.53099100	N	-3.22931200	4.37112300	-3.74177300
H	1.13867800	0.82066200	0.66638800	C	-1.94658100	4.24992200	-4.22122200
H	0.72248700	2.36172800	-0.14582300	C	0.19157100	5.40386500	-3.96948600
H	-5.62533700	0.30015400	-0.46022500	C	-1.39188200	3.33123800	-5.12630200
H	-5.06735300	1.08269600	1.00393300	C	0.74551800	4.49225300	-4.86380300
H	-5.85681800	1.07308400	-4.56252200	C	-0.04120200	3.46825600	-5.43934000
H	-5.51319300	0.31340000	-6.10557300	C	-0.84876300	3.72215200	7.68402500
H	-3.29077000	1.57049900	-6.18608900	C	-1.30624900	3.79299200	6.21374400
H	-3.59715000	2.13687600	-4.54948000	C	-1.13037900	2.49618800	5.41374000
H	-1.52353000	-0.67951700	-3.79440500	O	-0.15122800	2.31780400	4.69559800
H	-1.57881900	1.04593000	-3.94120600	N	-2.11888200	1.58411700	5.57241900
H	2.40050200	-1.35642600	-4.33622700	C	-0.23836700	-8.25848800	2.04255500
H	3.14127700	-0.95648800	-2.77085500	C	-0.39997200	-7.07007000	2.98249300
O	1.94050100	-2.15617700	-0.53996800	C	0.15081800	-5.76426000	2.50708000
H	10.79711900	-1.60037400	-4.71883500	N	0.12791800	-4.64692700	3.32031100
H	5.47038800	-5.58793000	-1.53610000	C	0.61296400	-5.32317500	1.29393600
H	2.07409000	8.27065800	-0.79977800	C	0.52426400	-3.58857300	2.60435400
H	1.81631700	2.87128200	7.30902600	N	0.83796400	-3.95961100	1.36314100
H	3.18474900	2.63936000	6.22787100	C	-3.99828000	-3.74543800	-0.40615400
H	0.78396800	0.31352600	7.57530700	C	-3.55014400	-2.57409500	-1.29526200

C	-2.11454200	-2.06684400	-1.13926300	O	7.12843000	0.43755900	-0.57229000
O	-1.24228300	-2.87775600	-0.65305700	O	7.51278800	0.04163800	-2.72826100
O	-1.82822900	-0.91587900	-1.50959700	C	-4.04955300	-0.71836200	3.51497400
C	-2.49638800	-1.70315200	-8.32204000	N	-5.27346500	1.79269500	1.02005100
C	-1.79834400	-2.34785600	-7.11740700	O	-2.89963100	-0.67771100	4.02624800
C	-0.76465100	-1.43504400	-6.45608100	C	-4.72648900	0.65245200	3.17481400
C	0.03871700	-2.12208700	-5.35212100	N	-0.78880100	1.18966900	-0.20182100
O	-0.09471700	-3.30330400	-5.07467100	O	-4.73203400	-1.72654500	3.24785000
N	0.94284700	-1.32388300	-4.71364800	C	-5.14731600	0.74109100	1.73863400
C	-3.24593400	-7.28352400	5.29815800	C	0.47356800	1.54868900	-0.90408800
C	-3.66497900	-5.89682500	4.79526100	C	-1.84128600	2.24275600	-0.38434100
C	-2.64567100	-4.77790900	5.00479100	C	-0.57594500	0.86524500	1.19894800
O	-1.50087800	-5.02008400	5.42789200	Fe	0.66531100	-2.62322500	-0.22040400
N	-3.04558900	-3.55049800	4.66400700	C	4.81795400	-1.48820900	-1.15859600
C	3.36925200	-7.94741600	-2.10028200	H	4.78904500	-2.33004900	-1.85909200
C	3.16848800	-6.87326000	-3.18252800	H	5.55008400	-1.73869800	-0.37855800
C	2.17634300	-5.83704600	-2.75405500	H	-6.30066900	1.71501500	-8.94105800
N	0.84359500	-5.82287500	-3.12594900	H	-5.13152500	2.49922400	-7.90706400
C	2.29108400	-4.82301600	-1.83833300	H	-4.99674200	0.76707100	-8.22172700
C	0.21829100	-4.82964900	-2.46076600	H	-1.75802900	-1.35124300	-9.01222200
N	1.06991500	-4.21055800	-1.66292200	H	-3.11401300	-2.43281700	-8.80241400
C	8.65795900	-0.90558200	2.08468700	H	-3.12131100	-0.85157100	-8.03110000
N	7.84329500	-0.13535000	3.03364300	H	-0.88484500	4.71978100	8.07341300
C	6.50477400	0.01998800	2.91576200	H	0.15900500	3.36107500	7.73959800
N	5.92043000	-0.11313200	1.74458500	H	-1.49139700	3.07369000	8.29462100
N	5.79009900	0.30967600	4.02511700	H	2.47141300	-8.50750600	-1.94220500
C	11.81130600	3.23904700	0.00977700	H	3.68348000	-7.50886700	-1.17621000
N	11.51197000	2.07358700	-0.81218200	H	4.14611100	-8.66087600	-2.41259800
C	10.26473400	1.62713400	-1.10043200	H	-0.65941600	-8.11051100	1.06999600
N	9.18991100	2.15334900	-0.52352500	H	0.78846200	-8.54361800	1.94696300
N	10.10159700	0.61275000	-1.95225700	H	-0.75858000	-9.12384900	2.47726900
C	-5.69002200	1.60104300	-8.06839600	H	-3.19187400	-7.30241900	6.36697600
C	-6.68534700	1.35845500	-6.90960000	H	-3.98631500	-7.98108000	4.96646200
C	-6.14307300	1.33805500	-5.49244700	H	-2.27125900	-7.59082500	4.91219700
C	-5.08997600	0.48373200	-5.11807200	H	-5.06040300	-3.74476600	-0.27436300
C	-6.72108600	2.11511900	-4.47598800	H	-3.68673100	-4.69944600	-0.77786000
C	-4.64166700	0.40307000	-3.80379500	H	-3.57563700	-3.63487400	0.60063900
C	-6.29405000	2.03750800	-3.14207600	H	4.82561900	0.60205000	3.94621100
C	-5.25097000	1.16531600	-2.78787000	H	6.14566800	0.11676200	4.95012600
O	-4.77340600	1.00393200	-1.54460900	H	4.90314100	-0.21141400	1.61470800
C	3.46091700	-1.35738400	-0.45741600	H	6.44096100	0.04943400	0.84206500
C	5.25436700	-0.20026200	-1.90706700	H	8.27768800	0.20441500	3.88034500
C	6.74978300	0.10215300	-1.75315600	H	8.86127800	-0.34999600	1.16414800
O	2.48630600	-1.97843900	-0.99946500	H	9.59907800	-1.17351300	2.57516200

H	9.13410300	0.35362500	-2.28236800	H	1.55252600	-0.75911600	1.00253200
H	10.90011600	0.12575600	-2.33112600	H	0.10134500	1.50842600	1.75497200
H	9.21239700	3.00903300	0.01561900	H	-1.39122900	0.36156000	1.70661100
H	8.30888300	1.58259700	-0.55482500	H	0.87658600	2.47634800	-0.48216500
H	12.24745800	1.77424100	-1.43920500	H	1.18070500	0.73057700	-0.76261300
H	12.81917100	3.13002700	0.42679600	H	0.26095500	1.69064800	-1.96673700
H	11.11393300	3.30893300	0.85042100	H	-3.66916200	-2.82424600	-2.36261900
H	-7.46611900	2.13182900	-6.96691300	H	-4.18593600	-1.69517600	-1.13803300
H	-7.21030500	0.40498600	-7.09526300	H	-2.53817600	-2.66448000	-6.36714000
H	-7.54346400	2.79238200	-4.71983000	H	-1.29309200	-3.26994100	-7.44004200
H	-4.61663500	-0.14851400	-5.86931700	H	-0.04536600	-1.06440900	-7.20678400
H	-3.82085600	-0.25561600	-3.52624700	H	-1.24780300	-0.53852900	-6.03681000
H	-6.78541900	2.63946800	-2.37484900	H	1.47761400	-1.70638100	-3.94583900
H	-5.22617700	1.47997500	-0.80694300	H	1.00081300	-0.33259100	-4.89094600
H	0.41441100	2.78282500	-6.15677000	H	5.00519400	-0.27429400	-2.97234800
H	1.79864900	4.57676400	-5.13840700	H	4.72234900	0.66929500	-1.49388100
H	-2.00178400	2.54971300	-5.57713000	O	3.37852900	-0.66599800	0.58022500
H	0.80624400	6.19838900	-3.54290400	H	11.77258900	4.12727200	-0.58571700
H	-4.23443200	5.72380500	-2.41686400	H	8.11212200	-1.79534100	1.84905200
H	-4.00303700	3.75841800	-3.96115800	H	-1.24437900	7.99948100	-2.69570600
H	-0.97498800	7.09720000	-1.21561400	H	-2.35778800	4.11977600	6.16882400
H	-2.57871800	7.77554600	-1.57210300	H	-0.71260100	4.55395700	5.68961300
H	-3.87751900	-5.92952700	3.71303700	H	-2.92041200	1.80815500	6.14379500
H	-4.61609200	-5.59531900	5.26150500	H	-2.20282500	0.73406800	4.99043500
H	-2.43229300	-2.74077400	4.73066000	O	0.65142400	-1.11977400	0.88014900
H	-3.92397200	-3.30078600	4.19892200	C	3.19687200	5.09511500	3.75612500
H	-1.46856500	-6.90778400	3.17439200	C	4.57554800	5.00356900	3.14057500
H	0.04157600	-7.30986400	3.96114900	C	4.78984900	4.31298800	1.93306200
H	0.77292300	-5.88150100	0.38044200	C	5.68621300	5.63260400	3.72368200
H	-0.31238100	-4.64016700	4.26766400	C	6.04581500	4.25521400	1.32744500
H	0.53646300	-2.56765900	2.97048800	C	6.95441900	5.57949600	3.13492600
H	4.12565400	-6.37719900	-3.39909400	C	7.13790100	4.89234200	1.93003000
H	2.84662400	-7.33647800	-4.12706300	O	8.36316200	4.81054500	1.31237900
H	0.42459000	-6.37321500	-3.86403200	H	8.95419300	5.46320400	1.70035200
H	3.16916100	-4.50708600	-1.28877300	H	7.79742800	6.08002600	3.61842100
H	-0.82761200	-4.58242300	-2.58577600	H	6.18279000	3.72811300	0.38437000
H	-5.63971200	0.70156100	3.79029900	H	5.56707500	6.18199700	4.65956300
H	-4.10004200	1.51215600	3.45004300	H	3.95040400	3.81463200	1.44294000
H	-1.15437000	0.30833500	-0.67764000	H	2.54676700	5.75440600	3.16011900
H	-5.35893700	-0.22127200	1.25341400	H	3.23565400	5.50721800	4.77226800
H	-5.08033300	2.64312800	1.55759900	H	2.69864400	4.11762600	3.81091000
H	-1.98347800	2.41785300	-1.45178400				
H	-2.77719400	1.88237300	0.04480600	57			
H	-1.51544600	3.16274100	0.11244800	C	1.54953300	7.69424700	-0.06641300

