

Supporting Information

Computational Insights into the Dual Reactivity of 1,2,3,4-Tetrazole: Metalloporphyrin-Catalyzed Click Reaction and Denitrogenative Annulation

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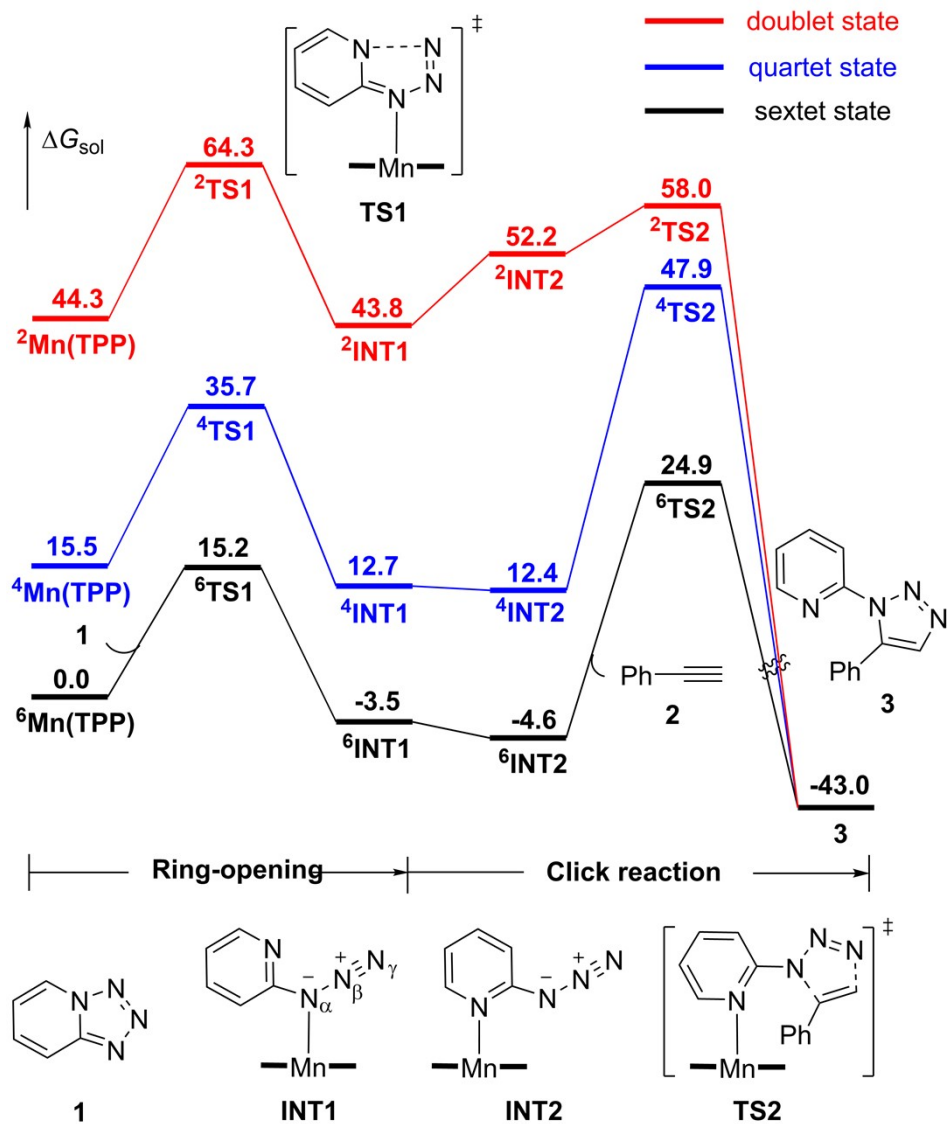


Fig. S1 Free energy profiles for Mn-porphyrin catalyzed click reaction of 1,2,3,4-tetrazole **1** and phenylacetylene **2**. The energies are shown in kcal mol⁻¹.

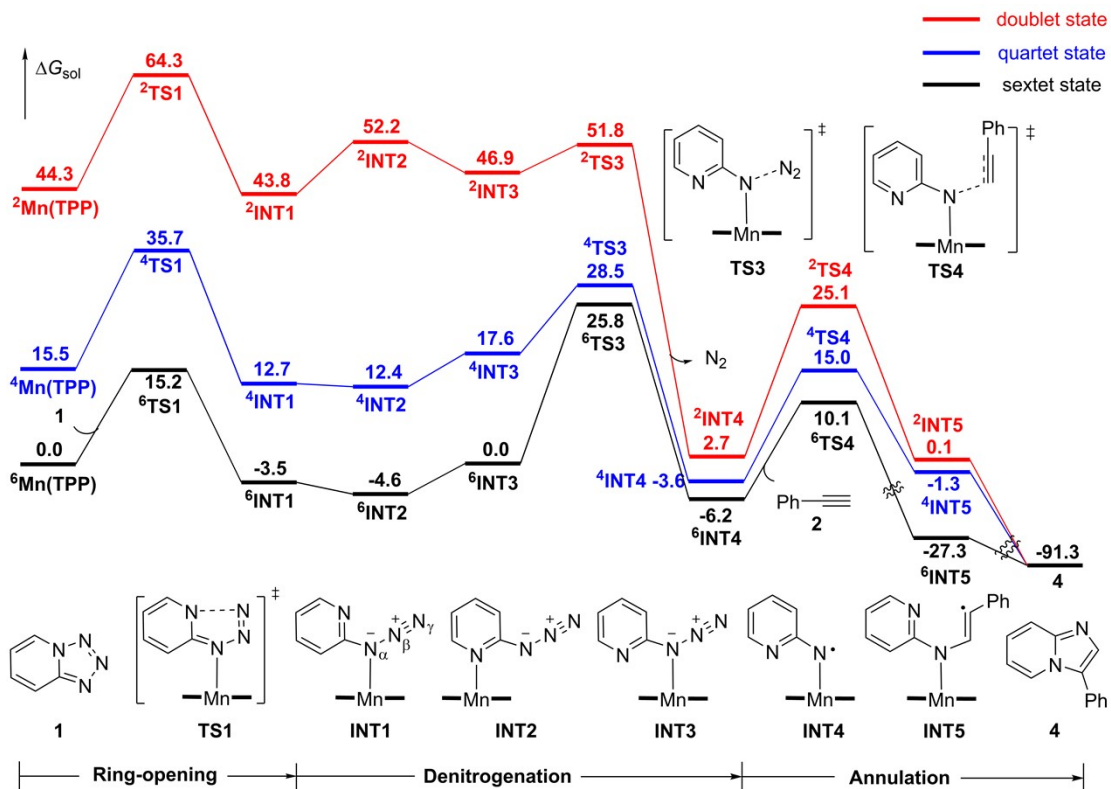


Fig. S2 Free energy profiles for Mn-porphyrin catalyzed denitrogenative annulation of **1**. The energies are shown in kcal mol⁻¹.

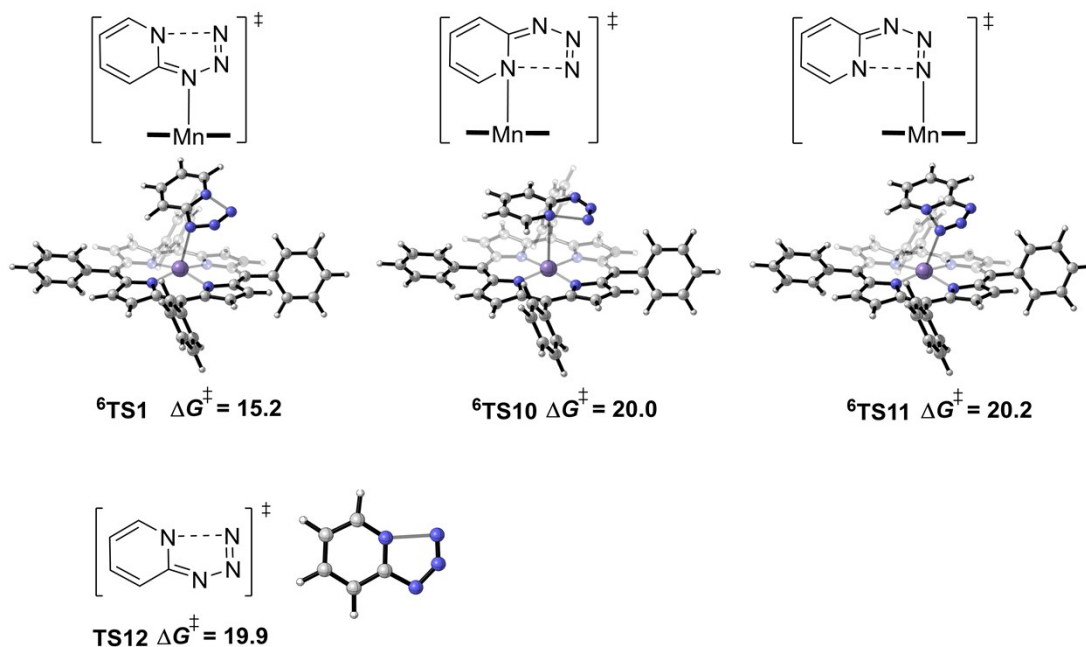


Fig. S3 Different conformers for the tetrazole ring-opening transition structures. The energies are shown in kcal mol⁻¹.

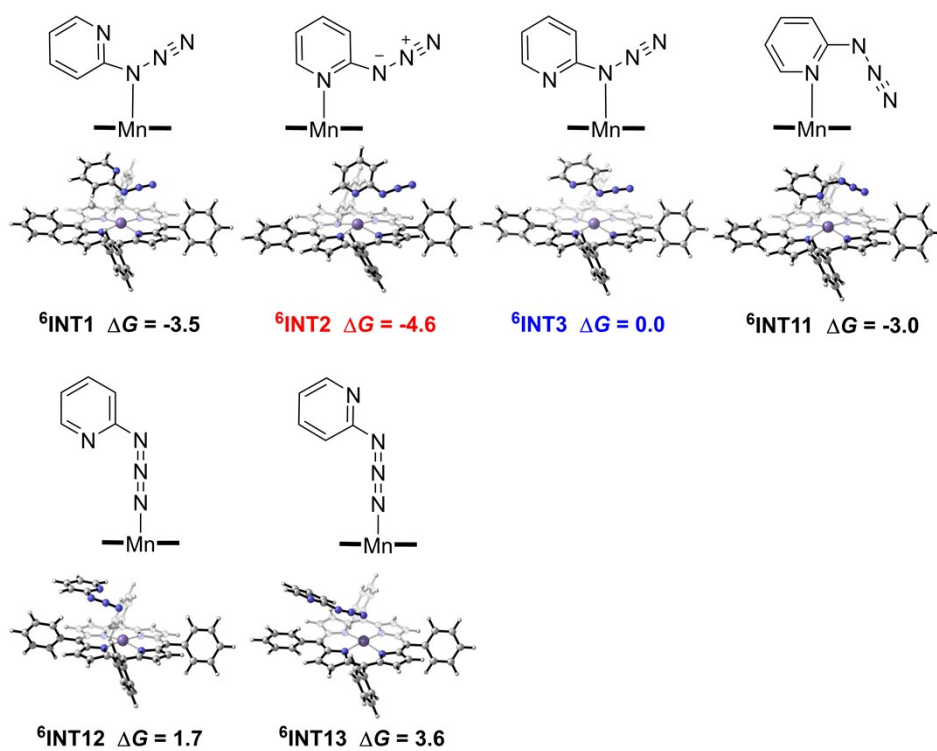


Fig. S4 Different conformers for the azide complex structures. The energies are shown in kcal mol⁻¹.

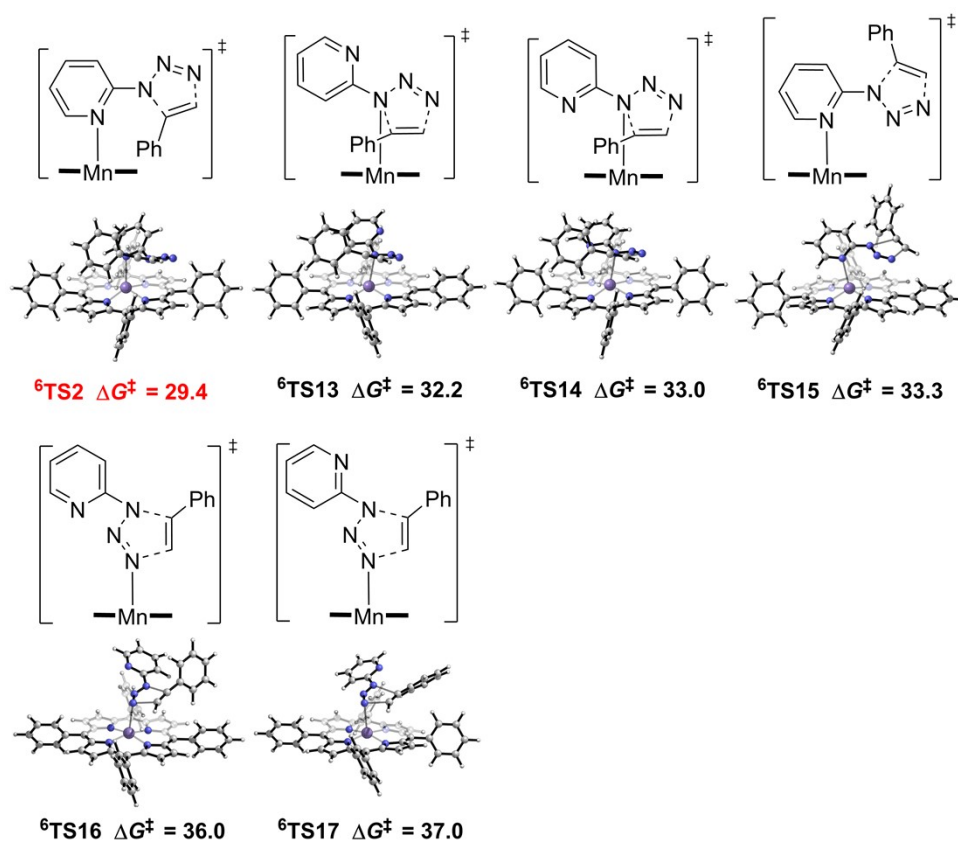


Fig. S5 Different conformers for the 1,5-regioisomer of tetrazole click reaction transition structures. The energies are shown in kcal mol⁻¹.

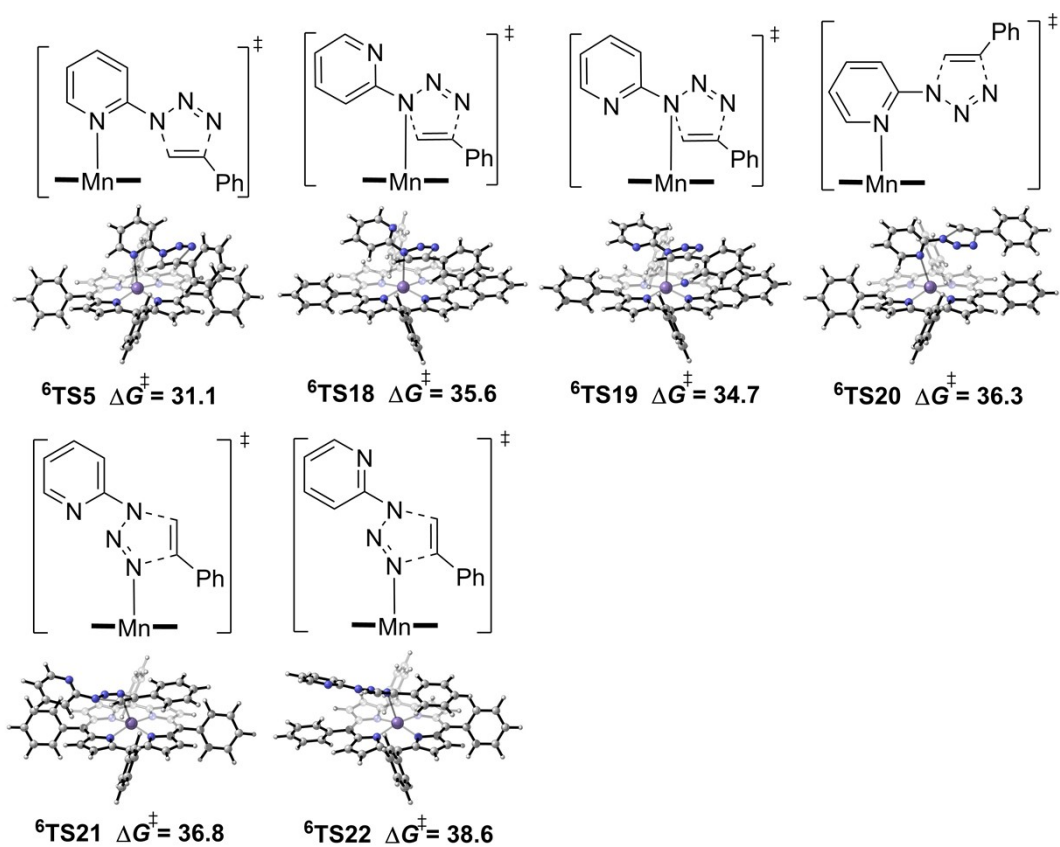


Fig. S6 Different conformers for the 1,4-regioisomer of tetrazole click reaction transition structures. The energies are shown in kcal mol⁻¹.

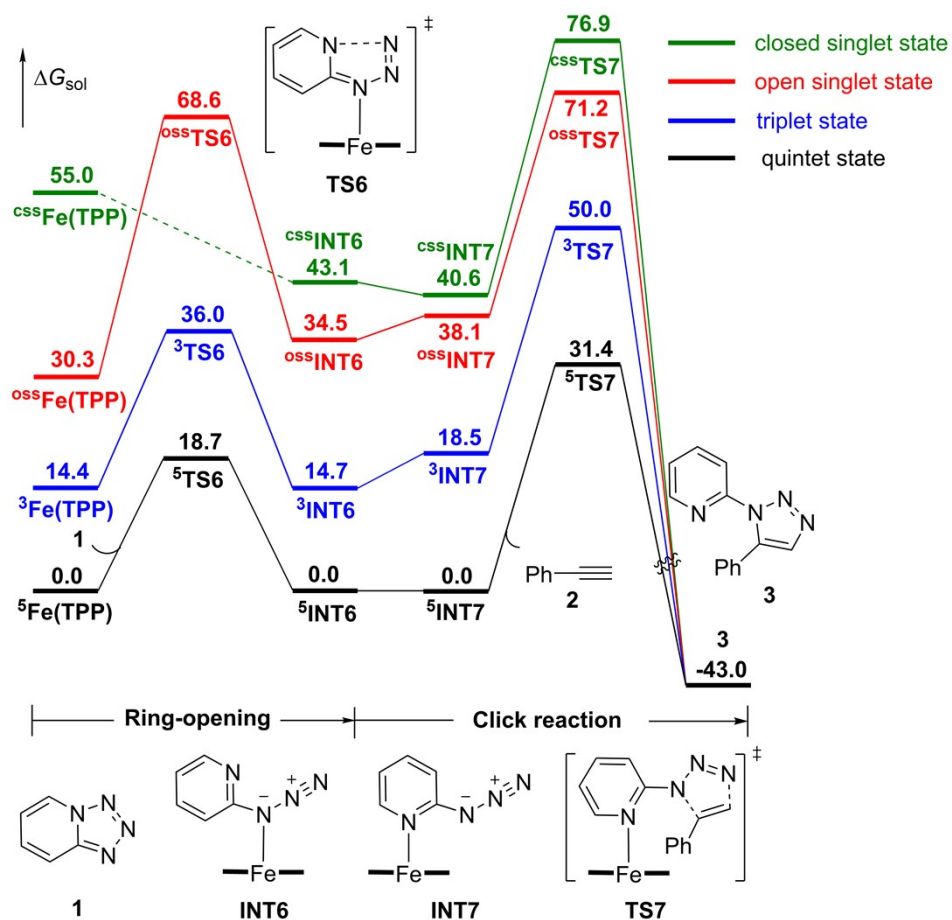


Fig. S7 Free energy profiles for Fe-porphyrin catalyzed click reaction of 1,2,3,4-tetrazole **1** and phenylacetylene **2**. The energies are shown in kcal mol⁻¹.

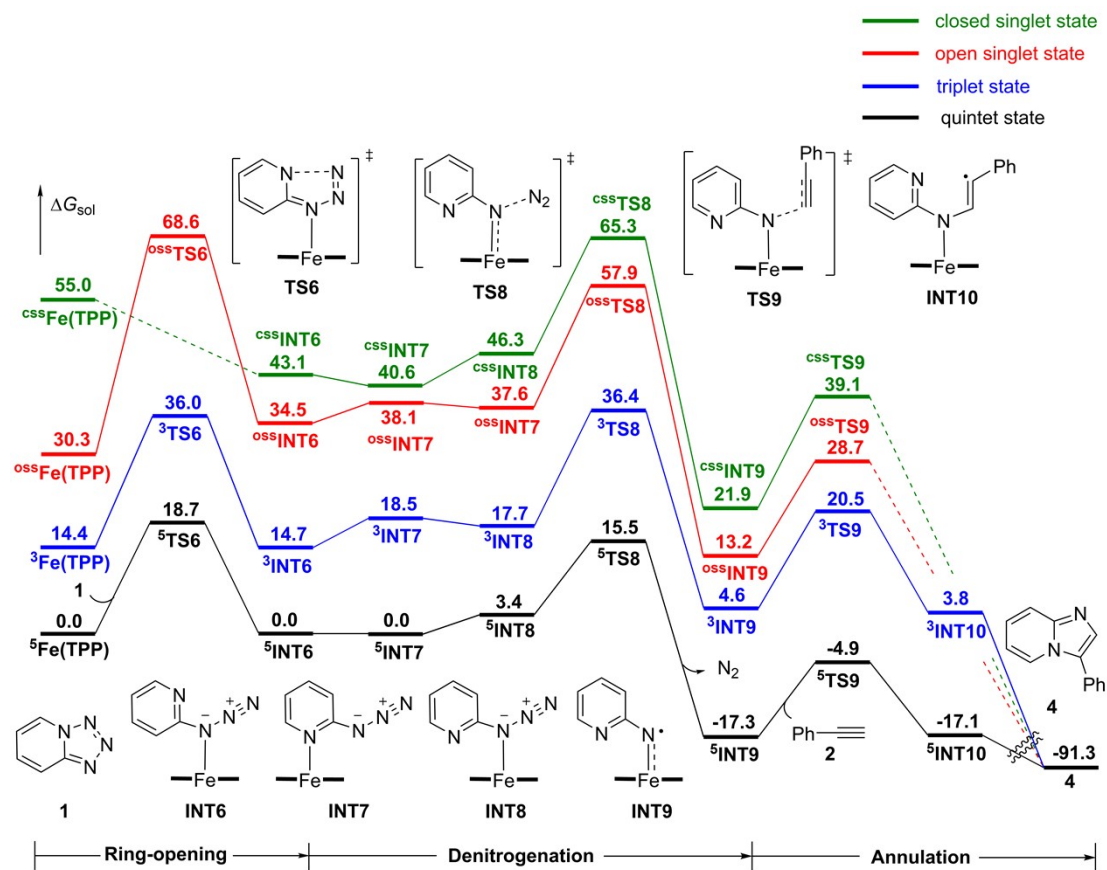


Fig. S8 Free energy profiles for Fe-porphyrin catalyzed denitrogenative annulation of **1**. The energies are shown in kcal mol⁻¹.

The bond orders and spin densities of ${}^6\text{INT4}$ and ${}^5\text{INT9}$ were calculated to confirm the structure. In ${}^6\text{INT4}$, the Mayer bond order value and Wiberg bond order value of the Mn–N bond are 0.44 and 0.71, respectively, suggesting a weaker bond strength compared to the Fe–N bond in ${}^5\text{INT9}$ with a Mayer bond order value of 0.75 and a Wiberg bond order value of 1.19. In addition, the spin densities on the N atom and Mn atom of ${}^6\text{INT4}$ are 1.17 and 4.06, respectively, while in ${}^5\text{INT9}$, the spin densities on the N atom and Fe atom are -0.64 and 4.47, respectively. These results indicate significant delocalization of the single electron over the Fe–N bond.

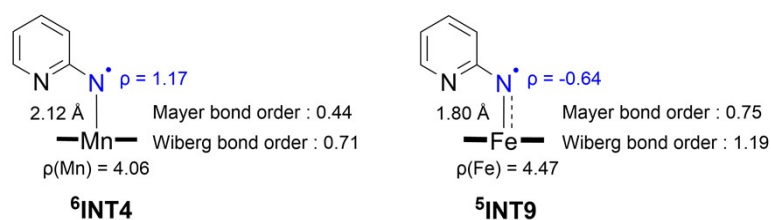


Fig. S9 M–N bond orders and spin densities (ρ) in ${}^6\text{INT4}$ and ${}^5\text{INT9}$.

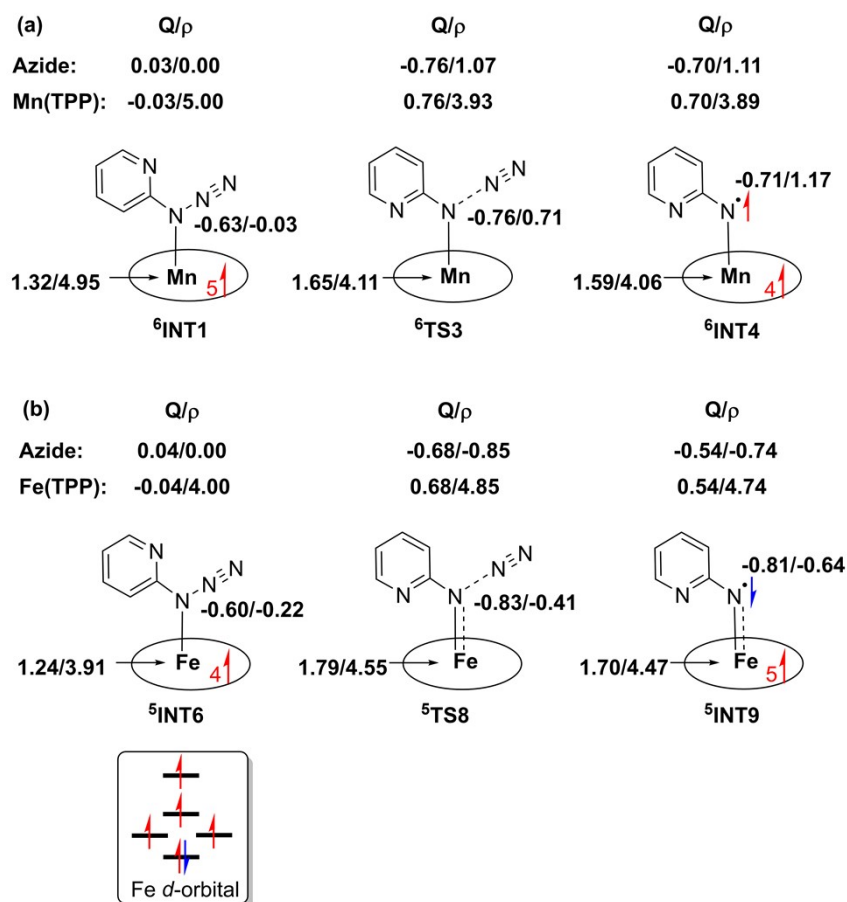


Fig. S10 Populations of Mulliken charges (Q in e) and spin densities (ρ) for the key structures of the denitrogenation process.

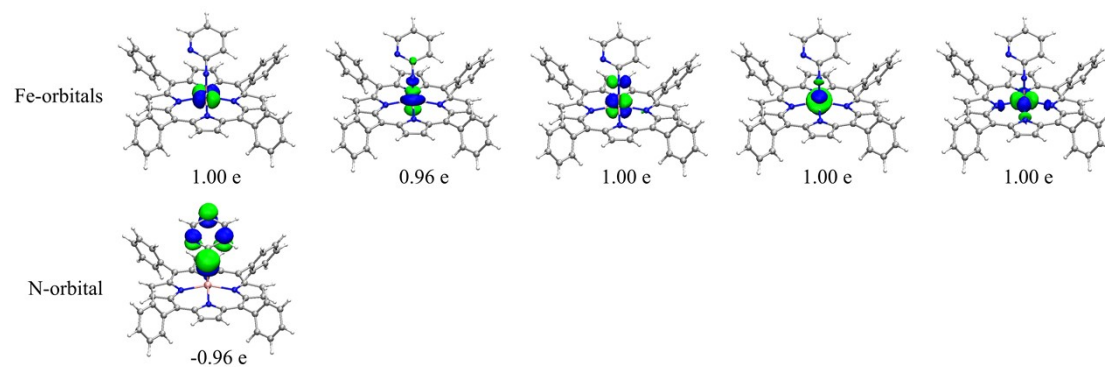


Fig. S11 SNOs of Fe-nitrene specie $^5\text{INT9}$ and their occupancies. The negative occupation number signifies a β -spin electron.

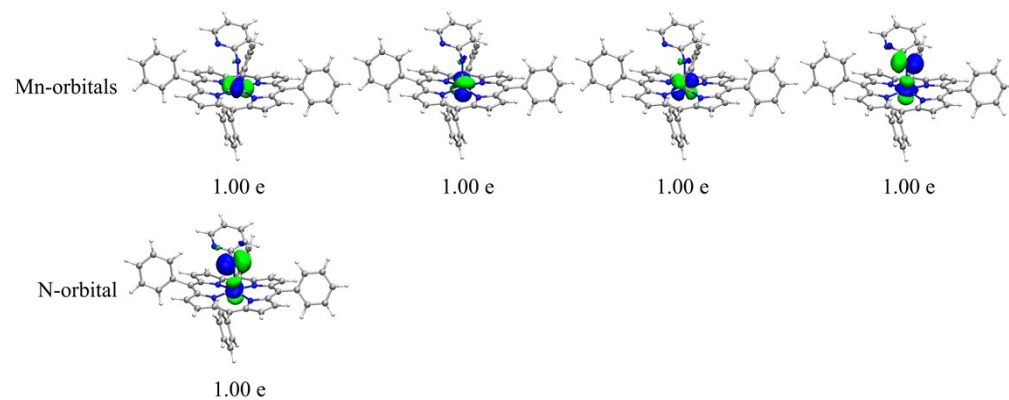


Fig. S12 SNOs of Mn-nitrene specie $^6\text{INT4}$ and their occupancies.

Table S1. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)M06/6-311+G(d,p)-SDD(SMD_{benzene})/(U)B3LYP-D3/6-31G(d)-LANL2DZ Level of Theory

Structures	ZPVE	TCE	TCH	TCG	E _{sol}	Gsol(E _{sol} +TCG)	Imaginary Frequency
1	0.093942	0.099606	0.100551	0.063950	-411.711218	-411.647268	
2	0.109556	0.116034	0.116978	0.079117	-308.231092	-308.151975	
²Mn(TPP)	0.599243	0.635908	0.636852	0.527490	-2016.013840	-2015.486350	
⁴Mn(TPP)	0.599259	0.635892	0.636836	0.527065	-2016.059402	-2015.532337	
⁶Mn(TPP)	0.597151	0.634291	0.635236	0.524298	-2016.081283	-2015.556985	
²TS1	0.691243	0.734867	0.735811	0.611063	-2427.712805	-2427.101742	243.00 <i>i</i>
⁴TS1	0.691670	0.735993	0.736937	0.609364	-2427.756781	-2427.147417	245.68 <i>i</i>
⁶TS1	0.689746	0.734503	0.735447	0.606898	-2427.786914	-2427.180016	237.70 <i>i</i>
²INT1	0.692487	0.737764	0.738708	0.609590	-2427.744098	-2427.134508	
⁴INT1	0.692350	0.737633	0.738577	0.608609	-2427.792692	-2427.184083	
⁶INT1	0.690472	0.736172	0.737116	0.606534	-2427.816341	-2427.209807	
²INT2	0.692804	0.738033	0.738977	0.609684	-2427.730736	-2427.121052	
⁴INT2	0.692763	0.738049	0.738993	0.608605	-2427.793106	-2427.184501	
⁶INT2	0.690642	0.736326	0.737270	0.605644	-2427.817246	-2427.211602	
²TS2	0.803197	0.855414	0.856358	0.712152	-2735.943071	-2735.230919	410.73 <i>i</i>
⁴TS2	0.803315	0.855429	0.856373	0.712211	-2735.992129	-2735.279918	409.59 <i>i</i>
⁶TS2	0.801084	0.853811	0.854756	0.707871	-2736.024481	-2735.316610	406.95 <i>i</i>
3	0.209339	0.221794	0.222738	0.168864	-720.036601	-719.867737	
²INT3	0.692018	0.737452	0.738397	0.608215	-2427.737688	-2427.129473	
⁴INT3	0.692053	0.737491	0.738435	0.607586	-2427.783736	-2427.176150	
⁶INT3	0.690113	0.735924	0.736868	0.605194	-2427.809431	-2427.204237	
²TS3	0.689411	0.734248	0.735192	0.607466	-2427.729099	-2427.121633	659.94 <i>i</i>
⁴TS3	0.688839	0.733926	0.734870	0.606000	-2427.764775	-2427.158775	701.21 <i>i</i>
⁶TS3	0.687978	0.733571	0.734515	0.603541	-2427.766708	-2427.163167	530.57 <i>i</i>
N₂	0.005599	0.007960	0.008904	-0.012850	-109.484696	-109.497546	
²INT4	0.682001	0.725043	0.725987	0.600430	-2318.302853	-2317.702423	

⁴INT4	0.681929	0.724925	0.725869	0.601186	-2318.313587	-2317.712401	
⁶INT4	0.680714	0.724200	0.725144	0.598848	-2318.315467	-2317.716619	
²TS4	0.793349	0.843302	0.844246	0.706032	-2626.524792	-2625.818760	497.44 <i>i</i>
⁴TS4	0.792809	0.842924	0.843869	0.704352	-2626.539078	-2625.834726	664.14 <i>i</i>
⁶TS4	0.791712	0.842377	0.843321	0.702055	-2626.544685	-2625.842630	406.22 <i>i</i>
²INT5	0.795782	0.845704	0.846648	0.707539	-2626.568346	-2625.860807	
⁴INT5	0.795950	0.845851	0.846795	0.707038	-2626.565554	-2625.858516	
⁶INT5	0.794753	0.845129	0.846073	0.702684	-2626.604864	-2625.902180	
4	0.199711	0.210270	0.211214	0.162687	-610.609889	-610.4472020	
²TS5	0.803586	0.8556930	0.8566370	0.712796	-2735.947129	-2735.234333	359.80 <i>i</i>
⁴TS5	0.803598	0.855722	0.856667	0.712127	-2735.993257	-2735.281130	373.32 <i>i</i>
⁶TS5	0.801147	0.853989	0.854933	0.706798	-2736.020657	-2735.313859	366.47 <i>i</i>
^{css}Fe(TPP)	0.599771	0.636354	0.637299	0.528475	-2035.558676	-2035.030201	
^{oss}Fe(TPP)	0.599549	0.636237	0.637181	0.528085	-2035.597571	-2035.069486	
³Fe(TPP)	0.599537	0.636283	0.637227	0.526567	-2035.621391	-2035.094824	
⁵Fe(TPP)	0.597442	0.634568	0.635512	0.524515	-2035.642295	-2035.117780	
^{oss}TS6	0.688115	0.732708	0.733652	0.688115	-2447.262505	-2446.655787	245.54 <i>i</i>
³TS6	0.692196	0.736464	0.737408	0.692196	-2447.317532	-2446.707608	249.16 <i>i</i>
⁵TS6	0.690014	0.734755	0.735699	0.690014	-2447.342230	-2446.735193	236.51 <i>i</i>
^{css}INT6	0.693449	0.738153	0.739098	0.612646	-2447.308950	-2446.696304	
^{oss}INT6	0.692965	0.738059	0.739003	0.611421	-2447.321521	-2446.710100	
³INT6	0.692994	0.738193	0.739137	0.609872	-2447.351557	-2446.741685	
⁵INT6	0.690880	0.736514	0.737458	0.606995	-2447.372034	-2446.765039	
^{css}INT7	0.694041	0.738593	0.739537	0.613717	-2447.314006	-2446.700289	
^{oss}INT7	0.693207	0.738193	0.739137	0.611599	-2447.315891	-2446.704292	
³INT7	0.692904	0.738104	0.739048	0.609550	-2447.345133	-2446.735583	
⁵INT7	0.691115	0.736709	0.737653	0.606699	-2447.371801	-2446.765102	
^{css}TS7	0.804891	0.856282	0.857226	0.716875	-2755.511286	-2754.794411	427.86 <i>i</i>
^{oss}TS7	0.803855	0.855804	0.856748	0.714424	-2756.440909	-2755.726485	418.97 <i>i</i>

³ TS7	0.803785	0.855887	0.856831	0.712656	-2755.549997	-2754.837341	409.44 <i>i</i>
⁵ TS7	0.801552	0.854177	0.855121	0.708262	-2755.575300	-2754.867038	416.21 <i>i</i>
^{css} INT8	0.692961	0.737870	0.738814	0.610557	-2447.301861	-2446.691304	
^{oss} INT8	0.692381	0.737711	0.738655	0.609414	-2447.314560	-2446.705146	
³ INT8	0.692445	0.737893	0.738837	0.607657	-2447.344522	-2446.736865	
⁵ INT8	0.690370	0.736158	0.737102	0.605725	-2447.365378	-2446.759653	
^{css} TS8	0.690644	0.735142	0.736086	0.610755	-2447.271715	-2446.660960	661.95 <i>i</i>
^{oss} TS8	0.689919	0.734598	0.735542	0.609748	-2447.282564	-2446.672816	514.98 <i>i</i>
³ TS8	0.689324	0.734255	0.735199	0.607340	-2447.314372	-2446.707032	624.99 <i>i</i>
⁵ TS8	0.686850	0.732709	0.733653	0.601358	-2447.341732	-2446.740374	531.78 <i>i</i>
^{css} INT9	0.683084	0.725832	0.726776	0.603786	-2337.836375	-2337.232589	
^{oss} INT9	0.681918	0.724986	0.725930	0.602526	-2337.849050	-2337.246524	
³ INT9	0.682613	0.725500	0.726444	0.601562	-2337.861782	-2337.260220	
⁵ INT9	0.680084	0.723501	0.724446	0.598800	-2337.893797	-2337.294997	
^{css} TS9	0.794812	0.844333	0.845277	0.709376	-2646.066593	-2645.357217	371.13 <i>i</i>
^{oss} TS9	0.793795	0.843696	0.844640	0.707609	-2646.081355	-2645.373746	408.90 <i>i</i>
³ TS9	0.793381	0.843433	0.844377	0.705259	-2646.092095	-2645.386836	461.39 <i>i</i>
⁵ TS9	0.790723	0.841684	0.842628	0.699777	-2646.127019	-2645.427242	357.46 <i>i</i>
³ INT10	0.796720	0.846400	0.847345	0.708453	-2646.121845	-2645.413392	
⁵ INT10	0.794941	0.845295	0.846239	0.704759	-2646.151426	-2645.446667	

ZPVE = zero-point vibrational energy; **TCE** = thermal correction to energy; **TCH** = thermal correction to enthalpy; **TCG** = thermal correction to Gibbs free energy.