C	0.39138500	7.01669100	-0.74328100	C	6.45231000	-5.16776500	-1.46954000
C	-0.94444800	7.10435200	-0.42515900	N	6.54606300	-4.55068100	-0.13760100
C	0.46015900	6.21144200	-1.94261000	C	5.52589600	-3.84974300	0.41569200
N	-1.70570800	6.41289800	-1.34694300	N	4.65766100	-3.22625200	-0.34668400
C	-0.87601100	5.85886500	-2.29179800	N	5.42661200	-3.81129600	1.76329600
C	1.51672500	5.77303600	-2.76724900	C	10.52850800	-2.53872800	-4.28018600
C	-1.17308700	5.10381100	-3.43701900	N	9.33631100	-3.07333900	-4.92975500
C	1.22608000	5.01716000	-3.89930800	C	8.06148900	-2.71212200	-4.63528000
C	-0.10768600	4.69054000	-4.23360500	N	7.78439000	-1.96167600	-3.57415200
C	3.25455200	1.39768700	8.00618500	N	7.05143200	-3.13884800	-5.39461200
C	2.37208500	2.07867300	6.94576100	C	-6.52429500	6.59443900	-4.38150500
C	1.17356500	1.22584000	6.54438200	C	-7.12323500	6.47319000	-2.95778000
O	1.25711000	0.43068400	5.59748700	C	-6.23550600	6.05014600	-1.80133300
N	0.07079800	1.39517900	7.28782200	C	-5.54073300	4.82708700	-1.77585100
C	-4.50487600	-7.18982500	1.54113000	C	-6.14470400	6.85707100	-0.65538000
C	-3.67485200	-6.33224800	2.49673000	C	-4.80576600	4.42034300	-0.66003900
C	-2.80971000	-5.26171000	1.89235900	C	-5.42305100	6.46238100	0.47519000
N	-1.93934300	-4.54977800	2.69541300	C	-4.75760900	5.22968500	0.48581300
C	-2.71049000	-4.67098800	0.65338900	O	-4.05484000	4.78109400	1.56349300
C	-1.36917400	-3.57652900	1.96319700	C	1.44423800	-2.20082500	-1.22490300
N	-1.81249000	-3.61672500	0.71216000	C	3.03544100	-1.46176900	-3.12728500
C	-5.74789600	-0.95185900	1.32901800	C	4.37321800	-1.97374700	-3.67395200
C	-4.98974000	0.09610200	0.49039000	O	0.23967200	-1.77739100	-1.37086400
C	-3.54697600	-0.34045100	0.25884600	O	5.25468600	-2.27879900	-2.78994800
O	-3.31933700	-1.06045200	-0.76549500	O	4.56746300	-2.07046200	-4.89621500
O	-2.65158300	-0.05784100	1.08135500	C	-3.36213800	-0.15310100	8.09626500
C	-5.89900500	2.43966400	-6.25808100	N	-1.45357600	2.12387800	9.94303900
C	-5.26158000	1.25168500	-5.52648900	O	-2.46603100	0.16257100	7.26177500
C	-3.75839700	1.45437800	-5.29903600	C	-3.44222900	0.70507200	9.40239600
C	-2.99909000	0.17211000	-4.95678800	N	-2.15261500	0.84258000	3.56439900
O	-3.39275700	-0.93198100	-5.30133400	O	-4.17882700	-1.08439100	8.00215100
N	-1.82448700	0.35080600	-4.29108800	C	-2.56212400	1.91974800	9.34589900
C	-5.32610400	-5.96740400	5.83346200	C	-1.12493500	1.91147200	3.51460600
C	-4.95036000	-4.48123700	5.73114800	C	-3.41938400	1.30339800	4.18654400
C	-3.44408400	-4.25095500	5.85732100	C	-1.67442300	-0.44723600	4.26729100
O	-2.63651800	-5.00589400	5.29137700	Fe	-1.58145800	-2.10807500	-0.75239900
N	-3.04230000	-3.19911100	6.57945000	C	2.16794400	-2.60224100	-2.52187800
C	-2.78941100	-7.34854400	-3.68412400	H	1.43230700	-2.93277700	-3.26443900
C	-2.66692300	-6.14168800	-4.61823800	H	2.79707700	-3.47005700	-2.28142500
C	-2.69372500	-4.84810100	-3.87498300	H	-7.20837100	7.23401600	-4.90169100
N	-3.72420500	-3.93132800	-3.92804700	H	-5.55107800	7.03867300	-4.38569800
C	-1.83543800	-4.35814100	-2.92392400	H	-6.46781900	5.63114200	-4.89908400
C	-3.46667700	-2.94147400	-3.04734100	H	-5.34291800	2.60027500	-7.15842000
N	-2.33112900	-3.18025100	-2.41789500	H	-6.92529200	2.25970600	-6.50068400

H	-5.84505000	3.36020800	-5.66405700	H	1.21790600	8.36640000	0.73507900
H	3.88508200	2.13028200	8.46735600	H	-5.25418800	-4.06434700	4.75586100
H	3.86154500	0.61405800	7.60108800	H	-5.48526500	-3.89574000	6.49185800
H	2.63758300	0.96517900	8.80689000	H	-2.04330300	-3.04460000	6.63920300
H	-3.74662100	-7.44990200	-3.21721700	H	-3.63675900	-2.48855800	7.05004200
H	-2.02164800	-7.40560100	-2.94125100	H	-4.34957400	-5.82209100	3.19631400
H	-2.67342400	-8.26509400	-4.28672600	H	-3.04534000	-6.97578100	3.12857600
H	-5.05265100	-6.57954700	0.85361200	H	-3.22704100	-4.92132600	-0.26624200
H	-3.88624900	-7.87259600	0.99727000	H	-1.90020400	-4.68395200	3.72067700
H	-5.22718100	-7.78556900	2.11418700	H	-0.66338400	-2.85360400	2.36211500
H	-4.96558300	-6.32912000	6.77415500	H	-1.72611600	-6.21262100	-5.18490600
H	-6.38541800	-6.10792100	5.78012400	H	-3.47123300	-6.16289900	-5.36771400
H	-4.84766100	-6.56287100	5.05090600	H	-4.48726100	-3.92882900	-4.59169900
H	-6.53733800	-0.50097100	1.89359100	H	-0.91112900	-4.79430500	-2.56115400
H	-6.13618600	-1.78024600	0.77355200	H	-4.10894900	-2.08629300	-2.88193200
H	-5.07065900	-1.38314800	2.08078100	H	-4.49484800	0.98795600	9.55256200
H	4.78103300	-3.16708800	2.19919700	H	-3.16515000	0.05115200	10.24434000
H	5.84977100	-4.51908100	2.34533700	H	-2.37059500	0.56297200	2.56968300
H	3.73162300	-2.87697200	-0.02603000	H	-2.89985800	2.71338700	8.66007300
H	4.91229800	-2.91523000	-1.31846800	H	-1.22850200	1.32684200	10.55079500
H	7.31347300	-4.81027500	0.46615600	H	-3.79673900	2.17255800	3.64162400
H	6.59619200	-4.43975300	-2.27336400	H	-4.15548600	0.49640700	4.14032500
H	7.20284100	-5.96115400	-1.54144300	H	-3.23594600	1.54377500	5.23751600
H	6.07665500	-2.75589200	-5.23960000	H	0.22679900	-0.40363600	4.56034200
H	7.22080500	-3.75703800	-6.17393300	H	-1.82309400	-0.27895500	5.34481000
H	8.51089100	-1.54458700	-3.01412500	H	-2.38847300	-1.20414300	3.92420400
H	6.78779300	-1.97090500	-3.22592500	H	-0.91566300	2.26607000	4.52891500
H	9.48066500	-3.47399100	-5.84747000	H	-0.21631600	1.50347900	3.06645200
H	11.35215300	-3.24860500	-4.41744600	H	-1.50338200	2.73310400	2.89753800
H	10.37151600	-2.42617400	-3.20233500	H	-5.48701500	0.25684300	-0.47511400
H	-7.55574400	7.44895000	-2.69296000	H	-4.97894700	1.05384000	1.02433700
H	-7.98446600	5.78467600	-3.00322700	H	-5.76097600	1.06751700	-4.56151400
H	-6.66316900	7.81786000	-0.63076600	H	-5.39752200	0.33584800	-6.11876700
H	-5.58296500	4.16286500	-2.63996700	H	-3.29251400	1.83783400	-6.22361500
H	-4.27211700	3.47089400	-0.65924700	H	-3.57508500	2.22158000	-4.53237100
H	-5.39020400	7.11352100	1.35250500	H	-1.27755300	-0.45982400	-4.03418300
H	-4.12852800	5.41735900	2.28184000	H	-1.52375000	1.25098300	-3.94854400
H	-0.30581200	4.11715700	-5.14129000	H	2.48647400	-0.94847300	-3.92573100
H	2.03618700	4.67974200	-4.54823100	H	3.27536800	-0.71957100	-2.35240200
H	-2.20358700	4.86934900	-3.70280500	O	2.03448300	-2.28600400	-0.14081900
H	2.55072200	6.02676600	-2.52793200	H	10.79707700	-1.60036500	-4.71884100
H	-1.42302000	7.63093000	0.39624500	H	5.47038700	-5.58792800	-1.53609800
H	-2.70974700	6.31413200	-1.31682400	H	2.07385400	8.27081700	-0.79982200
H	2.25834400	6.97118600	0.36612100	H	2.01338500	3.04253200	7.33654700

H	2.95160600	2.28901800	6.03788500	C	-4.38258000	-2.78518200	2.92441600
H	0.06107600	2.02963300	8.07988900	C	-4.07681100	-2.14222600	1.55982700
H	-0.78716600	0.82643800	7.20255300	C	-2.69319400	-2.56236400	1.07111700
O	-0.40769900	-0.79351400	3.90775100	O	-1.69738500	-1.80527400	1.47742600
C	5.51958900	0.83984200	3.36724700	O	-2.52783800	-3.56543500	0.39489200
C	6.58529900	0.56566800	2.32936500	C	-3.37415700	-7.75505700	-3.14983900
C	6.31986500	0.72518700	0.95670500	C	-2.59578700	-7.23249600	-1.92627600
C	7.88305900	0.17468000	2.69202500	C	-1.34049000	-6.43746500	-2.29949600
C	7.29873900	0.50584300	-0.01217800	C	-0.32422300	-6.29228000	-1.16800500
C	8.87544800	-0.05593100	1.73291900	O	-0.27861200	-7.04900600	-0.20700900
C	8.58685800	0.10876000	0.37262100	N	0.58781000	-5.29216500	-1.34220000
O	9.51286400	-0.11828300	-0.60998400	C	-3.73116700	0.98944600	8.70837300
H	10.38394000	-0.20289000	-0.21026700	C	-3.98018600	1.34583100	7.24205600
H	9.87624700	-0.36065500	2.05066400	C	-2.80746500	2.05258900	6.56154000
H	7.07339400	0.64496000	-1.06916000	O	-1.68173200	2.08872500	7.09129400
H	8.13437400	0.04529600	3.74694200	N	-3.05105700	2.58542000	5.36203400
H	5.32312100	1.03206300	0.63264100	C	2.31222600	-6.29978300	5.66228600
H	5.38770000	1.92218200	3.52021900	C	2.12280000	-6.61327000	4.16430400
H	5.77798700	0.40193900	4.34003600	C	1.31124500	-5.58255900	3.42369800
H	4.54184000	0.43753600	3.06672400	N	0.34621600	-5.89024100	2.48060000
				C	1.31558700	-4.20689900	3.47265700
				C	-0.19163700	-4.74596000	2.01426600
				N	0.37058900	-3.70167600	2.60106400
				C	8.45222000	0.37567600	2.08317500
				N	7.79738900	1.68665300	1.96637200
				C	6.46413300	1.83080300	1.78819700
				N	5.76650900	0.88143700	1.20145200
				N	5.87125900	2.96054900	2.23023300
				C	11.81505800	0.44762900	-2.40157600
				N	11.31392000	-0.80463600	-1.84803200
				C	10.00410200	-1.11649000	-1.68954300
				N	9.04979500	-0.21630100	-1.90632700
				N	9.65168900	-2.33422900	-1.27602200
				C	-6.24443500	-5.50509700	-5.95676100
				C	-7.10564900	-4.54502100	-5.10925800
				C	-6.32436100	-3.56360400	-4.25639800
				C	-5.52053500	-4.01748500	-3.19416200
				C	-6.37182200	-2.17892500	-4.47112900
				C	-4.77521700	-3.14709800	-2.40634800
				C	-5.64223000	-1.28118400	-3.67627200
				C	-4.82121000	-1.76027200	-2.64073100
				O	-4.05910400	-0.97466400	-1.85825800
				C	3.05542300	-1.39189900	1.04796700
				C	4.77686700	-2.10724100	-0.72345500
⁵TS₆₋₈							
C	-1.38980700	2.18508300	-7.47223100				
C	-1.69928000	0.92526600	-6.71298000				
C	-2.93232400	0.47470100	-6.29660000				
C	-0.75771300	-0.10783900	-6.34324400				
N	-2.81865100	-0.76356700	-5.69945700				
C	-1.50051200	-1.14975500	-5.71297600				
C	0.63633100	-0.26279500	-6.49355200				
C	-0.89022200	-2.32312700	-5.24268400				
C	1.24513800	-1.42372400	-6.02500900				
C	0.48737500	-2.44565800	-5.40786200				
C	-0.23573700	8.48361800	0.69671200				
C	-0.79760200	7.30571600	-0.11852900				
C	-0.75614100	5.96723300	0.62175100				
O	0.17917400	5.18316300	0.46534800				
N	-1.79190600	5.72558800	1.45502100				
C	-1.03534300	-2.58190600	7.95263200				
C	-1.05452400	-1.14792800	7.43424200				
C	-0.50271600	-0.92097000	6.06366100				
N	-0.27769500	0.35473100	5.58073600				
C	-0.25088300	-1.75954700	5.00995100				
C	0.06465900	0.27024100	4.28877300				
N	0.10810500	-1.00462100	3.90671600				

C	6.29529200	-1.97490100	-0.88806100	H	8.59259000	-0.10501800	1.11046000
O	1.99334200	-2.08704200	1.17223000	H	9.41927400	0.51214900	2.57713800
O	6.78784200	-0.82286700	-0.60220000	H	8.63233700	-2.61385100	-1.26896200
O	6.97338200	-2.93606300	-1.28088400	H	10.35358100	-3.01838700	-1.03590100
C	-3.72231900	2.84413700	2.22467200	H	9.24877400	0.68441000	-2.31282600
N	-4.14880200	1.70942000	-1.39317300	H	8.10210700	-0.40664000	-1.48889200
O	-2.53065600	3.19243900	2.48583200	H	11.95946500	-1.58346400	-1.85993200
C	-4.18307100	2.99486900	0.74788100	H	12.84226200	0.60077900	-2.05114100
N	-0.61360000	1.58896400	-0.79334200	H	11.22081500	1.29660200	-2.04834400
O	-4.56023000	2.38808000	3.01792400	H	-7.77690500	-3.98538100	-5.77809000
C	-3.70860700	1.87558400	-0.16643900	H	-7.76528300	-5.14166200	-4.45705000
C	0.65321600	2.32220300	-1.12261500	H	-7.00119700	-1.77830300	-5.26974100
C	-0.99227600	0.64678000	-1.88581100	H	-5.48534100	-5.08365500	-2.96757400
C	-1.64979300	2.55816700	-0.43409000	H	-4.15407600	-3.51661100	-1.59149200
Fe	0.12735100	-1.61156000	1.92176500	H	-5.72279900	-0.20700100	-3.85360300
C	4.34318900	-2.17125000	0.76714500	H	-4.23359300	-0.00373400	-1.93123700
H	4.21352400	-3.21477800	1.07598500	H	0.99060000	-3.35359900	-5.06938600
H	5.12093900	-1.73567100	1.40919600	H	2.32137300	-1.55809800	-6.14827900
H	-6.89794000	-6.12604200	-6.53629600	H	-1.47989800	-3.11295800	-4.77794500
H	-5.60106100	-4.95870300	-6.61379900	H	1.23123000	0.51238500	-6.97981700
H	-5.62346000	-6.15598000	-5.32988100	H	-3.90602400	0.94671400	-6.39767300
H	-2.65373100	-8.23256100	-3.78101000	H	-3.58374100	-1.27699000	-5.27957800
H	-4.08254900	-8.47944500	-2.80631900	H	-0.70179700	2.84292500	-6.91870700
H	-3.87715100	-6.96389500	-3.71370200	H	-2.30022500	2.75783800	-7.69081900
H	-0.15997000	9.33547800	0.05110400	H	-4.19349200	0.44089800	6.64734700
H	0.73801800	8.24261000	1.07413900	H	-4.88026200	1.97144900	7.14158200
H	-0.88168300	8.74336700	1.54633600	H	-2.29155600	2.98214900	4.81724300
H	1.38105500	-6.36612700	6.18506200	H	-3.87867100	2.41971400	4.77073200
H	2.72220400	-5.31929600	5.78674300	H	-2.09239900	-0.79160000	7.41591400
H	3.00806400	-7.02000200	6.11327800	H	-0.53291400	-0.48858500	8.14273200
H	-1.50344100	-3.28869600	7.29964900	H	-0.33764700	-2.83702900	4.96253400
H	-0.04551200	-2.91397000	8.18676600	H	-0.55634500	1.20822100	6.11036600
H	-1.59791000	-2.61722200	8.89665000	H	0.23362700	1.12051900	3.63776200
H	-3.61064200	1.88186800	9.28707700	H	3.10948700	-6.70692800	3.68040800
H	-4.54943500	0.42048400	9.09754500	H	1.64113200	-7.59534500	4.04701500
H	-2.81477700	0.40791600	8.83753700	H	0.14345700	-6.79283400	2.05957000
H	-5.41941800	-2.72398500	3.18269200	H	1.93884000	-3.55591900	4.07588100
H	-4.07850200	-3.81133200	2.91539700	H	-0.97616200	-4.69300000	1.26216300
H	-3.81525800	-2.28375700	3.72067900	H	-5.27926100	2.97561600	0.72288100
H	4.93347500	3.19309000	1.93401800	H	-3.86993000	3.96937200	0.34602200
H	6.31298900	3.56285100	2.90919600	H	-0.35852500	0.99135600	0.07331300
H	4.73955400	0.79824400	1.25437900	H	-3.33255500	0.96987700	0.32356900
H	6.21285200	0.19677600	0.53677000	H	-4.64112000	2.54416300	-1.72439300
H	8.33000800	2.51618400	2.18873200	H	-0.14125700	-0.01095000	-2.08460300

H	-1.85115000	0.04776400	-1.57970800	58			
H	-1.24208900	1.21031000	-2.78927400	C	1.54937500	7.69448700	-0.06650900
H	1.31425200	0.30767900	1.17282300	C	0.57843600	6.79142000	-0.77503300
H	-1.81918100	3.30422800	-1.21151400	C	-0.79606700	6.81091700	-0.70065400
H	-1.58715700	2.89807600	0.60436800	C	0.90631800	5.79449100	-1.77009700
H	0.53843400	2.82176000	-2.09107200	N	-1.33948900	5.89802100	-1.58373600
H	0.83203000	3.07396900	-0.34787000	C	-0.32366000	5.26450300	-2.25827300
H	1.47131800	1.59634300	-1.16906100	C	2.11648100	5.30604400	-2.30528400
H	-4.80158700	-2.48248300	0.81181800	C	-0.36843300	4.28540400	-3.26246900
H	-4.14627000	-1.05203200	1.63694600	C	2.07558800	4.32569300	-3.29295200
H	-3.23728800	-6.62263000	-1.27414100	C	0.84340100	3.82347200	-3.77065700
H	-2.27795800	-8.09219000	-1.31888600	C	3.25319500	1.39755700	8.00701500
H	-0.80018900	-6.95148700	-3.11435700	C	2.44025200	2.09176300	6.89773200
H	-1.60250500	-5.44428000	-2.69121200	C	1.62473100	1.14294600	6.01252400
H	1.27230300	-5.12094900	-0.61822800	O	2.10173300	0.67150500	4.98109900
H	0.45959800	-4.57575500	-2.04110500	N	0.37331300	0.86365900	6.44037700
H	4.42726800	-2.99796900	-1.25877400	C	-4.50489400	-7.18974500	1.54118100
H	4.33145600	-1.22515500	-1.20575200	C	-3.69628700	-6.40436500	2.56697000
O	3.10839500	-0.14513600	1.13553300	C	-2.71067200	-5.41597000	2.03054600
H	11.81573800	0.40664300	-3.47086500	N	-1.84834600	-4.74415900	2.87725200
H	7.81693800	-0.23117600	2.69413500	C	-2.51651100	-4.85757700	0.79386800
H	-0.92274200	1.92935000	-8.40038600	C	-1.20219400	-3.80572000	2.17559700
H	-1.82749600	7.52952000	-0.43884200	N	-1.57286700	-3.85012700	0.89626100
H	-0.19871400	7.17229000	-1.02913800	C	-6.07476300	-1.42224000	0.64588600
H	-2.55351200	6.38499700	1.52201300	C	-5.17801900	-0.17879500	0.63568400
H	-1.92295800	4.80828800	1.91615400	C	-3.79834700	-0.28241700	-0.01764500
O	0.35066200	0.13616800	1.19232000	O	-3.23811500	-1.46988000	0.01662600
C	4.16346400	6.46075600	-1.37151400	O	-3.24472100	0.69083100	-0.50737800
C	5.39391100	5.66709300	-1.75252900	C	-5.89890900	2.43962000	-6.25818500
C	5.33640700	4.28247600	-1.98721400	C	-5.33961800	1.20701000	-5.53220700
C	6.63823800	6.29555600	-1.92644000	C	-3.84313300	1.29861400	-5.22403300
C	6.46015600	3.55088800	-2.38011000	C	-3.20957900	-0.03857700	-4.83478700
C	7.77312800	5.58026600	-2.31686000	O	-3.72058000	-1.11731400	-5.09584100
C	7.68888400	4.20057200	-2.54916000	N	-1.98719800	0.05448200	-4.23292500
O	8.77324400	3.45544100	-2.92930100	C	-5.32616400	-5.96718400	5.83358900
H	9.48950900	4.04820900	-3.17710400	C	-4.99111900	-4.48161500	5.67695700
H	8.72562300	6.10151600	-2.44356900	C	-3.49587700	-4.17172200	5.60551100
H	6.38699900	2.47926700	-2.56593500	O	-2.65786300	-5.07463600	5.42775100
H	6.73053300	7.37056700	-1.75836800	N	-3.15155700	-2.88480300	5.70525300
H	4.38606800	3.75726000	-1.87109700	C	-2.78939200	-7.34883300	-3.68441400
H	3.72824700	6.95479400	-2.25446100	C	-2.68496100	-6.03263300	-4.47510000
H	4.40189900	7.25011200	-0.64531900	C	-2.75434100	-4.82406100	-3.58929800
H	3.38054400	5.82782700	-0.93543300	N	-3.82986700	-3.95762200	-3.53216000
				C	-1.88988600	-4.36659600	-2.62553200