Cartesian coordinates of the structures

(U)M06/6-311+G(d,p)-SDD(SMD_{benzene})/(U)B3LYP-D3/6-31G(d)-LANL2DZ

1

C	0.91768700	1.42689700	
0.00001900			
C	-0.31843400	0.73674300	-
0.00006600			
C	0.83019700	-1.40030600	
0.00004100			
C	2.02945700	-0.74389700	
0.00008000			
C	2.07321200	0.68376000	-
0.00008100			
H	0.91474800	2.51040400	
0.00007800			
H	0.69110800	-2.47371300	
0.00000800			
H	2.94733200	-1.32064000	
0.00005000			
H	3.03778300	1.18143800	-
0.00001800			
N	-1.59504600	1.13003400	
0.00003200			
N	-0.30807100	-0.64115100	-
0.00003400			
N	-1.59688700	-1.07867100	-
0.00008800			
N	-2.32623700	0.00169100	
0.00007800			

2

C	1.51251400	-1.20921000	
0.00001300			
C	0.11941400	-1.21383700	-
0.00001100			
C	-0.59425000	-0.00002100	-
0.00003100			
C	0.11939600	1.21382700	-
0.00001300			
C	1.51248000	1.20923100	

0.00001500			
C	2.21310200	0.00001100	
0.00002500			
H	2.05311900	-2.15178600	
0.00002300			
H	-0.42931200	-2.15060600	-
0.00002200			
H	-0.42937200	2.15057200	-
0.00002400			
H	2.05308400	2.15180800	
0.00002500			
H	3.29967000	0.00003400	
0.00004500			
C	-2.02358200	-0.00001200	-
0.00007300			
C	-3.23364100	0.00000400	-
0.00001500			
H	-4.29978900	0.00001500	
0.00049400			

²Mn (TPP)

Mn	0.00136500	-0.00005500	-
0.00027100			
N	1.46954000	1.39022000	
0.00856900			
C	-0.09233700	-3.45485300	
0.01597800			
C	3.45492700	-0.09461700	-
0.00081600			
C	3.40564900	-2.60465700	-
0.05874100			
C	2.41748800	-3.54075300	-
0.06649500			
C	2.76392600	-1.31354700	-
0.02952700			
C	1.16261900	-2.83108100	-
0.01981300			
H	2.52334200	-4.61513400	-
0.09755300			
H	4.47327000	-2.76770100	-
0.07312100			
N	-1.38868600	1.46845500	
0.00973900			
N	1.39124400	-1.46856700	-

0.00911700			
N	-1.46695300	-1.39033000	-
0.01016700			
C	0.09685300	3.45469400	-
0.01518700			
C	-3.45333500	0.09454000	-
0.00065300			
C	-3.53549700	-2.41182300	
0.15428900			
C	3.54309800	2.41431800	
0.05819400			
C	-3.39815300	2.60176800	-
0.15487400			
C	-2.59944300	-3.40020900	
0.15498900			
C	2.60767800	3.40310500	
0.06691100			
C	-2.40935900	3.53739200	-
0.15475500			
C	-2.82837700	-1.16019000	
0.03951300			
C	2.83167700	1.16029300	
0.02849200			
C	-2.76067800	1.31322600	-
0.04035700			
C	-1.31120800	-2.76208100	
0.04223900			
C	1.31583500	2.76322400	
0.02007500			
C	-1.15805700	2.82961900	-
0.04203600			
H	-2.76027400	-4.46482700	
0.24028400			
H	2.77227800	4.47003300	
0.09866000			
H	-2.51150700	4.60926600	-
0.23968800			
H	-4.60727400	-2.51482300	
0.23895600			
H	4.61805100	2.51863600	
0.07252700			
H	-4.46264400	2.76344100	-
0.23965800			
C	0.13509000	4.94941100	-

0.03218200			
C	-0.34663300	5.68912900	
1.05880800			
C	0.64994300	5.64116500	-
1.13945700			
C	-0.31350800	7.08421800	
1.04404800			
H	-0.74589400	5.15975300	
1.91940200			
C	0.68393200	7.03620900	-
1.15505700			
H	1.02140500	5.07478100	-
1.98884800			
C	0.20230800	7.76196700	-
0.06305000			
H	-0.68700300	7.64123400	
1.89929000			
H	1.08249700	7.55582300	-
2.02242600			
H	0.22843600	8.84828400	-
0.07493100			
C	4.95069700	-0.13568500	-
0.00155400			
C	5.65447900	-0.52999300	-
1.14934800			
C	5.67635000	0.21920500	
1.14548800			
C	7.04966500	-0.56965500	-
1.15031700			
H	5.09788900	-0.80463800	-
2.04109600			
C	7.07159900	0.18183600	
1.14498900			
H	5.13673800	0.52403600	
2.03786500			
C	7.76224600	-0.21326800	-
0.00303100			
H	7.57956000	-0.87492500	-
2.04877500			
H	7.61847600	0.45732500	
2.04289700			
H	8.84853000	-0.24327300	-
0.00358800			
C	-0.13596400	-4.94939200	

0.03487800			
C	-0.65805000	-5.66321700	-
1.05478800			
C	0.34021100	-5.66665500	
1.14323100			
C	-0.70236900	-7.05797000	-
1.03748900			
H	-1.02753800	-5.11412100	-
1.91632500			
C	0.29676700	-7.06140300	
1.16136900			
H	0.74279400	-5.12014200	
1.99145300			
C	-0.22479100	-7.76128700	
0.07081500			
H	-1.10636500	-7.59495800	-
1.89167600			
H	0.66616900	-7.60075600	
2.02959600			
H	-0.25909500	-8.84735200	
0.08471700			
C	-4.94744900	0.13546700	-
0.00132400			
C	-5.64941200	0.69279200	
1.07889300			
C	-5.67779200	-0.38229700	-
1.08240200			
C	-7.04432000	0.73171600	
1.07845500			
H	-5.09067200	1.09306900	
1.92018400			
C	-7.07271400	-0.34385500	-
1.08382300			
H	-5.14092500	-0.81291700	-
1.92295000			
C	-7.76030100	0.21344500	-
0.00317500			
H	-7.57160300	1.16293400	
1.92533800			
H	-7.62195100	-0.74525100	-
1.93140900			
H	-8.84657500	0.24362000	-
0.00391700			

⁴Mn (TPP)

Mn	-0.00134000	-0.00001800	-
0.00015100			
N	-1.44675700	1.41811600	
0.00849700			
C	0.03102200	-3.45667400	
0.01548700			
C	-3.45680400	-0.03333100	-
0.00061800			
C	-3.45274200	-2.54522600	-
0.05677400			
C	-2.48128800	-3.49875400	-
0.06508600			
C	-2.78818400	-1.26531200	-
0.02858500			
C	-1.21363500	-2.81141400	-
0.01939400			
H	-2.60649300	-4.57106100	-
0.09610800			
H	-4.52306300	-2.68962700	-
0.07045300			
N	1.41651200	1.44579600	
0.01179300			
N	-1.41913700	-1.44574000	-
0.00879100			
N	1.44411100	-1.41824900	-
0.01202800			
C	-0.03563000	3.45662000	-
0.01469700			
C	3.45507900	0.03330900	-
0.00053900			
C	3.49347400	-2.47547100	
0.15389400			
C	-3.50119300	2.47814200	
0.05633000			
C	3.44503900	2.54246100	-
0.15432700			
C	2.54001200	-3.44718300	
0.15407700			
C	-2.54833100	3.45023800	
0.06547300			
C	2.47297900	3.49556800	-
0.15382000			
C	2.80866100	-1.21114200	

0.03860500			
C	-2.81207100	1.21130400	
0.02782400			
C	2.78480400	1.26508900	-
0.03928200			
C	1.26296500	-2.78630900	
0.04085600			
C	-1.26764000	2.78750800	
0.01975000			
C	1.20897800	2.81011000	-
0.04053400			
H	2.68216400	-4.51445100	
0.23957900			
H	-2.69426700	4.51989700	
0.09703300			
H	2.59439700	4.56542300	-
0.23897100			
H	4.56317400	-2.59772200	
0.23933600			
H	-4.57410800	2.60184200	
0.06982400			
H	4.51214600	2.68543900	-
0.23996500			
C	0.04818100	-4.95177700	
0.03455000			
C	-0.44170400	-5.66058100	
1.14238800			
C	0.55862000	-5.67477100	-
1.05461600			
C	-0.42309200	-7.05587800	
1.16046000			
H	-0.83529600	-5.10708900	
1.99030200			
C	0.57810300	-7.07008700	-
1.03739800			
H	0.93867800	-5.13228900	-
1.91574300			
C	0.08697100	-7.76487900	
0.07035900			
H	-0.80285400	-7.58862000	
2.02830100			
H	0.97333300	-7.61411300	-
1.89123500			
H	0.10190700	-8.85138500	

0.08420000			
C	4.94969700	0.04772300	-
0.00103400			
C	5.66135500	0.59424300	
1.07839700			
C	5.67099100	-0.48480600	-
1.08105500			
C	7.05672900	0.60820500	
1.07826300			
H	5.10969700	1.00581200	
1.91890700			
C	7.06637100	-0.47132300	-
1.08218400			
H	5.12674700	-0.90713500	-
1.92106100			
C	7.76358700	0.07537700	-
0.00229300			
H	7.59143600	1.03132100	
1.92457900			
H	7.60852800	-0.88387100	-
1.92897600			
H	8.85022700	0.08609100	-
0.00279600			
C	-0.04729700	4.95179600	-
0.03245700			
C	0.44878200	5.68343100	
1.05757200			
C	-0.55077400	5.65210500	-
1.13960400			
C	0.44077400	7.07887800	
1.04199000			
H	0.83935200	5.14750300	
1.91809800			
C	-0.55965000	7.04751900	-
1.15604200			
H	-0.93323800	5.09199900	-
1.98827100			
C	-0.06388200	7.76515500	-
0.06499800			
H	0.82512200	7.62958500	
1.89651100			
H	-0.94968200	7.57369600	-
2.02333500			
H	-0.07042300	8.85176000	-

0.07753800			
C	-4.95309400	-0.04783100	-
0.00116000			
C	-5.66399300	-0.43371400	-
1.14746200			
C	-5.67227100	0.32407800	
1.14460000			
C	-7.05965700	-0.44851800	-
1.14823300			
H	-5.11251000	-0.72145000	-
2.03825000			
C	-7.06795600	0.31155200	
1.14431300			
H	-5.12722500	0.62250600	
2.03583300			
C	-7.76567200	-0.07535300	-
0.00222400			
H	-7.59499200	-0.74752200	-
2.04557300			
H	-7.60972500	0.59997800	
2.04125500			
H	-8.85231700	-0.08600500	-
0.00262600			
⁶Mn (TPP)			
Mn	0.00160800	-0.00007700	-
0.00108800			
N	1.41398500	-1.53840000	-
0.01083200			
C	0.15255100	3.47169600	-
0.00306000			
C	3.47342800	-0.14887200	-
0.00136300			
C	3.61714300	2.38941800	
0.03536200			
C	2.69504900	3.39534400	
0.04787000			
C	2.88828100	1.13846800	
0.01958500			
C	1.38525400	2.77845700	
0.01721100			
H	2.88580200	4.45833900	
0.07472900			
H	4.69315700	2.48640300	

0.03795500			
N	-1.53677400	-1.41243900	-
0.05753800			
N	1.54043000	1.41177600	
0.00892300			
N	-1.41025500	1.53874300	
0.05608700			
C	-0.14504900	-3.47199800	
0.00298900			
C	-3.47005800	0.14874800	-
0.00082400			
C	-3.38718500	2.68610700	-
0.15628500			
C	3.39944000	-2.69017200	-
0.03696200			
C	-3.60463100	-2.38626200	
0.15555500			
C	-2.38110900	3.60834700	-
0.15301400			
C	2.39463900	-3.61351000	-
0.04850300			
C	-2.68118200	-3.39123200	
0.15293200			
C	-2.77469800	1.38135200	-
0.02023500			
C	2.78028200	-1.38143200	-
0.02184500			
C	-2.88272400	-1.13882300	
0.01881900			
C	-1.13509300	2.88446700	-
0.01545600			
C	1.14243800	-2.88678300	-
0.01808200			
C	-1.37776100	-2.77674500	
0.01486300			
H	-2.47363100	4.67981600	-
0.25621500			
H	2.49370400	-4.68897100	-
0.07452300			
H	-2.86515700	-4.45076600	
0.25679400			
H	-4.44590900	2.87196100	-
0.26448900			
H	4.46320100	-2.87892200	-

0.03949200			
H	-4.67536000	-2.48070800	
0.26408000			
C	-0.21374500	-4.96589400	
0.03187900			
C	-0.78051600	-5.67630800	-
1.03811100			
C	0.28066600	-5.68766200	
1.12983400			
C	-0.84961500	-7.06978900	-
1.01229900			
H	-1.16433600	-5.12503000	-
1.89189700			
C	0.21238300	-7.08115000	
1.15653700			
H	0.71591500	-5.14506400	
1.96425000			
C	-0.35297100	-7.77675700	
0.08524100			
H	-1.28771400	-7.60312100	-
1.85185300			
H	0.59613000	-7.62284000	
2.01706800			
H	-0.40659900	-8.86192900	
0.10583600			
C	4.96906200	-0.21304700	-
0.00153900			
C	5.70323800	0.18801300	
1.12521400			
C	5.66594700	-0.67571500	-
1.12835700			
C	7.09761600	0.12897700	
1.12543200			
H	5.17027400	0.54521200	
2.00196800			
C	7.06023700	-0.73690500	-
1.12865100			
H	5.10414900	-0.98572200	-
2.00506800			
C	7.78042200	-0.33422700	-
0.00161700			
H	7.64994300	0.44051200	
2.00810500			
H	7.58364900	-1.09482700	-

2.01135500			
H	8.86610500	-0.38106700	-
0.00163200			
C	0.21192500	4.96606300	-
0.02919900			
C	-0.29157000	5.72022600	
1.04246200			
C	0.76632200	5.64502400	-
1.12582700			
C	-0.24028700	7.11453000	
1.01985100			
H	-0.72142400	5.20205800	
1.89504400			
C	0.81840100	7.03927100	-
1.14933800			
H	1.15302300	5.06890500	-
1.96169000			
C	0.31543400	7.77855900	-
0.07618900			
H	-0.63071200	7.68171600	
1.86073800			
H	1.24721500	7.54785400	-
2.00879400			
H	0.35560300	8.86435500	-
0.09428200			
C	-4.96328900	0.21275300	-
0.00112600			
C	-5.70520300	-0.33753500	-
1.05885500			
C	-5.65587500	0.82464200	
1.05623200			
C	-7.09916000	-0.27767600	-
1.05984000			
H	-5.17726000	-0.80902900	-
1.88284800			
C	-7.04982500	0.88468500	
1.05634300			
H	-5.08992900	1.24920900	
1.88052000			
C	-7.77617300	0.33370700	-
0.00198100			
H	-7.65601200	-0.70428900	-
1.88996800			
H	-7.56851600	1.35754600	

1.88614100			
H	-8.86185500	0.38040200	-
0.00231600			
²TS1			
N	-1.08656900	-1.35754300	
0.73157000			
C	3.76907600	0.08502800	
0.17882500			
C	0.34922800	-3.37421800	
0.63380500			
C	2.83175500	-3.39501400	
0.23325900			
C	3.78257900	-2.43137300	
0.09669800			
C	1.57659100	-2.71850400	
0.46214800			
C	3.11744000	-1.15687800	
0.24557300			
H	4.83626000	-2.56459300	-
0.09974700			
H	2.95911100	-4.46580100	
0.17103700			
N	-1.09781100	1.51174900	
0.66957600			
N	1.76916900	-1.35258100	
0.44999300			
N	1.75136500	1.51793000	
0.32503000			
C	-3.10526900	0.07007000	
0.88140700			
C	0.31901700	3.53635100	
0.43452100			
C	2.83447800	3.56026600	
0.36431700			
C	-2.13559100	-3.39723400	
1.02415000			
C	-2.19615300	3.54103400	
0.54013600			
C	3.79449300	2.59851300	
0.29584100			
C	-3.09910500	-2.43864800	
1.08692800			
C	-3.14858500	2.57592200	

0.67819300			
C	1.55877500	2.88258300	
0.37244100			
C	-0.88199000	-2.71908900	
0.78837700			
C	-0.91549300	2.87572200	
0.55258300			
C	3.11469500	1.32417600	
0.25788800			
C	-2.44161700	-1.16625900	
0.89225600			
C	-2.46051800	1.31167700	
0.76859700			
H	4.86626500	2.73243900	
0.28863200			
H	-4.15576800	-2.57188900	
1.26739000			
H	-4.22072900	2.70491400	
0.70319800			
H	2.97175800	4.62997900	
0.42430300			
H	-2.25245200	-4.46481500	
1.13987000			
H	-2.34423700	4.60566300	
0.43312600			
N	-0.07957100	-0.36109100	-
1.95108900			
N	0.15439600	-1.61896200	-
2.21603900			
N	-0.45671300	-2.47619100	-
2.72744500			
C	-1.37531000	-0.11406400	-
2.45276600			
C	-1.96611200	1.16036800	-
2.36466100			
C	-3.25817900	-1.01713900	-
3.48247100			
C	-3.25651500	1.29851900	-
2.84429400			
H	-1.42180200	1.97589400	-
1.90668900			
C	-3.92448000	0.19705600	-
3.41290400			
H	-3.70355800	-1.90759700	-

3.91595800			
H	-3.75482800	2.25982500	-
2.76808300			
H	-4.93718700	0.28597100	-
3.79093400			
N	-2.01012800	-1.13930400	-
3.00674600			
Mn	0.32957400	0.08402600	
0.42712500			
C	0.34335500	-4.86869000	
0.60956400			
C	-0.26170800	-5.55371500	-
0.45588600			
C	0.94146400	-5.61175400	
1.63814400			
C	-0.26915600	-6.94873300	-
0.48992500			
H	-0.71692200	-4.98010600	-
1.25846900			
C	0.93354900	-7.00712500	
1.60443200			
H	1.41031500	-5.08561200	
2.46504400			
C	0.32766100	-7.67946900	
0.54043700			
H	-0.73708400	-7.46491800	-
1.32420800			
H	1.39717700	-7.56862700	
2.41133800			
H	0.32147400	-8.76592700	
0.51402200			
C	5.25500000	0.08947400	
0.02049000			
C	5.84940700	0.61933800	-
1.13569700			
C	6.08642400	-0.43363700	
1.02342100			
C	7.23670800	0.62536900	-
1.28574900			
H	5.21189500	1.02390700	-
1.91674300			
C	7.47387200	-0.42795000	
0.87450300			
H	5.63370900	-0.84236200	

1.92238500			
C	8.05347400	0.10153900	-
0.28090100			
H	7.67915500	1.03531200	-
2.18991400			
H	8.10211800	-0.83297800	
1.66352200			
H	9.13396100	0.10605800	-
0.39728000			
C	0.31167300	5.02955300	
0.37955400			
C	0.75851500	5.70516800	-
0.76719300			
C	-0.14062900	5.78778500	
1.47117300			
C	0.75230600	7.09951000	-
0.82219400			
H	1.11123900	5.12522500	-
1.61551400			
C	-0.14758000	7.18214200	
1.41735600			
H	-0.48349100	5.27239600	
2.36386800			
C	0.29855300	7.84259900	
0.27011400			
H	1.09877500	7.60508900	-
1.71979800			
H	-0.49636500	7.75262500	
2.27419900			
H	0.29386500	8.92850800	
0.22818000			
C	-4.59674100	0.06336200	
0.97124900			
C	-5.36764400	-0.49832600	-
0.05907000			
C	-5.25776000	0.62056100	
2.07683000			
C	-6.76107000	-0.50139900	
0.01331600			
H	-4.86182200	-0.92670800	-
0.91888800			
C	-6.65155000	0.61882400	
2.14971200			
H	-4.66775600	1.05309200	

2.87989100			
C	-7.40796100	0.05807900	
1.11786100			
H	-7.34214400	-0.93833600	-
0.79496500			
H	-7.14628300	1.05068300	
3.01573300			
H	-8.49319400	0.05578600	
1.17504100			
4TS1			
N	-1.10388800	-1.33869200	
0.71357900			
C	3.78237900	0.04199600	
0.22132300			
C	0.30706900	-3.37333900	
0.59155900			
C	2.79440900	-3.42435500	
0.21749500			
C	3.76251900	-2.47330200	
0.11565400			
C	1.54595000	-2.73314100	
0.43968400			
C	3.11383300	-1.19159300	
0.27177300			
H	4.81711900	-2.61941900	-
0.06626000			
H	2.90669200	-4.49555300	
0.13608900			
N	-1.07650900	1.53131900	
0.66301700			
N	1.75968200	-1.37112200	
0.45272300			
N	1.78021100	1.49899100	
0.33269200			
C	-3.10039700	0.11595900	
0.90431000			
C	0.36564100	3.53295000	
0.39133000			
C	2.88220300	3.53006500	
0.34678800			
C	-2.17498000	-3.36639000	
0.99764600			
C	-2.15027700	3.56995100	

0.49736600			
C	3.83367900	2.55769000	
0.30728100			
C	-3.12413200	-2.39532500	
1.09156100			
C	-3.11346700	2.61931300	
0.66033900			
C	1.59984000	2.86507100	
0.35277200			
C	-0.91562100	-2.70330400	
0.75384500			
C	-0.87739100	2.88978700	
0.51852400			
C	3.14132800	1.29000000	
0.28278600			
C	-2.45412200	-1.12986400	
0.89912500			
C	-2.43989200	1.34857700	
0.77140900			
H	4.90668100	2.68140300	
0.30928100			
H	-4.17885500	-2.51797800	
1.28961400			
H	-4.18387000	2.76166700	
0.68689100			
H	3.02975700	4.59930000	
0.38869300			
H	-2.30552900	-4.43370800	
1.10068300			
H	-2.28670400	4.63377800	
0.36893000			
N	-0.06859200	-0.34694300	-
2.05376200			
N	0.14695100	-1.61134400	-
2.29943200			
N	-0.49686600	-2.47920600	-
2.75292200			
C	-1.39048300	-0.11243000	-
2.48230500			
C	-1.97764400	1.16307100	-
2.38115200			
C	-3.33106800	-1.03497500	-
3.37998800			
C	-3.29348500	1.29294400	-

2.78743800			
H	-1.40915100	1.98558000	-
1.96639000			
C	-3.99195600	0.18123900	-
3.29730600			
H	-3.80161000	-1.93381700	-
3.76725000			
H	-3.78849800	2.25477700	-
2.69783900			
H	-5.02499500	0.26358200	-
3.61738600			
N	-2.05744100	-1.14892400	-
2.97526700			
Mn	0.33583500	0.08008600	
0.44906400			
C	0.27862900	-4.86694200	
0.54595300			
C	-0.33930000	-5.52660400	-
0.52818700			
C	0.86587200	-5.63437800	
1.56296700			
C	-0.36932900	-6.92071500	-
0.58200500			
H	-0.78544200	-4.93407000	-
1.32195100			
C	0.83517000	-7.02876800	
1.50936100			
H	1.34400900	-5.12787700	
2.39679400			
C	0.21692400	-7.67580400	
0.43679100			
H	-0.84661100	-7.41723000	-
1.42290400			
H	1.29050800	-7.60923800	
2.30751900			
H	0.19300100	-8.76153000	
0.39484200			
C	5.27084200	0.02578000	
0.09019500			
C	5.89506000	0.54370900	-
1.05566000			
C	6.07480800	-0.50874300	
1.10933400			
C	7.28489300	0.52810800	-

1.17919300			
H	5.27885400	0.95562000	-
1.84983900			
C	7.46476600	-0.52470200	
0.98685200			
H	5.59879600	-0.90939400	
1.99987700			
C	8.07426300	-0.00615900	-
0.15805700			
H	7.75068200	0.92904300	-
2.07562900			
H	8.07156400	-0.93825600	
1.78813100			
H	9.15669700	-0.01849600	-
0.25390900			
C	0.37627900	5.02448500	
0.30186100			
C	0.83774600	5.66712200	-
0.85801000			
C	-0.07192100	5.81383400	
1.37293800			
C	0.84916600	7.05973300	-
0.94591700			
H	1.18754900	5.06292200	-
1.69045300			
C	-0.06105400	7.20651000	
1.28619500			
H	-0.42535800	5.32409600	
2.27588400			
C	0.39911600	7.83400600	
0.12607600			
H	1.20656300	7.53959100	-
1.85328700			
H	-0.40685700	7.80140500	
2.12749800			
H	0.40823400	8.91858700	
0.05850500			
C	-4.58877500	0.13367500	
1.03264300			
C	-5.39850100	-0.43716000	
0.03758900			
C	-5.20925000	0.72629000	
2.14366500			
C	-6.78910200	-0.41523900	

0.14963800			
H	-4.92474100	-0.89192400	-
0.82665200			
C	-6.60009800	0.74964800	
2.25618100			
H	-4.58966900	1.16659300	
2.91975300			
C	-7.39496300	0.17911200	
1.25919100			
H	-7.40008400	-0.85971700	-
0.63204100			
H	-7.06252000	1.20880700	
3.12599800			
H	-8.47799400	0.19640300	
1.34711900			
⁶TS1			
N	-1.23334000	-1.26069400	
0.73737800			
C	3.80717900	-0.25041900	
0.18881400			
C	0.05214300	-3.38151500	
0.63875500			
C	2.54656300	-3.65456300	
0.22200900			
C	3.59039200	-2.78518000	
0.10058700			
C	1.35601100	-2.86228000	
0.46061800			
C	3.05352300	-1.44688500	
0.25736900			
H	4.62501500	-3.02662200	-
0.09573500			
H	2.57746700	-4.73178300	
0.14471900			
N	-0.95693300	1.67601100	
0.69148900			
N	1.69886100	-1.53263600	
0.46075700			
N	1.95725500	1.40620700	
0.24584800			
C	-3.07010300	0.39050800	
0.94773000			
C	0.67575100	3.52722300	

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C	3.21167800	3.32546200	
0.37372000			
C	-2.43811500	-3.17923500	
1.11575600			
C	-1.85471500	3.78031900	
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C	4.08087800	2.27543000	
0.32497000			
C	-3.30639900	-2.13153800	
1.20677300			
C	-2.89314800	2.90991800	
0.66037200			
C	1.87209400	2.77361700	
0.32264800			
C	-1.13183200	-2.62622000	
0.81299800			
C	-0.63333200	3.00195700	
0.52016100			
C	3.28652700	1.06552600	
0.23890300			
C	-2.54436300	-0.92232100	
0.95693200			
C	-2.32419700	1.58559900	
0.79859600			
H	5.15964300	2.31407700	
0.37133400			
H	-4.35987800	-2.17065000	
1.44391600			
H	-3.94746300	3.14562400	
0.68054700			
H	3.45385300	4.37426700	
0.46794000			
H	-2.65476500	-4.22766400	
1.26214500			
H	-1.91389200	4.84929400	
0.33953300			
N	-0.22580700	-0.42180800	-
2.07325200			
N	-0.06366100	-1.68411700	-
2.36260800			
N	-0.72130200	-2.51083800	-
2.86020400			
C	-1.53435700	-0.10093200	-

2.50879200			
C	-2.05477900	1.19586200	-
2.35075400			
C	-3.50247100	-0.88325400	-
3.46456900			
C	-3.36040300	1.40890800	-
2.75945800			
H	-1.45245300	1.97087100	-
1.89379400			
C	-4.10528100	0.35882600	-
3.32671100			
H	-4.01241600	-1.73781200	-
3.89886200			
H	-3.80844100	2.38824200	-
2.62505600			
H	-5.13043300	0.50583900	-
3.64875700			
N	-2.24048400	-1.07965800	-
3.05572700			
Mn	0.33803300	0.06436600	
0.20723900			
C	-0.09720400	-4.86869500	
0.62121600			
C	-0.82947700	-5.49260000	-
0.40176200			
C	0.48670500	-5.66887700	
1.61548300			
C	-0.97368000	-6.88020600	-
0.42900200			
H	-1.27477700	-4.87798600	-
1.17914700			
C	0.34190400	-7.05664400	
1.58903700			
H	1.05153600	-5.19159100	
2.41131300			
C	-0.38910500	-7.66655700	
0.56675000			
H	-1.53866700	-7.34758100	-
1.23138600			
H	0.79612000	-7.66090100	
2.37000900			
H	-0.50184900	-8.74728200	
0.54604800			
C	5.28979000	-0.38628000	

0.06426900			
C	5.96592100	0.13036700	-
1.05315000			
C	6.04027300	-1.02973900	
1.06203200			
C	7.35060000	0.00602400	-
1.17078900			
H	5.39307000	0.62723400	-
1.83095600			
C	7.42502200	-1.15426200	
0.94559800			
H	5.52643500	-1.42677900	
1.93279900			
C	8.08504400	-0.63700600	-
0.17161300			
H	7.85510800	0.40748200	-
2.04581200			
H	7.98903200	-1.65055400	
1.73103200			
H	9.16363700	-0.73383000	-
0.26259700			
C	0.80968300	5.01327000	
0.31027400			
C	1.38110700	5.62686700	-
0.81678300			
C	0.37416000	5.82975500	
1.36718500			
C	1.51005500	7.01433100	-
0.88728200			
H	1.72172200	5.00337600	-
1.63862100			
C	0.50284800	7.21725100	
1.29793800			
H	-0.06049000	5.36383800	
2.24685100			
C	1.07057400	7.81458600	
0.16992300			
H	1.95064400	7.47034400	-
1.77006500			
H	0.16563400	7.83144700	
2.12882500			
H	1.17141400	8.89529200	
0.11607000			
C	-4.55214300	0.52899500	

1.07354400			
C	-5.40437300	-0.02946100	
0.10631800			
C	-5.12713900	1.22442900	
2.14948700			
C	-6.78912600	0.10519800	
0.21029500			
H	-4.96739000	-0.56476300	-
0.73090700			
C	-6.51200200	1.36027600	
2.25410900			
H	-4.47635000	1.65422400	
2.90552600			
C	-7.34821300	0.80170800	
1.28440700			
H	-7.43192400	-0.33152900	-
0.55000500			
H	-6.93816300	1.89745900	
3.09737500			
H	-8.42674300	0.90675000	
1.36647200			
²INT1			
Mn	-0.28972700	0.14899100	-
0.50200300			
N	-2.30353500	0.28226900	-
0.35611900			
C	1.95913500	-2.44650300	-
0.72383400			
C	-2.90805100	-2.11483000	-
0.56670100			
C	-1.28026100	-4.01183200	-
0.87922200			
C	0.07797500	-4.10626600	-
0.86982400			
C	-1.60649600	-2.61402000	-
0.72325700			
C	0.59286600	-2.76402800	-
0.74455000			
H	0.68334300	-4.99636700	-
0.96123600			
H	-1.99979300	-4.81155300	-
0.97463100			
N	-0.13789600	2.16209700	-

0.41736800				
N	-0.44905700	-1.86467100	-	
0.67792100				
N	1.71137600	0.01681600	-	
0.80750200				
C	-2.52262900	2.73001300	-	
0.03540500				
C	2.29612400	2.42506300	-	
0.81126300				
C	3.96017300	0.54302900	-	
0.89154600				
C	-4.52810300	-0.26469900	-	
0.04688700				
C	0.66234400	4.32514500	-	
0.57815800				
C	3.86888100	-0.81336600	-	
0.81849300				
C	-4.41734900	1.08070600		
0.12932600				
C	-0.67648100	4.40862700	-	
0.34381900				
C	2.61259400	1.05894500	-	
0.87124600				
C	-3.20811400	-0.76068100	-	
0.35339900				
C	0.99922400	2.92247700	-	
0.61181600				
C	2.46461000	-1.14067900	-	
0.78390600				
C	-3.03131600	1.42263600	-	
0.08567900				
C	-1.17361100	3.05784000	-	
0.24125100				
H	4.67566100	-1.53026600	-	
0.78124600				
H	-5.19832300	1.78008700		
0.38900900				
H	-1.28104900	5.30070300	-	
0.27011200				
H	4.85679700	1.14444800	-	
0.92175000				
H	-5.41557400	-0.87399500		
0.04177200				
H	1.35916000	5.13611500	-	

0.73196100			
N	0.02754300	-0.49045400	
2.05857000			
N	-0.61418000	-1.53243900	
2.30073500			
N	-1.31550500	-2.40933500	
2.45481400			
C	1.40216200	-0.51013100	
2.41519300			
C	2.10183200	0.69302400	
2.26388400			
C	3.25823700	-1.63843000	
3.10629500			
C	3.46151800	0.68249500	
2.54482100			
H	1.58823200	1.57298300	
1.89495800			
C	4.05890800	-0.50558000	
2.97940100			
H	3.68305000	-2.58599400	
3.43018700			
H	4.04963500	1.58538000	
2.40856700			
H	5.11978300	-0.55599200	
3.20134700			
N	1.94651900	-1.65481700	
2.82832300			
C	-3.47805700	3.84955300	
0.22401000			
C	-3.36948700	4.62283900	
1.39050800			
C	-4.49593100	4.15604700	-
0.69282200			
C	-4.25605600	5.67220200	
1.63567800			
H	-2.58426300	4.39101600	
2.10461400			
C	-5.38304500	5.20515300	-
0.44866800			
H	-4.58261600	3.56556400	-
1.60052700			
C	-5.26606100	5.96635800	
0.71673900			
H	-4.16013600	6.25715300	

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H	-6.16238200	5.43101100	-
1.17174300			
H	-5.95678100	6.78343100	
0.90707800			
C	-4.04065800	-3.08989900	-
0.56029400			
C	-5.00541100	-3.07350600	-
1.57894300			
C	-4.16492800	-4.03161000	
0.47340000			
C	-6.06691600	-3.97959500	-
1.56799300			
H	-4.91432600	-2.34543500	-
2.38025400			
C	-5.22660900	-4.93716900	
0.48450700			
H	-3.42476900	-4.04098600	
1.26837600			
C	-6.18008300	-4.91443000	-
0.53630600			
H	-6.80317100	-3.95719000	-
2.36717300			
H	-5.31149700	-5.65737600	
1.29406400			
H	-7.00661200	-5.61999300	-
0.52733100			
C	2.92669500	-3.57771900	-
0.59577800			
C	2.97368100	-4.30867800	
0.60251300			
C	3.79342900	-3.93055200	-
1.64006000			
C	3.87186800	-5.36606500	
0.75161400			
H	2.30721800	-4.02695000	
1.41279900			
C	4.69165200	-4.98881200	-
1.48989500			
H	3.75493200	-3.37164100	-
2.57099200			
C	4.73355900	-5.70881800	-
0.29364400			
H	3.89981300	-5.92172700	

1.68548200			
H	5.35433200	-5.25404400	-
2.30954000			
H	5.43219000	-6.53318900	-
0.17758900			
C	3.42176500	3.40322000	-
0.90007500			
C	4.18038300	3.52457500	-
2.07446300			
C	3.75677500	4.20743800	
0.20137700			
C	5.24446300	4.42477400	-
2.14593000			
H	3.92696900	2.90628600	-
2.93094600			
C	4.82034600	5.10808000	
0.13135400			
H	3.17239900	4.12095800	
1.11362600			
C	5.56818000	5.21897600	-
1.04329300			
H	5.81827600	4.50849400	-
3.06510400			
H	5.06673800	5.72022800	
0.99500300			
H	6.39670300	5.91985600	-
1.09925400			
⁴INT1			
Mn	-0.28305300	0.15047600	-
0.54107700			
N	1.70337000	-0.03725800	-
0.78718700			
C	-2.43552700	2.78017200	
0.01632300			
C	2.36129600	2.34985700	-
0.87177700			
C	0.78127400	4.28853700	-
0.60572600			
C	-0.55066200	4.40594300	-
0.32240300			
C	1.07949500	2.88661400	-
0.66095500			
C	-1.08133200	3.07737300	-

0.22026200				
H	-1.12712500	5.31297800	-	
0.21486700				
H	1.49570000	5.08176000	-	
0.76973800				
N	-0.49122800	-1.85424200	-	
0.67450700				
N	-0.07518600	2.15582300	-	
0.44011600				
N	-2.27025500	0.33692600	-	
0.35277000				
C	1.90447600	-2.50074400	-	
0.64865800				
C	-2.96084700	-2.02966800	-	
0.62851600				
C	-4.52169200	-0.14600000	-	
0.07645300				
C	3.97182600	0.42756100	-	
0.90452200				
C	-1.37877100	-3.96744300	-	
0.90146300				
C	-4.37133800	1.18298800	-	
0.14346700				
C	3.84880900	-0.91617800	-	
0.77462000				
C	-0.02024900	-4.10188700	-	
0.83761600				
C	-3.21261600	-0.67916500	-	
0.38905300				
C	2.63470900	0.98221100	-	
0.89468900				
C	-1.67061200	-2.56958800	-	
0.76158800				
C	-2.97107400	1.49483700	-	
0.05427100				
C	2.43393000	-1.21447200	-	
0.72741500				
C	0.52887700	-2.78421700	-	
0.69927900				
H	-5.13011900	1.90094300	-	
0.41727800				
H	4.63578200	-1.65292400	-	
0.71357300				
H	0.56115200	-5.01017100	-	

0.89966800			
H	-5.42561400	-0.73371500	-
0.01397900			
H	4.87980400	1.00899300	-
0.96533100			
H	-2.11742000	-4.74693400	-
1.01495200			
N	-0.01656000	-0.43600900	
2.08665400			
N	-0.70331800	-1.45047200	
2.31811200			
N	-1.44329000	-2.29693500	
2.46314500			
C	1.35616200	-0.51421700	
2.43647500			
C	2.10887300	0.65389500	
2.26119600			
C	3.16451700	-1.71207700	
3.13794000			
C	3.46773200	0.58768600	
2.53678700			
H	1.63358100	1.54901600	
1.87763200			
C	4.01411100	-0.61847700	
2.98879500			
H	3.54891300	-2.67231100	
3.47470200			
H	4.09506800	1.46069800	
2.38227200			
H	5.07281300	-0.71248800	
3.20687200			
N	1.85172600	-1.67488900	
2.86651500			
C	3.51071800	3.29565200	-
1.00089700			
C	4.23557100	3.38569900	-
2.19871200			
C	3.90186800	4.09712400	
0.08349400			
C	5.32280000	4.25386600	-
2.30993500			
H	3.93866400	2.76784900	-
3.04148200			
C	4.98829600	4.96589800	-

0.02636200			
H	3.34336100	4.03412100	
1.01366500			
C	5.70259700	5.04637400	-
1.22422700			
H	5.87093400	4.31354400	-
3.24648000			
H	5.27885600	5.57683400	
0.82430800			
H	6.54891500	5.72241900	-
1.31100800			
C	-3.35070200	3.92197300	
0.31992600			
C	-3.20290400	4.65328700	
1.50867500			
C	-4.36402600	4.29367900	-
0.57708000			
C	-4.04932300	5.72489000	
1.79595100			
H	-2.41913000	4.37173700	
2.20631600			
C	-5.21123400	5.36501100	-
0.29063700			
H	-4.47934700	3.73612300	-
1.50227000			
C	-5.05664400	6.08362000	
0.89714200			
H	-3.92411300	6.27703600	
2.72368300			
H	-5.98855800	5.64136700	-
0.99816400			
H	-5.71602600	6.91808200	
1.12034600			
C	-4.12429100	-2.96695100	-
0.66462700			
C	-5.05301400	-2.91379900	-
1.71444700			
C	-4.31431800	-3.90670700	
0.36055200			
C	-6.14483900	-3.78298700	-
1.74236800			
H	-4.91093000	-2.18588600	-
2.50848800			
C	-5.40596900	-4.77547500	

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H	-3.60140400	-3.94343700	
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C	-6.32369400	-4.71670600	-
0.71911200			
H	-6.85353400	-3.73237300	-
2.56482400			
H	-5.54240700	-5.49487800	
1.13589200			
H	-7.17370800	-5.39352000	-
0.74039900			
C	2.83686400	-3.65627700	-
0.48639600			
C	3.71535300	-4.04671200	-
1.50710700			
C	2.83335800	-4.37614300	
0.71948500			
C	4.57847200	-5.12894900	-
1.32511200			
H	3.71385500	-3.49797000	-
2.44482900			
C	3.69625900	-5.45763500	
0.90024200			
H	2.15539800	-4.06762100	
1.51008900			
C	4.57180500	-5.83649300	-
0.12081600			
H	5.25136100	-5.42264800	-
2.12651800			
H	3.68559400	-6.00420300	
1.83980600			
H	5.24297100	-6.67960500	
0.01999000			
6INT1			
Mn	-0.30720700	0.12732800	-
0.32404000			
N	-0.31372600	2.22374000	-
0.34279500			
C	-2.78072100	-2.33030800	-
0.48781000			
C	-2.76315500	2.56858700	-
0.08571200			
C	-4.55960400	0.77612700	