C	-3.59386900	-3.03273400	-2.58009100	H	-5.34292100	2.60022500	-7.15843100
N	-2.42660000	-3.25961700	-2.00339900	H	-6.92530800	2.25974400	-6.50064600
C	6.45231000	-5.16777100	-1.46953900	H	-5.83446400	3.34455000	-5.64264100
N	6.53883800	-4.49635700	-0.16360400	H	3.88573600	2.13003000	8.46685500
C	5.54047700	-3.74840000	0.36028500	H	3.86192600	0.61452400	7.60076100
N	4.66078800	-3.16417300	-0.42680600	H	2.60235200	0.96305200	8.77807400
N	5.46457600	-3.62271800	1.70245800	H	-3.74657000	-7.44978100	-3.21708600
C	10.52847100	-2.53871200	-4.28019400	H	-2.02172500	-7.40545700	-2.94116000
N	9.37193700	-3.10433600	-4.96466900	H	-2.66283300	-8.20574300	-4.36183400
C	8.08215100	-2.77209200	-4.71160800	H	-5.05261300	-6.57960100	0.85353700
N	7.76131500	-1.99413300	-3.68226500	H	-3.88625600	-7.87260800	0.99727700
N	7.10286000	-3.25333200	-5.47822500	H	-5.24711100	-7.80121900	2.07346800
C	-6.52447100	6.59460400	-4.38093000	H	-4.96561300	-6.32900800	6.77420900
C	-7.12982800	6.55550100	-2.95521600	H	-6.38537900	-6.10814400	5.77994500
C	-6.53347400	5.65152900	-1.89456700	H	-4.85648300	-6.57676600	5.05717500
C	-7.17474900	4.45252100	-1.53689400	H	-6.99090500	-1.21759000	1.16002400
C	-5.40779200	6.02069200	-1.14007000	H	-6.29186000	-1.76744800	-0.34359600
C	-6.73545500	3.66974300	-0.47217300	H	-5.58147100	-2.24804300	1.17612000
C	-4.94727200	5.24165700	-0.07178500	H	4.87846400	-2.91050100	2.11569100
C	-5.61558600	4.05590000	0.28529300	H	5.94410900	-4.25613800	2.32514200
O	-5.26909900	3.29255900	1.33587200	H	3.76399700	-2.78082500	-0.09751500
C	1.34577000	-2.40230700	-1.47020200	H	4.89301600	-2.90920100	-1.42443600
C	2.97688500	-1.67796000	-3.32757700	H	7.31663100	-4.71876300	0.44211100
C	4.35038600	-2.13647000	-3.82913600	H	6.61188000	-4.47439600	-2.30048500
O	0.08292600	-2.32488500	-1.64508500	H	7.19896500	-5.96720800	-1.49842000
O	5.22553600	-2.36656200	-2.91522200	H	6.11545100	-2.89867200	-5.35400000
O	4.57457600	-2.26191500	-5.04189800	H	7.30624700	-3.89668100	-6.22857800
C	-2.83593000	0.19591800	4.76762400	H	8.46347500	-1.53442000	-3.12412100
N	-2.65556100	3.23645500	2.46835300	H	6.76192400	-2.02077800	-3.35175500
O	-1.70798400	-0.36595800	4.87194900	H	9.55450400	-3.52701300	-5.86554000
C	-2.84009400	1.69123800	4.30630100	H	11.37035900	-3.23319900	-4.38167700
N	-0.05790600	1.42500600	1.61522400	H	10.33204700	-2.42096200	-3.20969700
O	-3.95255600	-0.29629700	5.00302000	H	-7.12618300	7.58808800	-2.56841200
C	-2.22548500	1.92742600	2.89035300	H	-8.19445100	6.29396800	-3.05524800
C	1.42427000	1.40985000	1.77490000	H	-4.90369000	6.96631000	-1.35834100
C	-0.47960100	2.29525700	0.48381400	H	-8.06419600	4.13581800	-2.08712800
C	-0.70395500	1.73375400	2.93617500	H	-7.26971700	2.76166500	-0.19392800
Fe	-1.49546400	-2.18222500	-0.32468900	H	-4.09829300	5.57579500	0.52664400
C	2.16378400	-2.83691200	-2.69097300	H	-4.34997400	3.44836600	1.64552200
H	1.49821600	-3.28083900	-3.43973100	H	0.84211100	3.07030900	-4.56080600
H	2.84070900	-3.63077300	-2.34533700	H	3.00624200	3.94694400	-3.71939700
H	-7.20827800	7.23396900	-4.90187100	H	-1.32069500	3.91421100	-3.64105900
H	-5.55105100	7.03861100	-4.38597600	H	3.07390600	5.69729000	-1.95695700
H	-6.49442400	5.61053300	-4.85889900	H	-1.44234100	7.43196500	-0.08611300

H	-2.32551700	5.71224000	-1.69640900	H	2.07409300	8.27068900	-0.79975100
H	2.29164000	7.13011100	0.51807100	H	1.78049000	2.85243300	7.34408400
H	1.03653800	8.38538600	0.61457300	H	3.12635900	2.62037100	6.22229600
H	-5.44094400	-4.07179700	4.75617600	H	0.00706200	1.30056200	7.27354000
H	-5.43623900	-3.89616500	6.49590000	H	-0.28518700	0.30705200	5.87265300
H	-2.18524400	-2.60781700	5.56161100	O	-0.40157500	-1.10412000	0.78789200
H	-3.78318600	-2.07643600	5.60938200	C	6.34121300	1.33872600	3.74877700
H	-4.38410600	-5.83920400	3.20925600	C	7.18243700	0.89305800	2.57326700
H	-3.17372100	-7.09999100	3.23967100	C	6.61874000	0.71744300	1.29633400
H	-3.00628000	-5.08669900	-0.14384500	C	8.56348800	0.67692900	2.69958800
H	-1.87078100	-4.86575800	3.91357500	C	7.38953200	0.34783400	0.19256600
H	-0.51868600	-3.07929600	2.60116000	C	9.35110000	0.30316600	1.60612700
H	-1.73556400	-6.00947600	-5.03098100	C	8.76694400	0.13853400	0.34404000
H	-3.47839000	-5.97992600	-5.23473300	O	9.49324600	-0.22994800	-0.75712000
H	-4.59840000	-3.91753900	-4.18917800	H	10.43040600	-0.18326100	-0.54438200
H	-0.92646400	-4.77000600	-2.33728500	H	10.42403100	0.14370600	1.74163200
H	-4.27118100	-2.22195900	-2.34685000	H	6.93066900	0.22866500	-0.78874400
H	-3.87458700	2.04247200	4.28667400	H	9.04488300	0.80558300	3.67111800
H	-2.29142500	2.29774400	5.04233800	H	5.54897900	0.88448900	1.15291300
H	-0.32229200	0.42296800	1.34216600	H	6.18081100	2.42818400	3.72320000
H	-2.66264800	1.18960800	2.20475800	H	6.82731000	1.10499500	4.70478700
H	-2.13519900	3.94064400	3.00751100	H	5.34962900	0.86780100	3.75201000
H	0.09785900	2.01421900	-0.40121900				
H	-1.53997900	2.13271700	0.27402900	⁵ TS ₈₋₉			
H	-0.28271200	3.34363600	0.72749700	C	-6.59992400	-2.57177800	-2.38615200
H	0.51921400	-1.37901200	0.60191800	C	-5.53063400	-1.03612800	-3.91157200
H	-0.21283100	2.62811800	3.34644300	C	-5.88707500	-1.37924700	-2.59522700
H	-0.48940300	0.88215300	3.59224400	O	-5.62023500	-0.61240900	-1.51975600
H	1.78731400	2.43806000	1.88759300	C	2.96485700	-1.57464700	1.02441800
H	1.68210300	0.83979300	2.67369700	C	4.74108400	-2.27411900	-0.69635200
H	1.87169800	0.95789400	0.88451600	C	6.26759800	-2.17722500	-0.79470400
H	-5.67616800	0.67529500	0.16583800	O	1.88333500	-2.24510400	1.09548700
H	-4.98850400	0.12895700	1.67472800	O	6.77785400	-1.05803000	-0.42351600
H	-5.89154600	1.03357700	-4.59478100	O	6.93501600	-3.13314300	-1.21766200
H	-5.50711900	0.31333600	-6.15030100	C	-3.80334200	2.61697100	2.22003100
H	-3.29300800	1.64815200	-6.11538000	N	-3.43049100	1.27710500	-1.38902000
H	-3.65049700	2.04511100	-4.43781800	O	-2.68116500	3.09899600	2.55177300
H	-1.55311700	-0.79666900	-3.90150100	C	-4.07570800	2.45558200	0.69078200
H	-1.66996600	0.92017900	-3.82363300	N	-0.58600800	1.65036800	-0.77705500
H	2.41424600	-1.22981400	-4.15526300	O	-4.72326700	2.26058400	2.97691500
H	3.16088400	-0.89574000	-2.57705100	C	-2.97103500	1.68686300	-0.05644400
O	1.93465300	-2.15575200	-0.39705600	C	0.64794700	2.45678800	-1.01305200
H	10.79711600	-1.60037300	-4.71883600	C	-1.01214700	0.90950000	-1.98096500
H	5.47038600	-5.58792600	-1.53610200	C	-1.67738400	2.49364700	-0.16969300

Fe	-0.01065700	-1.73910700	1.76342300	H	-5.01029100	-0.09513400	-4.09683200
C	4.24153200	-2.38137300	0.77048600	H	-4.88021800	0.01593800	-1.65068700
H	4.06842600	-3.43132500	1.03266600	H	2.13644300	-1.91864900	-4.20566200
H	5.00295100	-1.99436200	1.46135400	H	3.18553100	0.13272700	-5.12732200
H	-6.80337800	-5.34942000	-7.37697400	H	-0.32213300	-2.30709600	-4.43062400
H	-5.46459800	-4.22991600	-7.30560000	H	1.82444400	1.84186200	-6.30632000
H	-5.61710900	-5.49264600	-6.07092000	H	-3.27382800	0.99293800	-6.76028400
H	-2.77414100	-7.81504600	-4.59684100	H	-2.64674100	-1.08533200	-5.49198000
H	-4.25649600	-8.07875800	-3.71048000	H	-0.38873200	3.54768900	-6.87900400
H	-3.96046300	-6.50909400	-4.48692500	H	-1.95120700	3.22769100	-7.65928800
H	0.13656800	9.31244600	0.66771400	H	-4.49121500	0.12666400	6.36773600
H	0.94518800	8.11322200	1.64518000	H	-5.20679600	1.60801800	6.96129200
H	-0.67630600	8.64145300	2.07935000	H	-2.52303400	2.85844200	4.90273700
H	0.83191400	-6.84801100	5.65725000	H	-4.11999700	2.34256100	4.75108800
H	2.22635500	-5.82653800	5.40167300	H	-2.50218400	-1.25276900	7.13219400
H	2.43696100	-7.55653200	5.61088500	H	-0.98890300	-1.06255500	7.98443800
H	-1.99517200	-3.75375500	6.86807300	H	-0.59601900	-3.15951700	4.66253600
H	-0.57018700	-3.50182100	7.84728800	H	-0.85921000	0.79757600	6.08318200
H	-2.14460400	-3.20061700	8.50511200	H	0.11652200	0.87661300	3.68213200
H	-4.01649700	1.33189900	9.14295400	H	2.65722800	-7.07461400	3.21078700
H	-4.99498400	-0.07453200	8.80003500	H	1.14380500	-7.92934400	3.45361600
H	-3.25043100	-0.13343800	8.61438500	H	-0.29384800	-6.91649600	1.50807700
H	-5.68377800	-2.73622600	2.63004300	H	1.64863000	-3.92082500	3.74857700
H	-4.36993400	-3.85124800	2.34295600	H	-1.26922900	-4.71196500	0.82369400
H	-4.09930300	-2.40464800	3.27970800	H	-5.02027300	1.91943100	0.56025300
H	4.92751800	2.86943200	2.28246900	H	-4.19950600	3.45623500	0.24913100
H	6.25527200	3.09975200	3.36558000	H	-0.30885100	0.92974100	-0.01407600
H	4.68788000	0.54723900	1.39977300	H	-2.75066400	0.76491700	0.50063500
H	6.17707100	-0.07050700	0.73388400	H	-3.61060600	2.12604800	-1.93849400
H	8.27357300	2.03140700	2.68614600	H	-0.66997900	-0.12757600	-1.97408400
H	8.49398000	-0.50914100	1.41013400	H	-2.38271200	0.86309000	-1.87064800
H	9.27059300	-0.03531400	2.95447400	H	-0.80213200	1.44267000	-2.91155500
H	8.60406900	-2.86571200	-1.11385800	H	1.27316300	0.15175300	1.10072800
H	10.30118300	-3.32528400	-0.81239300	H	-1.82035000	3.37699400	-0.80883400
H	9.34907800	0.46463000	-1.94703700	H	-1.34593600	2.82167600	0.81983400
H	8.13827300	-0.63416200	-1.23056600	H	0.46991200	3.17031900	-1.82513300
H	11.98107900	-1.88774400	-1.49316200	H	0.88189200	3.01449900	-0.10127100
H	12.91334300	0.28631800	-1.48907300	H	1.46217500	1.77796800	-1.28513400
H	11.30605400	1.01359300	-1.51192800	H	-4.89272900	-2.35587900	0.30318700
H	-7.61856900	-3.21539500	-6.66927200	H	-4.32085200	-1.00010200	1.28423500
H	-7.94710300	-4.52209200	-5.55533000	H	-3.44858000	-6.33105700	-2.02934000
H	-5.65085400	-1.54524300	-5.99970800	H	-2.58735900	-7.86184300	-2.07622500
H	-7.52024900	-4.29485300	-3.26528900	H	-0.90286900	-6.70945400	-3.70189600
H	-6.8898300	-2.83947400	-1.37044800	H	-1.62130200	-5.18627200	-3.18385200