0.11231900				
C	-4.56505100	-0.58284000	-	
0.00927800				
C	-3.19959400	1.22193900	-	
0.11586500				
C	-3.20827200	-0.99226000	-	
0.31062200				
H	-5.40762200	-1.24848800		
0.11026200				
H	-5.39705900	1.41551100		
0.35112500				
N	1.73729900	0.16264400	-	
0.85073600				
N	-2.40801100	0.12450000	-	
0.35445200				
N	-0.33975400	-1.94616300	-	
0.66842600				
C	2.10860100	2.61434800	-	
0.73938600				
C	2.11207500	-2.29299900	-	
0.83013600				
C	0.34816300	-4.12139600	-	
0.92045800				
C	-1.03037300	4.40390100	-	
0.39242600				
C	3.93068800	-0.51902800	-	
0.87570300				
C	-1.01490300	-4.13170000	-	
0.85709800				
C	0.32197100	4.41749900	-	
0.57670200				
C	3.92976900	0.84507400	-	
0.88133700				
C	0.77113800	-2.74084500	-	
0.80014200				
C	-1.43036600	3.01934800	-	
0.24650600				
C	2.54734700	-0.94815000	-	
0.86396600				
C	-1.44544000	-2.75917500	-	
0.67347600				
C	0.77237400	3.04146500	-	
0.54806200				
C	2.54536700	1.27273600	-	

0.85292500				
H	-1.66917500	-4.98827300	-	
0.93012800				
H	0.95204900	5.27824300	-	
0.74931600				
H	4.78887600	1.50004400	-	
0.87211600				
H	1.00773800	-4.96645500	-	
1.05712900				
H	-1.69964900	5.25207000	-	
0.38654800				
H	4.78923600	-1.17461200	-	
0.86525600				
C	-3.80858400	3.61887800		
0.10858800				
C	-4.84552500	3.78552600	-	
0.82377700				
C	-3.77110500	4.46706900		
1.22719500				
C	-5.81789300	4.76942500	-	
0.64176300				
H	-4.87829900	3.13846100	-	
1.69565000				
C	-4.74314200	5.45112600		
1.41041200				
H	-2.97320000	4.34416700		
1.95409700				
C	-5.77025400	5.60536200		
0.47639900				
H	-6.60964900	4.88663500	-	
1.37703800				
H	-4.70047100	6.09432700		
2.28549500				
H	-6.52750600	6.37174600		
0.61839600				
C	-3.83282200	-3.39109000	-	
0.43490900				
C	-3.83250500	-4.34582900		
0.59488000				
C	-4.84327400	-3.45039800	-	
1.40744200				
C	-4.81584500	-5.33438700		
0.64865700				
H	-3.05719500	-4.30069200		

1.35438800			
C	-5.82658600	-4.43913200	-
1.35397000			
H	-4.84803600	-2.71558800	-
2.20763000			
C	-5.81564800	-5.38451000	-
0.32568100			
H	-4.80348200	-6.06265500	
1.45538100			
H	-6.59844400	-4.47341300	-
2.11840200			
H	-6.58124900	-6.15465800	-
0.28376700			
C	3.16841000	-3.34936200	-
0.76854200			
C	3.31421800	-4.11230400	
0.40165800			
C	4.02823500	-3.59511600	-
1.84883100			
C	4.29901700	-5.09715000	
0.48720300			
H	2.65635900	-3.91089200	
1.24246200			
C	5.01289300	-4.58107500	-
1.76276300			
H	3.91590800	-3.00961800	-
2.75713100			
C	5.15091100	-5.33458500	-
0.59465600			
H	4.40256600	-5.67799500	
1.40021500			
H	5.66849900	-4.76385000	-
2.61018000			
H	5.91698100	-6.10263800	-
0.52841300			
C	3.16004400	3.67430400	-
0.78562700			
C	3.37418100	4.51367700	
0.32060200			
C	3.96634400	3.84743900	-
1.92205600			
C	4.36629600	5.49447100	
0.29346300			
H	2.75201900	4.39013400	

1.20304600			
C	4.95861300	4.82802700	-
1.95071000			
H	3.80461800	3.20648600	-
2.78393400			
C	5.16284500	5.65424100	-
0.84286200			
H	4.51879100	6.13151000	
1.16081400			
H	5.56912300	4.95019800	-
2.84152000			
H	5.93557300	6.41790800	-
0.86566800			
C	1.56266400	-0.47814500	
2.41540000			
C	3.50274300	0.89753200	
2.53265200			
C	4.21426700	-0.23729600	
2.93462600			
C	3.52477500	-1.44231100	
3.05409900			
H	4.00152300	1.85349400	
2.40340500			
H	5.27922000	-0.19291300	
3.13720300			
H	4.04043900	-2.35169400	
3.35415600			
N	0.18202000	-0.58645800	
2.07886600			
N	-0.94760400	-2.63496400	
2.50600500			
N	-0.34907800	-1.68999500	
2.33288200			
C	2.14195700	0.78725500	
2.27542200			
H	1.54363700	1.62471300	
1.93525900			
N	2.21550800	-1.57448100	
2.79735300			
²INT2			
Mn	0.32875400	-0.13284300	-
0.43141100			
N	0.40140200	-2.13224600	-

0.73637500				
C	-2.16542100	2.25247900	-	
0.36467000				
C	-2.00788700	-2.56349600	-	
1.00548900				
C	-3.89157500	-0.90792800	-	
0.73679100				
C	-3.91615100	0.44909800	-	
0.55700100				
C	-2.48382200	-1.27229500	-	
0.80717300				
C	-2.55101800	0.91150000	-	
0.51518600				
H	-2.74193000	-3.34105400	-	
1.18596600				
H	-4.79280900	1.06747400	-	
0.42930600				
N	2.36279700	-0.06998800	-	
0.49057400				
N	-1.69306300	-0.15760000	-	
0.64927800				
N	0.28983300	1.90580600	-	
0.47903400				
C	2.83080900	-2.50942500	-	
0.51948600				
C	2.72091700	2.38182100	-	
0.55071800				
C	0.91144000	4.13279000	-	
0.43547800				
C	-0.24310800	-4.33328500	-	
1.01947100				
C	4.55754100	0.65494600	-	
0.57498800				
C	-0.44660900	4.09209000	-	
0.35624400				
C	1.10523000	-4.33275200	-	
0.82706500				
C	4.58392500	-0.70474000	-	
0.52365400				
C	1.36938300	2.76443600	-	
0.51323700				
C	-0.67591800	-2.96020300	-	
0.94818500				
C	3.16817400	1.05001500	-	

0.53929800			
C	-0.83268900	2.69906800	-
0.38316400			
C	1.50828900	-2.94938600	-
0.67526700			
C	3.21097200	-1.15548900	-
0.48023100			
H	-1.13086900	4.92601500	-
0.29830800			
H	1.77202100	-5.18205000	-
0.79481900			
H	5.44923600	-1.35102600	-
0.54880300			
H	1.54866700	5.00490300	-
0.44207500			
H	-0.89865600	-5.18120100	-
1.17466600			
H	5.39639500	1.33140500	-
0.64846000			
C	-0.55684700	-0.61149400	
4.02836800			
C	-0.47497200	-0.80862100	
2.64067900			
C	1.09260000	0.86151900	
2.42086200			
C	1.08502200	1.12620800	
3.78640600			
C	0.23538200	0.37494300	
4.60181600			
H	-1.22149600	-1.22196200	
4.63138600			
H	1.72538000	1.41726900	
1.74107100			
H	1.72435800	1.90192300	
4.19353300			
H	0.19260300	0.55054400	
5.67297800			
N	-1.20129300	-1.79190200	
1.95164200			
N	0.32478700	-0.07949200	
1.84807500			
N	-2.88083700	-3.13280500	
2.94587800			
N	-2.06006600	-2.44794500	

2.54924900			
C	-3.24165300	3.27939700	-
0.21695900			
C	-3.38210100	3.99613500	
0.98156800			
C	-4.13009500	3.55101200	-
1.26907200			
C	-4.38463800	4.95610600	
1.12618700			
H	-2.69649700	3.79233300	
1.79952100			
C	-5.13428800	4.50936800	-
1.12537600			
H	-4.02372900	3.00425200	-
2.20175700			
C	-5.26494300	5.21500000	
0.07304900			
H	-4.48056600	5.49886900	
2.06302400			
H	-5.81109200	4.70881400	-
1.95212800			
H	-6.04638300	5.96185900	
0.18500400			
C	3.75020700	3.46613600	-
0.58385900			
C	3.86863200	4.30486400	-
1.70283600			
C	4.61523900	3.67075200	
0.50215000			
C	4.82506100	5.32066400	-
1.73476600			
H	3.20352900	4.15166900	-
2.54799600			
C	5.57338300	4.68486100	
0.47131400			
H	4.53119500	3.02430700	
1.37157200			
C	5.68070200	5.51388200	-
0.64770700			
H	4.90461600	5.95818300	-
2.61138700			
H	6.23319700	4.82974700	
1.32283800			
H	6.42610400	6.30425500	-

0.67269200			
C	3.91597500	-3.53472800	-
0.44712500			
C	4.66861100	-3.68915900	
0.72754100			
C	4.21457900	-4.35309400	-
1.54774000			
C	5.68808400	-4.63914100	
0.80261700			
H	4.44555000	-3.05613800	
1.58197800			
C	5.23297800	-5.30443400	-
1.47364400			
H	3.64310200	-4.23269200	-
2.46369300			
C	5.97271900	-5.45096100	-
0.29785800			
H	6.25792600	-4.74718300	
1.72189500			
H	5.45266300	-5.92667100	-
2.33729200			
H	6.76648500	-6.19099200	-
0.24034400			
C	-5.05781200	-1.80132100	-
0.81730600			
C	-5.12644100	-2.99885500	-
0.08218900			
C	-6.16177100	-1.44299800	-
1.61154300			
C	-6.25548400	-3.81495900	-
0.15112300			
H	-4.30306600	-3.27288400	
0.57012000			
C	-7.29130700	-2.25714700	-
1.67654300			
H	-6.11560400	-0.52407300	-
2.18957000			
C	-7.34131400	-3.44963700	-
0.94979200			
H	-6.29034100	-4.73255400	
0.43041900			
H	-8.13137500	-1.96397700	-
2.30092400			
H	-8.22033700	-4.08635500	-

1.00290500

4INT2

Mn	0.45992000	-0.00996300	-
0.44026500			
N	-1.54915700	-0.26161200	-
0.66189300			
C	2.53345600	2.70500400	-
0.06071700			
C	-2.28678400	2.09771600	-
0.62611800			
C	-0.79712700	4.07735500	-
0.19681900			
C	0.53970200	4.24445300	-
0.00648100			
C	-1.01814600	2.66918800	-
0.43623700			
C	1.15249900	2.94304100	-
0.14895000			
H	1.06609300	5.16019700	
0.21899300			
H	-1.57099900	4.82984900	-
0.15489200			
N	0.76227900	-2.00559300	-
0.74203800			
N	0.18265100	1.99455800	-
0.39122600			
N	2.47259000	0.24318700	-
0.36323900			
C	-1.59577900	-2.71476400	-
0.73970200			
C	3.23086200	-2.09977700	-
0.69509600			
C	4.75448100	-0.10543500	-
0.46905500			
C	-3.82213600	0.10442800	-
0.77224600			
C	1.70745500	-4.11154000	-
0.84946400			
C	4.55986000	1.22786300	-
0.27275100			
C	-3.64834900	-1.25322800	-
0.70516600			
C	0.35416300	-4.27570200	-

0.85433100			
C	3.44929800	-0.72221600	-
0.51367200			
C	-2.51883700	0.71478900	-
0.70700500			
C	1.95746000	-2.68753600	-
0.78090400			
C	3.13336600	1.44239300	-
0.20769400			
C	-2.20927700	-1.46751700	-
0.67785600			
C	-0.22667400	-2.95955600	-
0.78485800			
H	-2.24466400	-3.58200400	-
0.78939200			
H	5.30959200	2.00250100	-
0.20463700			
H	-0.20922100	-5.19969800	-
0.89449700			
H	5.69345100	-0.62500100	-
0.59207400			
H	-4.76337200	0.63331200	-
0.80171800			
H	2.47001600	-4.87622000	-
0.87885100			
C	-1.40080900	-1.93442200	
3.28062800			
C	-0.98890000	-0.80269400	
2.55829200			
C	1.12393400	-1.64966100	
2.27454700			
C	0.82358900	-2.80537400	
2.98940000			
C	-0.47381200	-2.94986400	
3.48734500			
H	-2.41221900	-2.00846400	
3.66815000			
H	2.10116000	-1.49954500	
1.82770400			
H	1.57629400	-3.57306100	
3.13142100			
H	-0.76128100	-3.84164100	
4.03727900			
N	-1.82064800	0.31376600	

2.31985400			
N	0.23722400	-0.67037200	
2.04246900			
N	-4.14539600	0.28177000	
2.78196800			
N	-3.02385400	0.21883600	
2.58757600			
C	3.43475200	3.87417700	
0.17481300			
C	4.17998200	3.97070900	
1.36038600			
C	3.56164300	4.89228500	-
0.78312300			
C	5.02688100	5.05701300	
1.58402800			
H	4.08615200	3.18629100	
2.10612500			
C	4.40808300	5.97920100	-
0.56050800			
H	2.99219200	4.82142600	-
1.70552500			
C	5.14325200	6.06508900	
0.62412900			
H	5.59260900	5.11771500	
2.51009100			
H	4.49702300	6.75624300	-
1.31521000			
H	5.80264900	6.91129700	
0.79768200			
C	-3.45878600	3.02155900	-
0.72003200			
C	-3.58423700	3.89324400	-
1.81334600			
C	-4.44799000	3.04857000	
0.27549800			
C	-4.66998000	4.76433200	-
1.91142400			
H	-2.82149500	3.87986300	-
2.58685700			
C	-5.53516800	3.91802900	
0.17771200			
H	-4.36169900	2.38330800	
1.12894500			
C	-5.64986500	4.77884700	-

0.91613300				
H	-4.75175100	5.42907400	-	
2.76742700				
H	-6.28954700	3.92531000		
0.96002900				
H	-6.49602200	5.45653000	-	
0.99191000				
C	4.42133900	-2.99830200	-	
0.77925900				
C	5.28911400	-3.14686400		
0.31448200				
C	4.69187400	-3.72113100	-	
1.95200200				
C	6.39657900	-3.99226900		
0.23846100				
H	5.08720200	-2.59154300		
1.22638500				
C	5.79827600	-4.56804900	-	
2.02904700				
H	4.02709000	-3.60961500	-	
2.80386400				
C	6.65445000	-4.70636400	-	
0.93404700				
H	7.05540300	-4.09628500		
1.09665200				
H	5.99424400	-5.11580600	-	
2.94707100				
H	7.51661500	-5.36510700	-	
0.99421300				
C	-4.70466400	-2.27340500	-	
0.64394900				
C	-5.82783700	-2.18605100	-	
1.48498100				
C	-4.64590200	-3.32798700		
0.28566000				
C	-6.85342200	-3.12668800	-	
1.40625300				
H	-5.87916300	-1.37974000	-	
2.21142800				
C	-5.67054100	-4.27114300		
0.36041500				
H	-3.80146500	-3.38682700		
0.96686300				
C	-6.77742200	-4.17569700	-	

0.48601300			
H	-7.71109000	-3.04481700	-
2.06882700			
H	-5.60921600	-5.07612600	
1.08830500			
H	-7.57585300	-4.91043300	-
0.42724100			
⁶INT2			
Mn	0.16783600	0.18327300	-
0.14306700			
N	1.41242100	1.88583900	-
0.27081300			
C	-3.25017900	-0.30062300	-
0.79723700			
C	-0.35663300	3.62837700	-
0.24211600			
C	-2.87255400	3.25815300	-
0.20797100			
C	-3.67463400	2.16904500	-
0.37996700			
C	-1.50142400	2.80110200	-
0.33016900			
C	-2.80534500	1.02931800	-
0.60196700			
H	-4.75405400	2.13683300	-
0.34298200			
H	-3.18014500	4.27373000	-
0.00488600			
N	1.86443600	-1.01010900	-
0.65830900			
N	-1.49871500	1.44561200	-
0.54709200			
N	-1.06385000	-1.46269300	-
0.68323900			
C	3.61089900	0.74322500	-
0.42768200			
C	0.70347600	-3.20463600	-
0.73898800			
C	-1.77790200	-3.60419600	-
1.11132200			
C	2.14183200	4.05945200	-
0.41809000			
C	3.20866900	-2.86508700	-

0.47183900			
C	-2.87574300	-2.79574000	-
1.14972300			
C	3.24379400	3.25837700	-
0.47732200			
C	4.01749100	-1.76791900	-
0.38871400			
C	-0.63608300	-2.75840000	-
0.82171900			
C	0.98875700	3.19037600	-
0.28911200			
C	1.85377700	-2.38394000	-
0.65042000			
C	-2.42284300	-1.44669800	-
0.86629500			
C	2.78091700	1.88786500	-
0.38128900			
C	3.16674700	-0.60012900	-
0.50856800			
H	-3.89331500	-3.08148700	-
1.37383200			
H	4.27180500	3.56449100	-
0.60741900			
H	5.08791300	-1.75233800	-
0.24185800			
H	-1.73760300	-4.66782600	-
1.29831600			
H	2.10837300	5.13700400	-
0.49036400			
H	3.50365300	-3.90246000	-
0.40548500			
C	-0.58158000	5.09972400	-
0.11767600			
C	-1.27075000	5.81315600	-
1.11231300			
C	-0.09898200	5.80441900	-
0.99752900			
C	-1.47443600	7.18827700	-
0.99386500			
H	-1.63975800	5.27837400	-
1.98271900			
C	-0.30258500	7.17944800	-
1.11734700			
H	0.43488300	5.26072000	-

1.77175200			
C	-0.99163800	7.87629100	
0.12192900			
H	-2.00504100	7.72345000	-
1.77706400			
H	0.07366700	7.70575700	
1.99076500			
H	-1.15007600	8.94746600	
0.21430200			
C	-4.72181200	-0.50906000	-
0.95258100			
C	-5.44052400	-1.31512700	-
0.05462900			
C	-5.42150200	0.10075300	-
2.00733600			
C	-6.81472800	-1.50405600	-
0.20350400			
H	-4.91380700	-1.78702200	
0.76871500			
C	-6.79554900	-0.08752400	-
2.15801700			
H	-4.87404800	0.72139100	-
2.71074900			
C	-7.49759100	-0.89069400	-
1.25610900			
H	-7.35264100	-2.12553200	
0.50763000			
H	-7.31685900	0.38943700	-
2.98388600			
H	-8.56812400	-1.03696200	-
1.37248800			
C	0.91831700	-4.68275900	-
0.72971200			
C	0.39414700	-5.46429700	
0.31319000			
C	1.64341000	-5.32267200	-
1.74735400			
C	0.59005800	-6.84541400	
0.33890700			
H	-0.16432500	-4.97343900	
1.10558900			
C	1.83990500	-6.70402400	-
1.72279100			
H	2.04688200	-4.72594400	-

2.56038200			
C	1.31412200	-7.47005900	-
0.67953800			
H	0.17999400	-7.43385700	
1.15580200			
H	2.39876300	-7.18292700	-
2.52255800			
H	1.46645400	-8.54591500	-
0.66118000			
C	5.08610300	0.97046300	-
0.39193500			
C	5.68516000	1.63325100	
0.69238200			
C	5.90895900	0.52751600	-
1.44110100			
C	7.06359200	1.84548900	
0.72798400			
H	5.05748400	1.97815000	
1.50917500			
C	7.28742200	0.73941100	-
1.40670900			
H	5.45430200	0.02068400	-
2.28738800			
C	7.86991200	1.39883800	-
0.32161800			
H	7.50830400	2.35610000	
1.57824000			
H	7.90588900	0.39488800	-
2.23141300			
H	8.94363700	1.56440700	-
0.29482300			
C	-1.18262900	-1.91830200	
3.62555900			
C	-0.94766400	-0.89290400	
2.69896300			
C	1.24054400	-1.54509000	
2.40559200			
C	1.10872700	-2.58883900	
3.31747300			
C	-0.13298800	-2.78015200	
3.92714600			
H	-2.15631200	-2.03131300	
4.09143500			
H	2.17468600	-1.36551900	

1.88558500			
H	1.95178200	-3.23764500	
3.52702800			
H	-0.28403200	-3.58901300	
4.63636900			
N	-1.90801100	0.06168800	
2.31260200			
N	0.23281500	-0.71700000	
2.08796800			
N	-4.19564600	-0.13967800	
2.90287000			
N	-3.08414500	-0.10929000	
2.65942000			

²TS2

Mn	0.28837100	0.17816000	-
0.83129100			
N	-1.30129100	1.41703500	-
1.02719200			
C	3.72365100	0.63659800	-
0.67376500			
C	-0.15917300	3.60260600	-
0.78265000			
C	2.32035000	3.95435400	-
0.55742400			
C	3.40449600	3.12991100	-
0.55699400			
C	1.15361300	3.11685000	-
0.70066900			
C	2.90811100	1.77897100	-
0.67081900			
H	4.44637600	3.40698200	-
0.48945400			
H	2.30778100	5.03191900	-
0.48227100			
N	-0.90704800	-1.41756100	-
1.19277300			
N	1.53003700	1.79057100	-
0.75575400			
N	1.92367900	-1.04576000	-
0.92036400			
C	-3.09622100	-0.26412800	-
1.31236900			
C	0.77211200	-3.23234600	-

1.07023100				
C	3.25963100	-2.93138900	-	
0.85176100				
C	-2.63005200	3.30532200	-	
1.13047800				
C	-1.70456800	-3.58382800	-	
1.32680000				
C	4.08312900	-1.85355700	-	
0.74624700				
C	-3.45123500	2.22840700	-	
1.27543700				
C	-2.78163700	-2.75597900	-	
1.38986900				
C	1.91106300	-2.42206100	-	
0.95234800				
C	-1.28994400	2.79397000	-	
0.96328800				
C	-0.53472600	-2.74384100	-	
1.20836100				
C	3.24482000	-0.67664200	-	
0.79380500				
C	-2.61586500	1.05083500	-	
1.21861600				
C	-2.28088500	-1.40411200	-	
1.29283500				
H	5.15849700	-1.84932900	-	
0.64526000				
H	-4.52250500	2.22681000	-	
1.41362600				
H	-3.82192500	-3.02952700	-	
1.48604100				
H	3.53241900	-3.97654400	-	
0.86494300				
H	-2.90028800	4.35145500	-	
1.13678800				
H	-1.69762900	-4.66342600	-	
1.34897600				
C	-4.57567800	-0.46160300	-	
1.41290800				
C	-5.28699300	-1.01800500	-	
0.33810800				
C	-5.27944100	-0.09063000	-	
2.56839800				
C	-6.66967600	-1.19269900	-	

0.41624600			
H	-4.74498400	-1.31444900	
0.55514300			
C	-6.66215500	-0.26509100	-
2.64593500			
H	-4.73305300	0.33542200	-
3.40530800			
C	-7.36178700	-0.81563300	-
1.56930500			
H	-7.20617700	-1.62165000	
0.42626000			
H	-7.19208800	0.02503600	-
3.54946000			
H	-8.43834600	-0.95133800	-
1.62991000			
C	-0.36891300	5.08078900	-
0.68820300			
C	0.03050900	5.93479700	-
1.72694200			
C	-0.97702100	5.63943200	
0.44594300			
C	-0.17304600	7.31263800	-
1.63366600			
H	0.50009600	5.50817200	-
2.60889200			
C	-1.18264500	7.01648700	
0.54040800			
H	-1.28088700	4.98120900	
1.25406200			
C	-0.78093400	7.85747300	-
0.50007400			
H	0.13912000	7.95991800	-
2.44904700			
H	-1.65318300	7.43251100	
1.42756200			
H	-0.94054400	8.93000200	-
0.42819900			
C	5.19705600	0.82970100	-
0.50806600			
C	6.08579100	0.53710900	-
1.55361700			
C	5.72105900	1.30176900	
0.70547100			
C	7.46110100	0.70974500	-

1.38963900			
H	5.68755000	0.17265900	-
2.49635700			
C	7.09549600	1.47679200	
0.87088700			
H	5.03784500	1.53423700	
1.51792600			
C	7.97032300	1.18003200	-
0.17693000			
H	8.13445400	0.48113500	-
2.21156100			
H	7.48322900	1.84140300	
1.81862400			
H	9.04103000	1.31525100	-
0.04959800			
C	0.96338900	-4.71411000	-
1.01019600			
C	1.34823800	-5.32360200	
0.19387100			
C	0.75800100	-5.52134500	-
2.13848900			
C	1.52136000	-6.70599700	
0.26921900			
H	1.51057000	-4.69962400	
1.06840300			
C	0.92965000	-6.90468800	-
2.06413500			
H	0.46227200	-5.05466000	-
3.07393800			
C	1.31132900	-7.50103300	-
0.86007200			
H	1.81564400	-7.16293600	
1.21056500			
H	0.76884500	-7.51597700	-
2.94829100			
H	1.44455100	-8.57801000	-
0.80226900			
N	-1.07398900	-1.97222200	
1.79630600			
N	-1.41787000	-3.18733500	
1.92404500			
N	-2.39138300	-3.77461000	
2.21658300			
C	0.22447900	-1.56614300	

2.09671700			
C	1.12124300	-2.33578100	
2.86286200			
C	1.67339200	0.21962300	
2.07517200			
C	2.34025700	-1.77365000	
3.21655000			
H	0.84721300	-3.34047600	
3.16788300			
C	2.61733100	-0.45512700	
2.84249500			
H	1.85300900	1.22940500	
1.72398700			
H	3.05880600	-2.34995400	
3.79278500			
H	3.55020000	0.02769000	
3.11347000			
N	0.51642500	-0.32487100	
1.66881600			
C	-3.01622300	-1.15782100	
2.86676800			
C	-3.59993200	-2.25339700	
2.88965000			
C	-2.57165300	0.19559600	
2.99806300			
C	-3.06159200	1.19769800	
2.14290300			
C	-1.63575500	0.53372500	
3.99478100			
C	-2.62321700	2.51157600	
2.28770800			
H	-3.76999200	0.94000800	
1.36401700			
C	-1.20375100	1.84897000	
4.13189600			
H	-1.24654100	-0.24534100	
4.64318800			
C	-1.69515700	2.84103700	
3.27824000			
H	-3.00065500	3.27050200	
1.61089400			
H	-0.47902000	2.09994800	
4.90151800			
H	-1.35301500	3.86692600	

3.38656100			
H		-4.44449200	-2.85751200
3.14848500			
⁴TS2			
Mn	0.30467100	0.04680600	-
0.86986000			
N	-1.11705400	1.47899100	-
1.09657400			
C	0.33279900	-3.40690300	-
0.93112600			
C	-3.10965400	0.02896400	-
1.35486600			
C	-3.12351900	-2.48245800	-
1.35614700			
C	-2.16477400	-3.44063400	-
1.23917200			
C	-2.45022100	-1.20580600	-
1.30530200			
C	-0.89863100	-2.75571400	-
1.10429000			
H	-2.29672900	-4.51250200	-
1.23985300			
H	-4.19000800	-2.61960400	-
1.45808400			
N	1.73886600	1.48805200	-
0.82347800			
N	-1.09340200	-1.39450000	-
1.16205700			
N	1.76281000	-1.38590800	-
0.90756600			
C	0.29246600	3.50178000	-
0.86210200			
C	3.76671200	0.06216000	-
0.75434600			
C	3.80358900	-2.45424100	-
0.72510600			
C	-3.15330200	2.54229600	-
1.33917900			
C	3.77079400	2.57805300	-
0.66549000			
C	2.84482500	-3.41998400	-
0.73412600			
C	-2.20846700	3.51230900	-

1.18514400			
C	2.80162000	3.53427300	-
0.67619500			
C	3.12179900	-1.18302300	-
0.80952300			
C	-2.46835900	1.27313900	-
1.26836300			
C	3.10475100	1.30057900	-
0.76669100			
C	1.57145100	-2.74946000	-
0.86658500			
C	-0.93492400	2.84345400	-
1.04577600			
C	1.53289000	2.85068000	-
0.77545600			
H	2.98319600	-4.48903800	-
0.66790800			
H	-2.35803700	4.58188900	-
1.16978200			
H	2.93086500	4.60580900	-
0.63395000			
H	4.87367800	-2.58509000	-
0.65822700			
H	-4.21703100	2.66790700	-
1.48076000			
H	4.83957200	2.72022900	-
0.60001400			
C	0.38376000	-2.46710700	
2.91045800			
C	-0.22945900	-1.47045700	
2.12798200			
C	1.70672900	-0.23189500	
2.05958600			
C	2.39401100	-1.14920000	
2.84864400			
C	1.71856300	-2.30437100	
3.25554900			
H	-0.18622100	-3.33182500	
3.23379000			
H	2.19496500	0.65765900	
1.67635200			
H	3.42975300	-0.97231800	
3.11910400			
H	2.22286100	-3.06222100	

3.84872400			
N	-1.58904600	-1.44510100	
1.82732500			
N	0.43351300	-0.39355900	
1.67250500			
N	-3.43442200	-2.69980100	
2.24803300			
N	-2.31592500	-2.47450700	
1.97029300			
C	-3.15069100	-0.00712300	
2.85994200			
C	-4.07780800	-0.83201800	
2.86065400			
C	-2.25358600	1.09553900	
3.02548700			
C	-1.32907700	1.09282900	
4.08831600			
C	-2.27985800	2.18414200	
2.13779500			
C	-0.45366500	2.16135300	
4.25666800			
H	-1.29926600	0.24320900	
4.76376700			
C	-1.40363000	3.25141700	
2.31653200			
H	-2.97271100	2.18375700	
1.30482200			
C	-0.48859200	3.24328400	
3.37155700			
H	0.25865000	2.14894100	
5.07712100			
H	-1.42864400	4.08319000	
1.62072500			
H	0.19437200	4.07814800	
3.50564600			
H	-5.08891100	-1.10938400	
3.07353300			
C	0.28150600	4.99222000	-
0.74787200			
C	0.64629300	5.61102400	
0.45908300			
C	-0.08863400	5.80368100	-
1.83142900			
C	0.63241600	7.00098700	

0.58274000			
H		0.94302500	4.98770600
1.29766300			
C	-0.10400700	7.19385300	-
1.70871500			
H	-0.36272300	5.33411200	-
2.77187500			
C	0.25471500	7.79714800	-
0.50089100			
H		0.91386400	7.46120600
1.52633200			
H	-0.39083700	7.80619900	-
2.55958900			
H	0.24241500	8.87957300	-
0.40591700			
C	5.25776000	0.07305400	-
0.63340800			
C		5.88038500	-0.36589300
0.54515300			
C	6.06233000	0.52808800	-
1.68870800			
C		7.27044100	-0.35197200
0.66645700			
H		5.26139000	-0.72300900
1.36379500			
C	7.45289400	0.54496300	-
1.56841900			
H	5.58711300	0.86846700	-
2.60447600			
C	8.06120100	0.10488200	-
0.39056700			
H		7.73559400	-0.69405800
1.58738200			
H	8.06111400	0.89785300	-
2.39713200			
H	9.14381500	0.11718400	-
0.29721900			
C	0.31486800	-4.89458800	-
0.78663900			
C	0.88170700	-5.73010900	-
1.76080900			
C		-0.27956500	-5.48327700
0.34089900			
C	0.86110700	-7.11751000	-

1.60890400				
H	1.33640900	-5.28182300	-	
2.63976000				
C	-0.30265400	-6.86994800	-	
0.49284900				
H	-0.72919000	-4.84111100	-	
1.09306800				
C	0.26976500	-7.69167000	-	
0.48120300				
H	1.30158900	-7.74992800	-	
2.37527400				
H	-0.76677400	-7.30843800	-	
1.37250200				
H	0.25219200	-8.77190900	-	
0.36387800				
C	-4.60020500	0.02062600	-	
1.48579600				
C	-5.40891300	0.35065600	-	
0.38790500				
C	-5.21327500	-0.31927200	-	
2.70027600				
C	-6.79972100	0.34480500	-	
0.50436400				
H	-4.93796500	0.59221100	-	
0.56005400				
C	-6.60447800	-0.32598700	-	
2.81668900				
H	-4.59025800	-0.57694200	-	
3.55236600				
C	-7.40150300	0.00747300	-	
1.71910500				
H	-7.41358200	0.59956000	-	
0.35589100				
H	-7.06502400	-0.58874900	-	
3.76546500				
H	-8.48452300	0.00279400	-	
1.80961200				
⁶TS2				
Mn	0.02613100	0.13628200	-	
0.58397500				
N	-2.02151500	0.34060200	-	
1.13079000				
C	2.72325800	2.34081400	-	

0.96674800				
C	-2.15799800	2.81142300	-	
0.98122700				
C	-0.22454900	4.45598500	-	
0.86249100				
C	1.13461100	4.32689600	-	
0.87316500				
C	-0.77897700	3.11988300	-	
0.95792000				
C	1.42806900	2.91047000	-	
0.98342100				
H	1.86839000	5.11769200	-	
0.81222800				
H	-0.79891400	5.36984100	-	
0.80476900				
N	-0.15603600	-1.92826200	-	
1.08341500				
N	0.24756400	2.21229400	-	
1.02983000				
N	2.11714400	-0.06553000	-	
0.96774900				
C	-2.62933500	-2.06337100	-	
1.17822800				
C	2.24686000	-2.53992700	-	
1.04074300				
C	4.23211900	-0.95332100	-	
1.11531900				
C	-4.14013800	1.23428700	-	
1.16352600				
C	0.30885100	-4.18167300	-	
1.09445200				
C	4.36375700	0.40365000	-	
1.09734400				
C	-4.27157900	-0.12272100	-	
1.22578100				
C	-1.04613900	-4.04895400	-	
1.13791600				
C	2.81310700	-1.24382500	-	
1.02950200				
C	-2.72029900	1.52238800	-	
1.10529900				
C	0.86777500	-2.84214200	-	
1.07563500				
C	3.02677800	0.96013200	-	

1.00015700				
C	-2.93324400	-0.68233900	-	
1.20728200				
C	-1.33476700	-2.62643000	-	
1.12670600				
H	5.27681000	0.97686800	-	
1.17149700				
H	-5.18916200	-0.69135400	-	
1.27159200				
H	-1.78314600	-4.83776100	-	
1.18084000				
H	5.01748100	-1.69016300	-	
1.20486700				
H	-4.93094000	1.97096100	-	
1.15493100				
H	0.87908400	-5.09895300	-	
1.07863200				
C	-3.78338100	-3.01428600	-	
1.14582100				
C	-4.02583300	-3.78407300	-	
0.00374500				
C	-4.64715600	-3.15245600	-	
2.24265900				
C	-5.10606600	-4.66592000	-	
0.05530000				
H	-3.35708400	-3.68240000	-	
0.85464800				
C	-5.72802900	-4.03416800	-	
2.19128100				
H	-4.46161200	-2.56395100	-	
3.13684900				
C	-5.96128200	-4.79311900	-	
1.04194000				
H	-5.28198600	-5.25104000	-	
0.95436500				
H	-6.38508800	-4.13182400	-	
3.05158300				
H	-6.80277700	-5.47967000	-	
1.00229900				
C	-3.11015500	3.95476000	-	
0.82052000				
C	-3.89853500	4.40564100	-	
1.88904400				
C	-3.23497700	4.59147100	-	

0.42428000			
C	-4.79198600	5.46461300	-
1.71691800			
H	-3.80423500	3.91871800	-
2.85565700			
C	-4.12603300	5.65146300	
0.59733000			
H	-2.62659500	4.24244500	
1.25469400			
C	-4.90826800	6.09059000	-
0.47363700			
H	-5.39407600	5.80347600	-
2.55595300			
H	-4.21241200	6.13182800	
1.56864300			
H	-5.60332600	6.91526800	-
0.34035100			
C	3.87946700	3.28319100	-
0.87323300			
C	4.15831500	4.19917600	-
1.89943000			
C	4.71010200	3.27027800	
0.25925100			
C	5.23643400	5.07936200	-
1.79596600			
H	3.52309100	4.21147600	-
2.78059700			
C	5.78851500	4.14947900	
0.36337100			
H	4.49624200	2.56416800	
1.05679200			
C	6.05497500	5.05769700	-
0.66414400			
H	5.44052300	5.77830400	-
2.60289900			
H	6.41950200	4.12749600	
1.24836900			
H	6.89511600	5.74241000	-
0.58434200			
C	3.20106100	-3.69100500	-
1.01546200			
C	4.00410900	-3.92035400	
0.11272000			
C	3.31830700	-4.56058100	-

2.11073700			
C	4.89786600	-4.99109700	
0.14707100			
H	3.91399100	-3.25374900	
0.96540800			
C	4.21184000	-5.63211200	-
2.07782200			
H	2.70378600	-4.38602200	-
2.98936900			
C	5.00441900	-5.85093000	-
0.94857800			
H	5.50733300	-5.15680600	
1.03170500			
H	4.29234300	-6.29300500	-
2.93694100			
H	5.70016500	-6.68539800	-
0.92273900			
N	0.73981600	-1.65433800	
1.96063900			
N	1.30433100	-2.77295500	
2.17881500			
N	0.93765900	-3.85653400	
2.44625400			
C	1.33908100	-0.44286400	
2.26866600			
C	2.40643000	-0.27152400	
3.16526100			
C	1.07953300	1.83737100	
2.01999400			
C	2.80350200	1.02469700	
3.47155600			
H	2.89221600	-1.13807100	
3.60113300			
C	2.11554800	2.10561000	
2.91120700			
H	0.53364100	2.63687800	
1.53203500			
H	3.63193400	1.19110300	
4.15470800			
H	2.38798400	3.13081800	
3.13682000			
N	0.71237400	0.59464500	
1.67827800			
C	-1.33058700	-2.32743100	

2.89346800			
C	-1.04483100	-3.53613600	
2.89223600			
C	-1.82871900	-0.99579900	
3.05539600			
C	-2.74416000	-0.44883300	
2.14041200			
C	-1.36806300	-0.20480100	
4.12769000			
C	-3.17288800	0.86953600	
2.28388800			
H	-3.10166100	-1.05187100	
1.31576300			
C	-1.80293900	1.10972800	
4.26474900			
H	-0.65499800	-0.62574300	
4.83000300			
C	-2.69961300	1.65308800	
3.33847300			
H	-3.86508900	1.28232100	
1.55806000			
H	-1.43601400	1.71392400	
5.08991000			
H	-3.03258700	2.68269100	
3.44020100			
H	-1.30553100	-4.55632200	
3.08356100			
3			
N	-0.76627900	1.20106300	
0.02781600			
N	-1.35008100	2.44064400	
0.03993800			
N	-0.39832200	3.32170200	
0.02760500			
C	-1.60955300	0.05909700	-
0.07143500			
C	-3.66756600	-1.04217000	
0.41339600			
C	-1.92341300	-2.04342000	-
0.88817100			
C	-3.19265900	-2.13449700	-
0.31676300			
H	-4.64979700	-1.06852700	

0.87631400			
H	-1.51250100	-2.86809000	-
1.46683700			
H	-3.78897000	-3.03267000	-
0.44196300			
C	0.60253700	1.31219900	-
0.00049300			
C	0.80271600	2.68007800	
0.00068900			
C	1.59259400	0.23031900	
0.06473500			
C	1.43574000	-0.86570100	
0.92825300			
C	2.76374300	0.33104000	-
0.70138000			
C	2.42507800	-1.84168500	
1.01397400			
H	0.54140200	-0.94536500	
1.53797100			
C	3.75391000	-0.64729600	-
0.61215100			
H	2.88446600	1.17126000	-
1.37914400			
C	3.58708800	-1.73734000	
0.24373100			
H	2.29184500	-2.68373900	
1.68771200			
H	4.65271800	-0.55947100	-
1.21629400			
H	4.35707600	-2.50089200	
0.31209400			
H	1.73940600	3.21800200	
0.02022400			
C	-2.86173000	0.08383000	
0.55357100			
N	-1.14125500	-0.96273900	-
0.78227400			
H	-3.17498400	0.95808700	
1.11058900			
²INT3			
Mn	-0.27315600	0.11377900	-
0.48197900			
N	-0.10358700	-1.91246800	-

0.57537600				
C	-2.90810000	2.32391800	-	
0.20171100				
C	-2.49909300	-2.54073900	-	
0.45019900				
C	-4.41015900	-0.94972000	-	
0.08914100				
C	-4.52214800	0.40442500	-	
0.00506300				
C	-3.01797000	-1.24378800	-	
0.32793200				
C	-3.20082400	0.95120600	-	
0.20161900				
H	-5.41367100	0.98415100		
0.18379200				
H	-5.19157000	-1.68758400		
0.01859900				
N	1.72959300	0.28294400	-	
0.76316100				
N	-2.29066100	-0.07077000	-	
0.37729500				
N	-0.45225400	2.12278900	-	
0.46330700				
C	2.36242000	-2.11400100	-	
0.75256600				
C	1.93195000	2.75116300	-	
0.69172400				
C	0.02651000	4.38206200	-	
0.55589600				
C	-0.60043100	-4.16540600	-	
0.72582800				
C	3.86815900	1.15839200	-	
0.81025900				
C	-1.32290800	4.26412600	-	
0.42562000				
C	0.75514000	-4.04809700	-	
0.78688800				
C	3.99049300	-0.19709400	-	
0.80992700				
C	0.56712100	3.04353800	-	
0.57043800				
C	-1.13323200	-2.83322100	-	
0.57969100				
C	2.45675600	1.45457500	-	

0.77578000			
C	-1.61762800	2.85199300	-
0.35276200			
C	1.06269900	-2.64129200	-
0.69211400			
C	2.65382900	-0.74224600	-
0.78716900			
H	-2.05740300	5.05539200	-
0.39362600			
H	1.48235500	-4.83681900	-
0.91303400			
H	4.90069000	-0.77810200	-
0.80437200			
H	0.60755400	5.28790300	-
0.65033400			
H	-1.19093200	-5.06780100	-
0.78639600			
H	4.65896500	1.89406500	-
0.80669800			
C	1.97588800	-1.47962600	
2.77667100			
C	1.31925200	-0.28831100	
2.43707100			
C	3.23930500	0.93159900	
2.56032300			
C	3.99794500	-0.18671800	
2.90840100			
C	3.34461400	-1.41477300	
3.01905700			
H	1.43982100	-2.42239600	
2.81999300			
H	3.70725400	1.90646100	
2.44234400			
H	5.06672200	-0.09798800	
3.07238800			
H	3.89562200	-2.31666800	
3.26907100			
N	-0.06797800	-0.23960200	
2.10124300			
N	1.92283900	0.89309600	
2.33280000			
N	-1.51211500	-2.04859500	
2.63425500			
N	-0.76325300	-1.22175700	

2.41479400			
C	-4.04166700	3.28364700	-
0.03360000			
C	-5.03945500	3.39629500	-
1.01432100			
C	-4.12845300	4.09314100	
1.10984900			
C	-6.09639800	4.29367200	-
0.85605400			
H	-4.97685900	2.77500500	-
1.90332700			
C	-5.18480800	4.99103300	
1.26891300			
H	-3.36007200	4.00976000	
1.87328900			
C	-6.17229100	5.09392700	
0.28631900			
H	-6.85788400	4.37084800	-
1.62771900			
H	-5.23835900	5.60713300	
2.16269600			
H	-6.99509600	5.79303300	
0.40980400			
C	2.89584100	3.89275400	-
0.66504800			
C	3.65480000	4.23423900	-
1.79396200			
C	3.06646200	4.63588000	
0.51394600			
C	4.56342300	5.29300400	-
1.74613300			
H	3.52552700	3.66322200	-
2.70917200			
C	3.97487100	5.69422100	
0.56237600			
H	2.47887400	4.37144700	
1.38900100			
C	4.72629300	6.02558000	-
0.56794100			
H	5.14107600	5.54801000	-
2.63078700			
H	4.09755400	6.25825200	
1.48339600			
H	5.43347900	6.84994500	-

0.53120300			
C	3.50443300	-3.07690100	-
0.76525300			
C	4.36589400	-3.16854500	-
1.86958900			
C	3.73958700	-3.91335100	
0.33787700			
C	5.43520300	-4.06537400	-
1.86833600			
H	4.18711900	-2.53087700	-
2.73061500			
C	4.80724200	-4.81144300	
0.34054700			
H	3.07407400	-3.85055300	
1.19346400			
C	5.66036500	-4.88906600	-
0.76286500			
H	6.08893300	-4.12497200	-
2.73452500			
H	4.97417100	-5.44924400	
1.20485600			
H	6.49230900	-5.58816500	-
0.76255300			
C	-3.45935400	-3.68501200	-
0.39966600			
C	-4.38659500	-3.88949100	-
1.43265600			
C	-3.45418000	-4.57192600	
0.68819500			
C	-5.28492600	-4.95642000	-
1.38179100			
H	-4.39504400	-3.20530900	-
2.27659100			
C	-4.35231400	-5.63874800	
0.73942200			
H	-2.74497200	-4.40980600	
1.49451500			
C	-5.26978700	-5.83465800	-
0.29568100			
H	-5.99378600	-5.10347100	-
2.19245400			
H	-4.33906600	-6.31386600	
1.59116000			
H	-5.96921800	-6.66547800	-

0.25562600

4INT3

Mn	-0.27711500	0.11271100	-
0.49846000			
N	-0.46817100	2.12429700	-
0.46712200			
C	-2.48394400	-2.55486000	-
0.43836500			
C	-2.92621100	2.30901900	-
0.21612700			
C	-4.52837200	0.37970800	-
0.01405500			
C	-4.40680900	-0.97427100	-
0.08778100			
C	-3.21060700	0.93439300	-
0.21326900			
C	-3.01245300	-1.26059400	-
0.32469500			
H	-5.18311300	-1.71659800	
0.02608900			
H	-5.42388700	0.95443300	
0.17122300			
N	1.72893500	0.29547900	-
0.76834800			
N	-2.29428500	-0.08294000	-
0.38291900			
N	-0.09177400	-1.91253400	-
0.57030400			
C	1.91439800	2.76469400	-
0.68234300			
C	2.37508800	-2.09790100	-
0.76352000			
C	0.77934900	-4.04239800	-
0.78294300			
C	-1.35015900	4.25995400	-
0.42419700			
C	3.99189400	-0.17006400	-
0.82291400			
C	-0.57512500	-4.16820500	-
0.71267400			
C	-0.00040500	4.38550600	-
0.54533400			
C	3.86119300	1.18458800	-

0.81504000				
C	1.07905100	-2.63361600	-	
0.69303100				
C	-1.63795500	2.84587300	-	
0.35978200				
C	2.65855900	-0.72393600	-	
0.79825200				
C	-1.11609700	-2.83924700	-	
0.56796400				
C	0.54724200	3.04977500	-	
0.56389000				
C	2.44786300	1.47198800	-	
0.77520300				
H	-1.15982000	-5.07472200	-	
0.76766000				
H	0.57641500	5.29492200	-	
0.63104400				
H	4.64762100	1.92492300	-	
0.80862300				
H	1.51021400	-4.82713900	-	
0.91259100				
H	-2.08866000	5.04746900	-	
0.39209900				
H	4.90585900	-0.74512300	-	
0.82226100				
C	-4.06708400	3.26127800	-	
0.05490600				
C	-5.06069300	3.36516500	-	
1.04080000				
C	-4.16579900	4.07134900		
1.08717700				
C	-6.12499400	4.25496600	-	
0.88917400				
H	-4.98912900	2.74300300	-	
1.92852700				
C	-5.22952300	4.96165800		
1.23957300				
H	-3.40102700	3.99426300		
1.85487700				
C	-6.21259500	5.05613100		
0.25171500				
H	-6.88311900	4.32544500	-	
1.66477400				
H	-5.29231400	5.57831800		

2.13236000			
H	-7.04113400	5.74932100	
0.37006000			
C	-3.43623600	-3.70547800	-
0.38127600			
C	-3.42127200	-4.58964300	
0.70879400			
C	-4.36549000	-3.91909900	-
1.41069300			
C	-4.31189700	-5.66247900	
0.76556200			
H	-2.71070900	-4.42054900	
1.51238800			
C	-5.25625100	-4.99203900	-
1.35420800			
H	-4.38145600	-3.23720400	-
2.25637700			
C	-5.23143800	-5.86739600	-
0.26594300			
H	-4.29115900	-6.33529400	
1.61897000			
H	-5.96669300	-5.14605500	-
2.16218800			
H	-5.92496600	-6.70292600	-
0.22146600			
C	3.52310500	-3.05340800	-
0.78397800			
C	3.76704400	-3.89412300	
0.31411500			
C	4.38248200	-3.13346200	-
1.89090500			
C	4.84103500	-4.78459600	
0.30950500			
H	3.10283500	-3.84121400	
1.17135100			
C	5.45817800	-4.02258700	-
1.89691600			
H	4.19708700	-2.49279000	-
2.74829000			
C	5.69207800	-4.85030800	-
0.79629200			
H	5.01446800	-5.42574000	
1.17004000			
H	6.11006100	-4.07304400	-

2.76507100			
H	6.52901900	-5.54338200	-
0.80162000			
C	2.87154200	3.91163600	-
0.64172500			
C	3.03456200	4.64255400	
0.54599100			
C	3.63111300	4.27023300	-
1.76482000			
C	3.93658500	5.70560400	
0.60861600			
H	2.44613800	4.36489600	
1.41640600			
C	4.53328500	5.33380400	-
1.70276200			
H	3.50753800	3.70879200	-
2.68672300			
C	4.68886800	6.05401600	-
0.51599900			
H	4.05351100	6.26004200	
1.53617500			
H	5.11159500	5.60217200	-
2.58301800			
H	5.39106000	6.88206700	-
0.46821200			
C	2.00371400	-1.47162800	
2.76302200			
C	1.31972100	-0.28489800	
2.46220100			
C	3.22691300	0.95964900	
2.54152500			
C	4.01142800	-0.15273800	
2.84870300			
C	3.37854300	-1.39119000	
2.96155000			
H	1.48231800	-2.42235700	
2.81125600			
H	3.67808600	1.94226900	
2.42221000			
H	5.08370700	-0.05154600	
2.97904700			
H	3.94950200	-2.28891000	
3.17957700			
N	-0.07799300	-0.24674800	

2.17971600			
N	1.90464200	0.90626800	
2.35499700			
N	-1.46780000	-2.11209500	
2.65641000			
N	-0.74391400	-1.25826900	
2.45648000			

6INT3

Mn	-0.26900900	0.12502900	-
0.25930100			
N	-0.73452700	2.15814400	-
0.36384700			
C	-2.16592900	-2.80828300	-
0.46886300			
C	-3.20329100	1.98592300	-
0.17794400			
C	-4.58190500	-0.14431000	
0.01305900			
C	-4.29495000	-1.47536300	-
0.07398400			
C	-3.34019500	0.57650400	-
0.18453700			
C	-2.87245000	-1.59123900	-
0.32299000			
H	-4.98060800	-2.30291400	
0.03705200			
H	-5.54422800	0.30685400	
0.20700900			
N	1.73415500	0.56436100	-
0.75713200			
N	-2.32477200	-0.33114800	-
0.36677900			
N	0.15451000	-1.92649700	-
0.55785100			
C	1.57027900	3.04037100	-
0.62237500			
C	2.62229000	-1.75469400	-
0.79098700			
C	1.26412600	-3.90120400	-
0.93277100			
C	-1.88000200	4.14577000	-
0.42977200			
C	4.02197800	0.37057400	-

0.74448900				
C	-0.06741700	-4.19219400	-	
0.85792700				
C	-0.55286700	4.43807400	-	
0.54972000				
C	3.72751300	1.70234800	-	
0.71184000				
C	1.40170100	-2.47098700	-	
0.74505400				
C	-1.99155600	2.70562500	-	
0.30580800				
C	2.76249000	-0.34592900	-	
0.77891200				
C	-0.76489700	-2.94644700	-	
0.61458300				
C	0.16815200	3.18147600	-	
0.50494300				
C	2.28378500	1.82193000	-	
0.71397000				
H	-0.53598400	-5.15829200	-	
0.97832800				
H	-0.10454800	5.41212600	-	
0.68343500				
H	4.42505600	2.52609600	-	
0.66444000				
H	2.07483800	-4.58754000	-	
1.13100300				
H	-2.70879800	4.83869500	-	
0.44679700				
H	5.00201000	-0.08326500	-	
0.72429700				
C	-4.45438500	2.79108100	-	
0.03495500				
C	-5.46900700	2.72484500	-	
1.00357000				
C	-4.63875100	3.63575800	-	
1.07166500				
C	-6.63479600	3.47962100	-	
0.86903400				
H	-5.33197800	2.07848600	-	
1.86580800				
C	-5.80420000	4.39092100	-	
1.20720500				
H	-3.85942300	3.69142000	-	

1.82640800			
C	-6.80645400	4.31513500	
0.23719900			
H	-7.40665000	3.41911000	-
1.63185900			
H	-5.93092200	5.03520000	
2.07334100			
H	-7.71424700	4.90326900	
0.34217800			
C	-2.97212000	-4.06683500	-
0.45540300			
C	-2.79783300	-5.01700600	
0.56371900			
C	-3.91990300	-4.32417600	-
1.45869600			
C	-3.54981800	-6.19227900	
0.57825200			
H	-2.07345200	-4.81888700	
1.34801300			
C	-4.67191600	-5.49948800	-
1.44492400			
H	-4.05801600	-3.59465800	-
2.25168800			
C	-4.48892700	-6.43772900	-
0.42631900			
H	-3.40598400	-6.91397000	
1.37821400			
H	-5.39727800	-5.68431200	-
2.23295800			
H	-5.07448900	-7.35317900	-
0.41519300			
C	3.87621600	-2.56415200	-
0.84650400			
C	4.19216000	-3.45860200	
0.18984200			
C	4.76774600	-2.45319800	-
1.92587700			
C	5.36443500	-4.21384400	
0.15273600			
H	3.50629500	-3.55261500	
1.02613800			
C	5.94124400	-3.20715500	-
1.96442800			
H	4.52810300	-1.77238200	-

2.73750200			
C	6.24486700	-4.08922100	-
0.92462000			
H	5.59161000	-4.89835200	
0.96615200			
H	6.61537900	-3.11055800	-
2.81145100			
H	7.15825200	-4.67715700	-
0.95541500			
C	2.37698000	4.29813400	-
0.62202600			
C	2.37868600	5.13839900	
0.50344600			
C	3.15306300	4.66327500	-
1.73346000			
C	3.13640200	6.31009100	
0.51767900			
H	1.78114800	4.85959100	
1.36690400			
C	3.91073800	5.83507100	-
1.72018100			
H	3.15325600	4.02061700	-
2.60927400			
C	3.90528000	6.66209400	-
0.59430500			
H	3.12878900	6.94625800	
1.39898400			
H	4.50122300	6.10476700	-
2.59193100			
H	4.49496600	7.57489900	-
0.58418200			
C	2.16000700	-1.49331600	
2.83432500			
C	1.38189000	-0.37502000	
2.50924600			
C	3.16913500	1.03508300	
2.58133300			
C	4.04374100	-0.00081800	
2.91331800			
C	3.52127600	-1.28791900	
3.04235800			
H	1.72386100	-2.48534700	
2.89433200			
H	3.53201600	2.05123000	

2.44994700			
H	5.10180200	0.19548100	
3.05040700			
H	4.16677200	-2.12787900	
3.28103700			
N	-0.01348300	-0.45733400	
2.20189900			
N	1.85871600	0.86069500	
2.38575600			
N	-1.24403300	-2.43173000	
2.68744800			
N	-0.59759800	-1.52059500	
2.48397800			

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Mn	-0.21591300	0.08547900	-
0.25614400			
N	0.07694000	2.05793500	-
0.48248900			
C	-3.02520500	-1.92943000	-
0.58341700			
C	-2.23556500	2.85584100	-
0.10672200			
C	-4.27593000	1.39989000	-
0.13629400			
C	-4.49705800	0.07291300	-
0.33796600			
C	-2.85185200	1.60508400	-
0.20473700			
C	-3.20840700	-0.54881700	-
0.48900900			
H	-5.44103800	-0.45173400	-
0.35092000			
H	-5.00594100	2.17532800	
0.04214400			
N	1.72072400	-0.23773900	-
0.76090300			
N	-2.20497100	0.39965400	-
0.41592400			
N	-0.55260100	-1.89305100	-
0.53627600			
C	2.51697400	2.10608600	-
0.88368400			
C	1.78808400	-2.70081600	-

0.53604900				
C	-0.22985500	-4.18528700	-	
0.53078200				
C	-0.24572200	4.34834600	-	
0.38901500				
C	3.80764800	-1.24179300	-	
0.80095900				
C	-1.57231200	-3.96983500	-	
0.59288700				
C	1.07322300	4.13993100	-	
0.64756500				
C	4.00389000	0.09716700	-	
0.94199500				
C	0.40248000	-2.89075000	-	
0.50600400				
C	-0.86358300	3.05060300	-	
0.28911700				
C	2.38708500	-1.44934400	-	
0.69873700				
C	-1.76999700	-2.54314900	-	
0.57635300				
C	1.27579900	2.71329300	-	
0.68228200				
C	2.70695900	0.72117600	-	
0.89829100				
H	-2.36400300	-4.70245100	-	
0.64885000				
H	1.84279800	4.87971800	-	
0.81080200				
H	4.94235100	0.62359500	-	
1.03184200				
H	0.29476900	-5.12948900	-	
0.53423700				
H	-0.76706200	5.29030100	-	
0.30274900				
H	4.55361900	-2.02134400	-	
0.75866800				
C	-3.08248100	4.05808700		
0.15901400				
C	-3.99366400	4.52875600	-	
0.79830000				
C	-2.96268900	4.74621800		
1.37580100				
C	-4.77147600	5.65901300	-	

0.54281600			
H	-4.08421200	4.00367400	-
1.74511300			
C	-3.74116200	5.87587700	
1.63163900			
H	-2.25670900	4.38528600	
2.11843700			
C	-4.64776000	6.33504600	
0.67328900			
H	-5.47019700	6.01387300	-
1.29579600			
H	-3.64095000	6.39531300	
2.58092300			
H	-5.25349700	7.21501900	
0.87234900			
C	-4.23997400	-2.80054700	-
0.60167100			
C	-4.61795500	-3.50292200	
0.55221600			
C	-5.02195400	-2.91739700	-
1.75878800			
C	-5.75478200	-4.31230200	
0.54476900			
H	-4.01860200	-3.39621000	
1.45179300			
C	-6.15913900	-3.72753300	-
1.76521700			
H	-4.73212800	-2.37128500	-
2.65238500			
C	-6.52707900	-4.42750700	-
0.61396300			
H	-6.04028100	-4.84854200	
1.44591000			
H	-6.75558600	-3.81286200	-
2.66971900			
H	-7.41243200	-5.05770700	-
0.61887300			
C	2.66425200	-3.90475400	-
0.41305600			
C	2.73286700	-4.60225400	
0.80242100			
C	3.42425200	-4.36343900	-
1.49914700			
C	3.54547400	-5.72926700	

0.93057400			
H	2.14675600	-4.24849800	
1.64522200			
C	4.23751000	-5.49058500	-
1.37154000			
H	3.36957800	-3.83083800	-
2.44446100			
C	4.30080400	-6.17621700	-
0.15619400			
H	3.59034200	-6.25671200	
1.87979200			
H	4.81743800	-5.83580900	-
2.22333600			
H	4.93354700	-7.05407500	-
0.05715100			
C	3.72227300	2.98080200	-
0.99722800			
C	4.14784800	3.73552500	
0.10741400			
C	4.45740500	3.05143800	-
2.18927700			
C	5.28319300	4.54192200	
0.02092000			
H	3.57653600	3.68145300	
1.02989400			
C	5.59286100	3.85889400	-
2.27601000			
H	4.13158100	2.46914200	-
3.04672500			
C	6.00901000	4.60553500	-
1.17129400			
H	5.60265300	5.11784200	
0.88547000			
H	6.15002300	3.90705300	-
3.20786800			
H	6.89323500	5.23356300	-
1.23913100			
C	1.62134300	-1.44451300	
2.74808400			
C	1.19650500	-0.22515600	
2.18479800			
C	3.23832400	0.74116700	
2.58181400			
C	3.75203600	-0.41443900	

3.17004300			
C	2.91302800	-1.52745800	
3.25416000			
H	0.95162700	-2.29529100	
2.76489000			
H	3.86039700	1.62871700	
2.47651500			
H	4.77289600	-0.44161500	
3.53774000			
H	3.26879300	-2.45936500	
3.68594900			
N	-0.09763100	-0.03979700	
1.63724400			
N	1.99208600	0.85142000	
2.11222300			
N	-2.19387100	-1.02385300	
2.24062600			
N	-1.03948300	-0.93765600	
2.36573400			

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Mn	-0.23576100	0.06520800	-
0.29571600			
N	0.42874500	1.95684800	-
0.54301600			
C	-3.35290600	-1.37549500	-
0.64858300			
C	-1.67065300	3.15529900	
0.00616500			
C	-3.95122800	2.09713700	
0.05404200			
C	-4.41982700	0.84753400	-
0.21516500			
C	-2.51705800	2.04534900	-
0.06335500			
C	-3.27560100	0.00664900	-
0.45116200			
H	-5.44509600	0.50812800	-
0.21870800			
H	-4.52156200	2.98043800	
0.30042700			
N	1.62238600	-0.59909200	-
0.76320900			
N	-2.11473700	0.75297900	-

0.34941700				
N				
	-0.92189800	-1.80555500		-
0.50384200				
C				
	2.81203400	1.55328100		-
1.05886600				
C				
	1.23284600	-3.01577800		-
0.38952900				
C				
	-1.01908300	-4.11223600		-
0.54751000				
C				
	0.52268400	4.26364700		-
0.48478700				
C				
	3.49300900	-1.94968600		-
0.64610800				
C				
	-2.29214100	-3.65366800		-
0.70153900				
C				
	1.75415400	3.82191900		-
0.85550400				
C				
	3.92551900	-0.68609200		-
0.90704100				
C				
	-0.16485100	-2.95750300		-
0.43777000				
C				
	-0.30402400	3.09700000		-
0.29560500				
C				
	2.05478000	-1.89959800		-
0.58188700				
C				
	-2.23471700	-2.21508500		-
0.64059700				
C				
	1.70477000	2.38029000		-
0.84869900				
C				
	2.75993400	0.15882200		-
0.95518500				
H				
	-3.19461500	-4.23101900		-
0.83766300				
H				
	2.62110600	4.41192100		-
1.11270800				
H				
	4.94343400	-0.34335600		-
1.01765800				
H				
	-0.67556400	-5.13647400		-
0.54714800				
H				
	0.18392700	5.28394300		-
0.38106500				
H				
	4.08930700	-2.83888300		-
0.50637100				
C				
	-2.25095900	4.48809500		

0.35002400				
C	-3.14850400	5.13686600	-	
0.51153300				
C	-1.88375300	5.12190100		
1.54699400				
C	-3.67289300	6.38709100	-	
0.18046700				
H	-3.42672900	4.65587200	-	
1.44505800				
C	-2.40905600	6.37152300		
1.87842900				
H	-1.18606100	4.62389300		
2.21435500				
C	-3.30551600	7.00714000		
1.01610800				
H	-4.36372500	6.87886700	-	
0.86020200				
H	-2.11938800	6.84713600		
2.81164100				
H	-3.71396700	7.98058600		
1.27393800				
C	-4.70928800	-1.98971100	-	
0.76844800				
C	-5.22730100	-2.78211800		
0.26742300				
C	-5.49420900	-1.76593200	-	
1.90891000				
C	-6.49958700	-3.34507300		
0.15990500				
H	-4.62662300	-2.94145100		
1.15820400				
C	-6.76667000	-2.32957700	-	
2.01632900				
H	-5.09832400	-1.14856600	-	
2.71060400				
C	-7.27186600	-3.12163200	-	
0.98274200				
H	-6.89011900	-3.95277100		
0.97187700				
H	-7.36178600	-2.15151800	-	
2.90809800				
H	-8.26276400	-3.56000500	-	
1.06587100				
C	1.86514500	-4.35064700	-	

0.17291500			
C	1.69676600	-5.01051700	
1.05418900			
C	2.61962500	-4.97554300	-
1.17740800			
C	2.27476700	-6.26106000	
1.27484700			
H	1.11250500	-4.53002000	
1.83373100			
C	3.19751100	-6.22667800	-
0.95753400			
H	2.74462000	-4.47432400	-
2.13305400			
C	3.02765100	-6.87241200	
0.26947500			
H	2.13881900	-6.75665100	
2.23247000			
H	3.77542800	-6.69944500	-
1.74720200			
H	3.47750700	-7.84672600	
0.44023700			
C	4.14479900	2.18503900	-
1.28791100			
C	4.73754900	2.97778200	-
0.29187200			
C	4.84046700	1.97725100	-
2.48835200			
C	5.99363400	3.55043900	-
0.49354300			
H	4.20118200	3.13754000	
0.63890700			
C	6.09668200	2.55096000	-
2.69056300			
H	4.38749300	1.36309600	-
3.26165700			
C	6.67687200	3.33882300	-
1.69376400			
H	6.44069400	4.15805300	
0.28883800			
H	6.62033300	2.38479200	-
3.62825900			
H	7.65528600	3.78476400	-
1.85095600			
C	1.56058100	-1.40547700	

2.88194500			
C	1.26321600	-0.21426100	
2.18498400			
C	3.39692300	0.56805200	
2.51944200			
C	3.78168900	-0.56252600	
3.23810600			
C	2.82827900	-1.56736500	
3.42368300			
H	0.80740900	-2.17953700	
2.97126500			
H	4.11166100	1.36838600	
2.33278200			
H	4.79006300	-0.65410200	
3.62936000			
H	3.07848400	-2.47876700	
3.96077100			
N	0.01043100	0.00974400	
1.58812500			
N	2.17154300	0.76180600	
2.02062900			
N	-2.21778900	-0.81787800	
2.29135500			
N	-1.11011900	-0.64846800	
2.53350000			

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Mn	-0.23149800	0.10742300	-
0.32220200			
N	0.24593800	2.05159700	-
0.49887100			
C	-3.21644100	-1.61942900	-
0.72543000			
C	-1.96653600	3.03800800	
0.03460400			
C	-4.13630600	1.77125900	
0.01246400			
C	-4.48613700	0.48951400	-
0.28490800			
C	-2.70433200	1.85793000	-
0.10188300			
C	-3.26957100	-0.23615400	-
0.53467800			
H	-5.47442600	0.05424800	-

0.29655400			
H	-4.78517600	2.59109200	
0.28192800			
N	1.66861900	-0.38285600	-
0.83918300			
N	-2.18892800	0.61699400	-
0.42741300			
N	-0.75337400	-1.81896500	-
0.60053900			
C	2.65461700	1.88005400	-
1.05176000			
C	1.50835100	-2.82532200	-
0.48194100			
C	-0.63228300	-4.11951100	-
0.61224100			
C	0.13088700	4.34827000	-
0.36415800			
C	3.65326800	-1.55626800	-
0.77502200			
C	-1.94357200	-3.78335800	-
0.76832800			
C	1.40130400	4.02923600	-
0.73632900			
C	3.96259500	-0.25259600	-
1.01703000			
C	0.11224500	-2.89211700	-
0.52514100			
C	-0.59331600	3.11242200	-
0.22724900			
C	2.22071600	-1.63929000	-
0.67906600			
C	-2.02248400	-2.34677200	-
0.72574200			
C	1.48196500	2.59320000	-
0.79041700			
C	2.72643100	0.48409200	-
1.01961200			
H	-2.79006900	-4.44271700	-
0.89080800			
H	2.21720900	4.70144600	-
0.95646400			
H	4.94204100	0.18671800	-
1.13321900			
H	-0.19276000	-5.10612200	-

0.59448200			
H	-0.29717500	5.33043400	-
0.22849000			
H	4.32824600	-2.39180300	-
0.66520100			
C	-2.67309700	4.29788700	
0.41240500			
C	-3.61419000	4.89047100	-
0.44339600			
C	-2.38415000	4.92022900	
1.63669600			
C	-4.25757700	6.07429900	-
0.08005800			
H	-3.83228800	4.41918300	-
1.39766700			
C	-3.02821500	6.10369000	
1.99976700			
H	-1.65535900	4.46447000	
2.30094400			
C	-3.96695800	6.68334700	
1.14300800			
H	-4.98104000	6.52355500	-
0.75518800			
H	-2.79860100	6.57062700	
2.95374700			
H	-4.46807300	7.60510900	
1.42593100			
C	-4.50754500	-2.36653700	-
0.80655200			
C	-4.93757900	-3.15016700	
0.27519400			
C	-5.31530500	-2.27849700	-
1.94886300			
C	-6.14908500	-3.83937000	
0.20939600			
H	-4.31901500	-3.19890700	
1.16674800			
C	-6.52709600	-2.96881000	-
2.01356000			
H	-4.98620600	-1.66817500	-
2.78551000			
C	-6.94558600	-3.75180000	-
0.93534300			
H	-6.47394100	-4.43932900	

1.05526600				
H	-7.14225200	-2.89624500	-	
2.90651500				
H	-7.88909300	-4.28865600	-	
0.98548300				
C	2.26343600	-4.09339000	-	
0.25541300				
C	2.23150100	-4.69967500		
1.00921700				
C	3.00108300	-4.69895900	-	
1.28286600				
C	2.92687900	-5.88687300		
1.24136100				
H	1.67226500	-4.22043500		
1.80694100				
C	3.69564800	-5.88714700	-	
1.04997300				
H	3.02215100	-4.23427400	-	
2.26480600				
C	3.65988500	-6.48368300		
0.21265500				
H	2.89905900	-6.34356600		
2.22710400				
H	4.26040300	-6.34853100	-	
1.85571300				
H	4.20072700	-7.40865400		
0.39379900				
C	3.92458400	2.63985400	-	
1.24666800				
C	4.47264300	3.38017900	-	
0.18695700				
C	4.60479700	2.60367000	-	
2.47242800				
C	5.67268500	4.07231400	-	
0.35281000				
H	3.94959300	3.39948700		
0.76499800				
C	5.80483400	3.29731500	-	
2.63803200				
H	4.18529600	2.02934800	-	
3.29383000				
C	6.34139300	4.03330300	-	
1.57905700				
H	6.08803000	4.63717900		

0.47748100			
H	6.31876000	3.26455700	-
3.59501900			
H	7.27616400	4.57217200	-
1.70803900			
C	1.62900800	-1.51405800	
3.08424900			
C	1.26159900	-0.37614900	
2.31537000			
C	3.43452000	0.41178500	
2.40807800			
C	3.88836700	-0.67212500	
3.15727600			
C	2.94453700	-1.64730200	
3.49998400			
H	0.88724900	-2.26327400	
3.32939900			
H	4.12769800	1.19751400	
2.10559700			
H	4.92887300	-0.74950300	
3.45600900			
H	3.23845900	-2.51821300	
4.08197100			
N	0.00951500	-0.12350200	
1.79620900			
N	2.17411300	0.57717500	
2.00149400			
N	-2.19176300	-1.15858700	
2.26103800			
N	-1.05895400	-1.22987600	
2.43687700			
²INT4			
Mn	0.26134100	0.00942600	-
0.16837700			
N	0.85326700	-1.89336800	-
0.49867500			
C	1.93951000	3.02578300	-
0.10865800			
C	3.31156500	-1.64241800	-
0.32460700			
C	4.51017900	0.52191600	
0.07838800			
C	4.12483700	1.82335400	

0.16436400				
C	3.32205200	-0.25055200	-	
0.18908100				
C	2.70160900	1.85459800	-	
0.06632600				
H	4.74083000	2.68697500		
0.36695900				
H	5.50233800	0.11249800		
0.19865100				
N	-1.62139600	-0.53400100	-	
0.71186900				
N	2.22053300	0.57618600	-	
0.26120200				
N	-0.25837800	1.93645800	-	
0.49208400				
C	-1.36734300	-2.98394500	-	
0.55535900				
C	-2.70080600	1.68679400	-	
0.83254300				
C	-1.49089900	3.87725200	-	
0.75648900				
C	2.11769700	-3.83070900	-	
0.58283500				
C	-3.93489800	-0.49293300	-	
0.82162700				
C	-0.20110400	4.25003000	-	
0.53453000				
C	0.81072100	-4.20557800	-	
0.60184900				
C	-3.56308600	-1.79725000	-	
0.71964800				
C	-1.52808400	2.43842400	-	
0.70786900				
C	2.14166400	-2.39195900	-	
0.47753500				
C	-2.72509100	0.29117000	-	
0.80907700				
C	0.56324900	3.04199300	-	
0.35704500				
C	0.02811800	-2.99799200	-	
0.54503000				
C	-2.12474400	-1.81868800	-	
0.65940300				
H	0.20777900	5.24935800	-	

0.51245500				
H	0.40052500	-5.20276900	-	
0.66960000				
H	-4.19639900	-2.67149200	-	
0.68383900				
H	-2.34336200	4.51182400	-	
0.94916400				
H	2.99217500	-4.46240700	-	
0.63161600				
H	-4.93430200	-0.08805800	-	
0.88111800				
C	4.61894600	-2.36498700	-	
0.27108000				
C	5.56149300	-2.20885300	-	
1.29859000				
C	4.93026300	-3.20403700	-	
0.80976800				
C	6.78509200	-2.87824700	-	
1.24877700				
H	5.32571200	-1.55953700	-	
2.13715900				
C	6.15408300	-3.87271000	-	
0.86038600				
H	4.20571500	-3.32370700	-	
1.61023100				
C	7.08462900	-3.71217900	-	
0.16903100				
H	7.50260300	-2.75045200	-	
2.05499100				
H	6.38199500	-4.51551800	-	
1.70650900				
H	8.03753700	-4.23307100	-	
0.12961100				
C	2.63187400	4.33498700	-	
0.09250200				
C	2.36190200	5.11437000	-	
1.22768100				
C	3.55684800	4.81164500	-	
0.84888100				
C	3.00307700	6.33902200	-	
1.41868700				
H	1.64738400	4.74929000	-	
1.96006300				
C	4.19763800	6.03675800	-	

0.65900400			
H	3.76671600	4.21432400	-
1.73170900			
C	3.92281400	6.80371400	
0.47565000			
H	2.78673100	6.92804300	
2.30600800			
H	4.90825300	6.39370600	-
1.39976100			
H	4.42203900	7.75748200	
0.62386000			
C	-4.00054900	2.41388700	-
0.95170600			
C	-4.50216500	3.15224600	
0.13099400			
C	-4.74676200	2.36306600	-
2.13825300			
C	-5.71974700	3.82584100	
0.02928500			
H	-3.92989000	3.18575500	
1.05344100			
C	-5.96480300	3.03696100	-
2.24099800			
H	-4.36306500	1.79209300	-
2.97912700			
C	-6.45437000	3.77036000	-
1.15773100			
H	-6.09688100	4.39020600	
0.87813000			
H	-6.52926300	2.99164100	-
3.16857300			
H	-7.40274200	4.29481400	-
1.23770800			
C	-2.08308400	-4.28502300	-
0.38972800			
C	-2.13076500	-4.87375100	
0.88303300			
C	-2.71272500	-4.92563900	-
1.46467600			
C	-2.79750800	-6.08454400	
1.07432900			
H	-1.64876200	-4.36196900	
1.71165300			
C	-3.37850000	-6.13820600	-

1.27190200			
H	-2.67533900	-4.46983200	-
2.45039000			
C	-3.42179500	-6.71974900	-
0.00270800			
H	-2.83139700	-6.53137900	
2.06456800			
H	-3.86047100	-6.62895000	-
2.11340000			
H	-3.93989900	-7.66338600	
0.14647400			
C	-1.88213700	1.05203300	
2.48387500			
C	-1.19114900	-0.13523400	
2.15245200			
C	-2.84308500	-1.43668700	
3.06179800			
C	-3.61129300	-0.32977000	
3.42284700			
C	-3.10730100	0.94077800	
3.12606500			
H	-1.45367100	2.01092800	
2.21408100			
H	-3.19994100	-2.44452900	
3.26961700			
H	-4.56887100	-0.45973000	
3.91673300			
H	-3.66990400	1.83425400	
3.38519100			
N	0.04995700	-0.05292000	
1.53847100			
N	-1.65742500	-1.36436800	
2.44683600			
⁴INT4			
Mn	-0.28590900	-0.01445300	
0.22575600			
N	-2.09725300	0.91537300	
0.29348400			
C	0.72452900	-3.26380000	
0.38072900			
C	-3.60896100	-1.04823700	
0.37690800			
C	-2.86086700	-3.44551900	

0.42102900			
C	-1.65251400	-4.06261600	
0.34121400			
C	-2.60980500	-2.02319100	
0.43410100			
C	-0.64987200	-3.02692200	
0.37038100			
H	-1.44431000	-5.12140100	
0.29520800			
H	-3.83968300	-3.90053900	
0.45143500			
N	0.59762200	1.77736700	
0.53864500			
N	-1.25126100	-1.78832400	
0.43342600			
N	1.42543000	-0.91736800	
0.75765300			
C	-1.33024700	3.25593100	
0.04667300			
C	2.90957100	1.04802100	
1.02008400			
C	3.68457600	-1.33156000	
1.00263700			
C	-4.35577500	1.31450900	
0.01685600			
C	2.17717700	3.43858600	
0.81393600			
C	3.08022800	-2.52791000	
0.77184200			
C	-3.71777100	2.50673100	-
0.13309500			
C	1.00452200	4.05077800	
0.49609400			
C	2.65703300	-0.32325000	
0.96298800			
C	-3.34268600	0.32108500	
0.26697900			
C	1.92623300	2.01974900	
0.81527300			
C	1.67467400	-2.26785000	
0.60961400			
C	-2.31180600	2.25994700	
0.05893000			
C	0.01801400	3.01323100	

0.32379600			
H		3.53284000	-3.50710900
0.72023000			
H	-4.15334700	3.47060900	-
0.35043000			
H	0.80615600	5.10913300	
0.41313900			
H	4.73365900	-1.13363900	
1.16548000			
H	-5.41356400	1.11133100	-
0.06132200			
H	3.13047500	3.89581100	
1.03455400			
N	0.03153900	-0.07332500	-
1.50795300			
C	1.27629900	-0.08825300	-
2.08503000			
C	1.90599500	1.13415200	-
2.43854300			
C	3.06099000	-1.27832200	-
2.93909400			
C	3.14639400	1.11040900	-
3.06069400			
H	1.40228700	2.06471900	-
2.19983800			
C	3.75182000	-0.12362600	-
3.31731000			
H	3.50224200	-2.25861900	-
3.12061400			
H	3.63923400	2.03953100	-
3.33882200			
H	4.72450500	-0.19324300	-
3.79445100			
N	1.86487400	-1.28565400	-
2.34832400			
C	-1.74169800	4.66557200	-
0.23101200			
C	-1.32340900	5.30245200	-
1.40908900			
C	-2.53622700	5.37985500	
0.67835100			
C	-1.69488700	6.62122700	-
1.67420800			
H	-0.70848600	4.75271800	-

2.11615600			
C	-2.90744900	6.69891400	
0.41385500			
H	-2.85713300	4.89335200	
1.59520500			
C	-2.48817100	7.32291800	-
0.76346500			
H	-1.36737500	7.09889000	-
2.59375800			
H	-3.52004800	7.24023800	
1.12991900			
H	-2.77737700	8.34991800	-
0.96950300			
C	4.31921300	1.49591900	
1.23335400			
C	4.93603100	1.35106300	
2.48401200			
C	5.05014800	2.05544700	
0.17470500			
C	6.25606600	1.76338000	
2.67488400			
H	4.37314600	0.91499600	
3.30474100			
C	6.36964000	2.46697600	
0.36582900			
H	4.57605600	2.14941500	-
0.79770800			
C	6.97546100	2.32327000	
1.61658800			
H	6.72093500	1.64932900	
3.65055600			
H	6.92659700	2.89476500	-
0.46368900			
H	8.00314700	2.64379200	
1.76514500			
C	-5.03824900	-1.48564300	
0.37240900			
C	-5.87334500	-1.18764900	
1.45959700			
C	-5.57303500	-2.18591400	-
0.71962800			
C	-7.21101500	-1.58576700	
1.45815400			
H	-5.46461100	-0.64267400	