C	-6.55385700	5.64485800	-1.88836000	H	-4.85675300	-6.57706200	5.05728800
C	-7.17327000	4.41954800	-1.58231900	H	-6.99090500	-1.21759000	1.16002400
C	-5.48117200	6.03500200	-1.06994500	H	-6.29186000	-1.76744800	-0.34359600
C	-6.76487900	3.63403100	-0.50733100	H	-5.58189500	-2.24791700	1.17671600
C	-5.05246500	5.25340800	0.01076800	H	4.88447900	-2.93356100	2.13207800
C	-5.69965400	4.04122700	0.31701100	H	5.95141800	-4.27961000	2.33164100
O	-5.39037900	3.27471100	1.37647800	H	3.76540400	-2.79443700	-0.07998600
C	1.34471000	-2.41549800	-1.45590600	H	4.89466200	-2.91081300	-1.40817000
C	2.97489000	-1.67947100	-3.30848200	H	7.32085400	-4.73088700	0.44317600
C	4.34942200	-2.13331000	-3.81173900	H	6.60942200	-4.46913300	-2.29650600
O	0.08224900	-2.33151800	-1.63407900	H	7.19921400	-5.96670700	-1.50538200
O	5.22617900	-2.36134300	-2.89909200	H	6.11154100	-2.89309700	-5.34153600
O	4.57181200	-2.25777400	-5.02500200	H	7.29968600	-3.88849000	-6.22254000
C	-2.87547100	0.23054500	4.62842800	H	8.46644100	-1.53753700	-3.11305100
N	-2.67078500	3.27883500	2.24702900	H	6.76369400	-2.01861500	-3.33972100
O	-1.73336700	-0.29864200	4.78209400	H	9.54808700	-3.52432100	-5.86310400
C	-2.91859100	1.70037100	4.11590600	H	11.36894000	-3.23442700	-4.38486200
N	-0.03432300	1.37286300	1.56700900	H	10.33563700	-2.42144900	-3.20898000
O	-3.97852900	-0.30244900	4.85639200	H	-7.12112600	7.58742800	-2.56627100
C	-2.25642800	1.95349400	2.74693900	H	-8.19906300	6.30470300	-3.05962100
C	1.44450500	1.37987800	1.77500100	H	-4.99963700	7.00150900	-1.24393900
C	-0.42490000	2.11278500	0.38970200	H	-8.02315200	4.08443000	-2.18204600
C	-0.73725200	1.76613700	2.85841600	H	-7.28446500	2.70577600	-0.27103900
Fe	-1.49474900	-2.19209900	-0.31837100	H	-4.25410600	5.61264800	0.66235700
C	2.16476900	-2.84345100	-2.67708900	H	-4.46803700	3.40446600	1.70360900
H	1.50121000	-3.28650000	-3.42815700	H	0.57987600	3.22286500	-4.66033900
H	2.84376000	-3.63636000	-2.33353000	H	2.78948000	4.03380700	-3.87617600
H	-7.20827800	7.23396900	-4.90187100	H	-1.53178100	4.07743800	-3.63438600
H	-5.55105100	7.03861100	-4.38597600	H	2.95753400	5.73046600	-2.06962000
H	-6.49478800	5.61085300	-4.85963300	H	-1.45062900	7.50178700	0.01313400
H	-5.34292100	2.60022500	-7.15843100	H	-2.42838900	5.85737000	-1.62200800
H	-6.92530800	2.25974400	-6.50064600	H	2.28809600	7.09368600	0.48549200
H	-5.83495300	3.34519900	-5.64353900	H	1.07866700	8.38611200	0.64370300
H	3.88573600	2.13003000	8.46685500	H	-5.46681400	-4.07076300	4.75966300
H	3.86192600	0.61452400	7.60076100	H	-5.43246300	-3.89538300	6.49808400
H	2.60485300	0.96145300	8.77950700	H	-2.19984800	-2.59483100	5.48235000
H	-3.74657000	-7.44978100	-3.21708600	H	-3.79385200	-2.05094600	5.48900500
H	-2.02172500	-7.40545700	-2.94116000	H	-4.38899900	-5.84439700	3.21301300
H	-2.66284600	-8.20528300	-4.36240200	H	-3.17935600	-7.10642100	3.24404900
H	-5.05261300	-6.57960100	0.85353700	H	-3.00792600	-5.09303100	-0.13581900
H	-3.88625600	-7.87260800	0.99727700	H	-1.87863800	-4.86620200	3.92450600
H	-5.24854700	-7.80272100	2.06999900	H	-0.52935500	-3.07783100	2.61244200
H	-4.96561300	-6.32900800	6.77420900	H	-1.73555500	-6.00724500	-5.02898300
H	-6.38537900	-6.10814400	5.77994500	H	-3.47852900	-5.97734400	-5.23273600

H	-4.60332200	-3.92256700	-4.17367500	H	10.44106200	-0.20550500	-0.52301800
H	-0.92397100	-4.77402000	-2.33572700	H	10.44093200	0.10665300	1.76500300
H	-4.27446600	-2.23361000	-2.32515400	H	6.94118400	0.21168400	-0.75565600
H	-3.96462100	2.00822000	4.03953200	H	9.06753500	0.75712000	3.70237900
H	-2.44174400	2.34339600	4.87315200	H	5.56518000	0.85603200	1.19411200
H	-0.29319900	0.34257800	1.35353800	H	6.21283900	2.38281700	3.77881100
H	-2.64576700	1.21714400	2.03236900	H	6.84929500	1.04305400	4.74407800
H	-2.40904400	4.00400900	2.91458400	H	5.36950300	0.82881500	3.78929700
H	-1.31208700	1.76152100	-0.13796200				
H	-2.20062100	3.49898800	1.37065600				
H	0.13320200	3.00993300	0.13298500	⁵ TS ₉₋₁₀			
H	0.52628900	-1.41246800	0.62035800	C	-1.11655500	3.64819000	-6.95411800
H	-0.25708500	2.68551100	3.22203600	C	-1.30307700	2.27929500	-6.36286900
H	-0.53902300	0.94705400	3.56108100	C	-2.48986000	1.60854900	-6.17472200
H	1.79184800	2.41509900	1.87264300	C	-0.26031000	1.35401400	-5.97759500
H	1.67456700	0.83736500	2.69878100	N	-2.25284800	0.33178600	-5.70239500
H	1.92202500	0.90890700	0.91051700	C	-0.89723400	0.14184900	-5.57917300
H	-5.67868500	0.67875700	0.17576600	C	1.14820500	1.42328000	-5.94415700
H	-4.98805900	0.12414000	1.67953100	C	-0.16798400	-0.98631400	-5.17408200
H	-5.89026600	1.03371600	-4.59444200	C	1.87377400	0.30948000	-5.52887000
H	-5.50226900	0.31413200	-6.14886100	C	1.22112200	-0.88684800	-5.15203900
H	-3.29111300	1.65184500	-6.11352300	C	0.16819200	8.12178000	2.32341100
H	-3.65411900	2.05879800	-4.43957800	C	-0.45946900	7.17762500	1.27763900
H	-1.52798200	-0.76783200	-3.90630900	C	-0.55589000	5.70434400	1.68895700
H	-1.62716700	0.95364000	-3.88248500	O	0.31490100	4.89226000	1.36092400
H	2.41124800	-1.22962000	-4.13453600	N	-1.63679300	5.36102600	2.41861900
H	3.15645100	-0.89963100	-2.55495800	C	-8.40678500	3.12691600	1.32949400
O	1.93029100	-2.17995100	-0.37882800	C	-7.76333800	4.36612400	0.74445900
H	10.79711600	-1.60037300	-4.71883600	C	-7.05484800	5.27082900	1.55689100
H	5.47038600	-5.58792600	-1.53610200	C	-7.81918500	4.64622200	-0.62893900
H	2.07409300	8.27068900	-0.79975100	C	-6.42924200	6.40007300	1.02847300
H	1.77044400	2.84602000	7.35454500	C	-7.19546100	5.77315000	-1.17629800
H	3.11426600	2.62768800	6.22891700	C	-6.49348000	6.65995200	-0.34866000
H	-0.03940300	1.38156100	7.19656200	O	-5.86169100	7.77239900	-0.81875700
H	-0.31175100	0.36656400	5.80905200	C	-1.25306600	-4.12250800	7.20133400
O	-0.39293800	-1.13305800	0.81081400	C	-1.17371100	-2.61773700	6.97219700
C	6.36472500	1.29189500	3.79110500	C	-0.50757100	-2.16379600	5.71233400
C	7.20223800	0.85369300	2.61014800	N	-0.27812000	-0.82196100	5.47884500
C	6.63517700	0.68718800	1.33351100	C	-0.14626800	-2.80106800	4.55242800
C	8.58349200	0.63538000	2.73127900	C	0.15965000	-0.67714400	4.21998700
C	7.40271000	0.32411600	0.22521400	N	0.26426500	-1.86194000	3.62176900
C	9.36781300	0.26809600	1.63330400	C	-4.51457900	-3.15678300	2.20532900
C	8.78025000	0.11231700	0.37164900	C	-4.22329100	-2.22298700	1.02718900
O	9.50334200	-0.24989800	-0.73377300	C	-2.78083700	-2.08176400	0.54183600
				O	-1.85339700	-2.40180600	1.38969300