2.30602300			
C	-6.91067400	-2.58370900	-
0.72135000			
H	-4.93217900	-2.41096000	-
1.56736500			
C	-7.73300500	-2.28548300	
0.36780400			
H	-7.84404400	-1.35147600	
2.30989200			
H	-7.31125200	-3.12194300	-
1.57623600			
H	-8.77461700	-2.59516200	
0.36609900			
C	1.22284500	-4.64034400	
0.08391800			
C	1.14487600	-5.68273800	
1.01614800			
C	1.79216700	-4.88293800	-
1.17593300			
C	1.62692000	-6.95337300	
0.69366300			
H	0.70986800	-5.49172200	
1.99353300			
C	2.27223100	-6.15348700	-
1.49528900			
H	1.83979700	-4.06302100	-
1.88831400			
C	2.19099500	-7.19070200	-
0.56187900			
H	1.56512600	-7.75550500	
1.42442300			
H	2.70790700	-6.33489800	-
2.47440500			
H	2.56603800	-8.17970600	-
0.81167100			
⁶INT4			
Mn	0.33122600	-0.01804200	-
0.28774000			
N	1.22003700	-1.81843100	-
0.41859000			
C	1.45057000	3.21796800	
0.00663300			
C	3.60487100	-1.14957100	-

0.40072200				
C	4.42381600	1.19068800	-	
0.04392400				
C	3.82138100	2.39859100		
0.13326100				
C	3.38180800	0.22812300	-	
0.29034000				
C	2.40646000	2.19793500	-	
0.04113200				
H	4.28760500	3.34504000		
0.36312600				
H	5.47622500	0.95682600		
0.01905100				
N	-1.43409700	-0.87814400	-	
0.78611500				
N	2.15486800	0.86225700	-	
0.29181900				
N	-0.51932900	1.79703500	-	
0.50296200				
C	-0.80992700	-3.23301300	-	
0.35876200				
C	-2.84551800	1.13619200	-	
1.05871000				
C	-2.05102000	3.49617800	-	
0.77600000				
C	2.77309200	-3.51977500	-	
0.39037600				
C	-3.69884200	-1.21912500	-	
1.06883700				
C	-0.86632600	4.07332100	-	
0.42666700				
C	1.54246100	-4.09577900	-	
0.28721700				
C	-3.13747700	-2.43222900	-	
0.81623900				
C	-1.84022800	2.07502100	-	
0.80240300				
C	2.57375500	-2.09461500	-	
0.42900500				
C	-2.63887400	-0.24430500	-	
1.01342800				
C	0.09171900	3.01303800	-	
0.26420700				
C	0.57290200	-3.03532400	-	

0.33451900				
C	-1.72665400	-2.21483300	-	
0.62944300				
H	-0.64582500	5.12488200	-	
0.31724500				
H	1.30219200	-5.14622900	-	
0.21422500				
H	-3.62328400	-3.39483000	-	
0.75433100				
H	-2.98859700	3.98375500	-	
0.99843300				
H	3.73487000	-4.00994400	-	
0.41687200				
H	-4.73894200	-0.98724700	-	
1.24329200				
C	5.02002900	-1.62982900	-	
0.41623800				
C	5.84589600	-1.36111600	-	
1.51810200				
C	5.55233800	-2.33894500		
0.67148200				
C	7.17164400	-1.79693100	-	
1.53546300				
H	5.43939200	-0.80931700	-	
2.36121100				
C	6.87782100	-2.77513900		
0.65393600				
H	4.91995300	-2.53949600		
1.53166700				
C	7.69070500	-2.50603600	-	
0.44980000				
H	7.79748100	-1.58487200	-	
2.39822900				
H	7.27667300	-3.31975600		
1.50553200				
H	8.72294300	-2.84528400	-	
0.46285200				
C	1.89720700	4.61015800		
0.31256600				
C	1.48654500	5.23526800		
1.49996000				
C	2.71608100	5.32117100	-	
0.57789700				
C	1.88987300	6.53870900		

1.79254700			
H	0.85310500	4.68818900	
2.19257700			
C	3.11949600	6.62469200	-
0.28530600			
H	3.02928200	4.84519700	-
1.50291600			
C	2.70786400	7.23668900	
0.90097100			
H	1.56802100	7.00700000	
2.71882100			
H	3.75052200	7.16372500	-
0.98691300			
H	3.02190400	8.25171300	
1.12867600			
C	-4.23425500	1.62924700	-
1.30627600			
C	-4.98159800	2.19120900	-
0.26049800			
C	-4.81576000	1.51920800	-
2.57725200			
C	-6.28325900	2.64063800	-
0.48544100			
H	-4.53636300	2.25270400	
0.72759500			
C	-6.11789800	1.96986700	-
2.80137200			
H	-4.24002300	1.08020400	-
3.38751600			
C	-6.85393500	2.53280900	-
1.75621300			
H	-6.85435800	3.06890200	
0.33409500			
H	-6.55576400	1.88285400	-
3.79219800			
H	-7.86789500	2.88280000	-
1.93041400			
C	-1.35419600	-4.58322100	-
0.02535600			
C	-1.95026500	-4.76080000	
1.23346100			
C	-1.29471900	-5.65981600	-
0.91931100			
C	-2.47523000	-6.00388200	

1.58853300			
H	-1.98083400	-3.91354200	
1.91463000			
C	-1.82228500	-6.90224700	-
0.56004600			
H	-0.84009500	-5.51755900	-
1.89618200			
C	-2.41290800	-7.07595700	
0.69372600			
H	-2.93157600	-6.13616500	
2.56605400			
H	-1.77542500	-7.73163000	-
1.26088400			
H	-2.82349800	-8.04300900	
0.97200900			
C	-2.01142300	1.14817100	
2.57100400			
C	-1.37318000	-0.08485600	
2.22823900			
C	-3.31566000	-1.24217100	
2.70579300			
C	-4.02464900	-0.09024800	
3.03993100			
C	-3.33415500	1.13043100	
2.97161400			
H	-1.44753300	2.07237300	
2.49399400			
H	-3.80903300	-2.21431300	
2.74712600			
H	-5.06429400	-0.14386200	
3.34606000			
H	-3.83242500	2.06183000	
3.23481500			
N	-0.09673200	-0.07710600	
1.79210400			
N	-2.03812000	-1.27321700	
2.31287600			
²TS4			
Mn	0.58353700	0.25147300	
0.56075000			
N	0.92242700	2.25219500	
0.56457000			
C	-2.09927300	-1.72779200	

1.34004300			
C	-1.33802700	3.08010400	
1.12034500			
C	-3.29925500	1.63530900	
1.70406800			
C	-3.52488400	0.29303800	
1.70332400			
C	-1.91437200	1.82821400	
1.34920900			
C	-2.26990900	-0.34181000	
1.39117500			
H	-4.44558200	-0.23218200	
1.91152800			
H	-4.00046300	2.42981200	
1.91421600			
N	2.59879200	-0.04623300	
0.52150600			
N	-1.28651500	0.60610900	
1.20925500			
N	0.35781400	-1.68936300	
1.12090600			
C	3.30794200	2.24588300	-
0.09890900			
C	2.68452500	-2.49759100	
0.86647200			
C	0.70728000	-3.96736700	
1.33441900			
C	0.58652600	4.53835700	
0.43766600			
C	4.63200100	-1.08799500	
0.15375900			
C	-0.63576300	-3.76149300	
1.39992500			
C	1.87905600	4.30218600	
0.08001200			
C	4.79799000	0.22863100	-
0.14646100			
C	1.32130900	-2.67963200	
1.11804500			
C	-0.00507100	3.25963600	
0.73992800			
C	3.25879800	-1.25686900	
0.56252800			
C	-0.84735400	-2.34188800	

1.28426500			
C	2.08454000	2.87661500	
0.15872400			
C	3.53304300	0.87871000	
0.09368900			
H	-1.41647700	-4.49608100	
1.53108300			
H	2.63314500	5.02329000	-
0.19930800			
H	5.69101500	0.71978900	-
0.50373400			
H	1.23871100	-4.90448000	
1.40722600			
H	0.07500700	5.48793400	
0.49810300			
H	5.36211800	-1.88109000	
0.08758200			
N	0.30473300	0.08013900	-
1.20513200			
C	0.10694500	-1.19119800	-
1.74233200			
C	1.24970700	-1.83969300	-
2.26963200			
C	-1.22791600	-2.97464500	-
2.31689200			
C	1.10654300	-3.10730000	-
2.81628600			
H	2.20997000	-1.33852600	-
2.22179000			
C	-0.16125900	-3.69974000	-
2.84520600			
H	-2.23559800	-3.38879700	-
2.31800300			
H	1.97198200	-3.62556100	-
3.22227600			
H	-0.31799600	-4.68862200	-
3.26463500			
N	-1.11292000	-1.75879800	-
1.77103600			
C	-5.78006000	0.12425300	-
1.73158400			
C	-5.94499300	-0.84963800	-
2.72092500			
C	-4.86024100	-1.20355400	-

3.53285400			
C	-3.62171400	-0.59586700	-
3.35795900			
C	-3.44048100	0.38248300	-
2.35298600			
C	-4.54562700	0.74070500	-
1.54913400			
H	-6.61599300	0.40001500	-
1.09450200			
H	-6.91031100	-1.32886400	-
2.86018300			
H	-4.98190400	-1.96123000	-
4.30251400			
H	-2.77258400	-0.88371800	-
3.96738500			
H	-4.41087800	1.48213900	-
0.77078700			
C	-2.18166800	0.99351500	-
2.15481300			
C	-1.02982600	1.39540100	-
1.93275700			
H	-0.32144200	2.19712600	-
1.94359800			
C	-2.21888300	4.28506300	
1.20012300			
C	-2.09571500	5.20809100	
2.24764100			
C	-3.18432400	4.50895700	
0.20622100			
C	-2.92499600	6.33007300	
2.30437400			
H	-1.34823200	5.03822100	
3.01771000			
C	-4.01268000	5.63034000	
0.26278400			
H	-3.26899200	3.79983800	-
0.61307200			
C	-3.88567700	6.54313900	
1.31309100			
H	-2.82213400	7.03562200	
3.12460400			
H	-4.75386700	5.79317900	-
0.51524800			
H	-4.53091600	7.41642700	

1.35794200			
C	4.44196600	3.09228500	-
0.58094500			
C	4.39856900	3.67613200	-
1.85616000			
C	5.56295400	3.32554100	
0.23003100			
C	5.45147000	4.47128900	-
2.31081000			
H	3.53251800	3.49898800	-
2.48777600			
C	6.61637600	4.12046900	-
0.22401900			
H	5.59979500	2.87977000	
1.22011300			
C	6.56368100	4.69541800	-
1.49596600			
H	5.40408200	4.91267300	-
3.30281300			
H	7.47583500	4.29437900	
0.41805500			
H	7.38368200	5.31467600	-
1.84954400			
C	3.57078100	-3.70127100	
0.84893700			
C	4.57322700	-3.86739600	
1.81592600			
C	3.42352800	-4.67927200	-
0.14706400			
C	5.40763900	-4.98609300	
1.79006800			
H	4.69220100	-3.11242100	
2.58816200			
C	4.25724100	-5.79780700	-
0.17280800			
H	2.64878700	-4.55088400	-
0.89733900			
C	5.25196300	-5.95447900	
0.79560800			
H	6.17676500	-5.10246000	
2.54905500			
H	4.13250800	-6.54528200	-
0.95202700			
H	5.90151500	-6.82546800	

0.77539400			
C	-3.32828300	-2.57401100	
1.28978200			
C	-3.73407500	-3.37770700	
2.36362000			
C	-4.10298600	-2.55193300	
0.11865400			
C	-4.89320500	-4.15106600	
2.26802800			
H	-3.14056300	-3.38844000	
3.27388400			
C	-5.26120200	-3.32383000	
0.02657800			
H	-3.78410800	-1.92962700	-
0.71112100			
C	-5.65874600	-4.12597800	
1.09957900			
H	-5.20078800	-4.76767800	
3.10862200			
H	-5.85058500	-3.29043800	-
0.88556600			
H	-6.56176300	-4.72672800	
1.02785400			
⁴TS4			
Mn	0.57128700	0.27661100	
0.65435200			
N	0.82173700	2.27391700	
0.61870800			
C	-2.03992300	-1.82649600	
1.28723500			
C	-1.46690200	3.00599000	
1.21847600			
C	-3.39175300	1.47249400	
1.70672800			
C	-3.56594100	0.12511900	
1.64873500			
C	-2.00386200	1.73092700	
1.40291800			
C	-2.27790400	-0.45296000	
1.35727000			
H	-4.47139800	-0.44247300	
1.80543800			
H	-4.12826300	2.23337400	

1.91940700			
N	2.58739400	0.05787300	
0.51626900			
N	-1.33011500	0.53833300	
1.24088000			
N	0.42473600	-1.66904200	
1.16807900			
C	3.17226300	2.36489300	-
0.16063000			
C	2.79201600	-2.37132400	
0.94133600			
C	0.87577500	-3.92441700	
1.38183900			
C	0.38580000	4.54034000	
0.51506600			
C	4.66213800	-0.89404800	
0.15833900			
C	-0.47754400	-3.78294400	
1.39482300			
C	1.66841200	4.35816200	
0.09579900			
C	4.75515400	0.41414500	-
0.20175700			
C	1.43741800	-2.61214700	
1.18611300			
C	-0.14491100	3.23964900	
0.83049900			
C	3.30513300	-1.11645800	
0.59585300			
C	-0.75692700	-2.37736900	
1.27655700			
C	1.93808700	2.94413600	
0.15535900			
C	3.46476600	1.01281700	
0.03980200			
H	-1.22701300	-4.55432800	
1.49104000			
H	2.37884400	5.10934000	-
0.21654300			
H	5.61621200	0.93622700	-
0.59195900			
H	1.44868400	-4.83529200	
1.46913300			
H	-0.16252100	5.46692600	

0.60079400			
H		5.43002500	-1.65227300
0.11681200			
N	0.23335800	0.06668600	-
1.09850300			
C	0.18235700	-1.18423100	-
1.70060800			
C	1.38333500	-1.74715300	-
2.19429500			
C	-1.00900000	-3.03586200	-
2.38297200			
C	1.35049400	-3.00740700	-
2.77717000			
H	2.30525000	-1.18533500	-
2.09425000			
C	0.12704700	-3.67849200	-
2.87695000			
H	-1.98592500	-3.51502800	-
2.44337200			
H	2.26461800	-3.45788300	-
3.15714100			
H	0.05320000	-4.66384100	-
3.32696800			
N	-0.99766500	-1.83173100	-
1.80415600			
C	-5.76973400	-0.08242400	-
1.81012100			
C	-5.87358400	-1.07045400	-
2.79448400			
C	-4.75820600	-1.37588500	-
3.58417400			
C	-3.55330200	-0.70755900	-
3.39470100			
C	-3.43267700	0.28729400	-
2.39479400			
C	-4.57024700	0.59458200	-
1.61261800			
H	-6.62863700	0.15846900	-
1.18908600			
H	-6.81283800	-1.59537500	-
2.94671600			
H	-4.82910600	-2.14406100	-
4.35019800			
H	-2.68196900	-0.95918200	-

3.98874500			
H	-4.48670300	1.34891400	-
0.83877200			
C	-2.20771300	0.95527000	-
2.18246100			
C	-1.05486800	1.33140100	-
1.90920900			
H	-0.35381600	2.14209100	-
1.91325600			
C	-2.38683900	4.17939300	
1.32482400			
C	-2.30667500	5.07011600	
2.40353400			
C	-3.34236100	4.40583200	
0.32207700			
C	-3.17066500	6.16431000	
2.48289800			
H	-1.56583300	4.89800200	
3.17958100			
C	-4.20518600	5.49942100	
0.40189800			
H	-3.39167700	3.72151500	-
0.52090900			
C	-4.12200300	6.38046000	
1.48337100			
H	-3.10175500	6.84571300	
3.32672100			
H	-4.93893400	5.66551800	-
0.38237300			
H	-4.79415800	7.23207500	
1.54586000			
C	4.24209600	3.25532000	-
0.70502900			
C	4.11078900	3.81445900	-
1.98518900			
C	5.38545000	3.55656200	
0.05021500			
C	5.10155400	4.65170000	-
2.49992900			
H	3.22647700	3.58479000	-
2.57304500			
C	6.37649800	4.39380800	-
0.46421600			
H	5.48888400	3.13123100	

1.04456100			
C	6.23736900	4.94326200	-
1.74091100			
H	4.98715300	5.07342500	-
3.49494600			
H	7.25458900	4.62063800	
0.13461100			
H	7.00884200	5.59540700	-
2.14137200			
C	3.73498800	-3.53136000	
0.94925800			
C	4.72707700	-3.63993500	
1.93430000			
C	3.65461600	-4.51934400	-
0.04437800			
C	5.61726600	-4.71527300	
1.92969700			
H	4.79457600	-2.87542000	
2.70342000			
C	4.54417200	-5.59428200	-
0.04844800			
H	2.88894000	-4.43264300	-
0.80998900			
C	5.52786000	-5.69531600	
0.93858600			
H	6.37822600	-4.78842600	
2.70213300			
H	4.47176000	-6.35086600	-
0.82540200			
H	6.22081500	-6.53239000	
0.93496900			
C	-3.22378500	-2.72921400	
1.18214800			
C	-3.62558600	-3.56729500	
2.23110800			
C	-3.95956300	-2.72210400	-
0.01386300			
C	-4.74382200	-4.39122800	
2.08628000			
H	-3.06250900	-3.56455100	
3.16065400			
C	-5.07717600	-3.54517200	-
0.15407000			
H	-3.64194000	-2.07424900	-

0.82440700			
C	-5.47122900	-4.38186900	
0.89340500			
H	-5.04975900	-5.03443500	
2.90730700			
H	-5.63798200	-3.52235600	-
1.08407400			
H	-6.34289700	-5.02184300	
0.78317100			
⁶TS4			
Mn	0.64540800	0.27412700	
0.62045900			
N	0.92309100	2.27835700	
0.57521500			
C	-2.00599300	-1.78319200	
1.27715300			
C	-1.34119300	3.05131300	
1.21108700			
C	-3.27193800	1.54615300	
1.75468300			
C	-3.47236600	0.19980700	
1.69709000			
C	-1.89315200	1.78351100	
1.41509700			
C	-2.20809700	-0.40200100	
1.36848700			
H	-4.38539400	-0.34924600	
1.87296100			
H	-3.99106800	2.31800700	
1.98670200			
N	2.65149700	0.01872700	
0.48922000			
N	-1.24827900	0.57782800	
1.23300100			
N	0.45949200	-1.68678100	
1.12626100			
C	3.28076700	2.32017300	-
0.18962100			
C	2.81327000	-2.42314200	
0.90376300			
C	0.86128000	-3.95064500	
1.29913100			
C	0.53358600	4.54837300	

0.47827900			
C	4.70586300	-0.96789900	
0.14425700			
C	-0.48868400	-3.78096900	
1.31398900			
C	1.81201000	4.34099900	
0.05581600			
C	4.82353500	0.34076000	-
0.21466700			
C	1.45133900	-2.64657800	
1.13067600			
C	-0.02237200	3.25987600	
0.79872800			
C	3.34618800	-1.17230900	
0.57074800			
C	-0.73795400	-2.36626500	
1.22785200			
C	2.05541400	2.92264100	
0.11705500			
C	3.54602800	0.96159300	
0.01684400			
H	-1.25415300	-4.53848600	
1.38863000			
H	2.53680400	5.07768600	-
0.25778700			
H	5.69540500	0.84664700	-
0.60186200			
H	1.41363000	-4.87603700	
1.36198300			
H	0.00459300	5.48600000	
0.56637000			
H	5.46084500	-1.73879400	
0.10052600			
N	0.27030000	-0.03672900	-
1.41653400			
C	0.03030300	-1.28240000	-
1.88991900			
C	1.15924200	-2.05950600	-
2.30567700			
C	-1.36971400	-3.06704900	-
2.35891400			
C	0.97026000	-3.36564400	-
2.71820800			
H	2.14514700	-1.60715100	-

2.27318600			
C	-0.32626600	-3.90295600	-
2.74893800			
H	-2.39809200	-3.43067100	-
2.37643100			
H	1.82381600	-3.96293300	-
3.03389200			
H	-0.51758000	-4.92096500	-
3.07296100			
N	-1.22461100	-1.80891400	-
1.93017700			
C	-5.96559700	0.15674200	-
1.59822300			
C	-6.14868300	-0.84178300	-
2.55927100			
C	-5.07882100	-1.21593300	-
3.38073200			
C	-3.83602400	-0.60488500	-
3.24291300			
C	-3.63774500	0.39918500	-
2.26929900			
C	-4.72723900	0.77717700	-
1.45618600			
H	-6.79056400	0.45071200	-
0.95461900			
H	-7.11637000	-1.32440700	-
2.66815600			
H	-5.21331400	-1.99344600	-
4.12828700			
H	-2.99493800	-0.91193800	-
3.85267000			
H	-4.57972600	1.54142800	-
0.70165000			
C	-2.36957400	1.01416000	-
2.11104200			
C	-1.21255700	1.40934500	-
1.95864300			
H	-0.44585900	2.15186900	-
1.94542100			
C	-2.24447300	4.23689700	
1.31825200			
C	-2.13403700	5.14470400	
2.37991500			
C	-3.21687900	4.45652300	

0.32986600			
C	-2.98507900	6.24924800	
2.45698100			
H	-1.38070900	4.97734500	
3.14491600			
C	-4.06666800	5.56031000	
0.40771000			
H	-3.28722100	3.75944600	-
0.50121400			
C	-3.95346300	6.45836700	
1.47244000			
H	-2.89303300	6.94398000	
3.28759900			
H	-4.81336200	5.72131400	-
0.36530000			
H	-4.61553000	7.31792900	
1.53342300			
C	4.37043200	3.18846600	-
0.72989300			
C	4.25803400	3.74363700	-
2.01365500			
C	5.51332200	3.47326400	
0.03255300			
C	5.26683700	4.56156100	-
2.52444800			
H	3.37511700	3.52491700	-
2.60770200			
C	6.52257500	4.29065300	-
0.47834400			
H	5.60199900	3.05122400	
1.02977400			
C	6.40197600	4.83680400	-
1.75835600			
H	5.16724200	4.98029400	-
3.52227800			
H	7.40016900	4.50489000	
0.12579700			
H	7.18755000	5.47358700	-
2.15606500			
C	3.73959700	-3.59595100	
0.91128800			
C	4.72546400	-3.72287000	
1.90057800			
C	3.64903500	-4.57824600	-

0.08718600			
C	5.59977900	-4.81108800	
1.89534500			
H	4.80027800	-2.96307600	
2.67373700			
C	4.52276200	-5.66603300	-
0.09142900			
H	2.88863600	-4.47607900	-
0.85592400			
C	5.50027400	-5.78556600	
0.89967500			
H	6.35599900	-4.89874200	
2.67091000			
H	4.44299800	-6.41779600	-
0.87224100			
H	6.18087700	-6.63269500	
0.89561400			
C	-3.21632100	-2.65330200	
1.21196100			
C	-3.57583100	-3.51377300	
2.25875500			
C	-4.02338800	-2.59187600	
0.06449700			
C	-4.72138200	-4.30584600	
2.15890200			
H	-2.95834200	-3.55260800	
3.15221800			
C	-5.16808200	-3.38343300	-
0.03088200			
H	-3.73569700	-1.93082700	-
0.74594200			
C	-5.51934800	-4.24235100	
1.01371500			
H	-4.99337500	-4.96632000	
2.97813300			
H	-5.78202000	-3.32010100	-
0.92461100			
H	-6.41192200	-4.85805600	
0.93821800			
²INT5			
Mn	0.57586700	0.27401400	
0.61958600			
N	0.73487400	2.28673800	

0.66239800			
C	-1.88473800	-1.96095600	
1.42648600			
C	-1.56229100	2.90155500	
1.35201500			
C	-3.39776800	1.26667400	
1.86082800			
C	-3.49869800	-0.09028500	
1.81920100			
C	-2.03199000	1.59615000	
1.53119900			
C	-2.18687100	-0.59811200	
1.50587500			
H	-4.36797900	-0.70307700	
2.00918700			
H	-4.17190400	1.98464700	
2.08764700			
N	2.58877700	0.15290100	
0.43047900			
N	-1.29537600	0.44149900	
1.36201700			
N	0.55230100	-1.68554700	
1.15446900			
C	3.05121900	2.50364700	-
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C	2.93723000	-2.26726900	
0.83044600			
C	1.13066800	-3.91192900	
1.40386800			
C	0.21080100	4.54019000	
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C	4.68606200	-0.69700200	-
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C	-0.22549800	-3.83963900	
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C	1.48806700	4.42519100	
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C	4.70423300	0.62297600	-
0.38161000			
C	1.60938600	-2.57571700	
1.14459800			
C	-0.25937100	3.20671700	
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C	3.36651400	-0.98736500	

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C	-0.57928100	-2.45086800	
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C	1.80980800	3.02076300	
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C	3.40546600	1.15710300	-
0.05761300			
H	-0.92707200	-4.64516300	
1.64798900			
H	2.15937700	5.21626900	-
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H	5.52127700	1.18857200	-
0.80456700			
H	1.75323900	-4.79028100	
1.48543700			
H	-0.36756600	5.44215600	
0.79962900			
H	5.48403300	-1.41773400	-
0.14932600			
N	0.01959700	0.12257900	-
1.21523900			
C	0.02970300	-1.19800100	-
1.70781000			
C	1.26517000	-1.72728200	-
2.12928000			
C	-1.06114400	-3.13949300	-
2.28343300			
C	1.30182000	-3.01852000	-
2.63918500			
H	2.15453800	-1.11350000	-
2.04939700			
C	0.11308300	-3.75187100	-
2.71889600			
H	-2.01102400	-3.67074500	-
2.31962400			
H	2.24224300	-3.44432800	-
2.97989800			
H	0.09518800	-4.76495900	-
3.10881500			
N	-1.11156400	-1.89904900	-
1.78541300			
C	-5.76972600	-0.50957000	-
2.27379500			
C	-5.88765200	-0.78935600	-

3.64399600			
C	-4.78542500	-0.58126900	-
4.48801300			
C	-3.58380500	-0.10991700	-
3.98285800			
C	-3.43914600	0.17525800	-
2.58830700			
C	-4.57967700	-0.03113900	-
1.74738600			
H	-6.61887600	-0.66891800	-
1.61332600			
H	-6.82428500	-1.16222600	-
4.04884000			
H	-4.87067000	-0.79777400	-
5.55022400			
H	-2.72737400	0.03589100	-
4.63411100			
H	-4.48507200	0.18254100	-
0.68792300			
C	-2.24520300	0.61358300	-
2.05909600			
C	-1.08118200	0.95209800	-
1.55456000			
H	-0.85650000	2.00287800	-
1.36882200			
C	-2.53046900	4.02807300	
1.51697600			
C	-2.40848700	4.93689100	
2.57766700			
C	-3.57535200	4.19588800	
0.59479500			
C	-3.31349100	5.99087200	
2.71559800			
H	-1.60085100	4.80996600	
3.29337000			
C	-4.47988100	5.24918200	
0.73336900			
H	-3.66922700	3.49315200	-
0.22894700			
C	-4.35113800	6.14937600	
1.79412900			
H	-3.20959800	6.68545500	
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H	-5.28234900	5.36847000	

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H	-5.05541800	6.96991700	
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C	4.06101600	3.45618300	-
0.74570600			
C	3.84615000	4.06730800	-
1.99050300			
C	5.23064800	3.76448000	-
0.03460600			
C	4.78082400	4.96170100	-
2.51387400			
H	2.94118100	3.83268900	-
2.54394800			
C	6.16530700	4.65935900	-
0.55742600			
H	5.39888800	3.29903800	
0.93254200			
C	5.94319200	5.25990100	-
1.79887800			
H	4.60195200	5.42305300	-
3.48144000			
H	7.06433800	4.89089900	
0.00759400			
H	6.67086200	5.95675900	-
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C	3.94486500	-3.37097300	
0.81972900			
C	5.00907800	-3.37313300	
1.73402300			
C	3.85591500	-4.41431500	-
0.11512500			
C	5.95931600	-4.39524700	
1.71712800			
H	5.08405600	-2.56702900	
2.45857300			
C	4.80588200	-5.43611200	-
0.13238200			
H	3.03453800	-4.41398000	-
0.82539100			
C	5.86047800	-5.42969900	
0.78379500			
H	6.77473400	-4.38479400	
2.43549800			
H	4.72454200	-6.23521700	-

0.86459300			
H	6.60042000	-6.22540600	
0.77035100			
C	-3.02967600	-2.91780400	
1.36855400			
C	-3.36510300	-3.76240600	
2.43477800			
C	-3.80328000	-2.95042900	
0.19674800			
C	-4.45538800	-4.62962000	
2.33068100			
H	-2.77439200	-3.73044200	
3.34642700			
C	-4.89434900	-3.81363900	
0.09749300			
H	-3.53364500	-2.29697400	-
0.62708300			
C	-5.22232200	-4.65637800	
1.16326500			
H	-4.70970500	-5.27802500	
3.16509300			
H	-5.48719300	-3.82183000	-
0.81354700			
H	-6.07264300	-5.32897900	
1.08648800			
4INT5			
Mn	0.56906300	0.27974000	
0.62317100			
N	0.70151200	2.29164700	
0.66386100			
C	-1.85764800	-1.98887300	
1.41773600			
C	-1.59932000	2.87670000	
1.37207400			
C	-3.41441500	1.21505100	
1.87175700			
C	-3.49784600	-0.14279000	
1.81861700			
C	-2.05317000	1.56496400	
1.54468300			
C	-2.17922200	-0.63115200	
1.50359600			
H	-4.35926900	-0.76842700	

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H	-4.19805800	1.92104000	
2.10348000			
N	2.58180500	0.18763200	
0.42789800			
N	-1.30126000	0.42126800	
1.36762600			
N	0.57691300	-1.67739300	
1.15958700			
C	3.00683900	2.54103300	-
0.20976600			
C	2.97040400	-2.22400800	
0.84411700			
C	1.18619700	-3.89512900	
1.41228300			
C	0.14632200	4.53787100	
0.67028800			
C	4.69160800	-0.63227300	-
0.04816800			
C	-0.17156300	-3.84286700	
1.48710300			
C	1.42047300	4.44050300	
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C	4.68723500	0.68444900	-
0.39513000			
C	1.64678700	-2.55231700	
1.15508500			
C	-0.30340600	3.19826400	
0.95094100			
C	3.37830600	-0.93969700	
0.46117500			
C	-0.54476600	-2.45946700	
1.35123200			
C	1.76168800	3.04095300	
0.19109000			
C	3.38141200	1.20066100	-
0.07103100			
H	-0.86257800	-4.65848900	
1.64112000			
H	2.07796200	5.24062800	-
0.10695800			
H	5.49378100	1.25935900	-
0.82557600			
H	1.82106600	-4.76420600	

1.49820300			
H	-0.44319900	5.43173800	
0.81160000			
H	5.50093000	-1.34088800	-
0.14518200			
N	0.00348700	0.10400600	-
1.20035200			
C	0.05371500	-1.20857600	-
1.70862300			
C	1.30499600	-1.71076800	-
2.11576400			
C	-0.98858700	-3.17028700	-
2.30685600			
C	1.37603700	-3.00056000	-
2.62597400			
H	2.18024400	-1.07867900	-
2.02478300			
C	0.20463500	-3.75895300	-
2.72349500			
H	-1.92733300	-3.71961100	-
2.36157300			
H	2.32996200	-3.40528500	-
2.95476000			
H	0.21328700	-4.77113100	-
3.11605500			
N	-1.07232100	-1.93206900	-
1.80842800			
C	-5.77173900	-0.57455300	-
2.29224600			
C	-5.89340000	-0.83087800	-
3.66704400			
C	-4.79639400	-0.59879800	-
4.51201500			
C	-3.59732700	-0.12429900	-
4.00442900			
C	-3.44736100	0.13508900	-
2.60461200			
C	-4.58278700	-0.09869900	-
1.76201600			
H	-6.61674900	-0.75290100	-
1.63126400			
H	-6.82865900	-1.20440000	-
4.07444900			
H	-4.88491500	-0.79693000	-

5.57756500			
H	-2.74592200	0.04298100	-
4.65711900			
H	-4.48438800	0.09483800	-
0.69896000			
C	-2.25621000	0.57075200	-
2.07141300			
C	-1.10790300	0.91566800	-
1.53760700			
H	-0.90901800	1.96785500	-
1.32923700			
C	-2.57788500	3.99187100	
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C	-2.45596400	4.89421000	
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C	-3.63180400	4.15622100	
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C	-3.37003200	5.93820200	
2.77154500			
H	-1.64111600	4.77018000	
3.32645300			
C	-4.54542600	5.19954100	
0.79352400			
H	-3.72562700	3.45888500	-
0.18848500			
C	-4.41677200	6.09316900	
1.85980800			
H	-3.26600200	6.62779500	
3.60505000			
H	-5.35484900	5.31625900	
0.07786900			
H	-5.12810400	6.90595400	
1.97926000			
C	3.99746000	3.50611200	-
0.77622600			
C	3.76212200	4.10857300	-
2.02154800			
C	5.16828800	3.83549600	-
0.07666900			
C	4.67831600	5.01491200	-
2.55689800			
H	2.85602200	3.85775600	-
2.56596700			
C	6.08440900	4.74237300	-

0.61148800			
H	5.35208000	3.37710600	
0.89101700			
C	5.84219600	5.33398300	-
1.85346900			
H	4.48384000	5.46931500	-
3.52473300			
H	6.98463200	4.99023400	-
0.05536900			
H	6.55544700	6.04016200	-
2.26992000			
C	3.99654100	-3.31051400	
0.84191800			
C	5.05841400	-3.28873600	
1.75866200			
C	3.92815900	-4.36038500	-
0.08733600			
C	6.02639100	-4.29416500	
1.74987300			
H	5.11761000	-2.47728400	
2.47869900			
C	4.89594100	-5.36543500	-
0.09648300			
H	3.10893800	-4.37829200	-
0.79983700			
C	5.94793700	-5.33543800	
0.82221100			
H	6.83976700	-4.26533900	
2.47004800			
H	4.83048700	-6.16985700	-
0.82443900			
H	6.70171200	-6.11813100	
0.81503300			
C	-2.98863900	-2.96163600	
1.35082700			
C	-3.32220900	-3.80853400	
2.41577700			
C	-3.75101700	-3.00634200	
0.17209100			
C	-4.40030600	-4.68989500	
2.30390200			
H	-2.73984600	-3.76729500	
3.33243000			
C	-4.83009200	-3.88367400	

0.06529100			
H	-3.48151800	-2.35196700	-
0.65109400			
C	-5.15663200	-4.72840800	
1.12991000			
H	-4.65349800	-5.34010400	
3.13725000			
H	-5.41488700	-3.90121900	-
0.85078500			
H	-5.99764300	-5.41191000	
1.04705300			
6INT5			
Mn	0.63730800	0.29496500	
0.61636600			
N	0.30170400	2.28075700	
0.70285300			
C	-1.22762100	-2.48030500	
1.22785900			
C	-2.01800000	2.31545500	
1.58240600			
C	-3.35880600	0.26543900	
2.15076400			
C	-3.16108800	-1.06973200	
1.96952900			
C	-2.14727100	0.93187900	
1.74108400			
C	-1.81073600	-1.23667700	
1.49785600			
H	-3.85049800	-1.88014000	
2.15550300			
H	-4.24800500	0.76377400	
2.50689700			
N	2.60681800	0.66298700	
0.37144900			
N	-1.19334800	-0.00965900	
1.41450400			
N	1.08630100	-1.63598800	
1.02242100			
C	2.44958300	3.04994600	-
0.27029300			
C	3.54835300	-1.59749400	
0.76923400			
C	2.16149300	-3.67168800	

1.07388600			
C	-0.76063500	4.32379400	
0.74630100			
C	4.86341000	0.39239700	-
0.00851400			
C	0.82271000	-3.92449900	
1.07737900			
C	0.46585300	4.51879500	
0.18423100			
C	4.54361800	1.66363700	-
0.37812900			
C	2.32513800	-2.24388100	
0.98381600			
C	-0.86707500	2.92496500	
1.06530400			
C	3.65053100	-0.23946900	
0.44443400			
C	0.15246800	-2.65270800	
1.08566300			
C	1.13073600	3.24361700	
0.16124800			
C	3.13999100	1.84386400	-
0.11256200			
H	0.32683200	-4.88318000	
1.10081000			
H	0.89457200	5.44386700	-
0.17190100			
H	5.19732500	2.42080000	-
0.78483100			
H	2.96977700	-4.38713400	
1.09437700			
H	-1.53368100	5.05656800	
0.92406400			
H	5.82675500	-0.09275900	-
0.06350100			
N	-0.11959800	-0.03981800	-
1.33303800			
C	0.10715800	-1.27819200	-
1.89843900			
C	1.44713300	-1.70056600	-
2.10063000			
C	-0.67609200	-3.27576000	-
2.76025900			
C	1.68752200	-2.95587900	-

2.62905100			
H	2.25358300	-1.02551700	-
1.83731400			
C	0.60360000	-3.78165000	-
2.96591500			
H	-1.55262700	-3.87300400	-
3.01041100			
H	2.70903000	-3.29019900	-
2.79670700			
H	0.74901500	-4.77354300	-
3.38224200			
N	-0.93055200	-2.06755200	-
2.24379700			
C	-6.13184000	-0.69659000	-
1.70931100			
C	-6.53715900	-0.59147800	-
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C	-5.58678800	-0.26640600	-
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C	-4.26049900	-0.04910300	-
3.69224800			
C	-3.82284500	-0.14394200	-
2.33159600			
C	-4.81022400	-0.48268300	-
1.34797100			
H	-6.86070300	-0.94967400	-
0.94221500			
H	-7.57412600	-0.76229400	-
3.32431500			
H	-5.89316900	-0.18545400	-
5.07103200			
H	-3.52662400	0.19409600	-
4.45484200			
H	-4.49774900	-0.56831400	-
0.31263400			
C	-2.50069500	0.03427900	-
1.97904400			
C	-1.37503400	0.54771000	-
1.51867600			
H	-1.37961600	1.59825600	-
1.21326700			
C	-3.21180900	3.17165900	
1.85063500			
C	-3.20873400	4.11263200	

2.89035800			
C	-4.35454300	3.05192800	
1.04243600			
C	-4.32687100	4.91557100	
3.12208200			
H	-2.32603000	4.20739100	
3.51693500			
C	-5.47087700	3.85555500	
1.27549700			
H	-4.35922600	2.32838700	
0.23122500			
C	-5.46017400	4.78862000	
2.31551900			
H	-4.31334500	5.63698300	
3.93472800			
H	-6.34657000	3.75462400	
0.64015400			
H	-6.33021800	5.41416300	
2.49600300			
C	3.16486900	4.21701300	-
0.87003700			
C	2.78742400	4.69537000	-
2.13386500			
C	4.20535500	4.86138200	-
0.18424300			
C	3.44057500	5.79024700	-
2.70160900			
H	1.98093700	4.19977600	-
2.66707100			
C	4.85899100	5.95573200	-
0.75263500			
H	4.49435100	4.50050700	
0.79898200			
C	4.47846400	6.42252800	-
2.01297500			
H	3.14015500	6.14678100	-
3.68315300			
H	5.66109400	6.44680100	-
0.20813100			
H	4.98685300	7.27501300	-
2.45517700			
C	4.80353300	-2.40838800	
0.77701400			
C	5.76865300	-2.21152000	

1.77566300			
C	5.05000700	-3.36024700	-
0.22433200			
C	6.95089300	-2.95353800	
1.77680200			
H	5.58409100	-1.47325400	
2.55119100			
C	6.23117000	-4.10292900	-
0.22260400			
H	4.30714200	-3.51005200	-
1.00238700			
C	7.18481500	-3.90166100	
0.77822900			
H	7.68727200	-2.79270200	
2.55962100			
H	6.40881400	-4.83430400	-
1.00650300			
H	8.10514400	-4.47931100	
0.77905700			
C	-2.14636400	-3.64635300	
1.08535200			
C	-2.17963400	-4.69894300	
2.01050400			
C	-3.02535500	-3.66507500	-
0.01138900			
C	-3.07222000	-5.75915700	
1.84007600			
H	-1.51375900	-4.67576400	
2.86903800			
C	-3.91673000	-4.72520700	-
0.17623500			
H	-2.98399900	-2.85460200	-
0.73339900			
C	-3.94186100	-5.77424500	
0.74685500			
H	-3.09368600	-6.56775100	
2.56598800			
H	-4.59203800	-4.72746200	-
1.02759200			
H	-4.63783300	-6.59889200	
0.61718700			
4			
N	1.82299500	2.06980900	