O	-2.55028200	-1.64682900	-0.58827000	C	-3.58506300	2.22708600	2.45372300
C	-3.61817600	-6.85139900	-4.73422100	N	-3.63757900	1.53490800	-1.34487700
C	-2.90505000	-6.54409600	-3.40888300	O	-2.43552800	2.66167300	2.77483900
C	-1.76817900	-5.52601300	-3.53104100	C	-3.99279900	2.36606700	0.95691200
C	-0.82393500	-5.51580300	-2.32652400	N	-0.39029900	1.86076400	-0.24908500
O	-0.65294300	-6.49091500	-1.61144300	O	-4.42123100	1.70185400	3.20908600
N	-0.11786900	-4.35850500	-2.15165600	C	-2.99308500	1.73249300	-0.03449900
C	-3.80089900	-0.65175000	8.63531000	C	0.65710700	2.78323500	-0.78640300
C	-4.02071400	-0.00087500	7.26406500	C	-0.39098500	0.54159800	-0.86919000
C	-2.81188800	0.76276200	6.72003500	C	-1.71862300	2.59650500	-0.07831500
O	-1.69317000	0.65937800	7.25379900	Fe	0.06955800	-2.11403800	1.55136300
N	-3.01130400	1.51120700	5.63025900	C	4.20572700	-2.32130500	0.23635000
C	1.96700100	-7.45998500	4.24033400	H	4.06255400	-3.40396100	0.32471900
C	1.81513800	-7.49366500	2.71053200	H	4.96999900	-2.03216500	0.97021800
C	1.00290100	-6.34432100	2.19416300	H	-7.00434800	-4.41290000	-7.75537500
N	-0.27616200	-6.45404400	1.68385600	H	-5.65569300	-3.31615600	-7.58509300
C	1.25787700	-4.99472700	2.19795300	H	-5.78203000	-4.72167200	-6.50883700
C	-0.73761600	-5.21815800	1.39712400	H	-2.90839500	-7.22625900	-5.44207000
N	0.16784000	-4.30898100	1.70824200	H	-4.36415500	-7.59571200	-4.54942000
C	8.46104800	-0.49992500	2.12925200	H	-4.10144600	-5.96334700	-5.15784600
N	7.89060700	0.84672300	2.30269800	H	0.29334800	9.08103400	1.86270900
C	6.57845400	1.13716400	2.14939800	H	1.12326800	7.76432200	2.65324600
N	5.81632700	0.40475900	1.36143500	H	-0.47524200	8.23679900	3.20679000
N	6.06926400	2.18925300	2.82513100	H	1.02447000	-7.58565500	4.73086300
C	11.90426500	0.31009200	-2.21988000	H	2.41777700	-6.54467900	4.56276500
N	11.31125200	-0.98927400	-1.93123900	H	2.61766300	-8.28294500	4.57172700
C	9.97968200	-1.22998100	-1.85519800	H	-1.74015400	-4.66129500	6.41547100
N	9.09766700	-0.23613700	-1.90372800	H	-0.28333400	-4.54099400	7.37261200
N	9.53071300	-2.47486600	-1.69224400	H	-1.83462100	-4.30897200	8.11345600
C	-6.33472000	-3.95254000	-7.05721700	H	-3.65125200	0.09993900	9.38247100
C	-7.28771200	-3.13695100	-6.14539500	H	-4.65045000	-1.24802100	8.89494100
C	-6.76473700	-2.42806800	-4.90752200	H	-2.91427800	-1.29128400	8.64491300
C	-7.10890500	-2.88923000	-3.62359300	H	-5.55214000	-3.09965200	2.46172500
C	-6.05170300	-1.21846400	-4.97283000	H	-4.25627900	-4.17346400	1.99316200
C	-6.79001500	-2.17706700	-2.46860200	H	-3.94055900	-2.85320500	3.08851200
C	-5.71778200	-0.49377400	-3.82128600	H	5.16619700	2.56816600	2.57607400
C	-6.09623800	-0.95581300	-2.54671900	H	6.54366400	2.59157400	3.62026100
O	-5.87061600	-0.27897700	-1.40754300	H	4.79047300	0.43890200	1.37984400
C	2.91363500	-1.60321300	0.63287400	H	6.22070700	-0.14180500	0.55190000
C	4.67503900	-1.96480900	-1.19785600	H	8.47506500	1.56414200	2.70930400
C	6.20127500	-1.92306100	-1.30783500	H	8.57755500	-0.76374900	1.07403800
O	1.86048300	-2.32561800	0.63257600	H	9.43058200	-0.53102400	2.63446900
O	6.77036800	-0.90443000	-0.76460400	H	8.49473500	-2.66980600	-1.76720000
O	6.81954700	-2.82679800	-1.88866700	H	10.17524200	-3.24357300	-1.58262600

H	9.36892900	0.70678200	-2.13365300	H	-2.74283100	0.73744700	0.34969800
H	8.12987600	-0.42929500	-1.53737300	H	-3.92076300	2.43267700	-1.73687200
H	11.90266300	-1.79356100	-2.09541500	H	-1.29864700	-0.06829700	-0.90720700
H	12.93209500	0.32096500	-1.83995600	H	-2.99438300	1.11064400	-2.01019400
H	11.35999000	1.11056100	-1.70734700	H	0.47588900	0.31157400	-1.48272100
H	-6.05174200	7.87725200	-1.75551800	H	0.95397600	-0.04841900	1.06845900
H	-7.26651300	5.96380000	-2.25070200	H	-1.77443900	3.33649000	-0.88674300
H	-5.89364800	7.09820700	1.67302400	H	-1.61154800	3.10430100	0.88451700
H	-8.36485300	3.97406300	-1.29474600	H	0.43951600	2.99654300	-1.83888900
H	-6.98734400	5.08798000	2.63132200	H	0.63596800	3.69528600	-0.17626200
H	-7.66740600	2.32185300	1.44782400	H	1.63162400	2.29251700	-0.70018500
H	-9.20661600	2.74766100	0.68067600	H	-4.82635300	-2.47453700	0.14754400
H	-7.78689900	-2.38630700	-6.78101400	H	-4.53098500	-1.20322200	1.30201900
H	-8.09288200	-3.81388500	-5.82194500	H	-3.63196200	-6.18274200	-2.66369900
H	-5.79121800	-0.79764700	-5.94833100	H	-2.48603800	-7.47373300	-2.99768600
H	-7.67122500	-3.82090100	-3.52345900	H	-1.13499100	-5.76600600	-4.40332800
H	-7.09585200	-2.54344400	-1.48861400	H	-2.16683600	-4.51610600	-3.71428000
H	-5.20790400	0.46639100	-3.90752300	H	0.47901300	-4.29066000	-1.33764700
H	-5.12563100	0.36622700	-1.46561700	H	-0.44644300	-3.48923000	-2.54416100
H	1.81504000	-1.75245600	-4.85210600	H	4.27259300	-2.68489500	-1.92019200
H	2.96447500	0.35144500	-5.50947000	H	4.30819700	-0.96491900	-1.47042700
H	-0.67362900	-1.91354100	-4.90673900	O	2.94047800	-0.38817300	0.92087700
H	1.66544100	2.33394600	-6.25100700	H	11.92246000	0.48408500	-3.27555600
H	-3.50626100	1.94460900	-6.36229800	H	7.78848300	-1.18620200	2.60022500
H	-2.96479400	-0.35142900	-5.49024900	H	-0.64466900	3.56174600	-7.91058700
H	-0.48687000	4.29020200	-6.32058500	H	-8.82351800	3.32227300	2.29547200
H	-2.07870600	4.15698300	-7.09614500	H	-1.45913200	7.55309900	1.00771400
H	-4.28219100	-0.75974900	6.50673000	H	0.14635100	7.19410200	0.36161100
H	-4.88468700	0.68085900	7.29256300	H	-2.35530600	6.04290800	2.61475400
H	-2.21719700	1.97343200	5.20019300	H	-1.84544200	4.37183600	2.64819100
H	-3.81827600	1.48868200	4.98841400	O	-0.01334100	-0.22413700	1.12149300
H	-2.19092500	-2.20525300	6.95444600	C	4.52555800	6.40888500	-0.06824700
H	-0.67915600	-2.13966000	7.83051400	C	5.73134700	5.66379400	-0.59722200
H	-0.18774800	-3.85674800	4.31566000	C	5.63596200	4.34040000	-1.06058100
H	-0.58526000	-0.07552300	6.13799900	C	6.98857400	6.28444100	-0.68582700
H	0.34455900	0.28243000	3.75128900	C	6.73530300	3.66009000	-1.59052800
H	2.80860000	-7.46594600	2.23821800	C	8.10003600	5.61914500	-1.20975700
H	1.35821500	-8.44239800	2.39348800	C	7.97859100	4.29991100	-1.66828600
H	-0.74292100	-7.31402800	1.42601200	O	9.03848300	3.60362800	-2.18427700
H	2.15059700	-4.47972600	2.53452200	H	9.77285900	4.20929400	-2.32404700
H	-1.71203900	-5.02206300	0.96935300	H	9.06320800	6.13333200	-1.26364800
H	-4.96687300	1.88901000	0.81852600	H	6.63138200	2.63756300	-1.95313800
H	-4.11688600	3.43649700	0.72661400	H	7.11017700	7.31375400	-0.34190200
H	-0.09316900	1.59573300	0.70755200	H	4.67416600	3.82487800	-1.01965600

H	4.07825200	7.03707800	-0.85473100	C	1.83911800	-7.57069100	2.71457400
H	4.79538500	7.07649500	0.76154900	C	1.01176300	-6.46844700	2.13300500
H	3.74137100	5.72797300	0.28647800	N	-0.23690000	-6.62661700	1.56408500
510				C	1.22825800	-5.11427000	2.12317800
C	-1.11658900	3.64819900	-6.95412500	C	-0.71677500	-5.40448500	1.23439800
C	-1.12174800	2.29250300	-6.30247300	N	0.14957600	-4.46798900	1.56855000
C	-2.18943400	1.43476000	-6.16980100	C	8.46104700	-0.49992500	2.12925100
C	0.03004200	1.57092300	-5.80672500	N	7.84909600	0.83383100	2.21541700
N	-1.77985000	0.23729500	-5.61139200	C	6.53618900	1.07124300	1.98945800
C	-0.42201300	0.28479200	-5.38959800	N	5.83259000	0.26757900	1.22176300
C	1.40144700	1.87952100	-5.69100400	N	5.96715100	2.14749400	2.57538400
C	0.45150900	-0.68392500	-4.87165400	C	11.90426600	0.31009100	-2.21988000
C	2.27111700	0.92062100	-5.17949700	N	11.39277900	-1.02358100	-1.93185800
C	1.79979100	-0.34965100	-4.77587400	C	10.07798000	-1.34781100	-1.86016900
C	0.16814900	8.12178200	2.32344600	N	9.13606500	-0.41039300	-1.91747300
C	-0.47892700	7.11609100	1.36343800	N	9.70870500	-2.61811400	-1.70013100
C	-0.41642200	5.70698200	1.94726100	C	-6.33471400	-3.95253900	-7.05720400
O	0.63890200	5.09204800	2.01718600	C	-7.31711900	-3.17091600	-6.15151500
N	-1.58665400	5.19628000	2.41645600	C	-6.81090700	-2.31409400	-5.00906000
C	-1.25306500	-4.12250600	7.20132500	C	-7.13078000	-2.62950200	-3.67664900
C	-1.16157300	-2.62232400	6.93997200	C	-6.13699900	-1.10298400	-5.23324500
C	-0.47396800	-2.20492800	5.67680300	C	-6.81298300	-1.77939800	-2.61880000
N	-0.21188200	-0.87279900	5.41973800	C	-5.81037400	-0.23955600	-4.18353400
C	-0.10036100	-2.86674400	4.53293700	C	-6.15005400	-0.56383200	-2.85641100
C	0.26494700	-0.76668400	4.16532100	O	-5.89659300	0.24810200	-1.81245900
N	0.35262600	-1.95903000	3.59414600	C	3.06468900	-1.84990900	0.63343900
C	-4.51455500	-3.15677300	2.20535300	C	4.84354900	-2.38535500	-1.13745400
C	-4.22444500	-2.26410600	0.98967100	C	6.36657700	-2.27634700	-1.24656200
C	-2.76104900	-2.13748700	0.54684200	O	1.99363900	-2.51968900	0.63685000
O	-1.87769100	-2.22531500	1.47559400	O	6.88723500	-1.21845000	-0.73156100
O	-2.49672200	-1.91771000	-0.64518600	O	7.02778600	-3.15575800	-1.81811500
C	-3.61816400	-6.85135700	-4.73426500	C	-3.11999100	2.12612200	1.59193300
C	-2.89690600	-6.47990000	-3.43054600	N	-3.58787400	1.82292100	-2.22161200
C	-1.95780400	-5.27163800	-3.57441400	O	-1.84577900	1.98087100	1.93651700
C	-0.86324200	-5.21781300	-2.50691900	C	-3.45062500	2.42316300	0.12788600
O	-0.19814000	-6.20245000	-2.22107200	N	-0.33340200	1.73374400	-0.26093800
N	-0.62132700	-3.99275100	-1.95436100	O	-3.99059700	2.11143500	2.43443500
C	-3.80088300	-0.65176500	8.63531400	C	-2.75689400	1.65331800	-1.01667600
C	-4.06924100	-0.01021200	7.27156800	C	0.86204600	2.58247300	-0.29617500
C	-2.89951200	0.76531700	6.67241000	C	0.01653000	0.30799900	-0.29476200
O	-1.75954600	0.70776800	7.13598200	C	-1.30194400	2.08541500	-1.31066800
N	-3.18876400	1.49859300	5.57434100	Fe	0.10791600	-2.29534200	1.49652300
C	1.96698000	-7.45995400	4.24032500	C	4.35773900	-2.60454900	0.32058500
				H	4.20359300	-3.67413800	0.50167000