0.33941500			
C	2.22416700	0.81598300	
0.13565300			
C	3.52674400	0.27567700	
0.04253600			
C	1.29131000	-1.38954800	-
0.29953700			
C	3.69225300	-1.06459600	-
0.21205300			
H	4.36293300	0.95383600	
0.17025500			
C	2.55481400	-1.90215000	-
0.39556800			
H	0.39015900	-1.96831000	-
0.45238600			
H	4.68829700	-1.48959500	-
0.28513500			
H	2.67532200	-2.95594300	-
0.62174200			
N	1.12217100	-0.05507800	-
0.01125000			
C	-3.70011800	0.57767300	-
0.66660100			
C	-4.08405300	-0.61129100	-
0.04093500			
C	-3.12841000	-1.37170300	
0.63686000			
C	-1.80055200	-0.94929300	
0.68967600			
C	-1.39766600	0.23752600	
0.04874400			
C	-2.37084500	0.99434100	-
0.62937100			
H	-4.43594100	1.17652500	-
1.19668200			
H	-5.11865500	-0.94065400	-
0.07901100			
H	-3.41961700	-2.28996100	
1.14003500			
H	-1.07729400	-1.52493300	
1.26031400			
H	-2.06889700	1.90521800	-
1.13846000			
C	-0.02040100	0.72880400	

0.11073000			
C		0.46692700	2.01405300
0.31736000			
H		-0.13747600	2.89784300
0.48070500			

²TS5

Mn	1.00572000	0.19679600	-0.69385400	
N	0.89719200		2.23319600	-
0.64019700				
C	3.54569400		-2.11671300	-
0.29131000				
C	3.28014600		2.74538200	-
0.11825100				
C	5.16708000		1.08295800	-
0.02839200				
C	5.23843600		-0.27221400	-
0.06522000				
C	3.77400900		1.44129500	-
0.19044600				
C	3.89317900		-0.76440000	-
0.27884000				
H		6.11682600	-0.89069500	
0.04454900				
H		5.97852100	1.78332600	
0.10245500				
N	-0.96581300		0.09376200	-
1.15020100				
N	3.01114900		0.29821600	-
0.37608500				
N	1.11419900		-1.83867500	-
0.74748700				
C	-1.53509700		2.50310800	-
1.08325200				
C	-1.25615000		-2.35764400	-
1.32079800				
C	0.50833500		-4.05693100	-
0.71868500				
C	1.38317600		4.40854100	-
0.06920200				
C	-3.02005900		-0.66682800	-
1.91564900				
C	1.86273200		-3.99203100	-
0.44394100				

C	0.02633500	4.33858200	-
0.33039000			
C	-3.09130500	0.68718100	-
1.85216800			
C	0.07036800	-2.72450200	-
0.92924200			
C	1.90642600	3.10576400	-
0.27736000			
C	-1.70211100	-1.04231200	-
1.45146100			
C	2.21802800	-2.61809000	-
0.46714300			
C	-0.24850200	2.99499400	-
0.69410100			
C	-1.82219700	1.16210500	-
1.34695500			
H	2.53581600	-4.81681100	-
0.26349000			
H	-0.69910300	5.13593800	-
0.26566400			
H	-3.91304800	1.32402800	-
2.13326100			
H	-0.11028100	-4.93997500	-
0.77632800			
H	1.94819700	5.27327700	
0.24568800			
H	-3.78085000	-1.35577800	-
2.25047500			
C	-2.64121400	3.49296100	-
1.20579000			
C	-3.76830000	3.40679900	-
0.37269300			
C	-2.58357600	4.52747300	-
2.15408300			
C	-4.81857200	4.31672400	-
0.49285700			
H	-3.81802600	2.62563500	
0.37813200			
C	-3.63541300	5.43523000	-
2.27807500			
H	-1.71166000	4.60678100	-
2.79669600			
C	-4.75670300	5.33219100	-
1.44974800			

H	-5.68022600	4.22734800	
0.16339100			
H	-3.58107100	6.22229000	-
3.02548100			
H	-5.57432900	6.04114500	-
1.54818200			
C	4.24001000	3.84920800	
0.16474100			
C	4.43577300	4.87918700	-
0.77027800			
C	4.95680300	3.88971500	
1.37159600			
C	5.33558000	5.91236100	-
0.51079600			
H	3.87812800	4.85839400	-
1.70183600			
C	5.84997600	4.92871200	
1.63492900			
H	4.80261000	3.10228500	
2.10379200			
C	6.04447200	5.94140100	
0.69315000			
H	5.48356300	6.69537300	-
1.24963900			
H	6.39065800	4.94832800	
2.57738900			
H	6.74191600	6.74942800	
0.89656500			
C	4.63566800	-3.11837500	-
0.10760200			
C	5.62726300	-3.28334500	-
1.08731200			
C	4.69249200	-3.91341800	
1.04774000			
C	6.64991300	-4.21697800	-
0.91450200			
H	5.58679400	-2.67489500	-
1.98628200			
C	5.71685900	-4.84367500	
1.22319000			
H	3.92544900	-3.79556800	
1.80696100			
C	6.69893300	-4.99880100	
0.24175600			

H	7.40657800	-4.33521600	-
1.68548700			
H	5.74897200	-5.44607900	
2.12716400			
H	7.49584500	-5.72496500	
0.37684100			
C	-2.20721700	-3.46064800	-
1.63083200			
C	-3.38597800	-3.62936100	-
0.88657700			
C	-1.93552000	-4.35272500	-
2.68275900			
C	-4.27155100	-4.66390700	-
1.19013400			
H	-3.59695000	-2.96624800	-
0.05629300			
C	-2.82851500	-5.37762900	-
2.99175100			
H	-1.02248500	-4.22954800	-
3.25777400			
C	-3.99914700	-5.53748400	-
2.24481300			
H	-5.17185300	-4.78633700	-
0.59439600			
H	-2.61040000	-6.05131200	-
3.81619200			
H	-4.69194600	-6.34045800	-
2.48217800			
N	-1.94822000	-1.14426600	
2.02023600			
N	-2.61581100	-2.27964500	
2.36693800			
N	-3.88298800	-2.03694900	
2.24134400			
C	-0.54348300	-1.05928400	
2.20886200			
C	0.18282400	-2.19912000	
2.56510500			
C	1.30288800	0.28618500	
2.28506200			
C	1.54390200	-2.03679000	
2.80150000			
H	-0.30977700	-3.15885800	
2.64310900			

C	2.12219600	-0.77292500	
2.67321400			
H	1.70683700	1.28210600	
2.12758500			
H	2.14584400	-2.89590900	
3.08025000			
H	3.18411600	-0.61466700	
2.82589400			
N	-0.01343000	0.15367300	
2.05241500			
C	-4.06932300	-0.74070200	
1.80728800			
C	-2.82408600	-0.16265000	
1.66332900			
C	-5.42559000	-0.17145400	
1.71856800			
C	-6.32845500	-0.47895500	
2.75316000			
C	-5.85833600	0.66623800	
0.67953400			
C	-7.61442600	0.05602500	
2.76613300			
H	-6.00179600	-1.13997100	
3.54971500			
C	-7.14624100	1.20976600	
0.70333400			
H	-5.25061300	0.88154300	-
0.19208200			
C	-8.02662300	0.91515300	
1.74453400			
H	-8.29211400	-0.19253900	
3.57856900			
H	-7.46230900	1.85562500	-
0.11209100			
H	-9.02643300	1.34086400	
1.75513300			
H	-2.48317300	0.81493000	
1.36833900			

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Mn	0.82662100	0.23574700	-0.69656300
N	1.23811400	2.21431700	-
0.54164000			

C	2.69387900	-2.64788500	-
0.58293700			
C	3.70857100	2.11609500	-
0.34964400			
C	5.11301500	0.02405100	-
0.47302900			
C	4.82583200	-1.30755600	-
0.49047600			
C	3.85193100	0.72820300	-
0.51889700			
C	3.39066600	-1.42936400	-
0.59309200			
H	5.51983400	-2.13410000	-
0.44425500			
H	6.08611400	0.48963200	-
0.41709300			
N	-1.11647700	0.66592400	-
1.06662400			
N	2.81806500	-0.17629700	-
0.63116000			
N	0.42550200	-1.73179300	-
0.96725600			
C	-1.06343600	3.11164400	-
0.67192900			
C	-1.99359200	-1.61271300	-
1.48860400			
C	-0.70522500	-3.74112400	-
1.07558000			
C	2.31030200	4.17867500	
0.02701400			
C	-3.29696600	0.51968300	-
1.81119900			
C	0.59951000	-4.02864800	-
0.80777000			
C	0.97608000	4.44892400	-
0.01963100			
C	-3.04416200	1.83475800	-
1.56172900			
C	-0.80701500	-2.30510300	-
1.19208800			
C	2.47123400	2.78227100	-
0.30694200			
C	-2.10182600	-0.21300600	-
1.46687900			

C	1.30586400	-2.77007200	-
0.75518000			
C	0.31135000	3.22727800	-
0.40965100			
C	-1.68642400	1.91887300	-
1.07940400			
H	1.04912200	-5.00141900	-
0.67117100			
H	0.48435400	5.38827900	
0.18689500			
H	-3.70556500	2.67621000	-
1.70926100			
H	-1.52692300	-4.43357900	-
1.18486300			
H	3.11385800	4.85489300	
0.28027000			
H	-4.20857100	0.08302500	-
2.19081900			
C	-1.93280400	4.31551000	-
0.51942400			
C	-2.97975300	4.30657200	
0.41829900			
C	-1.74576300	5.46349600	-
1.30491200			
C	-3.81375500	5.41461900	
0.56799700			
H	-3.13005500	3.42269300	
1.03251300			
C	-2.57975600	6.57269400	-
1.15554100			
H	-0.94604300	5.47461200	-
2.03994300			
C	-3.61597600	6.55197600	-
0.21903000			
H	-4.61521800	5.38998300	
1.30170600			
H	-2.42411800	7.45080400	-
1.77680300			
H	-4.26546900	7.41564600	-
0.10418900			
C	4.94314000	2.93795600	-
0.16169800			
C	5.30804900	3.90141600	-
1.11511400			

C	5.75460800	2.77677200	
0.97238200			
C	6.45412300	4.67858200	-
0.94200600			
H	4.68396700	4.03377800	-
1.99440000			
C	6.90110500	3.55273400	
1.14702200			
H	5.47683500	2.03733300	
1.71848200			
C	7.25473600	4.50628900	
0.18952800			
H	6.72323800	5.41644000	-
1.69323700			
H	7.51472700	3.41638000	
2.03370800			
H	8.14715700	5.11141400	
0.32486000			
C	3.47777300	-3.90325500	-
0.36787300			
C	4.33873800	-4.40283200	-
1.35581100			
C	3.35743200	-4.60594500	
0.84080800			
C	5.06624100	-5.57445000	-
1.13901100			
H	4.43135100	-3.86573900	-
2.29571300			
C	4.08151500	-5.77914600	
1.05692000			
H	2.69074600	-4.21970500	
1.60659800			
C	4.93950100	-6.26620900	
0.06783300			
H	5.72738600	-5.94983300	-
1.91569800			
H	3.97835000	-6.31159900	
1.99906600			
H	5.50426600	-7.17936600	
0.23568500			
C	-3.21305400	-2.40879200	-
1.81984100			
C	-4.36806400	-2.31357900	-
1.02653900			

C	-3.23140700	-3.26754200	-
2.93106600			
C	-5.50883300	-3.05406200	-
1.33460900			
H	-4.36588000	-1.66043600	-
0.16316000			
C	-4.37255000	-4.00925200	-
3.23955100			
H	-2.34456200	-3.34387300	-
3.55393800			
C	-5.51533900	-3.90500500	-
2.44231200			
H	-6.38780500	-2.96432400	-
0.70163900			
H	-4.37036100	-4.66438900	-
4.10687400			
H	-6.40367900	-4.48283100	-
2.68375200			
N	-1.09173400	-1.22405400	
1.84491000			
N	-1.95501000	-2.11925100	
2.08056200			
N	-3.11765300	-2.19814300	
2.12958500			
C	0.21977700	-1.30150600	
2.31087800			
C	0.70549500	-2.31637600	
3.15473100			
C	2.23199800	-0.19333100	
2.34451900			
C	2.02337400	-2.22790200	
3.58512600			
H	0.05984800	-3.13654500	
3.44917800			
C	2.80634600	-1.13856200	
3.18884200			
H	2.80083500	0.65563700	
1.97982800			
H	2.43465200	-2.99843700	
4.23162400			
H	3.83742500	-1.03434600	
3.50831500			
N	0.97372500	-0.27519000	
1.88850300			

C	-3.56319700	0.01883000
1.87904900		
C	-2.41812300	0.48873000
1.81531700		
C	-5.00363800	0.05258600
1.78618000		
C	-5.83076700	-0.86462500
2.45690000		
C	-5.59854800	1.04022700
0.97472100		
C	-7.21643900	-0.79265300
2.32036200		
H	-5.37997600	-1.63351700
3.07306600		
C	-6.98295000	1.10076400
0.83820700		
H	-4.95974800	1.73648500
0.44259300		
C	-7.79804300	0.18535800
1.50989900		
H	-7.84368300	-1.50778800
2.84583500		
H	-7.42595200	1.86330700
0.20307100		
H	-8.87814200	0.23274400
1.40066000		
H	-1.57825200	1.13982800
1.70757000		

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Mn	0.78011200	0.23089600	-
0.41038900			
N	0.93710900	2.33481500	-
0.60739200			
C	3.11152100	-2.33750900	-
0.60170700			
C	3.38841500	2.55102200	-
0.28352700			
C	5.10451000	0.67254000	-
0.22382900			
C	5.02259000	-0.68866600	-
0.28190400			
C	3.75902700	1.18844200	-
0.38844600			

C	3.63189600	-1.02415000	-
0.51721000			
H	5.83137500	-1.39783900	-
0.18011200			
H	5.99235700	1.27051700	-
0.07635300			
N	-1.21516100	0.39885500	-
1.11541900			
N	2.89997300	0.13599200	-
0.58660100			
N	0.71063800	-1.81620200	-
0.94071500			
C	-1.46962200	2.85647100	-
0.88391700			
C	-1.69254300	-2.00461300	-
1.51115100			
C	-0.05353100	-3.94240900	-
1.35443400			
C	1.70987700	4.45835100	-
0.18582300			
C	-3.35577300	-0.10787300	-
1.78345500			
C	1.28104600	-4.03644200	-
1.08611500			
C	0.35605000	4.54219700	-
0.32965800			
C	-3.29005900	1.24478600	-
1.62275100			
C	-0.40911600	-2.53984300	-
1.26043100			
C	2.07460600	3.06648700	-
0.36917200			
C	-2.04390200	-0.63799600	-
1.46912100			
C	1.76184200	-2.68964200	-
0.83865100			
C	-0.12604500	3.20505200	-
0.61615400			
C	-1.94290000	1.55818200	-
1.18883400			
H	1.89204700	-4.92784200	-
1.09101700			
H	-0.25947800	5.42669200	-
0.24933000			

H	-4.07419600	1.96744800	-
1.79799100			
H	-0.73261500	-4.74268300	-
1.61233300			
H	2.39788900	5.26280300	
0.03146100			
H	-4.21002800	-0.69316300	-
2.09138700			
C	-2.49421800	3.94405400	-
0.84106000			
C	-3.51288800	3.90639900	
0.12582900			
C	-2.47783400	5.00671900	-
1.75706600			
C	-4.49081800	4.90017700	
0.17306600			
H	-3.52790900	3.09161600	
0.84428900			
C	-3.45436300	6.00324600	-
1.70930100			
H	-1.69713000	5.03979400	-
2.51174400			
C	-4.46457100	5.95239600	-
0.74576900			
H	-5.26984600	4.85253900	
0.92955700			
H	-3.42990700	6.81594200	-
2.43061000			
H	-5.22568500	6.72734400	-
0.71132400			
C	4.48602900	3.53951000	-
0.04177700			
C	4.82654700	4.48164500	-
1.02483200			
C	5.19237500	3.55201700	
1.17098500			
C	5.84571700	5.40881100	-
0.80251200			
H	4.28429900	4.47851400	-
1.96616600			
C	6.21278100	4.47733400	
1.39471400			
H	4.93223800	2.82964300	
1.93990400			

C	6.54274100	5.40919200	
0.40792600			
H	6.09773600	6.12838100	-
1.57711000			
H	6.74601300	4.47383400	
2.34186700			
H	7.33662200	6.13074600	
0.58134000			
C	4.07173500	-3.46717300	-
0.41031300			
C	5.10294500	-3.71672100	-
1.32857600			
C	3.95015300	-4.30646800	
0.70888400			
C	5.99162900	-4.77482000	-
1.13157500			
H	5.19836000	-3.07549100	-
2.20029000			
C	4.83725400	-5.36526100	
0.90606800			
H	3.15355000	-4.11501000	
1.42278200			
C	5.86178100	-5.60232300	-
0.01363300			
H	6.78175900	-4.95661600	-
1.85541200			
H	4.73037000	-6.00393300	
1.77926600			
H	6.55293200	-6.42702600	
0.13866100			
C	-2.76838500	-2.97234500	-
1.89873900			
C	-3.33053700	-3.84274300	-
0.95366700			
C	-3.23101000	-3.02534000	-
3.22254600			
C	-4.33153200	-4.74292400	-
1.32279000			
H	-2.99088900	-3.79929000	
0.07560100			
C	-4.23198700	-3.92477300	-
3.59230400			
H	-2.79728500	-2.35482400	-
3.95926600			

C	-4.78505000	-4.78726700	-
2.64280900			
H	-4.76143200	-5.40477400	-
0.57547100			
H	-4.57675000	-3.95394800	-
4.62269500			
H	-5.56509600	-5.48757100	-
2.92961100			
N	-1.06974900	-1.24779000	
1.87514800			
N	-1.95283500	-2.12460900	
2.12746700			
N	-3.11831200	-2.16811900	
2.18305000			
C	0.22559200	-1.36660700	
2.37531400			
C	0.63508000	-2.34732700	
3.29544500			
C	2.31081100	-0.38262600	
2.38639100			
C	1.94693700	-2.31414300	
3.74952500			
H	-0.06591300	-3.10458600	
3.62848700			
C	2.80414400	-1.30316100	
3.30382200			
H	2.94136600	0.40097600	
1.98199800			
H	2.29537100	-3.06494000	
4.45332500			
H	3.83373300	-1.24118900	
3.63779600			
N	1.05584100	-0.41746600	
1.90641100			
C	-3.57392500	-0.00818500	
1.94225600			
C	-2.44172500	0.48243400	
1.82976900			
C	-5.01822800	-0.00193300	
1.97515000			
C	-5.74388000	-0.77830600	
2.89397400			
C	-5.71631800	0.83039700	
1.07963500			

C	-7.13568600	-0.71306000
2.92324700		
H	-5.21031700	-1.42960500
3.57733800		
C	-7.10797800	0.88383300
1.11031300		
H	-5.15726000	1.41651700
0.35984800		
C	-7.82299900	0.11526600
2.03252300		
H	-7.68551800	-1.31567000
3.64116300		
H	-7.63428100	1.52747200
0.41044900		
H	-8.90852400	0.15893800
2.05484900		
H	-1.62255000	1.14968400
1.67866700		

cssFe (TPP)

Fe	-0.00138100	-0.00000800	-
0.00004800			
N	1.41913800	-1.41978800	
0.00285500			
C	-3.44964700	-0.00095100	-
0.00026800			
C	-0.00118300	-3.44953000	
0.01695200			
C	-2.50635600	-3.46616400	-
0.08594500			
C	-3.46701900	-2.50553000	-
0.07894700			
C	-1.23298700	-2.78900900	-
0.02971500			
C	-2.78888100	-1.23238700	-
0.03988700			
H	-4.53895100	-2.63558500	-
0.09833500			
H	-2.63716400	-4.53754000	-
0.12080600			
N	1.41836500	1.42054500	-
0.00285600			
N	-1.42090700	-1.42077500	-
0.01638100			

N	-1.42168800	1.41999600	
0.01629400			
C	3.44820000	0.00094100	-
0.00022500			
C	-0.00307400	3.44952000	-
0.01651500			
C	-2.50828800	3.46476200	
0.08612300			
C	2.50036000	-3.46131900	
0.17201000			
C	2.49841700	3.46270800	-
0.17178800			
C	-3.46841100	2.50359300	
0.07872400			
C	3.46102300	-2.50050700	
0.17106700			
C	3.45961700	2.50243200	-
0.17130200			
C	-1.23453400	2.78832900	
0.02989800			
C	1.23009000	-2.78687900	
0.05477300			
C	1.22854500	2.78753800	-
0.05453000			
C	-2.78956500	1.23083600	
0.03957100			
C	2.78640600	-1.23040500	
0.05164000			
C	2.78572900	1.23193500	-
0.05188600			
H	-4.54042300	2.63304200	
0.09798900			
H	4.52996200	-2.62856500	
0.25568600			
H	4.52846400	2.63112500	-
0.25609900			
H	-2.63972400	4.53604900	
0.12119500			
H	2.62827800	-4.53023100	
0.25765900			
H	2.62569000	4.53171500	-
0.25722500			
C	0.00179200	-4.94475000	
0.03378700			

C	0.50229100	-5.67069400	-
1.05778000			
C	-0.49214100	-5.65002900	
1.14183300			
C	0.50815800	-7.06619100	-
1.04271500			
H	0.88602300	-5.13054400	-
1.91874500			
C	-0.48705200	-7.04550300	
1.15786900			
H	-0.87891500	-5.09390600	
1.99117000			
C	0.01319000	-7.75775600	
0.06535000			
H	0.89600600	-7.61281100	-
1.89827700			
H	-0.86998600	-7.57585600	
2.02578000			
H	0.01753600	-8.84438200	
0.07754400			
C	4.94294900	0.00134900	-
0.00048400			
C	5.65910600	0.53668100	
1.08128800			
C	5.65899800	-0.53346400	-
1.08257900			
C	7.05459300	0.53744500	
1.08149900			
H	5.11105900	0.95075500	
1.92294100			
C	7.05448900	-0.53313800	-
1.08347000			
H	5.11085400	-0.94794200	-
1.92396900			
C	7.75655400	0.00244100	-
0.00116300			
H	7.59313400	0.95225200	
1.92949600			
H	7.59293800	-0.94753100	-
1.93172700			
H	8.84325400	0.00287800	-
0.00142900			
C	-0.00089900	4.94475200	-
0.03277900			

C	0.49893000	5.67049500	
1.05922500			
C	-0.49512200	5.65023700	-
1.14056500			
C	0.50371800	7.06600500	
1.04490700			
H	0.88293100	5.13016700	
1.91995900			
C	-0.49111300	7.04572300	-
1.15585400			
H	-0.88131500	5.09428800	-
1.99028100			
C	0.00836300	7.75777800	-
0.06285500			
H	0.89101700	7.61246700	
1.90081900			
H	-0.87429200	7.57624900	-
2.02355100			
H	0.01183800	8.84441400	-
0.07445700			
C	-4.94591300	-0.00139400	-
0.00055000			
C	-5.66024700	-0.35302100	-
1.15547200			
C	-5.66096500	0.34975600	
1.15407500			
C	-7.05602400	-0.35468100	-
1.15604400			
H	-5.11160600	-0.62503900	-
2.05293400			
C	-7.05674100	0.35043600	
1.15406600			
H	-5.11289400	0.62213700	
2.05177700			
C	-7.75822400	-0.00236700	-
0.00113300			
H	-7.59437000	-0.62730700	-
2.05996100			
H	-7.59565500	0.62267900	
2.05776100			
H	-8.84492700	-0.00275500	-
0.00134900			

^{oss}Fe (TPP)

Fe	-0.00120900	-0.00002500	-
0.00004600			
N	1.43672800	-1.39793700	-
0.00419600			
C	-3.45030400	-0.04919400	-
0.00009200			
C	0.04682000	-3.45039200	
0.01483900			
C	-2.45475800	-3.49862100	-
0.08809700			
C	-3.42977400	-2.55038500	-
0.07908000			
C	-1.19289000	-2.80503100	-
0.03035400			
C	-2.77040100	-1.27002000	-
0.03813200			
H	-4.49970300	-2.69609100	-
0.09927100			
H	-2.57155600	-4.57153500	-
0.12571900			
N	1.39629100	1.43830700	
0.00411400			
N	-1.39894700	-1.43849500	-
0.01400300			
N	-1.43939900	1.39801800	
0.01393300			
C	3.44875900	0.04915600	-
0.00007400			
C	-0.05155700	3.45030800	-
0.01478200			
C	-2.55350900	3.42720700	
0.08817900			
C	2.54452000	-3.42362100	
0.17616000			
C	2.44585400	3.49476500	-
0.17614000			
C	-3.50109000	2.45155700	
0.07907700			
C	3.49269900	-2.44831600	
0.17686400			
C	3.42147100	2.54690600	-
0.17693900			
C	-1.27237700	2.76988000	
0.03036300			

C	1.26746300	-2.76839600	
0.05219900			
C	1.18801900	2.80337600	-
0.05222500			
C	-2.80549100	1.19051800	
0.03803900			
C	2.80201500	-1.19012600	
0.05114400			
C	2.76695700	1.26951200	-
0.05123500			
H	-4.57473800	2.56669000	
0.09934500			
H	4.56276400	-2.56198300	
0.26778300			
H	4.48785400	2.69109200	-
0.26781800			
H	-2.70088600	4.49634300	
0.12589600			
H	2.68783900	-4.49020300	
0.26653200			
H	2.55864900	4.56500900	-
0.26647900			
C	0.07098000	-4.94501200	
0.03198700			
C	0.58565900	-5.66362800	-
1.05795300			
C	-0.41648400	-5.65706700	
1.13868400			
C	0.61148500	-7.05887500	-
1.04255300			
H	0.96368400	-5.11802800	-
1.91799800			
C	-0.39126200	-7.05229800	
1.15484300			
H	-0.81316600	-5.10638300	
1.98698600			
C	0.12282700	-7.75730200	
0.06402800			
H	1.00979700	-7.59997600	-
1.89679200			
H	-0.76911400	-7.58804700	
2.02164500			
H	0.14279400	-8.84374000	
0.07640800			

C	4.94288100	0.07046000	-
0.00024200			
C	5.65121000	0.62258300	
1.07839700			
C	5.66640300	-0.46112800	-
1.07910900			
C	7.04652100	0.64277300	
1.07859200			
H	5.09725100	1.03328700	
1.91781400			
C	7.06171700	-0.44115100	-
1.07983000			
H	5.12416000	-0.88759000	-
1.91831800			
C	7.75597900	0.11093400	-
0.00076200			
H	7.57911400	1.07004700	
1.92412700			
H	7.60606400	-0.85294100	-
1.92556200			
H	8.84255500	0.12658900	-
0.00097400			
C	-0.07002600	4.94501500	-
0.03149500			
C	0.42375400	5.67764200	
1.05878400			
C	-0.57765400	5.64325600	-
1.13793000			
C	0.40937100	7.07306000	
1.04404900			
H	0.81729300	5.14273100	
1.91858200			
C	-0.59263900	7.03864400	-
1.15342500			
H	-0.95824000	5.08180100	-
1.98654800			
C	-0.09919200	7.75764600	-
0.06221400			
H	0.79189600	7.62500500	
1.89856500			
H	-0.98569600	7.56369700	-
2.02000800			
H	-0.11057600	8.84421400	-
0.07405800			

C	-4.94620400	-0.07055900	-
0.00031400			
C	-5.65535600	-0.42855000	-
1.15651100			
C	-5.66571200	0.26697900	
1.15563700			
C	-7.05098100	-0.44969800	-
1.15690600			
H	-5.10291600	-0.68941600	-
2.05495300			
C	-7.06137200	0.24814000	
1.15554600			
H	-5.12130000	0.54352400	
2.05429200			
C	-7.75784400	-0.11082600	-
0.00080100			
H	-7.58558500	-0.72686800	-
2.06164200			
H	-7.60401000	0.50985700	
2.06010100			
H	-8.84442700	-0.12639500	-
0.00098400			
³Fe (TPP)			
Fe	-0.00000500	0.00000000	-
0.00076400			
N	-0.37131200	-1.96976200	-
0.00070300			
C	-1.94517700	2.84885500	-
0.00076100			
C	-2.84885400	-1.94517000	-
0.00010000			
C	-4.27147600	0.11326600	-
0.00402800			
C	-4.01959000	1.44957300	
0.00404000			
C	-2.99489100	-0.55504500	
0.00311200			
C	-2.58730600	1.60729400	-
0.00382300			
H	-4.73195700	2.26122200	
0.01247800			
H	-5.23044300	-0.38335300	-
0.01204400			

N	1.96975100	-0.37130800	-
0.00076400			
N	-1.96976300	0.37130800	-
0.00058400			
N	0.37130300	1.96976300	-
0.00084500			
C	1.94516800	-2.84885400	-
0.00078300			
C	2.84884200	1.94516900	-
0.00049600			
C	1.44957500	4.01959000	
0.00307900			
C	-1.44958000	-4.01958900	
0.00360400			
C	4.27146500	-0.11326300	-
0.00438100			
C	0.11326800	4.27147400	-
0.00534000			
C	-0.11327500	-4.27147400	-
0.00493100			
C	4.01958100	-1.44957200	
0.00374200			
C	1.60729000	2.58730300	-
0.00412400			
C	-1.60729900	-2.58730300	-
0.00376400			
C	2.99487900	0.55504500	
0.00281300			
C	-0.55504900	2.99489400	
0.00230600			
C	0.55504200	-2.99489300	
0.00246900			
C	2.58729600	-1.60729200	-
0.00399500			
H	-0.38334500	5.23044000	-
0.01387600			
H	0.38333600	-5.23044200	-
0.01339400			
H	4.73194800	-2.26122000	
0.01215000			
H	2.26122500	4.73195600	
0.01132600			
H	-2.26122800	-4.73195700	
0.01204200			

H	5.23042900	0.38336100	-
0.01247200			
C	4.08415600	2.78864600	
0.00015200			
C	4.44832700	3.52348500	-
1.13807900			
C	4.90017000	2.85988000	
1.13911500			
C	5.60032200	4.31150100	-
1.13750500			
H	3.82077800	3.47073400	-
2.02339200			
C	6.05312100	3.64649700	
1.14006900			
H	4.62199000	2.29394600	
2.02382500			
C	6.40614000	4.37487600	
0.00167700			
H	5.87006000	4.87245400	-
2.02842300			
H	6.67294800	3.69325000	
2.03157800			
H	7.30342700	4.98788800	
0.00227300			
C	-2.78867100	4.08415200	-
0.00038300			
C	-2.85946200	4.90074900	
1.13819300			
C	-3.52400400	4.44771800	-
1.13849200			
C	-3.64611700	6.05367300	
1.13888600			
H	-2.29315500	4.62303700	
2.02281000			
C	-4.31205200	5.59969100	-
1.13818100			
H	-3.47160600	3.81971600	-
2.02350300			
C	-4.37497800	6.40608900	
0.00061500			
H	-3.69252500	6.67395000	
2.03010000			
H	-4.87338200	5.86895600	-
2.02900400			

H	-4.98801900	7.30335600	
0.00100800			
C	-4.08416200	-2.78865300	
0.00069900			
C	-4.90016100	-2.85972400	
1.13968300			
C	-4.44833900	-3.52367400	-
1.13741400			
C	-6.05310300	-3.64635200	
1.14077300			
H	-4.62197400	-2.29365300	
2.02430400			
C	-5.60032800	-4.31170000	-
1.13670500			
H	-3.82080400	-3.47105500	-
2.02274200			
C	-6.40613100	-4.37490800	
0.00249700			
H	-6.67291700	-3.69297700	
2.03229800			
H	-5.87007200	-4.87279200	-
2.02753300			
H	-7.30341200	-4.98792900	
0.00319900			
C	2.78867100	-4.08414500	-
0.00043300			
C	3.52384200	-4.44777900	-
1.13862500			
C	2.85964500	-4.90065800	
1.13819100			
C	4.31190500	-5.59974200	-
1.13834900			
H	3.47130600	-3.81984100	-
2.02367200			
C	3.64631500	-6.05357100	
1.13884900			
H	2.29346900	-4.62288900	
2.02287400			
C	4.37501200	-6.40606000	
0.00049500			
H	4.87310900	-5.86906300	-
2.02923500			
H	3.69286600	-6.67378200	
2.03010100			

H	4.98806500	-7.30331800	
0.00086100			
⁵Fe (TPP)			
Fe	0.00003400	0.00001300	
0.00002100			
N	-2.08130600	0.00012900	-
0.04388100			
C	2.45802000	-2.44587700	-
0.00928100			
C	-2.45829900	-2.44552300	
0.00930400			
C	-0.68269700	-4.24595000	-
0.00479700			
C	0.68215000	-4.24604800	
0.00540400			
C	-1.11215500	-2.86864400	
0.00329700			
C	1.11182300	-2.86880100	-
0.00316300			
H	1.33840600	-5.10386500	
0.01654300			
H	-1.33910900	-5.10364800	-
0.01559100			
N	0.00016000	2.05077800	
0.00003700			
N	-0.00011300	-2.05077800	-
0.00009000			
N	2.08137300	-0.00013200	
0.04389000			
C	-2.45798900	2.44586000	
0.00933800			
C	2.45836000	2.44553900	-
0.00931400			
C	4.27750800	0.68015200	-
0.09471300			
C	-4.27747600	-0.68019200	
0.09415600			
C	0.68273500	4.24594400	
0.00529600			
C	4.27741500	-0.68071400	-
0.09474100			
C	-4.27739700	0.68067300	
0.09419300			

C	-0.68211600	4.24603700	-
0.00484800			
C	2.89418000	1.10640900	-
0.00424300			
C	-2.89411600	-1.10641400	
0.00406800			
C	1.11220400	2.86864600	-
0.00313900			
C	2.89402200	-1.10678900	-
0.00422300			
C	-2.89398100	1.10677100	
0.00408000			
C	-1.11178600	2.86879200	
0.00337600			
H	5.12933000	-1.34089100	-
0.16819100			
H	-5.12934100	1.34084000	
0.16740200			
H	-1.33836300	5.10386200	-
0.01574500			
H	5.12951300	1.34022200	-
0.16812900			
H	-5.12948200	-1.34030000	
0.16728500			
H	1.33912500	5.10365500	
0.01631700			
C	-3.51262300	-3.50664900	
0.03335500			
C	-4.37322600	-3.68291900	-
1.06115500			
C	-3.66706200	-4.34105200	
1.15133800			
C	-5.36127000	-4.66825700	-
1.03956200			
H	-4.25909200	-3.04077600	-
1.92998900			
C	-4.65422200	-5.32717000	
1.17368300			
H	-3.00740900	-4.20736700	
2.00410500			
C	-5.50444000	-5.49383300	
0.07798200			
H	-6.01638700	-4.79330900	-
1.89769600			

H	-4.76216500	-5.96169000	
2.04942800			
H	-6.27356800	-6.26132400	
0.09521700			
C	-3.51217700	3.50710500	
0.03339400			
C	-4.37293900	3.68333400	-
1.06101500			
C	-3.66640000	4.34167200	
1.15128800			
C	-5.36094400	4.66870200	-
1.03937500			
H	-4.25894600	3.04111800	-
1.92981400			
C	-4.65352500	5.32782200	
1.17368200			
H	-3.00661800	4.20806300	
2.00396700			
C	-5.50392600	5.49439200	
0.07811300			
H	-6.01617400	4.79369500	-
1.89743200			
H	-4.76130200	5.96243400	
2.04938100			
H	-6.27304300	6.26189200	
0.09540400			
C	3.51217900	-3.50715000	-
0.03332000			
C	4.37324700	-3.68308800	
1.06089600			
C	3.66601800	-4.34207500	-
1.15100100			
C	5.36120200	-4.66850600	
1.03926000			
H	4.25953800	-3.04059800	
1.92952700			
C	4.65309700	-5.32827100	-
1.17339000			
H	3.00597300	-4.20870800	-
2.00351200			
C	5.50381800	-5.49453700	-
0.07802200			
H	6.01667900	-4.79327700	
1.89716100			

H	4.76059200	-5.96315800	-
2.04892300			
H	6.27289500	-6.26207800	-
0.09530300			
C	3.51264200	3.50668700	-
0.03341100			
C	3.66654400	4.34157000	-
1.15111800			
C	4.37371600	3.68259300	
1.06079800			
C	4.65365300	5.32773400	-
1.17351100			
H	3.00651100	4.20820300	-
2.00364000			
C	5.36170500	4.66798000	
1.03915900			
H	4.25998000	3.04011400	
1.92943600			
C	5.50435600	5.49399800	-
0.07812600			
H	4.76117800	5.96260300	-
2.04905400			
H	6.01718400	4.79272700	
1.89706100			
H	6.27344200	6.26152900	-
0.09539700			
CSS			
TS6			
Fe	-0.33030200	0.06281800	-
0.45822200			
N	-1.89443300	1.32931500	-
0.36128200			
C	0.01409300	-3.36721000	-
0.69498200			
C	-3.75095800	-0.29330600	-
0.12939900			
C	-3.46460500	-2.79313800	
0.04944500			
C	-2.41207700	-3.65458400	-
0.13037100			
C	-2.95560800	-1.47231300	-
0.16774700			
C	-1.27435400	-2.85616400	-
0.44627300			

H	-2.41570400	-4.73059200	-
0.03827100			
H	-4.48227700	-3.03758000	
0.31347600			
N	0.94091900	1.63298700	-
0.63509200			
N	-1.61215200	-1.50778000	-
0.44167300			
N	1.21915000	-1.20303300	-
0.76930800			
C	-0.70016500	3.49610900	-
0.46386900			
C	3.09532100	0.41241000	-
0.83098300			
C	3.32292400	-2.06591800	-
1.19903300			
C	-4.04269900	2.19109100	-
0.39722200			
C	2.86212600	2.90151600	-
0.50530400			
C	2.45987300	-3.12022200	-
1.17495400			
C	-3.19279700	3.24857700	-
0.50228200			
C	1.79656000	3.76422200	-
0.38994200			
C	2.54554700	-0.88223300	-
0.92357400			
C	-3.22590400	1.00526600	-
0.28605300			
C	2.31389100	1.59288200	-
0.67600400			
C	1.15808200	-2.59045800	-
0.88283400			
C	-1.85616000	2.72018400	-
0.45287300			
C	0.61515100	2.97760400	-
0.49109300			
H	2.68266900	-4.16283400	-
1.34736900			
H	-3.44605800	4.29217400	-
0.61661300			
H	1.82748000	4.83437200	-
0.24715800			

H	4.38326400	-2.08039300	-
1.40161400			
H	-5.12208400	2.20327900	-
0.41158800			
H	3.91367100	3.14220000	-
0.46786800			
N	0.08905600	-0.37432500	
1.95189800			
N	-0.04432100	-1.65326500	
2.18757600			
N	0.64038300	-2.46849100	
2.67718600			
C	1.36424100	-0.04256200	
2.45284400			
C	1.86187500	1.27245600	
2.38868100			
C	3.31482200	-0.82786900	
3.45736400			
C	3.14051200	1.49409400	
2.86878400			
H	1.26048400	2.05613400	
1.94607600			
C	3.88930800	0.43335600	
3.41345800			
H	3.82631400	-1.69298000	
3.86877700			
H	3.56797800	2.48979900	
2.80722100			
H	4.89485900	0.58820100	
3.78924700			
N	2.07756100	-1.03037000	
2.98108100			
C	-0.85118700	4.97912000	-
0.44082300			
C	-1.47146400	5.61816700	
0.64449800			
C	-0.37136200	5.76220400	-
1.50316100			
C	-1.60739900	7.00658700	
0.66768700			
H	-1.84138400	5.01645600	
1.46943000			
C	-0.51820400	7.14897600	-
1.48447400			