H	5.11755500	-2.25566600	1.03252600	H	3.33622700	1.14510000	-5.09686200
H	-7.00434900	-4.41290100	-7.75537300	H	0.09287600	-1.66446300	-4.55908200
H	-5.65570500	-3.31614500	-7.58509600	H	1.78059300	2.85192700	-6.00962300
H	-5.77519300	-4.71887400	-6.51143400	H	-3.22807200	1.58216400	-6.45206000
H	-2.90840900	-7.22627400	-5.44207600	H	-2.37338000	-0.56423400	-5.45587800
H	-4.36413300	-7.59572800	-4.54939600	H	-0.56224600	4.38977400	-6.36134800
H	-4.11878000	-5.98111500	-5.17698100	H	-2.13465400	4.02873000	-7.10788200
H	0.29337700	9.08102500	1.86269900	H	-4.34360600	-0.78029700	6.52989600
H	1.12327900	7.76433100	2.65322400	H	-4.94310000	0.65840700	7.32916000
H	-0.45644100	8.26159500	3.21781700	H	-2.43483100	1.92913000	5.05673600
H	1.02447400	-7.58567100	4.73086600	H	-4.07559500	1.44886600	5.09173400
H	2.41779000	-6.54468700	4.56276900	H	-2.17657100	-2.20350600	6.90365900
H	2.61610100	-8.27001700	4.60833700	H	-0.67037100	-2.13006900	7.79290800
H	-1.74015800	-4.66129700	6.41547500	H	-0.15738800	-3.92676200	4.31552000
H	-0.28333300	-4.54099100	7.37261300	H	-0.49940900	-0.10802200	6.04439000
H	-1.83805600	-4.29308600	8.11580000	H	0.49779300	0.17900400	3.68866900
H	-3.65125900	0.09994600	9.38246600	H	2.83792300	-7.55037900	2.25296300
H	-4.65045600	-1.24801300	8.89493800	H	1.40491000	-8.54492800	2.44654300
H	-2.91295300	-1.28867600	8.62345600	H	-0.68259100	-7.50708700	1.34201000
H	-5.55214300	-3.09966300	2.46171400	H	2.09177600	-4.56972300	2.48659100
H	-4.25629800	-4.17346700	1.99315400	H	-1.67648900	-5.24766100	0.75759900
H	-3.92760300	-2.83500500	3.07513900	H	-4.52919100	2.26783100	0.03797200
H	5.06829700	2.48410100	2.25933900	H	-3.28329100	3.50519900	-0.00397200
H	6.39962700	2.62160700	3.35420400	H	-1.21991100	1.92556600	1.14039400
H	4.80165700	0.23779100	1.20682600	H	-2.77749400	0.57808600	-0.78979600
H	6.28363300	-0.34435000	0.48944500	H	-3.66341400	2.80809300	-2.47386200
H	8.39736600	1.59174900	2.59753100	H	-0.88500400	-0.27580800	-0.51518400
H	8.63140800	-0.81036100	1.09409500	H	-3.14619000	1.36192400	-3.01379300
H	9.40909700	-0.48139100	2.67584000	H	0.75588900	0.11033000	-1.09120500
H	8.68398200	-2.87935300	-1.74646200	H	1.51502600	-0.13630800	0.93100900
H	10.40059000	-3.34229100	-1.57724200	H	-0.99363800	1.66040500	-2.28220600
H	9.36241200	0.55156800	-2.11457400	H	-1.27873300	3.17852700	-1.43532400
H	8.18615100	-0.66032200	-1.53429300	H	1.39665000	2.49939500	-1.25934800
H	12.03440500	-1.78938900	-2.09082900	H	0.59334600	3.62767800	-0.11953800
H	12.92612300	0.38704100	-1.83044900	H	1.54085700	2.28821900	0.51099900
H	11.30687700	1.07530500	-1.71433200	H	-4.79800100	-2.59068600	0.11408800
H	-7.92169500	-2.52343300	-6.80977200	H	-4.56320100	-1.23639500	1.19444500
H	-8.03245600	-3.89862300	-5.73855700	H	-3.63263600	-6.26940300	-2.63686100
H	-5.89910500	-0.80095300	-6.25668400	H	-2.30321900	-7.34006000	-3.08765400
H	-7.66565700	-3.55760700	-3.46046700	H	-1.41344600	-5.34362300	-4.53137500
H	-7.08712600	-2.03454000	-1.59544900	H	-2.52942000	-4.33225700	-3.61122900
H	-5.33592200	0.71921900	-4.39514400	H	0.09512400	-3.96887400	-1.23876200
H	-5.17853400	0.88931200	-2.02681700	H	-1.33041900	-3.26568300	-1.89346500
H	2.50530000	-1.08740600	-4.39052300	H	4.48414700	-3.19409400	-1.78408900

H	4.44011600	-1.43871200	-1.52592500	C	-1.15411300	-1.07074000	7.38251900
O	3.12780700	-0.60900300	0.85462900	C	-0.51817900	-0.87757100	6.04384200
H	11.92245800	0.48408500	-3.27555600	N	-0.28242800	0.38904900	5.54149700
H	7.78848300	-1.18620200	2.60022500	C	-0.19489800	-1.74010100	5.02995000
H	-0.64463800	3.56170000	-7.91056700	C	0.12468200	0.27901900	4.27314500
H	-1.51007800	7.41485100	1.12264400	N	0.20465300	-1.00666200	3.92509300
H	0.08095600	7.08795100	0.41759700	C	-4.53737300	-2.51888900	2.83179200
H	-2.46677600	5.68312500	2.33707200	C	-4.22727500	-1.85576900	1.48296400
H	-1.59268700	4.24751100	2.77152100	C	-2.80337100	-1.96890600	0.94398200
O	0.52061600	-0.11924600	0.94753100	O	-1.84348300	-1.81174600	1.83762800
C	4.25506700	6.22218100	-0.47186300	O	-2.56053700	-2.15072300	-0.23788300
C	5.54890500	5.51727800	-0.81501200	C	-3.74885200	-7.54784400	-3.22617300
C	5.54605900	4.24517200	-1.41847800	C	-3.00257100	-6.98520000	-2.00680800
C	6.79730700	6.10855100	-0.57200600	C	-1.82053800	-6.08564300	-2.37811100
C	6.72834600	3.59176200	-1.76723200	C	-0.83996100	-5.83863400	-1.23098400
C	7.99322600	5.46703600	-0.91266400	O	-0.83217700	-6.50095400	-0.20386300
C	7.96427500	4.20481100	-1.51728400	N	0.08161800	-4.85707900	-1.46126700
O	9.10437100	3.53517200	-1.87239300	C	-3.73488300	1.22049200	8.61990100
H	9.85286300	4.13623700	-1.80823100	C	-3.96127200	1.57712300	7.14737700
H	8.94828100	5.96028400	-0.71339800	C	-2.75018700	2.19187300	6.44486100
H	6.70066300	2.61276200	-2.24613000	O	-1.62849900	2.20162800	6.98908600
H	6.84810000	7.09701400	-0.11103700	N	-2.95427500	2.67645200	5.21836900
H	4.59507800	3.75405300	-1.63518300	C	1.91069900	-6.41122300	5.64990500
H	3.67089100	6.43478200	-1.38011700	C	1.72894200	-6.72351500	4.15298000
H	4.43907800	7.17931900	0.03221900	C	0.93784100	-5.66945900	3.43305100
H	3.61802900	5.61613900	0.18744900	N	-0.31539800	-5.87185300	2.88490700
				C	1.19745800	-4.33813800	3.21780300
				C	-0.76038300	-4.70961200	2.36887700
				N	0.13281000	-3.75410900	2.56325500
				C	8.46783800	-0.10798000	2.13638500
				N	7.90595600	1.24614900	2.02279900
				C	6.59204100	1.49620000	1.82472100
				N	5.82491500	0.59901000	1.23841300
				N	6.08550300	2.67211100	2.25084300
				C	11.88047000	-0.23767200	-2.30928000
				N	11.28547800	-1.45139300	-1.76183100
				C	9.95556600	-1.66923700	-1.61680900
				N	9.07019900	-0.70144200	-1.83593700
				N	9.51195400	-2.86075600	-1.21371800
				C	-6.45174000	-5.13997900	-6.06798200
				C	-7.39719700	-4.15148000	-5.33864800
				C	-6.85531100	-3.19599500	-4.29212000
				C	-7.06044500	-3.44621700	-2.92334500
				C	-6.25664800	-1.97103400	-4.62960800
⁵TS₉₋₁₀(dehydrogenation)							
C	-1.14238300	2.25418200	-7.53360800				
C	-1.46974700	1.00642500	-6.76115100				
C	-2.70773400	0.57159900	-6.34537400				
C	-0.54038600	-0.03963900	-6.39466200				
N	-2.60707700	-0.67003600	-5.74697800				
C	-1.29459500	-1.07601500	-5.77098300				
C	0.85096600	-0.21202500	-6.54892800				
C	-0.70124700	-2.26505600	-5.32027900				
C	1.44461600	-1.38645300	-6.09421300				
C	0.67422000	-2.40591100	-5.48932300				
C	0.28074500	8.48759900	0.64290300				
C	-0.36445900	7.34102900	-0.16007800				
C	-0.38858600	5.98843100	0.56650800				
O	0.59281500	5.24742900	0.55468200				
N	-1.54061500	5.68243300	1.20533300				
C	-1.24196500	-2.50223000	7.89836500				