H	0.11101900	5.27218200	-
2.34353000			
C	-1.13397300	7.77551100	-
0.39783000			
H	-2.08261500	7.48698100	
1.51877400			
H	-0.15247500	7.74032300	-
2.31961000			
H	-1.24384700	8.85650600	-
0.38186500			
C	-5.21736400	-0.44016600	
0.06773700			
C	-5.85557100	0.15545200	
1.16942400			
C	-5.99870500	-1.17282500	-
0.84277400			
C	-7.23123600	0.02118800	
1.35620700			
H	-5.25953300	0.72055900	
1.88018000			
C	-7.37506400	-1.30135900	-
0.65954500			
H	-5.51537300	-1.63560700	-
1.69813900			
C	-7.99640000	-0.70640300	
0.44157700			
H	-7.70493500	0.48223700	
2.21894300			
H	-7.96359700	-1.86379500	-
1.37964500			
H	-9.06858300	-0.80937800	
0.58563300			
C	0.17140700	-4.84973800	-
0.71308200			
C	0.93440400	-5.48940900	
0.27635900			
C	-0.44745000	-5.62553700	-
1.70482000			
C	1.07592600	-6.87734100	
0.27126900			
H	1.39963300	-4.88861500	
1.05227100			
C	-0.29481400	-7.01227200	-
1.71490900			

H	-1.04310600	-5.13193500	-
2.46704600			
C	0.46570900	-7.64167400	-
0.72624500			
H	1.66106000	-7.36166900	
1.04849500			
H	-0.77023600	-7.60089200	-
2.49494600			
H	0.58003100	-8.72236500	-
0.73201100			
C	4.57462600	0.55348600	-
0.87292800			
C	5.37593900	-0.06563700	
0.10227700			
C	5.20585900	1.30943000	-
1.87554300			
C	6.76379200	0.06968000	
0.07771300			
H	4.89585300	-0.64637200	
0.88358400			
C	6.59418500	1.44057900	-
1.90301900			
H	4.59617600	1.78940400	-
2.63541800			
C	7.37865300	0.82298000	-
0.92542900			
H	7.36573200	-0.41197400	
0.84422000			
H	7.06429000	2.02199900	-
2.69182700			
H	8.46018300	0.92693300	-
0.94644800			
oss-TS6			
Fe	-0.33030200	0.06281800	-
0.45822200			
N	-1.89443300	1.32931500	-
0.36128200			
C	0.01409300	-3.36721000	-
0.69498200			
C	-3.75095800	-0.29330600	-
0.12939900			
C	-3.46460500	-2.79313800	
0.04944500			

C	-2.41207700	-3.65458400	-
0.13037100			
C	-2.95560800	-1.47231300	-
0.16774700			
C	-1.27435400	-2.85616400	-
0.44627300			
H	-2.41570400	-4.73059200	-
0.03827100			
H	-4.48227700	-3.03758000	
0.31347600			
N	0.94091900	1.63298700	-
0.63509200			
N	-1.61215200	-1.50778000	-
0.44167300			
N	1.21915000	-1.20303300	-
0.76930800			
C	-0.70016500	3.49610900	-
0.46386900			
C	3.09532100	0.41241000	-
0.83098300			
C	3.32292400	-2.06591800	-
1.19903300			
C	-4.04269900	2.19109100	-
0.39722200			
C	2.86212600	2.90151600	-
0.50530400			
C	2.45987300	-3.12022200	-
1.17495400			
C	-3.19279700	3.24857700	-
0.50228200			
C	1.79656000	3.76422200	-
0.38994200			
C	2.54554700	-0.88223300	-
0.92357400			
C	-3.22590400	1.00526600	-
0.28605300			
C	2.31389100	1.59288200	-
0.67600400			
C	1.15808200	-2.59045800	-
0.88283400			
C	-1.85616000	2.72018400	-
0.45287300			
C	0.61515100	2.97760400	-
0.49109300			

H	2.68266900	-4.16283400	-
1.34736900			
H	-3.44605800	4.29217400	-
0.61661300			
H	1.82748000	4.83437200	-
0.24715800			
H	4.38326400	-2.08039300	-
1.40161400			
H	-5.12208400	2.20327900	-
0.41158800			
H	3.91367100	3.14220000	-
0.46786800			
N	0.08905600	-0.37432500	
1.95189800			
N	-0.04432100	-1.65326500	
2.18757600			
N	0.64038300	-2.46849100	
2.67718600			
C	1.36424100	-0.04256200	
2.45284400			
C	1.86187500	1.27245600	
2.38868100			
C	3.31482200	-0.82786900	
3.45736400			
C	3.14051200	1.49409400	
2.86878400			
H	1.26048400	2.05613400	
1.94607600			
C	3.88930800	0.43335600	
3.41345800			
H	3.82631400	-1.69298000	
3.86877700			
H	3.56797800	2.48979900	
2.80722100			
H	4.89485900	0.58820100	
3.78924700			
N	2.07756100	-1.03037000	
2.98108100			
C	-0.85118700	4.97912000	-
0.44082300			
C	-1.47146400	5.61816700	
0.64449800			
C	-0.37136200	5.76220400	-
1.50316100			

C	-1.60739900	7.00658700	
0.66768700			
H	-1.84138400	5.01645600	
1.46943000			
C	-0.51820400	7.14897600	-
1.48447400			
H	0.11101900	5.27218200	-
2.34353000			
C	-1.13397300	7.77551100	-
0.39783000			
H	-2.08261500	7.48698100	
1.51877400			
H	-0.15247500	7.74032300	-
2.31961000			
H	-1.24384700	8.85650600	-
0.38186500			
C	-5.21736400	-0.44016600	
0.06773700			
C	-5.85557100	0.15545200	
1.16942400			
C	-5.99870500	-1.17282500	-
0.84277400			
C	-7.23123600	0.02118800	
1.35620700			
H	-5.25953300	0.72055900	
1.88018000			
C	-7.37506400	-1.30135900	-
0.65954500			
H	-5.51537300	-1.63560700	-
1.69813900			
C	-7.99640000	-0.70640300	
0.44157700			
H	-7.70493500	0.48223700	
2.21894300			
H	-7.96359700	-1.86379500	-
1.37964500			
H	-9.06858300	-0.80937800	
0.58563300			
C	0.17140700	-4.84973800	-
0.71308200			
C	0.93440400	-5.48940900	
0.27635900			
C	-0.44745000	-5.62553700	-
1.70482000			

C	1.07592600	-6.87734100	
0.27126900			
H	1.39963300	-4.88861500	
1.05227100			
C	-0.29481400	-7.01227200	-
1.71490900			
H	-1.04310600	-5.13193500	-
2.46704600			
C	0.46570900	-7.64167400	-
0.72624500			
H	1.66106000	-7.36166900	
1.04849500			
H	-0.77023600	-7.60089200	-
2.49494600			
H	0.58003100	-8.72236500	-
0.73201100			
C	4.57462600	0.55348600	-
0.87292800			
C	5.37593900	-0.06563700	
0.10227700			
C	5.20585900	1.30943000	-
1.87554300			
C	6.76379200	0.06968000	
0.07771300			
H	4.89585300	-0.64637200	
0.88358400			
C	6.59418500	1.44057900	-
1.90301900			
H	4.59617600	1.78940400	-
2.63541800			
C	7.37865300	0.82298000	-
0.92542900			
H	7.36573200	-0.41197400	
0.84422000			
H	7.06429000	2.02199900	-
2.69182700			
H	8.46018300	0.92693300	-
0.94644800			
³TS6			
Fe	-0.33226400	0.08293100	-
0.46410700			
N	-1.88496500	1.34744600	-
0.33746300			

C	0.01366000	-3.34075800	-
0.51873000			
C	-3.76448100	-0.26387700	-
0.32415500			
C	-3.51795900	-2.75644500	-
0.19430800			
C	-2.46282800	-3.61241800	-
0.22880500			
C	-2.98200000	-1.42397800	-
0.34064300			
C	-1.27585800	-2.81114800	-
0.41140100			
H	-2.47528900	-4.68807200	-
0.13235300			
H	-4.56330400	-2.99350000	-
0.06275300			
N	0.93388200	1.63878600	-
0.62976100			
N	-1.60844000	-1.47363400	-
0.45807000			
N	1.21789300	-1.18269600	-
0.70198100			
C	-0.66161500	3.49951400	-
0.26380100			
C	3.07394800	0.43213200	-
0.97017000			
C	3.32155200	-2.06261900	-
1.10477900			
C	-4.02500100	2.23168500	-
0.32990600			
C	2.86779000	2.90886000	-
0.65310500			
C	2.47130800	-3.11181700	-
0.94753900			
C	-3.15936600	3.27821900	-
0.28302400			
C	1.83209800	3.75927200	-
0.41302300			
C	2.54145200	-0.86081300	-
0.93137600			
C	-3.22771500	1.02829000	-
0.33895900			
C	2.30529100	1.58892800	-
0.79057900			

C	1.16175800	-2.55997100	-
0.69690900			
C	-1.82600600	2.72301100	-
0.28199200			
C	0.62514900	2.96901500	-
0.42516100			
H	2.69496600	-4.16631300	-
1.01634700			
H	-3.39151300	4.33303500	-
0.27358800			
H	1.87511300	4.82503300	-
0.24318500			
H	4.37762100	-2.09104600	-
1.32833400			
H	-5.10396200	2.26189200	-
0.36253500			
H	3.91997200	3.14486500	-
0.71255900			
N	0.04836300	-0.28600300	
2.07117800			
N	-0.22344300	-1.53309900	
2.34722500			
N	0.39171300	-2.42275000	
2.80138900			
C	1.38961400	-0.11264600	
2.46322500			
C	2.03476300	1.13308600	
2.34231100			
C	3.30472900	-1.12151000	
3.32523700			
C	3.36258400	1.20348600	
2.72274300			
H	1.49581400	1.98101600	
1.94017400			
C	4.01954100	0.06214700	
3.22344400			
H	3.74085300	-2.03982700	
3.70695300			
H	3.89977300	2.14124800	
2.62028900			
H	5.06073700	0.09860400	
3.52558500			
N	2.01832700	-1.17612400	
2.95024800			

C	-0.80546900	4.97651300	-
0.09096700			
C	-1.31189700	5.50567500	
1.10662400			
C	-0.44662500	5.86309000	-
1.11850900			
C	-1.45219800	6.88391900	
1.27428200			
H	-1.59448500	4.82478300	
1.90466800			
C	-0.58653900	7.24148800	-
0.95189700			
H	-0.06097100	5.46035000	-
2.05079300			
C	-1.08913200	7.75627400	
0.24551500			
H	-1.84250700	7.27609800	
2.20976800			
H	-0.30842200	7.91286100	-
1.76008600			
H	-1.19874300	8.82964700	
0.37523500			
C	-5.24964800	-0.41706200	-
0.26138900			
C	-5.96814800	0.00257500	
0.86896600			
C	-5.95377400	-0.99090600	-
1.33129400			
C	-7.35452100	-0.14536200	
0.92716800			
H	-5.42831200	0.44307600	
1.70240900			
C	-7.34021000	-1.13924900	-
1.27404500			
H	-5.40353500	-1.31818000	-
2.20902300			
C	-8.04486800	-0.71655000	-
0.14450000			
H	-7.89457700	0.18108700	
1.81206300			
H	-7.86999900	-1.58163300	-
2.11360900			
H	-9.12450800	-0.83205800	-
0.09938300			

C	0.18382800	-4.82296900	-
0.43221400			
C	0.82506900	-5.39227200	
0.67888300			
C	-0.28615300	-5.66735000	-
1.44900400			
C	0.99144000	-6.77491000	
0.76963000			
H	1.17908700	-4.73998700	
1.47182700			
C	-0.11887800	-7.05010500	-
1.35831200			
H	-0.78082100	-5.22983300	-
2.31174100			
C	0.52094600	-7.60755600	-
0.24870900			
H	1.48464200	-7.20230300	
1.63885300			
H	-0.48453500	-7.69106800	-
2.15629900			
H	0.65120500	-8.68419800	-
0.17786100			
C	4.54653900	0.59242600	-
1.16230500			
C	5.45226500	0.10741700	-
0.20518900			
C	5.05421600	1.24378000	-
2.29728900			
C	6.82735100	0.26857400	-
0.37891900			
H	5.06529500	-0.39274000	
0.67711200			
C	6.42933000	1.40616000	-
2.47126800			
H	4.35965800	1.62051300	-
3.04279000			
C	7.32073400	0.91910900	-
1.51237600			
H	7.51393200	-0.11101700	
0.37365300			
H	6.80436600	1.90900200	-
3.35879000			
H	8.39160400	1.04485000	-
1.64800100			

⁵TS6

Fe	-0.31446500	0.08329600	-
0.34425000			
N	-1.78384400	1.52405200	-
0.30499500			
C	-0.31564800	-3.37686800	-
0.64207100			
C	-3.77957200	0.04345700	-
0.18450000			
C	-3.79166000	-2.49916400	-
0.14484300			
C	-2.82758000	-3.45093100	-
0.27463500			
C	-3.13480900	-1.20840600	-
0.26192900			
C	-1.56883400	-2.75538500	-
0.47371300			
H	-2.94884000	-4.52364500	-
0.23231500			
H	-4.84753300	-2.65008600	
0.02674300			
N	1.13097500	1.56452300	-
0.68863200			
N	-1.79004900	-1.40219800	-
0.44289700			
N	1.12986800	-1.35453400	-
0.75725100			
C	-0.33966900	3.54482500	-
0.42981300			
C	3.12599000	0.11639000	-
0.90587300			
C	3.14336800	-2.41018500	-
1.09739700			
C	-3.82641700	2.57471900	-
0.28372700			
C	3.16057300	2.64774700	-
0.71209500			
C	2.18581900	-3.37891600	-
1.02640000			
C	-2.87172700	3.54726200	-
0.34882800			
C	2.19649800	3.60104700	-
0.56936600			

C	2.47891400	-1.13823100	-
0.91511300			
C	-3.14046300	1.30261000	-
0.24633500			
C	2.48533300	1.36797200	-
0.79743100			
C	0.92160800	-2.71447000	-
0.79892500			
C	-1.58672800	2.88497900	-
0.35554600			
C	0.91703400	2.91708400	-
0.56857000			
H	2.31905600	-4.44587100	-
1.13114100			
H	-3.02463600	4.61485300	-
0.41127200			
H	2.33573100	4.66771400	-
0.46878700			
H	4.20100600	-2.54224900	-
1.27417600			
H	-4.89867800	2.70609200	-
0.28158700			
H	4.23035100	2.79478900	-
0.74878300			
N	0.07552400	-0.36600000	
1.92131400			
N	-0.19982500	-1.60786000	
2.22440900			
N	0.36817400	-2.46269600	
2.78253600			
C	1.36497700	-0.12950700	
2.45174100			
C	1.98527900	1.12772600	
2.33501700			
C	3.20057700	-1.03944300	
3.55389800			
C	3.26923700	1.25180000	
2.83683600			
H	1.46954900	1.94004500	
1.84046300			
C	3.89860700	0.15508400	
3.45505000			
H	3.61448600	-1.92391900	
4.02865800			

H	3.79123100	2.19841100	
2.73892900			
H	4.90537800	0.23279300	
3.85099700			
N	1.95983200	-1.14863900	
3.05655100			
C	-0.35532700	5.03837900	-
0.36923500			
C	-0.81605500	5.70354900	
0.77837400			
C	0.08899600	5.80785700	-
1.45650300			
C	-0.83052800	7.09754400	
0.83864000			
H	-1.16265000	5.11555100	
1.62363500			
C	0.07527800	7.20191500	-
1.39742700			
H	0.44133300	5.30114200	-
2.35042500			
C	-0.38416800	7.85151300	-
0.24926200			
H	-1.18723600	7.59446700	
1.73708100			
H	0.41804500	7.78060400	-
2.25120200			
H	-0.39564300	8.93720800	-
0.20325400			
C	-5.26721500	0.04151100	-
0.03798300			
C	-5.87397600	0.57050300	
1.11241000			
C	-6.08851700	-0.48788500	-
1.04618100			
C	-7.26234200	0.56916900	
1.25182600			
H	-5.24505400	0.97995100	
1.89785400			
C	-7.47703600	-0.48979000	-
0.90779100			
H	-5.62691200	-0.89479700	-
1.94138500			
C	-8.06857800	0.03867000	
0.24199100			

H	-7.71387000	0.97847800	
2.15179500			
H	-8.09685600	-0.89959900	-
1.70100500			
H	-9.14993300	0.03741200	
0.35007800			
C	-0.28602100	-4.87228300	-
0.62079400			
C	0.32013300	-5.55057000	
0.44831300			
C	-0.86445600	-5.62264700	-
1.65531700			
C	0.34826100	-6.94539000	
0.48030800			
H	0.76018800	-4.97212500	
1.25593400			
C	-0.83635800	-7.01783600	-
1.62368400			
H	-1.33395600	-5.10212200	-
2.48536700			
C	-0.22926800	-7.68314400	-
0.55598500			
H	0.81702400	-7.45595700	
1.31759000			
H	-1.28512900	-7.58465200	-
2.43526900			
H	-0.20724000	-8.76943100	-
0.53126800			
C	4.61845600	0.11701100	-
0.98454600			
C	5.38363400	-0.44450500	
0.05059000			
C	5.28673700	0.68479100	-
2.08041500			
C	6.77765900	-0.43777900	-
0.00821400			
H	4.87265100	-0.88053200	
0.90376500			
C	6.68115900	0.69305400	-
2.13956800			
H	4.70166700	1.11727200	-
2.88708200			
C	7.43143600	0.13191900	-
1.10347100			

H	7.35385700	-0.87480600	
0.80351800			
H	7.18129400	1.13293600	-
2.99843000			
H	8.51716200	0.13733000	-
1.15009700			
CSSINT6			
Fe	-0.20464400	0.11867100	-
0.42921100			
N	1.70586000	-0.40415500	-
0.75747600			
C	-3.21705400	-1.54299500	-
0.70194900			
C	1.46939600	-2.84980600	-
0.51974800			
C	-0.69111100	-4.10133600	-
0.78412600			
C	-1.99369200	-3.73427500	-
0.91819400			
C	0.07376000	-2.88584000	-
0.62924000			
C	-2.03893600	-2.29460500	-
0.79333300			
H	-2.85186000	-4.37132400	-
1.07370400			
H	-0.27059100	-5.09609000	-
0.81719700			
N	0.33658700	2.04750900	-
0.44685100			
N	-0.76160600	-1.79184400	-
0.66256400			
N	-2.13502100	0.65819800	-
0.35380500			
C	2.74498900	1.83045100	-
0.97365200			
C	-1.85660800	3.07685100	
0.06974200			
C	-4.05519300	1.85181500	
0.14447500			
C	3.66601000	-1.63387500	-
0.68044600			
C	0.25245500	4.36019200	-
0.38514200			

C	-4.43809800	0.57762400	-
0.13515500			
C	4.01533500	-0.33591000	-
0.88761900			
C	1.51993700	4.01767600	-
0.73769500			
C	-2.62084200	1.90732600	-
0.02452300			
C	2.22337100	-1.67696100	-
0.63287500			
C	-0.48403500	3.12905900	-
0.21133700			
C	-3.23757000	-0.16557200	-
0.44118300			
C	2.79029200	0.43023300	-
0.91856700			
C	1.57869000	2.57349400	-
0.74752600			
H	-5.43516600	0.16270000	-
0.11451900			
H	5.00873200	0.07758700	-
0.98233300			
H	2.34253700	4.67471300	-
0.97897700			
H	-4.68055500	2.68379800	
0.43264800			
H	4.31712300	-2.48991100	-
0.58129900			
H	-0.16536400	5.35143200	-
0.28633000			
C	2.17804100	-4.14228400	-
0.27908000			
C	2.02647100	-4.78459600	
0.95998200			
C	2.98801800	-4.73771500	-
1.25667700			
C	2.67562000	-5.99288200	
1.21621900			
H	1.40127900	-4.31899500	
1.71703800			
C	3.63688200	-5.94696400	-
1.00018700			
H	3.10102800	-4.24767800	-
2.21971900			

C	3.48288600	-6.57722900	
0.23688400			
H	2.55189100	-6.47790200	
2.18113500			
H	4.25793000	-6.39929900	-
1.76896600			
H	3.98735800	-7.51912000	
0.43558200			
C	-2.54263500	4.35897700	
0.41320800			
C	-3.50367600	4.92134500	-
0.44155600			
C	-2.21856400	5.03774100	
1.59825800			
C	-4.12941500	6.12546300	-
0.11629000			
H	-3.75166100	4.40762400	-
1.36596700			
C	-2.84393400	6.24171200	
1.92486100			
H	-1.47169100	4.61081600	
2.26184100			
C	-3.80236200	6.78889100	
1.06871600			
H	-4.86813600	6.54836600	-
0.79208800			
H	-2.58422900	6.75078100	
2.84936800			
H	-4.28950200	7.72670900	
1.32201800			
C	4.02786300	2.55933600	-
1.20439200			
C	4.58171500	3.37885400	-
0.20778700			
C	4.71978900	2.41849800	-
2.41739900			
C	5.79052800	4.04299100	-
0.41893800			
H	4.05380000	3.49156800	
0.73537400			
C	5.92899200	3.08186300	-
2.63005000			
H	4.29900300	1.78392800	-
3.19219900			

C	6.46820600	3.89648800	-
1.63163900			
H	6.20507100	4.67117400	
0.36524600			
H	6.44817600	2.96481500	-
3.57763600			
H	7.40972100	4.41322700	-
1.79719000			
C	-4.52816100	-2.25195700	-
0.80828300			
C	-5.38672500	-2.00021300	-
1.88900800			
C	-4.93309400	-3.16631400	
0.17646800			
C	-6.61695900	-2.65196400	-
1.98735200			
H	-5.08003800	-1.28983600	-
2.65171300			
C	-6.16313600	-3.81803100	
0.07883900			
H	-4.27625300	-3.35568700	
1.02064600			
C	-7.00824200	-3.56352800	-
1.00401700			
H	-7.26823900	-2.44933200	-
2.83353900			
H	-6.46363400	-4.52033400	
0.85199100			
H	-7.96628700	-4.07088700	-
1.08000200			
C	2.15674900	0.49008500	
2.18348900			
C	1.13142500	-0.44988000	
2.30334700			
C	2.38009200	-1.84122800	
3.60216300			
C	3.48849400	-1.00066400	
3.52111300			
C	3.36690100	0.18956200	
2.79690000			
H	1.99870700	1.39092900	
1.60610900			
H	2.42558500	-2.77224500	
4.16255800			

H	4.41883200	-1.27194100
4.00923200		
H	4.20437800	0.87499700
2.70615000		
N	-0.08815200	-0.18620200
1.59735800		
N	1.21153200	-1.58154100
2.99745500		
N	-2.04245500	-1.32657800
2.35613300		
N	-1.08451400	-0.82388000
2.03228400		

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Fe	-0.24541700	0.14585900	-
0.48676600			
N	1.70988100	-0.21261300	-
0.78211900			
C	-3.10478300	-1.78145200	-
0.68253200			
C	1.68367600	-2.67617100	-
0.58071600			
C	-0.36543800	-4.10572200	-
0.81488300			
C	-1.69800500	-3.85379400	-
0.92198600			
C	0.29375900	-2.83031600	-
0.66338800			
C	-1.86663200	-2.42622700	-
0.78699600			
H	-2.49979200	-4.56310100	-
1.06433000			
H	0.13874100	-5.06011900	-
0.86120700			
N	0.13471400	2.11196900	-
0.43940300			
N	-0.63522100	-1.81437800	-
0.66999700			
N	-2.21325500	0.50765800	-
0.35289700			
C	2.56087300	2.10715800	-
0.93257600			
C	-2.14479200	2.94482800	-
0.06325600			

C	-4.22308000	1.53031100	
0.16072700			
C	3.76453900	-1.27305900	-
0.72739000			
C	-0.14331800	4.40546600	-
0.33693400			
C	-4.49619100	0.22441000	-
0.10314900			
C	4.00436500	0.05475700	-
0.90125600			
C	1.15690600	4.17644900	-
0.66439400			
C	-2.80211300	1.71090700	-
0.02621900			
C	2.33201000	-1.44017900	-
0.68281500			
C	-0.77893300	3.11611700	-
0.20136000			
C	-3.24038200	-0.41198800	-
0.42043800			
C	2.72124600	0.71513500	-
0.91628800			
C	1.33474100	2.74457500	-
0.70413900			
H	-5.45199900	-0.27701500	-
0.06358500			
H	4.95978900	0.55266400	-
0.97735000			
H	1.92811800	4.90420700	-
0.86957900			
H	-4.91486600	2.30602900	
0.45407600			
H	4.48589200	-2.07176800	-
0.63842900			
H	-0.64252700	5.35688500	-
0.22568800			
C	2.50419400	-3.90562000	-
0.36862100			
C	2.40662900	-4.59062300	
0.85342200			
C	3.36806300	-4.40073500	-
1.35616600			
C	3.16212900	-5.74107700	
1.08277400			

H	1.74067600	-4.20142000	
1.61833600			
C	4.12341300	-5.55204500	-
1.12597900			
H	3.43872600	-3.87926500	-
2.30666100			
C	4.02316300	-6.22458400	
0.09422900			
H	3.07909400	-6.25969200	
2.03450000			
H	4.78520900	-5.92683700	-
1.90242300			
H	4.61054400	-7.12144500	
0.27242300			
C	-2.94493900	4.16044000	
0.40162100			
C	-3.94496300	4.63446400	-
0.46192300			
C	-2.69624000	4.86261100	
1.59131400			
C	-4.68067700	5.77613100	-
0.14160700			
H	-4.13674800	4.10158200	-
1.38889600			
C	-3.43148700	6.00428900	
1.91270300			
H	-1.92174600	4.50268300	
2.26284400			
C	-4.42675400	6.46418000	
1.04727400			
H	-5.44834900	6.13133500	-
0.82405600			
H	-3.22883800	6.53245300	
2.84073300			
H	-4.99951500	7.35337100	
1.29672900			
C	3.78204200	2.94654700	-
1.11983900			
C	4.25889200	3.76355800	-
0.08224800			
C	4.49254700	2.91499600	-
2.32963300			
C	5.41196500	4.53119900	-
0.25028300			

H	3.71517400	3.79194600	
0.85825700			
C	5.64614500	3.68192800	-
2.49901500			
H	4.13082400	2.28342700	-
3.13609500			
C	6.10942900	4.49252000	-
1.46001800			
H	5.76775900	5.15583300	
0.56493500			
H	6.18110300	3.64867200	-
3.44445700			
H	7.00761100	5.08976800	-
1.59196600			
C	-4.34912300	-2.60468500	-
0.76234000			
C	-5.24645900	-2.43863600	-
1.82786800			
C	-4.65167700	-3.54352600	
0.23627600			
C	-6.41530900	-3.19818100	-
1.89822700			
H	-5.01865300	-1.70995700	-
2.60092000			
C	-5.82045800	-4.30268000	
0.16630900			
H	-3.96489900	-3.66563400	
1.06897600			
C	-6.70498700	-4.13303500	-
0.90165900			
H	-7.09788500	-3.06125500	-
2.73284300			
H	-6.04280800	-5.02266500	
0.94954100			
H	-7.61521000	-4.72430400	-
0.95587200			
C	2.16087000	0.53820100	
2.22111000			
C	1.25240000	-0.51280500	
2.38775800			
C	2.81852900	-1.87913100	
3.32136900			
C	3.81567100	-0.91606400	
3.18403100			

C	3.47248900	0.31725200
2.61969900		
H	1.83703300	1.46092100
1.75579800		
H	3.04153100	-2.85304300
3.75140100		
H	4.83120500	-1.12922100
3.50114800		
H	4.21934600	1.09306800
2.47896600		
N	-0.06540000	-0.29624200
1.89594500		
N	1.54984000	-1.69387700
2.92800900		
N	-1.77502500	-1.86627800
2.40900500		
N	-0.91087300	-1.16295500
2.20941000		

³INT6

Fe	-0.27160100	0.16073200	-
0.52536800			
N	-2.24753700	0.44524700	-
0.36276500			
C	1.76861700	-2.59151300	-
0.61835800			
C	-3.05170500	-1.88099300	-
0.65854900			
C	-1.56950300	-3.89385400	-
0.91167400			
C	-0.22712200	-4.09417200	-
0.82524500			
C	-1.79065900	-2.47467800	-
0.77478600			
C	0.38511500	-2.79534800	-
0.68223600			
H	0.31262600	-5.02840600	-
0.87831800			
H	-2.34596300	-4.63320300	-
1.03993900			
N	0.03570100	2.13574800	-
0.43669400			
N	-0.58174500	-1.81438100	-
0.67471500			

N	1.69733500	-0.12509600	-
0.78999400			
C	-2.27729500	2.88594900	
0.04335500			
C	2.46688700	2.22604800	-
0.89912000			
C	3.98083600	0.22931000	-
0.90707300			
C	-4.51490500	0.07139200	-
0.08625000			
C	0.98881600	4.23731100	-
0.62359400			
C	3.79023800	-1.10920800	-
0.75842900			
C	-4.29297700	1.39037100	
0.15902300			
C	-0.32473000	4.41723900	-
0.31952200			
C	2.67552400	0.84176700	-
0.90699700			
C	-3.23792400	-0.51647800	-
0.40831200			
C	1.21708400	2.81431900	-
0.67564700			
C	2.36609600	-1.33039600	-
0.71142700			
C	-2.88283600	1.62636100	-
0.04116800			
C	-0.91679400	3.10633500	-
0.20557300			
H	4.54025800	-1.88233000	-
0.68284300			
H	-5.01240000	2.14100000	
0.45106100			
H	-0.85903000	5.34926600	-
0.20773500			
H	4.91690800	0.76383700	-
0.97282200			
H	-5.44857900	-0.46861900	-
0.03109900			
H	1.73849000	4.99313200	-
0.80560100			
N	-0.04837000	-0.44501300	
2.08504100			

N	-0.76341200	-1.44301500	
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N	-1.52908200	-2.26942100	
2.42611300			
C	1.31979200	-0.56597500	
2.43630000			
C	2.11054600	0.57629000	
2.25705600			
C	3.08740800	-1.81907700	
3.14660600			
C	3.46563800	0.46738500	
2.53736200			
H	1.66466200	1.48285300	
1.86546300			
C	3.97190700	-0.75380700	
2.99622800			
H	3.43980700	-2.79039700	
3.48666400			
H	4.12165800	1.31876200	
2.38091200			
H	5.02644700	-0.88067700	
3.21792200			
N	1.77712300	-1.74039300	
2.87211500			
C	-3.12811100	4.06969800	
0.37038900			
C	-2.92116500	4.78405500	
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C	-4.13795900	4.49942200	-
0.50475600			
C	-3.70591900	5.89549400	
1.87086400			
H	-2.14037000	4.45733800	
2.24190900			
C	-4.92312300	5.61084600	-
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H	-4.29855600	3.95601500	-
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C	-4.70987300	6.31197900	
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H	-3.53519800	6.43369400	
2.79952700			
H	-5.69780700	5.93218600	-
0.88690500			

H	-5.32117800	7.17757400	
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C	3.65915200	3.11266900	-
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C	4.37729500	3.14486000	-
2.25860000			
C	4.09976700	3.91217200	
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C	5.50448400	3.95655800	-
2.39456400			
H	4.04309200	2.52738300	-
3.08755200			
C	5.22648000	4.72431300	-
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H	3.54826100	3.89200400	
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C	5.93257700	4.74861300	-
1.32657400			
H	6.04632500	3.97255400	-
3.33651400			
H	5.55480500	5.33464900	
0.71577500			
H	6.81023700	5.38050700	-
1.43259900			
C	2.63864400	-3.79082800	-
0.43245000			
C	3.50949200	-4.23607800	-
1.43749600			
C	2.58254000	-4.49753700	
0.77997700			
C	4.31277800	-5.35962400	-
1.23402700			
H	3.54803300	-3.69795300	-
2.38055300			
C	3.38606300	-5.62029700	
0.98216500			
H	1.91292300	-4.14556700	
1.55938800			
C	4.25389100	-6.05400400	-
0.02341800			
H	4.97957600	-5.69579200	-
2.02375200			
H	3.33493900	-6.15611600	
1.92657000			

H	4.87862200	-6.92923500	
0.13411400			
C	-4.26172300	-2.75603800	-
0.71114300			
C	-5.18026700	-2.64162700	-
1.76517200			
C	-4.50884700	-3.69389400	
0.30359600			
C	-6.31673100	-3.45077900	-
1.80846300			
H	-4.99471600	-1.91417900	-
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C	-5.64543300	-4.50233000	
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H	-3.80463800	-3.77645700	
1.12662700			
C	-6.55185900	-4.38387800	-
0.79600600			
H	-7.01654400	-3.35383000	-
2.63434900			
H	-5.82552200	-5.22110500	
1.05559500			
H	-7.43687300	-5.01371400	-
0.82918900			
⁵INT6			
Fe	-0.28731700	0.13056400	-
0.40281500			
N	-0.17063100	2.20726800	-
0.37673600			
C	-2.88252100	-2.17686600	-
0.51990500			
C	-2.57676700	2.70818400	-
0.06391500			
C	-4.45571900	1.01773900	
0.13180800			
C	-4.54141100	-0.33609800	-
0.01447900			
C	-3.07734300	1.38735700	-
0.09631500			
C	-3.21558800	-0.81844500	-
0.32507000			
H	-5.41987700	-0.95496200	
0.09575600			

H	-5.25247100	1.70216200	
0.38399000			
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0.83770600			
N	-2.34444800	0.25096400	-
0.35358500			
N	-0.42846700	-1.93721300	-
0.66882400			
C	2.26082500	2.45985700	-
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C	1.98889400	-2.44165400	-
0.77162100			
C	0.12501200	-4.15967900	-
0.88918100			
C	-0.74787800	4.43552800	-
0.39444900			
C	3.88823200	-0.77224000	-
0.83109300			
C	-1.23438900	-4.08435200	-
0.86166500			
C	0.59547400	4.36683800	-
0.60653600			
C	3.96268400	0.58941500	-
0.87236600			
C	0.62757500	-2.80467200	-
0.76730600			
C	-1.22821400	3.07478000	-
0.25071600			
C	2.48779300	-1.12390100	-
0.82062400			
C	-1.57893200	-2.68430300	-
0.69339700			
C	0.95818100	2.96310800	-
0.59290400			
C	2.60841300	1.09284800	-
0.86315000			
H	-1.94260200	-4.89576200	-
0.94443100			
H	1.27770000	5.18563900	-
0.78382500			
H	4.85526200	1.19767200	-
0.87598400			
H	0.73781700	-5.04247900	-
1.00281700			

H	-1.36600100	5.32114200	-
0.36566400			
H	4.70775400	-1.47514000	-
0.79810200			
N	0.07705300	-0.51075800	
1.98387400			
N	-0.53056100	-1.56711500	
2.26567200			
N	-1.19550000	-2.46286000	
2.45698600			
C	1.44147100	-0.46352900	
2.39137200			
C	2.09258200	0.76676200	
2.25506300			
C	3.31554300	-1.51077300	
3.15325100			
C	3.44241000	0.81328700	
2.57969400			
H	1.55390400	1.62298800	
1.86685200			
C	4.07293100	-0.34647700	
3.04195800			
H	3.76651900	-2.43730500	
3.50154400			
H	3.99676800	1.73914700	
2.45672200			
H	5.12719100	-0.35176100	
3.29839200			
N	2.01588300	-1.58217400	
2.83152600			
C	3.37690300	3.45035000	-
0.85857000			
C	3.66365100	4.28253700	
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C	4.17261400	3.56103400	-
2.00975900			
C	4.71605000	5.19723900	
0.18322300			
H	3.05002600	4.20650500	
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C	5.22524700	4.47549500	-
2.06437000			
H	3.95594000	2.92348200	-
2.86210500			

C	5.50115300	5.29600000	-
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H	4.92441400	5.83019600	
1.04188600			
H	5.82724500	4.55030000	-
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H	6.32091100	6.00802000	-
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C	-3.55823000	3.81329900	
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C	-3.45770000	4.64233900	
1.28498400			
C	-4.59347200	4.05343900	-
0.76174400			
C	-4.36765600	5.67956600	
1.49249500			
H	-2.66004600	4.46266600	
2.00025700			
C	-5.50385000	5.09044400	-
0.55533300			
H	-4.67405200	3.42154100	-
1.64162000			
C	-5.39425000	5.90674100	
0.57294800			
H	-4.27701900	6.30742300	
2.37502800			
H	-6.29545600	5.26426200	-
1.27947900			
H	-6.10317800	6.71449300	
0.73386600			
C	-4.00409900	-3.16520000	-
0.48826300			
C	-4.09010100	-4.11364700	
0.54333900			
C	-4.99389000	-3.15934000	-
1.48313700			
C	-5.13834300	-5.03415900	
0.57667100			
H	-3.33045900	-4.11720100	
1.31976800			
C	-6.04190900	-4.08028000	-
1.45021900			
H	-4.93220100	-2.42762900	-
2.28384800			

C	-6.11696300	-5.02075600	-
0.42013500			
H	-5.19291300	-5.75889300	
1.38480900			
H	-6.79730900	-4.06536400	-
2.23151400			
H	-6.93302300	-5.73797600	-
0.39407400			
C	2.98267300	-3.55334500	-
0.66832000			
C	3.06822300	-4.28925900	
0.52468000			
C	3.83853800	-3.88009500	-
1.72987200			
C	3.99141900	-5.32790400	
0.65103300			
H	2.41281500	-4.02507500	
1.35002500			
C	4.76141300	-4.91999700	-
1.60287800			
H	3.77184600	-3.31542200	-
2.65570200			
C	4.84018100	-5.64638900	-
0.41231400			
H	4.04940600	-5.88750300	
1.58114900			
H	5.41498200	-5.16574000	-
2.43581100			
H	5.55812400	-6.45638700	-
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CSS-INT7			
Fe	-0.13139400	0.00038900	-
0.33636500			
N	-1.66705500	-1.28326600	-
0.47181100			
C	3.24032700	-0.30379700	-
0.98406800			
C	-0.42687400	-3.40495600	-
0.17433400			
C	2.08066000	-3.63646200	-
0.28120900			
C	3.09066100	-2.78124900	-
0.59452700			

C	0.85891200	-2.86266800	-
0.29201400			
C	2.50065500	-1.47073300	-
0.74782700			
H	4.14349000	-3.00318100	-
0.69190300			
H	2.14665800	-4.69574900	-
0.08080400			
N	-1.41920400	1.53885600	-
0.47446600			
N	1.14207100	-1.53566100	-
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N	1.38905500	1.28050900	-
0.56854000			
C	-3.54738300	0.30074500	-
0.74245000			
C	0.17376400	3.40591900	-
0.20902600			
C	2.62769400	3.23066400	-
0.71719900			
C	-2.90610600	-3.23626700	-
0.54548400			
C	-2.33518300	3.64178800	-
0.16414600			
C	3.46541600	2.20243100	-
1.01535100			
C	-3.76714700	-2.21004000	-
0.77906500			
C	-3.36779000	2.78518400	-
0.38792400			
C	1.32991300	2.65036000	-
0.45107100			
C	-1.59677700	-2.65371100	-
0.35846300			
C	-1.11841700	2.86715500	-
0.25583000			
C	2.69871300	0.98326400	-
0.88528700			
C	-2.99828100	-0.98869000	-
0.69357600			
C	-2.79246400	1.47264000	-
0.57574400			
H	4.50607200	2.25492300	-
1.29994100			

H	-4.82432700	-2.26622400	-
0.99297500			
H	-4.42466900	3.00831400	-
0.40349800			
H	2.84547900	4.28884600	-
0.71844900			
H	-3.12006000	-4.29522600	-
0.53729100			
H	-2.38549400	4.70261800	
0.03249900			
C	0.72250400	0.03551000	
3.90755900			
C	0.86075800	-0.01748100	
2.51102300			
C	-1.42329200	0.11346500	
2.23159500			
C	-1.64494200	0.17037300	
3.60023300			
C	-0.54578600	0.13218000	
4.45920100			
H	1.60633400	-0.00218600	
4.53607000			
H	-2.24976200	0.14160000	
1.53901500			
H	-2.65996500	0.24536100	
3.97425800			
H	-0.67219300	0.17507700	
5.53694900			
N	2.10383300	-0.12424400	
1.88316300			
N	-0.19685300	0.02418000	
1.67124100			
N	4.17576100	-0.13011700	
3.02733600			
N	3.13495100	-0.12126600	
2.56053000			
C	-0.57742000	-4.87096100	
0.06890300			
C	-1.19001200	-5.32965900	
1.24574400			
C	-0.13818600	-5.81686200	-
0.87086000			
C	-1.34991800	-6.69553600	
1.48241700			