C	-6.70480700	-2.52430200	-1.94223900	H	-3.95464100	-2.04926300	3.63543100
C	-5.88625800	-1.03533800	-3.65503000	H	5.18909600	2.99558300	1.91362700
C	-6.11330800	-1.29603700	-2.28990400	H	6.58217500	3.26179200	2.90238000
O	-5.84032500	-0.42443200	-1.30522300	H	4.79882900	0.62597000	1.26593200
C	2.94689000	-1.52282100	1.04398300	H	6.22055300	-0.11587100	0.57051500
C	4.65400800	-2.28598700	-0.72225200	H	8.49917000	2.03364400	2.24476400
C	6.18035000	-2.26509000	-0.86709500	H	8.58196600	-0.59083800	1.16152600
O	1.86470500	-2.18016700	1.22231000	H	9.43859400	-0.03855200	2.63687700
O	6.75222700	-1.15583000	-0.55915300	H	8.47632600	-3.06714300	-1.22257200
O	6.79121800	-3.26832900	-1.26333600	H	10.16025300	-3.59853100	-0.98182900
C	-3.49760800	2.60290500	2.03660200	H	9.34046300	0.18775400	-2.22657500
N	-3.70216600	1.40738800	-1.64623800	H	8.10732400	-0.82532300	-1.43036300
O	-2.36863300	3.11487000	2.29945500	H	11.87376700	-2.27438300	-1.76922600
C	-3.90739200	2.50517600	0.53874200	H	12.91103600	-0.15529700	-1.94524500
N	-0.48894800	1.33098900	-0.86888500	H	11.34203700	0.65120400	-1.96470300
O	-4.33171700	2.17932500	2.86239200	H	-7.91015400	-3.55737300	-6.11307100
C	-3.00991200	1.62907100	-0.35848400	H	-8.19308100	-4.74515200	-4.86327600
C	0.70587800	2.13094300	-1.24149700	H	-6.11888900	-1.71665000	-5.68428800
C	-0.78561500	0.29903800	-1.81184200	H	-7.54098800	-4.37820700	-2.61571500
C	-1.62044500	2.26349000	-0.49744200	H	-6.90458000	-2.72956400	-0.89083100
Fe	0.03267900	-1.65234600	1.97963000	H	-5.47459900	-0.06931000	-3.95143000
C	4.20090000	-2.35316300	0.76126400	H	-5.15369900	0.24721800	-1.54182800
H	4.02621900	-3.39512900	1.05207400	H	1.16474100	-3.32510000	-5.16323400
H	4.98829100	-1.95813500	1.41812900	H	2.51876600	-1.53347200	-6.22002600
H	-7.13319600	-5.72245600	-6.65458200	H	-1.30276500	-3.05514500	-4.87071500
H	-5.77002600	-4.63227800	-6.71776600	H	1.45571800	0.55991000	-7.02776600
H	-5.90232800	-5.79012700	-5.37984500	H	-3.67620200	1.05364000	-6.44967000
H	-3.05012200	-8.06723200	-3.84856500	H	-3.37721200	-1.19746000	-5.36163700
H	-4.50194700	-8.22947200	-2.89021300	H	-0.44322200	2.90719600	-6.98922800
H	-4.22472000	-6.75736700	-3.81801400	H	-2.04349400	2.83753100	-7.76139500
H	0.41312800	9.33255900	-0.00253700	H	-4.24467800	0.68284000	6.56611800
H	1.23446400	8.19102200	1.03174700	H	-4.81426600	2.26500500	7.04274500
H	-0.35182200	8.79146400	1.48871100	H	-2.16895600	3.02556700	4.67659700
H	0.97127200	-6.42268700	6.16188100	H	-3.75316300	2.46978300	4.59343500
H	2.37532000	-5.45591700	5.77822100	H	-2.16707500	-0.65491200	7.30680100
H	2.55630200	-7.16697600	6.11899800	H	-0.63476500	-0.44105300	8.11955000
H	-1.74264300	-3.18166300	7.24047600	H	-0.25279700	-2.82069300	5.00894000
H	-0.27577500	-2.89072300	8.14411800	H	-0.57303100	1.25830500	6.04864100
H	-1.81779100	-2.50020600	8.83481300	H	0.30548200	1.11791700	3.61040200
H	-3.56941800	2.10521600	9.19918000	H	2.71425700	-6.81834200	3.67155700
H	-4.58908300	0.70033900	8.99998700	H	1.23884500	-7.69959200	4.02494400
H	-2.85609300	0.58471500	8.75669100	H	-0.76860400	-6.76591200	2.74420900
H	-5.57178200	-2.39720800	3.07821800	H	2.07527500	-3.76731700	3.49714800
H	-4.29319800	-3.56087500	2.82725300	H	-1.70578000	-4.60539000	1.85323100

N	-2.90670200	-3.07381200	5.54431500	C	2.30127200	-2.64363700	-2.27310500
C	-2.78939000	-7.34884000	-3.68443400	H	1.60858900	-3.06165500	-3.01229900
C	-2.66077600	-6.02450300	-4.46019200	H	2.98899500	-3.44740400	-1.98066600
C	-2.68038300	-4.81902900	-3.56465300	H	-7.20828000	7.23396300	-4.90187500
N	-3.71249100	-3.90340800	-3.52594600	H	-5.55104700	7.03860200	-4.38597400
C	-1.80917100	-4.39553200	-2.58610000	H	-6.49176900	5.61197300	-4.86179000
C	-3.44211000	-2.98644300	-2.57008900	H	-5.34292000	2.60022700	-7.15843000
N	-2.29641400	-3.26112200	-1.97537400	H	-6.92530900	2.25974500	-6.50064400
C	6.45231000	-5.16777100	-1.46953800	H	-5.83689300	3.34545100	-5.64343700
N	6.59428300	-4.62038000	-0.10997700	H	3.88576100	2.13002300	8.46683200
C	5.63570000	-3.88956700	0.50735900	H	3.86195300	0.61454600	7.60076000
N	4.78921200	-3.16365600	-0.19025200	H	2.59330600	0.96319800	8.76969900
N	5.57484100	-3.92060500	1.85712100	H	-3.74656500	-7.44977900	-3.21707600
C	10.52847000	-2.53871200	-4.28019600	H	-2.02173300	-7.40545300	-2.94115200
N	9.32254600	-3.06363700	-4.90817900	H	-2.66338100	-8.20094300	-4.36783700
C	8.06179600	-2.67543700	-4.59325900	H	-5.05261300	-6.57960700	0.85353100
N	7.82599100	-1.89448600	-3.54370700	H	-3.88625100	-7.87259800	0.99727000
N	7.02697800	-3.10023800	-5.31856400	H	-5.25856700	-7.80566600	2.05438100
C	-6.52447700	6.59462400	-4.38093100	H	-4.96562400	-6.32900000	6.77421600
C	-7.12727300	6.54800000	-2.95393200	H	-6.38538000	-6.10814200	5.77996800
C	-6.50558900	5.67782100	-1.87710600	H	-4.87484400	-6.60946000	5.07142700
C	-7.09055600	4.44812100	-1.52439700	H	-6.99092500	-1.21758100	1.15998500
C	-5.42516800	6.11273200	-1.09198400	H	-6.29188000	-1.76743700	-0.34359500
C	-6.64451900	3.70148700	-0.43648300	H	-5.57765900	-2.24413000	1.17784400
C	-4.96054700	5.37191800	0.00282200	H	5.00572200	-3.24838900	2.35285000
C	-5.57448600	4.15520000	0.35650900	H	5.98675700	-4.67258500	2.38984600
O	-5.22929300	3.42861000	1.43351700	H	3.89126300	-2.80199200	0.17862200
C	1.51361400	-2.22678000	-1.02312400	H	5.02160900	-2.83342100	-1.16297000
C	3.08591300	-1.46500600	-2.91019500	H	7.35537400	-4.95633900	0.46382300
C	4.42352100	-1.92144100	-3.49603600	H	6.57396400	-4.39654500	-2.23589400
O	0.28796900	-1.95492600	-1.21790200	H	7.20194700	-5.95316400	-1.60554100
O	5.34054400	-2.18847800	-2.63376900	H	6.06228000	-2.70579300	-5.13574000
O	4.58306500	-2.02019000	-4.72203800	H	7.16550400	-3.73855100	-6.08772300
C	-2.40196200	0.18348500	4.21481300	H	8.57796000	-1.49942500	-3.00156400
N	-2.48980100	3.55426000	2.27251000	H	6.84461700	-1.89473700	-3.15505600
O	-1.26894100	-0.35335200	3.94688200	H	9.44538700	-3.48130000	-5.82139700
C	-2.57579700	1.70079500	3.91296100	H	11.34530800	-3.25237400	-4.43737400
N	0.30247000	2.07085000	1.39875000	H	10.39376600	-2.43352000	-3.19866200
O	-3.36940000	-0.37527500	4.74427100	H	-7.15765300	7.58389000	-2.57765300
C	-1.97273100	2.21174200	2.59287300	H	-8.18299200	6.25155600	-3.05143700
C	1.71345100	2.47264000	1.50856200	H	-4.96443400	7.08181800	-1.30339500
C	-0.17238600	1.54087700	0.33156100	H	-7.94394600	4.07731900	-2.09738100
C	-0.44239500	2.14850100	2.67754800	H	-7.13756900	2.76876900	-0.16482200
Fe	-1.44038200	-2.24360800	-0.18875800	H	-4.16115700	5.77007700	0.63000000

H	-4.30682300	3.59319600	1.73922900	H	-2.11587800	0.86394300	-3.25856900
H	0.82428500	2.83246100	-4.30874700	H	2.48274600	-0.98280800	-3.68865300
H	2.99443100	3.75030700	-3.52301000	H	3.31961600	-0.71253300	-2.14269600
H	-1.33058800	3.74200800	-3.44777700	O	2.10178800	-2.15431600	0.07982700
H	3.07017400	5.59911300	-1.86419400	H	10.79711800	-1.60037300	-4.71883400
H	-1.43904600	7.47584100	-0.11623700	H	5.47038600	-5.58792600	-1.53610300
H	-2.33268800	5.69565000	-1.65230200	H	2.07409500	8.27068600	-0.79975200
H	2.29634600	7.14394500	0.52531100	H	1.69349700	2.76132500	7.32861300
H	1.03456000	8.39030200	0.60840600	H	3.14850600	2.76621000	6.32801400
H	-5.32540200	-4.08392400	4.71454200	H	0.20181700	0.79270800	7.02786500
H	-5.28693100	-3.87171500	6.45090600	H	0.11963000	0.11129500	5.42908700
H	-1.90696100	-2.96515800	5.43392600	O	-0.38798900	-1.02846000	1.42958400
H	-3.42263800	-2.20702500	5.35120500	C	6.74469100	1.06239100	4.15531400
H	-4.40058100	-5.80613800	3.17761400	C	7.54549700	0.64589700	2.94135900
H	-3.27663800	-7.14237100	3.30807200	C	6.94405300	0.47454400	1.68306600
H	-2.99406600	-5.00324700	-0.03786000	C	8.93427600	0.44859400	3.02107800
H	-1.63701600	-5.22836400	3.93139100	C	7.68529100	0.12793600	0.55027000
H	-0.09924200	-3.58877300	2.66285800	C	9.69087600	0.09809400	1.90021600
H	-1.71893700	-6.02614200	-5.02997900	C	9.06861600	-0.06278900	0.65442700
H	-3.46171400	-5.93912600	-5.20932300	O	9.76394100	-0.40945500	-0.47249100
H	-4.47547500	-3.83893400	-4.18700600	H	10.70637000	-0.37938900	-0.28154600
H	-0.87413300	-4.84906500	-2.27620300	H	10.76964000	-0.04827300	1.99976500
H	-4.09704500	-2.15652200	-2.33637900	H	7.19570300	0.00843600	-0.41571900
H	-3.64761700	1.91940900	3.91157200	H	9.44399500	0.57347300	3.97870300
H	-2.14487400	2.25521300	4.76351500	H	5.86713800	0.62273900	1.57665200
H	-0.69647800	-0.89045600	2.36146100	H	6.88447900	2.13433800	4.36627400
H	-2.33107500	1.54807700	1.79611100	H	7.06037200	0.51417700	5.05423600
H	-2.29994900	4.20519000	3.03395500	H	5.66991500	0.89444900	4.01710000
H	-1.21715900	1.20117800	0.24714100				
H	-2.03038500	3.92921000	1.44543800				
H	0.48834400	1.43646700	-0.52762000				
H	0.53901900	-1.31138200	1.42694700				
H	-0.04705900	3.01704300	3.22026700				
H	-0.16729700	1.23760300	3.23074200				
H	1.76351200	3.55825000	1.65147700				
H	2.14489500	1.97144000	2.38368500				
H	2.25378500	2.19855400	0.59890000				
H	-5.59708800	0.62094100	0.01778500				
H	-5.12011100	0.24009700	1.65015700				
H	-5.91623400	1.01429200	-4.61226200				
H	-5.46245000	0.32161100	-6.16566000				
H	-3.28572600	1.69227700	-6.04538100				
H	-3.70232500	2.07684600	-4.37717600				
H	-1.77121300	-0.79162600	-3.56474600				