H	-1.53955100	-4.60288800	
1.97389400			
C	-0.29764300	-7.18308400	-
0.63565200			
H	0.32387100	-5.47000100	-
1.79061100			
C	-0.90262500	-7.62701600	
0.54259300			
H	-1.82225800	-7.03209900	
2.40170300			
H	0.04472200	-7.90069100	-
1.37669800			
H	-1.02725600	-8.69099500	
0.72547100			
C	4.69677600	-0.45259700	-
1.28243900			
C	5.11726700	-1.07766900	-
2.46682000			
C	5.67259100	0.00360200	-
0.38201900			
C	6.47512500	-1.23608000	-
2.74709100			
H	4.36775800	-1.43719800	-
3.16620800			
C	7.03064800	-0.15488900	-
0.66060200			
H	5.35925200	0.47765200	
0.54367200			
C	7.43640500	-0.77420500	-
1.84503700			
H	6.78182500	-1.71802500	-
3.67175000			
H	7.77114000	0.19990800	
0.05148600			
H	8.49398400	-0.89803200	-
2.06234900			
C	0.34010300	4.87207300	
0.02167000			
C	1.02050900	5.33224000	
1.16007100			
C	-0.15135400	5.81694700	-
0.89296600			
C	1.19618700	6.69824000	
1.38424800			

H	1.41079100	4.60629100	
1.86803500			
C	0.02343400	7.18336000	-
0.67009900			
H	-0.66589400	5.46915200	-
1.78408800			
C	0.69647600	7.62864500	
0.47011000			
H	1.72193000	7.03574100	
2.27370300			
H	-0.35997300	7.90008000	-
1.39165700			
H	0.83336000	8.69275700	
0.64315000			
C	-5.02268000	0.44531000	-
0.92806500			
C	-5.53363600	1.08924400	-
2.06604100			
C	-5.92696500	-0.03997400	
0.02977000			
C	-6.90951300	1.23894100	-
2.24409000			
H	-4.84013100	1.47014100	-
2.81038100			
C	-7.30310600	0.10859100	-
0.14689200			
H	-5.54014600	-0.53517500	
0.91608700			
C	-7.79897600	0.74846600	-
1.28522200			
H	-7.28658500	1.73583000	-
3.13411900			
H	-7.98763500	-0.27094200	
0.60729400			
H	-8.87056700	0.86476400	-
1.42351800			
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Fe	0.13297400	0.01290100	-
0.39396000			
N	1.66065200	1.32133900	-
0.47818100			
C	-3.26382000	0.26466900	-
0.95571400			

C	0.37760700	3.42606400	-
0.23542800			
C	-2.13368900	3.61763300	-
0.30246400			
C	-3.14093900	2.74454700	-
0.57468400			
C	-0.90141400	2.86298200	-
0.34265400			
C	-2.53580900	1.44362200	-
0.74098800			
H	-4.19987000	2.94958400	-
0.63497700			
H	-2.21051300	4.67624400	-
0.10233200			
N	1.45600500	-1.50748000	-
0.51162400			
N	-1.17232400	1.53222900	-
0.57554400			
N	-1.37680900	-1.29336700	-
0.60439900			
C	3.57138000	-0.23340500	-
0.70761700			
C	-0.11656200	-3.40273600	-
0.29914400			
C	-2.58083700	-3.26227700	-
0.76890300			
C	2.86623000	3.29373900	-
0.55637600			
C	2.39325500	-3.59888700	-
0.20504000			
C	-3.44579500	-2.24424700	-
1.02010700			
C	3.75055400	2.27947900	-
0.75197500			
C	3.41959700	-2.72309300	-
0.38304600			
C	-1.28821800	-2.66340400	-
0.51730300			
C	1.56287700	2.69136000	-
0.38918900			
C	1.16822000	-2.84192500	-
0.31957700			
C	-2.69799700	-1.01405200	-
0.88390800			

C	3.00021800	1.04673200	-
0.66967700			
C	2.83023700	-1.41816100	-
0.57131200			
H	-4.49241900	-2.31067700	-
1.27842500			
H	4.81157000	2.35112300	-
0.94062600			
H	4.47966600	-2.93020900	-
0.36663800			
H	-2.77972700	-4.32395400	-
0.78783000			
H	3.06257800	4.35606800	-
0.55913600			
H	2.45455000	-4.66116200	-
0.01957300			
C	-0.73874600	-0.15027700	
4.01675800			
C	-0.86649500	-0.03665100	
2.62264100			
C	1.41510400	-0.13177000	
2.33947500			
C	1.63880800	-0.24698900	
3.70672200			
C	0.53400400	-0.25898800	
4.56046900			
H	-1.62158500	-0.14903500	
4.64808500			
H	2.23598200	-0.11965400	
1.63558500			
H	2.65189000	-0.32753200	
4.08518100			
H	0.66006800	-0.34906100	
5.63561900			
N	-2.10263500	0.09332600	
1.97371800			
N	0.19039400	-0.03298200	
1.79394300			
N	-4.18900900	0.00184100	
3.08995700			
N	-3.14402700	0.03577300	
2.63439500			
C	0.50002900	4.89886300	-
0.01862100			

C	1.10272800	5.39296500	
1.14910700			
C	0.03878400	5.81749400	-
0.97491300			
C	1.23313000	6.76617400	
1.35985500			
H	1.46755500	4.68783200	
1.89084000			
C	0.16860500	7.19100400	-
0.76556600			
H	-0.41748700	5.44343300	-
1.88688300			
C	0.76507100	7.67000000	
0.40325600			
H	1.69819000	7.13005100	
2.27242100			
H	-0.19038300	7.88696700	-
1.51928300			
H	0.86664500	8.73967200	
0.56608700			
C	-4.73081600	0.38953600	-
1.20970100			
C	-5.19771500	1.02258500	-
2.37248400			
C	-5.67150000	-0.10005200	-
0.28954100			
C	-6.56584600	1.15725100	-
2.61190900			
H	-4.47596100	1.40697800	-
3.08763900			
C	-7.03983300	0.03458900	-
0.52732800			
H	-5.32302100	-0.58181100	
0.61931000			
C	-7.49163100	0.66279800	-
1.69018200			
H	-6.90829800	1.64584800	-
3.52038300			
H	-7.75233200	-0.34583900	
0.19991500			
H	-8.55724200	0.76806700	-
1.87569400			
C	-0.25402900	-4.87732800	-
0.10469100			

C	-0.92539700	-5.38113400	
1.02060800			
C	0.26134900	-5.78790500	-
1.04076800			
C	-1.07070000	-6.75592500	
1.21010000			
H	-1.33256400	-4.68214800	
1.74595000			
C	0.11704700	-7.16305600	-
0.85255300			
H	0.77110100	-5.40631500	-
1.92076500			
C	-0.54843000	-7.65173400	
0.27425500			
H	-1.59000400	-7.12729500	
2.08979200			
H	0.51858800	-7.85270400	-
1.59044500			
H	-0.66158900	-8.72264800	
0.42038200			
C	5.05344900	-0.35260700	-
0.85117700			
C	5.60919700	-0.98799600	-
1.97295800			
C	5.92068800	0.15024000	
0.13171500			
C	6.99215100	-1.11294700	-
2.11051200			
H	4.94478300	-1.38160900	-
2.73693300			
C	7.30384100	0.02653400	-
0.00450900			
H	5.49923400	0.63950700	
1.00545800			
C	7.84424700	-0.60552700	-
1.12683600			
H	7.40398700	-1.60352000	-
2.98856000			
H	7.95908800	0.41935800	
0.76864700			
H	8.92134900	-0.70246700	-
1.23367100			

³INT7

Fe	0.18245400	0.19438300	-
0.45980400			
N	2.00385600	1.02690300	-
0.36554200			
C	-3.02816300	1.39469400	-
0.84541700			
C	1.33858800	3.37810200	
0.04257000			
C	-1.02474600	4.23799200	
0.06491400			
C	-2.23396400	3.69591600	-
0.23934500			
C	-0.04323700	3.18793400	-
0.08010200			
C	-2.00603500	2.30198300	-
0.53703000			
H	-3.19959200	4.17972800	-
0.23800300			
H	-0.80872700	5.25402400	
0.36054600			
N	1.03992300	-1.61991900	-
0.65698300			
N	-0.66575900	2.00522200	-
0.41594100			
N	-1.62637000	-0.63567900	-
0.69656400			
C	3.42897000	-0.96662400	-
0.71443900			
C	-0.99149600	-3.02367100	-
0.53097500			
C	-3.32240600	-2.18713200	-
0.94127600			
C	3.70099100	2.59425700	-
0.28216700			
C	1.36486400	-3.89890700	-
0.44473900			
C	-3.88114300	-0.95720700	-
1.10319900			
C	4.28221000	1.39384000	-
0.54868500			
C	2.59531100	-3.32893100	-
0.56194800			
C	-1.91454900	-1.98174800	-
0.69420500			

C	2.28040700	2.36156100	-
0.17007500			
C	0.39576300	-2.83370400	-
0.53520300			
C	-2.82793500	0.01083000	-
0.90828200			
C	3.22475600	0.41149100	-
0.57023100			
C	2.38854600	-1.90639000	-
0.68365700			
H	-4.91113000	-0.72016700	-
1.32404100			
H	5.32799500	1.18577100	-
0.71973600			
H	3.55886800	-3.81655100	-
0.53938000			
H	-3.80476700	-3.15107300	-
1.01307300			
H	4.17894400	3.55922900	-
0.19706400			
H	1.12915400	-4.94456200	-
0.31229100			
C	-1.18094000	-1.93522600	
3.28144500			
C	-1.04033200	-0.75776700	
2.52892100			
C	1.22099400	-1.06575400	
2.31233400			
C	1.19471600	-2.24344800	
3.05389500			
C	-0.03966400	-2.68872200	
3.53329800			
H	-2.15229400	-2.24396400	
3.65550100			
H	2.14141700	-0.69235200	
1.87512300			
H	2.10722600	-2.80293500	
3.22732000			
H	-0.11494600	-3.61237600	
4.10005200			
N	-2.11740000	0.10878300	
2.23217600			
N	0.12791500	-0.34067900	
2.03462600			

N	-4.37366700	-0.53213400	
2.57407700			
N	-3.26635400	-0.29530200	
2.43825400			
C	1.85027200	4.74477900	
0.36083500			
C	2.54963400	4.97800200	
1.55550400			
C	1.65975000	5.81619300	-
0.52607700			
C	3.03984600	6.24881500	
1.85856800			
H	2.70178900	4.15277200	
2.24545300			
C	2.14999700	7.08729200	-
0.22415600			
H	1.12770000	5.64128700	-
1.45681400			
C	2.84095700	7.30780200	
0.96968400			
H	3.57416200	6.41225100	
2.79082500			
H	1.99717300	7.90402700	-
0.92477000			
H	3.22289100	8.29764900	
1.20490400			
C	-4.40148100	1.93952200	-
1.06875900			
C	-4.65047300	2.78923000	-
2.15861500			
C	-5.46131600	1.63525500	-
0.19993100			
C	-5.92405600	3.31517500	-
2.37779600			
H	-3.83448800	3.03182500	-
2.83351500			
C	-6.73534600	2.16112700	-
0.41834700			
H	-5.28144600	0.98550400	
0.65085400			
C	-6.97134300	3.00214000	-
1.50814400			
H	-6.09844400	3.96706200	-
3.22978800			

H	-7.54207700	1.91713000	
0.26785900			
H	-7.96357900	3.41168200	-
1.67769900			
C	-1.52846900	-4.40745100	-
0.37116200			
C	-2.29525800	-4.73275100	
0.75914500			
C	-1.29525900	-5.40210200	-
1.33338300			
C	-2.81010200	-6.01850200	
0.92674300			
H	-2.47824500	-3.96524600	
1.50575900			
C	-1.80943800	-6.68884000	-
1.16674500			
H	-0.71214300	-5.15501900	-
2.21590600			
C	-2.56767200	-7.00138700	-
0.03591300			
H	-3.39932600	-6.25347100	
1.80944800			
H	-1.62345900	-7.44548800	-
1.92444900			
H	-2.96908900	-8.00300300	
0.09274900			
C	4.82598300	-1.47771200	-
0.84557100			
C	5.76140100	-1.30488100	
0.18712200			
C	5.22561000	-2.16174700	-
2.00462200			
C	7.06133300	-1.79640500	
0.06271200			
H	5.45883400	-0.78218100	
1.09024600			
C	6.52521000	-2.65401500	-
2.13024600			
H	4.50680000	-2.30153200	-
2.80701900			
C	7.44759700	-2.47238200	-
1.09709300			
H	7.77071600	-1.65586700	
0.87410100			

H	6.81812500	-3.17620900	-
3.03727400			
H	8.45985500	-2.85543700	-
1.19465800			
⁵INT7			
Fe	0.11157000	0.04073800	-
0.28076600			
N	1.70902900	1.40469400	-
0.42327100			
C	-3.32511500	0.27657600	-
0.77105800			
C	0.37495300	3.49115300	-
0.41641500			
C	-2.15155000	3.67666400	-
0.34006600			
C	-3.17803400	2.78558000	-
0.46178500			
C	-0.92042400	2.92702400	-
0.44902700			
C	-2.59024900	1.47665400	-
0.63398700			
H	-4.23711000	2.99472900	-
0.41918900			
H	-2.22342200	4.74277400	-
0.18131900			
N	1.48010400	-1.50630900	-
0.57751100			
N	-1.22008700	1.59205300	-
0.60503600			
N	-1.45109000	-1.32586200	-
0.57829600			
C	3.59390800	-0.19052900	-
0.55160400			
C	-0.12204700	-3.41159900	-
0.54873800			
C	-2.62850000	-3.27330000	-
0.93320900			
C	2.89850400	3.36282800	-
0.65824200			
C	2.39308000	-3.60112200	-
0.32023200			
C	-3.51671700	-2.24564500	-
1.01524400			

C	3.79452000	2.33985800	-
0.71452400			
C	3.42603900	-2.70957100	-
0.34318400			
C	-1.32721200	-2.68797200	-
0.66033500			
C	1.58567700	2.76947400	-
0.47622200			
C	1.17179100	-2.84603200	-
0.48465000			
C	-2.77259900	-1.01997600	-
0.78172600			
C	3.04180400	1.10808400	-
0.55816400			
C	2.85144200	-1.39431500	-
0.51196900			
H	-4.57223500	-2.30322400	-
1.23844500			
H	4.86106300	2.40524700	-
0.87424300			
H	4.47982300	-2.92297500	-
0.23748900			
H	-2.82233000	-4.32639000	-
1.07746900			
H	3.09691900	4.41967000	-
0.76364700			
H	2.45426800	-4.67220300	-
0.19380500			
C	-0.67264700	-0.41396000	
4.20210300			
C	-0.80488200	-0.14697700	
2.83078700			
C	1.47342500	-0.25468300	
2.51246200			
C	1.70517100	-0.52529800	
3.85735900			
C	0.60488900	-0.60930100	
4.71381500			
H	-1.54857100	-0.46190900	
4.84123800			
H	2.28618100	-0.17876500	
1.80002200			
H	2.71809400	-0.66703800	
4.21782900			

H	0.73843000	-0.81987800	
5.77106700			
N	-2.03367300	0.09116300	
2.19164500			
N	0.24522900	-0.07761100	
2.00057100			
N	-4.12425500	-0.12578600	
3.28535200			
N	-3.08066000	-0.04219200	
2.83486700			
C	0.47689900	4.98022700	-
0.34756100			
C	1.11446800	5.60185900	
0.73842200			
C	-0.04907500	5.79017000	-
1.36729100			
C	1.21942600	6.99153100	
0.80606300			
H	1.52533800	4.98262200	
1.53083100			
C	0.05561900	7.17988500	-
1.30121800			
H	-0.53622500	5.31770300	-
2.21534900			
C	0.68961600	7.78556400	-
0.21371400			
H	1.71195100	7.45416100	
1.65744900			
H	-0.35284300	7.78942800	-
2.10306400			
H	0.77142300	8.86801300	-
0.16219000			
C	-4.80796200	0.39652400	-
0.90885700			
C	-5.67121500	-0.18106700	
0.03665600			
C	-5.37270800	1.09472100	-
1.98915500			
C	-7.05546900	-0.06301000	-
0.09180600			
H	-5.24907300	-0.72038200	
0.87916600			
C	-6.75668200	1.21266600	-
2.11954200			

H	-4.71352300	1.54103700	-
2.72811200			
C	-7.60338000	0.63434200	-
1.17079000			
H	-7.70507400	-0.51144900	
0.65531200			
H	-7.17370000	1.75233900	-
2.96582800			
H	-8.68149900	0.72665500	-
1.27150200			
C	5.08288200	-0.30490200	-
0.58092900			
C	5.86743500	0.25024700	
0.44336600			
C	5.73276900	-0.97025500	-
1.63346700			
C	7.25830300	0.14359700	
0.41776100			
H	5.37446600	0.76784200	
1.26166200			
C	7.12348700	-1.07817100	-
1.66039200			
H	5.13491000	-1.39840300	-
2.43283700			
C	7.89140900	-0.52187500	-
0.63457800			
H	7.84716700	0.57674900	
1.22217700			
H	7.60769500	-1.59215300	-
2.48661200			
H	8.97470700	-0.60537600	-
0.65569400			
C	-0.22554700	-4.90201700	-
0.52938100			
C	-0.92603800	-5.55475100	
0.49800800			
C	0.36124300	-5.68251500	-
1.53885800			
C	-1.03335200	-6.94572600	
0.51904400			
H	-1.38504900	-4.95853400	
1.28164000			
C	0.25478200	-7.07354000	-
1.51923700			

H	0.89715900	-5.18600200	-
2.34263700			
C	-0.44234300	-7.71021800	-
0.48961200			
H	-1.57587600	-7.43250100	
1.32539000			
H	0.71105800	-7.65978800	-
2.31263200			
H	-0.52589600	-8.79364600	-
0.47450900			
CSS-TS7			
Fe	-0.35112700	0.14373400	-
0.73017600			
N	-2.00914600	-1.01147200	-
0.80356800			
C	0.23787400	3.51879100	-
0.66671800			
C	-3.75989900	0.74056800	-
0.77344700			
C	-3.34021800	3.20055700	-
0.47173800			
C	-2.22262500	3.96796600	-
0.37387600			
C	-2.89795600	1.84020100	-
0.68111300			
C	-1.09187600	3.09059500	-
0.57998000			
H	-2.16256000	5.03295300	-
0.20491400			
H	-4.37111900	3.51565200	-
0.40273400			
N	0.76762900	-1.50116600	-
1.04598700			
N	-1.52233700	1.79188500	-
0.74628400			
N	1.23813700	1.29915200	-
1.10774900			
C	-0.95991300	-3.25278000	-
0.79060100			
C	2.95068100	-0.43494700	-
1.51888800			
C	3.37253200	2.03700200	-
1.61991000			

C	-4.21523900	-1.72613900	-
0.86032600			
C	2.57833800	-2.91218400	-
1.35489300			
C	2.62945800	3.13695900	-
1.32952300			
C	-3.43530800	-2.83803500	-
0.81324900			
C	1.49270600	-3.69962000	-
1.12795100			
C	2.51162600	0.88988700	-
1.44154500			
C	-3.32513800	-0.58817600	-
0.84698600			
C	2.12001000	-1.54217300	-
1.31010500			
C	1.29977600	2.67004000	-
1.00632100			
C	-2.06153900	-2.38898200	-
0.77792400			
C	0.36054800	-2.81588400	-
0.96019400			
H	2.93446500	4.17280100	-
1.35528800			
H	-3.75136800	-3.87083100	-
0.82419200			
H	1.45623800	-4.77798900	-
1.08115600			
H	4.40898500	1.99525300	-
1.92037400			
H	-5.29328500	-1.67034400	-
0.90033400			
H	3.59798800	-3.22134900	-
1.53229300			
C	4.39509900	-0.68530300	-
1.81349800			
C	4.79008900	-1.27308900	-
3.02468300			
C	5.38201400	-0.34121200	-
0.87693100			
C	6.13869300	-1.51196000	-
3.29393800			
H	4.03006900	-1.54002900	-
3.75377800			

C	6.73033700	-0.57934700	-
1.14619700			
H	5.08193800	0.11339400	
0.06174000			
C	7.11310600	-1.16592200	-
2.35484400			
H	6.42797400	-1.96422000	-
4.23902000			
H	7.48216900	-0.30853700	-
0.40927100			
H	8.16338900	-1.35111800	-
2.56415800			
C	0.55503700	4.95755800	-
0.42272800			
C	1.36332200	5.31665000	
0.66784800			
C	0.07912300	5.97086000	-
1.26885000			
C	1.67916000	6.65345500	
0.91199300			
H	1.74466800	4.53445500	
1.31872100			
C	0.39418600	7.30854900	-
1.02528600			
H	-0.53471700	5.69945500	-
2.12297500			
C	1.19360700	7.65419500	
0.06678900			
H	2.30446000	6.91341900	
1.76221100			
H	0.02089300	8.08011800	-
1.69361500			
H	1.43993100	8.69574000	
0.25535600			
C	-5.23440900	0.99262100	-
0.74312600			
C	-5.86826400	1.38918100	
0.44385200			
C	-6.01216000	0.82665600	-
1.89829800			
C	-7.24462700	1.61810000	
0.47573700			
H	-5.26968800	1.51957400	
1.34159800			

C	-7.38950500	1.05186700	-
1.86762800			
H	-5.52714200	0.51848100	-
2.82037000			
C	-8.00962900	1.44896900	-
0.68073100			
H	-7.71984400	1.92430000	
1.40412500			
H	-7.97730600	0.92070300	-
2.77236600			
H	-9.08165600	1.62551700	-
0.65706400			
C	-1.22781400	-4.71827700	-
0.67370600			
C	-0.95843100	-5.60081800	-
1.73141800			
C	-1.77854800	-5.24027700	
0.50861400			
C	-1.21601900	-6.96666100	-
1.60484500			
H	-0.54869000	-5.20506800	-
2.65618600			
C	-2.03701900	-6.60562600	
0.63660600			
H	-2.00149800	-4.56014600	
1.32566900			
C	-1.75341600	-7.47439600	-
0.41965200			
H	-1.00312700	-7.63364400	-
2.43615000			
H	-2.45863400	-6.99036800	
1.56163300			
H	-1.95354400	-8.53797300	-
0.32174200			
N	2.01435100	0.71201300	
1.55387500			
N	2.92350700	1.58616600	
1.69931500			
N	4.05607700	1.59831000	
2.02204100			
C	0.71822200	0.96130700	
1.99377400			
C	0.49292500	1.64714100	
3.20072100			

C	-1.49982100	0.33811100
1.89600700		
C	-0.77829700	1.66820100
3.75182700		
H	1.33485900	2.12055500
3.69510000		
C	-1.79010500	0.95825900
3.10305900		
H	-2.26722700	-0.17982500
1.34174300		
H	-0.96817900	2.19653400
4.68165200		
H	-2.79626200	0.90123200
3.50418000		
N	-0.28683000	0.37253800
1.30248100		
C	3.25391500	-0.89876600
2.81834200		
C	4.31426500	-0.25130700
2.78787700		
C	2.14698500	-1.77081500
3.04018300		
C	1.87267400	-2.82082200
2.14783200		
C	1.29885000	-1.56224200
4.14714000		
C	0.77484600	-3.64831100
2.36136200		
H	2.50612500	-2.96401200
1.28113900		
C	0.19675700	-2.38948700
4.34643100		
H	1.50816800	-0.74695200
4.83197300		
C	-0.06781600	-3.43428200
3.45533700		
H	0.56683400	-4.45001600
1.66124700		
H	-0.45637200	-2.21858100
5.19780500		
H	-0.92763100	-4.08009900
3.61287100		
H	5.35326300	-0.17653500
3.03681300		

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Fe	-0.31693800	0.08349200	-
0.85303000			
N	-2.11211800	-0.84100900	-
0.82857000			
C	0.71311800	3.36260700	-
0.86768300			
C	-3.61688000	1.12654100	-
0.78492800			
C	-2.87479600	3.51993800	-
0.62902600			
C	-1.66472100	4.13926600	-
0.59780900			
C	-2.61776600	2.10683300	-
0.77958500			
C	-0.66229700	3.11402300	-
0.77741200			
H	-1.46300500	5.19364800	-
0.48008100			
H	-3.85368600	3.96916900	-
0.54795700			
N	0.58704900	-1.70171300	-
1.10363200			
N	-1.26211300	1.87787300	-
0.87504200			
N	1.43313900	1.01328700	-
1.17121600			
C	-1.36171200	-3.20076200	-
0.81422300			
C	2.92007400	-0.94471000	-
1.44079100			
C	3.67458000	1.44428100	-
1.56029400			
C	-4.39054400	-1.26031600	-
0.77066600			
C	2.20722000	-3.34509300	-
1.27390000			
C	3.06366600	2.64315100	-
1.37416400			
C	-3.76055700	-2.46461000	-
0.74598500			
C	1.01557500	-3.97446500	-
1.08385100			

C	2.65904200	0.42822000	-
1.40353200			
C	-3.36077700	-0.24917200	-
0.82282000			
C	1.93446100	-1.92739100	-
1.28841100			
C	1.66668700	2.36788300	-
1.12095600			
C	-2.34009300	-2.19972100	-
0.78036000			
C	0.00516900	-2.94590300	-
0.99305600			
H	3.50425700	3.62812100	-
1.41979500			
H	-4.20894500	-3.44697100	-
0.72362000			
H	0.83435500	-5.03628700	-
1.00561500			
H	4.71408100	1.25509500	-
1.78304700			
H	-5.45272000	-1.06461600	-
0.75771500			
H	3.18437900	-3.79205800	-
1.38300000			
C	4.33665700	-1.38888700	-
1.61478200			
C	4.74717200	-2.05461300	-
2.77942300			
C	5.28102100	-1.14922500	-
0.60450800			
C	6.07055200	-2.47172600	-
2.93139200			
H	4.02017200	-2.24053600	-
3.56519000			
C	6.60403900	-1.56550800	-
0.75691900			
H	4.96512300	-0.63857300	-
0.29990600			
C	7.00300700	-2.22824900	-
1.92021400			
H	6.37377700	-2.98242400	-
3.84166900			
H	7.32302700	-1.37472600	-
0.03573900			

H	8.03362700	-2.55227400	-
2.03852900			
C	1.20273700	4.76248500	-
0.68821700			
C	2.01719200	5.08259400	
0.40995500			
C	0.87603400	5.77701800	-
1.60088500			
C	2.48615000	6.38345000	
0.59486700			
H	2.28337200	4.29816500	
1.11311300			
C	1.34403400	7.07895900	-
1.41639300			
H	0.25579400	5.53421800	-
2.45905700			
C	2.14921300	7.38657100	-
0.31719700			
H	3.11458000	6.61352300	
1.45137200			
H	1.08502300	7.85145300	-
2.13574700			
H	2.51477800	8.40000200	-
0.17458300			
C	-5.04240300	1.57094900	-
0.69208500			
C	-5.54773300	2.09474900	
0.50736000			
C	-5.90182100	1.46470100	-
1.79517200			
C	-6.87824100	2.50492500	
0.60219500			
H	-4.88400900	2.18086300	
1.36376600			
C	-7.23390000	1.87168000	-
1.70134200			
H	-5.51636700	1.05965800	-
2.72672600			
C	-7.72576800	2.39339400	-
0.50265800			
H	-7.25389700	2.90778300	
1.53925400			
H	-7.88618100	1.78476300	-
2.56633300			

H	-8.76240100	2.71129100	-
0.42997300			
C	-1.80943400	-4.61837700	-
0.66521900			
C	-1.66753000	-5.54393000	-
1.71084400			
C	-2.39162700	-5.05133900	
0.53764200			
C	-2.08444200	-6.86656500	-
1.55436400			
H	-1.22940700	-5.21548400	-
2.64895900			
C	-2.80918400	-6.37347800	
0.69542700			
H	-2.51430500	-4.33642700	
1.34615600			
C	-2.65458900	-7.28651200	-
0.35015200			
H	-1.96931600	-7.56803600	-
2.37650500			
H	-3.25289400	-6.69033200	
1.63569600			
H	-2.97862400	-8.31661200	-
0.22884000			
N	2.03871200	0.76017500	
1.68010100			
N	3.03487000	1.53010400	
1.83850900			
N	4.15483700	1.42410400	
2.17914400			
C	0.75592200	1.16336700	
2.04090000			
C	0.51288600	2.14104500	
3.02382200			
C	-1.47344200	0.59810400	
1.96544200			
C	-0.78751200	2.32764600	
3.47014700			
H	1.34090400	2.71451300	
3.42756200			
C	-1.80292800	1.51475000	
2.95752900			
H	-2.22944100	-0.01983400	
1.49776800			

H	-1.00314800	3.07983200
4.22389500		
H	-2.82905900	1.60255800
3.29879100		
N	-0.23203900	0.44301200
1.47736700		
C	3.03217900	-0.99260600
2.91567800		
C	4.16606800	-0.48679000
2.93889600		
C	1.82352600	-1.73635300
3.08624700		
C	1.48132800	-2.77050800
2.19908400		
C	0.94954700	-1.41202600
4.14328500		
C	0.29330600	-3.47458300
2.37608300		
H	2.13662100	-3.00356400
1.36826400		
C	-0.24092200	-2.11470900
4.30554500		
H	1.20827800	-0.60138000
4.81739900		
C	-0.57102400	-3.14869400
3.42385300		
H	0.03611700	-4.26866500
1.68371000		
H	-0.91212600	-1.85460800
5.11944500		
H	-1.49912300	-3.69917600
3.55383100		
H	5.19731800	-0.52752800
3.22299900		

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Fe	0.31836300	0.03991300	-
0.93573700			
N	1.81182600	1.38320400	-
0.84517100			
C	0.14577500	-3.39826000	-
0.89332300			
C	3.76798400	-0.13602800	-
0.77935700			

C	3.65682700	-2.63956100	-
0.70095300			
C	2.64402900	-3.54570600	-
0.67899400			
C	3.04894800	-1.33516200	-
0.80917200			
C	1.41214900	-2.80576100	-
0.82202200			
H	2.71718600	-4.61903300	-
0.58619700			
H	4.71819200	-2.82779500	-
0.63665600			
N	-1.01103500	1.53168100	-
1.15650700			
N	1.67651700	-1.45496900	-
0.89230700			
N	-1.14991400	-1.30517700	-
1.16377700			
C	0.48514300	3.47435100	-
0.82247200			
C	-3.08599300	0.21160300	-
1.43909900			
C	-3.22627900	-2.28822600	-
1.45734200			
C	3.90110500	2.36471100	-
0.65795500			
C	-2.99229600	2.71369400	-
1.34844900			
C	-2.32739400	-3.29316800	-
1.29217300			
C	2.98314700	3.36786100	-
0.63731900			
C	-1.99881700	3.62324900	-
1.15711300			
C	-2.49169000	-1.04995100	-
1.35828700			
C	3.16851400	1.12848200	-
0.78895500			
C	-2.37284800	1.41037600	-
1.34080100			
C	-1.03519600	-2.67574100	-
1.09966800			
C	1.68226300	2.75318000	-
0.75563000			

C	-0.76398500	2.88303800	-
1.04500000			
H	-2.51016000	-4.35727500	-
1.30922200			
H	3.16244500	4.43037300	-
0.56261300			
H	-2.08890300	4.69734400	-
1.08834000			
H	-4.28877800	-2.36703300	-
1.63274800			
H	4.97586200	2.44515900	-
0.58903900			
H	-4.04990100	2.89790600	-
1.46665200			
C	-4.57198500	0.28604500	-
1.58553500			
C	-5.15923100	0.74219100	-
2.77454900			
C	-5.40291400	-0.09295000	-
0.52012000			
C	-6.54780000	0.81734600	-
2.89723900			
H	-4.51879600	1.03593800	-
3.60173400			
C	-6.79089300	-0.01803600	-
0.64348600			
H	-4.94803600	-0.43959300	
0.40315500			
C	-7.36737900	0.43711500	-
1.83186600			
H	-6.98889600	1.16914700	-
3.82620900			
H	-7.42237600	-0.31176000	
0.19112400			
H	-8.44840600	0.49531200	-
1.92742200			
C	0.04042100	-4.88132300	-
0.74302900			
C	-0.62184500	-5.43078500	
0.36635000			
C	0.58757400	-5.75197200	-
1.69788600			
C	-0.72765000	-6.81338000	
0.52089700			

H	-1.06132100	-4.76251900	
1.10106100			
C	0.48363100	-7.13520700	-
1.54341700			
H	1.09222600	-5.33403100	-
2.56437800			
C	-0.17286700	-7.67032000	-
0.43262800			
H	-1.24351500	-7.22081600	
1.38650600			
H	0.90986200	-7.79459000	-
2.29495500			
H	-0.25522300	-8.74733000	-
0.31326800			
C	5.25836400	-0.20369600	-
0.67568100			
C	5.87204200	-0.66161500	
0.50022000			
C	6.07108500	0.19990400	-
1.74534600			
C	7.26241400	-0.71753800	
0.60430600			
H	5.24569600	-0.97763600	
1.32992300			
C	7.46212600	0.14658300	-
1.64219300			
H	5.60221500	0.55626700	-
2.65832200			
C	8.06189300	-0.31252600	-
0.46724300			
H	7.72123600	-1.07330400	
1.52320200			
H	8.07708800	0.46006500	-
2.48168000			
H	9.14481600	-0.35471200	-
0.38718600			
C	0.54739000	4.95576500	-
0.63700200			
C	0.25132500	5.83733800	-
1.68756600			
C	0.90571300	5.49242700	
0.61015500			
C	0.30318300	7.21866000	-
1.49396100			

H	-0.01891600	5.42974300	-
2.65760300			
C	0.95856700	6.87328700	
0.80465900			
H	1.14171900	4.81232400	
1.42336700			
C	0.65536700	7.74099800	-
0.24711900			
H	0.07342500	7.88712500	-
2.31953300			
H	1.23354500	7.27083800	
1.77817200			
H	0.69522200	8.81650400	-
0.09704900			
N	-1.60875600	-1.41420400	
1.83290300			
N	-2.31413800	-2.45733500	
1.97212500			
N	-3.41931900	-2.71518000	
2.27426100			
C	-0.24133800	-1.42121000	
2.10719400			
C	0.40690600	-2.44002400	
2.83112100			
C	1.66508300	-0.14216800	
2.05460100			
C	1.74477000	-2.26426500	
3.15698300			
H	-0.13619100	-3.33293000	
3.12233000			
C	2.38734300	-1.07745800	
2.78993000			
H	2.12873700	0.77272600	
1.70110900			
H	2.27704100	-3.03763300	
3.70388000			
H	3.42407700	-0.88951400	
3.04907600			
N	0.38871300	-0.31316800	
1.68511700			
C	-3.16964800	-0.02299100	
2.92189100			
C	-4.07939100	-0.86649500	
2.94987100			

C	-2.28551900	1.09167600
3.07343900		
C	-2.28024600	2.14372300
2.14204200		
C	-1.40102500	1.13139700
4.16884300		
C	-1.41411000	3.22034700
2.31432600		
H	-2.94114500	2.10504300
1.28402100		
C	-0.53571900	2.20938200
4.33004900		
H	-1.39610300	0.30853800
4.87728700		
C	-0.54131700	3.25689000
3.40441600		
H	-1.41202300	4.02540400
1.58743800		
H	0.14435600	2.23150900
5.17726500		
H	0.13066800	4.10119200
3.53393500		
H	-5.07585400	-1.16324200
3.20257800		

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N	-1.63107500	1.15105600	-
1.13011800			
C	3.51808800	0.98746600	-
0.89444200			
C	-0.73174800	3.44669600	-
0.96829400			
C	1.70116200	4.12033700	-
0.80536600			
C	2.88485500	3.43860100	-
0.80417900			
C	0.64597700	3.14193300	-
0.93461800			
C	2.57010800	2.03410500	-
0.93895600			
H	3.87919700	3.85093500	-
0.71287100			
H	1.55544600	5.18847200	-
0.72951500			

N	-0.85738100	-1.66042300	-
1.16256300			
N	1.20345400	1.88633300	-
1.02120800			
N	1.96936200	-0.94061100	-
0.92502000			
C	-3.17697800	-0.77105300	-
1.23707800			
C	1.06293200	-3.23541400	-
1.02891000			
C	3.53048400	-2.63075500	-
1.01562400			
C	-3.18590000	2.84882100	-
1.20208200			
C	-1.37326600	-3.90310600	-
1.12035500			
C	4.21351900	-1.45400000	-
0.98287600			
C	-3.86870000	1.67307600	-
1.28620400			
C	-2.55017600	-3.21899000	-
1.17825500			
C	2.11648100	-2.30006000	-
0.97855200			
C	-1.77596300	2.51516000	-
1.10862200			
C	-0.30927100	-2.92272600	-
1.11625100			
C	3.22446400	-0.39089300	-
0.92356000			
C	-2.88377200	0.60637600	-
1.24421400			
C	-2.22385500	-1.80966800	-
1.19196200			
H	5.28367100	-1.31004800	-
1.02231100			
H	-4.93734000	1.53500500	-
1.36573000			
H	-3.54917000	-3.62885400	-
1.20585700			
H	3.93614500	-3.62974800	-
1.08680200			
H	-3.59263200	3.85012300	-
1.20412400			

H	-1.23654800	-4.97344300	-
1.07535300			
C	-4.62089100	-1.16311000	-
1.22230800			
C	-5.18155700	-1.73388500	-
0.06828900			
C	-5.44206600	-0.95780100	-
2.34067800			
C	-6.53115600	-2.08754100	-
0.03438200			
H	-4.54730300	-1.89730100	
0.79900000			
C	-6.79226000	-1.31077400	-
2.30637600			
H	-5.01223200	-0.52026700	-
3.23749500			
C	-7.34092700	-1.87623100	-
1.15290300			
H	-6.95109000	-2.52488800	
0.86785800			
H	-7.41434100	-1.14798100	-
3.18267100			
H	-8.39201100	-2.15116300	-
1.12647100			
C	-1.11622500	4.88381000	-
0.80273500			
C	-1.59751500	5.64043400	-
1.88046200			
C	-1.00952400	5.49475700	
0.45634100			
C	-1.96712300	6.97525000	-
1.70331900			
H	-1.67970900	5.17329000	-
2.85791700			
C	-1.37618400	6.82946900	
0.63430800			
H	-0.63796700	4.90904700	
1.29305900			
C	-1.85736500	7.57341300	-
0.44588100			
H	-2.33691700	7.54891200	-
2.54916500			
H	-1.28990300	7.28731200	
1.61642900			

H	-2.14448100	8.61249300	-
0.30865400			
C	4.95623300	1.37284000	-
0.76656400			
C	5.61533900	2.07797200	-
1.78522000			
C	5.67518400	1.03526700	
0.39152900			
C	6.95724200	2.43686500	-
1.64985800			
H	5.06594700	2.33899700	-
2.68534000			
C	7.01687600	1.39330600	
0.52753900			
H	5.16669600	0.49192500	
1.18332500			
C	7.66227800	2.09577400	-
0.49310700			
H	7.45358600	2.97824500	-
2.45100200			
H	7.55786500	1.12650500	
1.43189800			
H	8.70745100	2.37445600	-
0.38840800			
C	1.43778500	-4.68116000	-
0.96683500			
C	2.01665100	-5.20943500	
0.19758300			
C	1.22332000	-5.53588600	-
2.05872800			
C	2.37021100	-6.55711300	
0.26998100			
H	2.17910400	-4.55243300	
1.04730200			
C	1.57694800	-6.88408000	-
1.98781100			
H	0.77881700	-5.13222500	-
2.96406100			
C	2.15136800	-7.39882800	-
0.82314300			
H	2.81182700	-6.95092500	
1.18173700			
H	1.40772500	-7.53133100	-
2.84439100			

H	2.42630800	-8.44876800	-
0.76776900			
N	-0.29423500	-1.85020600	
1.87253700			
N	-0.30016100	-3.09541200	
2.12947900			
N	-1.10902100	-3.88458800	
2.45188500			
C	0.78186100	-1.03713200	
2.19893000			
C	1.75416400	-1.35642700	
3.16226500			
C	1.59605000	1.10640200	
1.98041000			
C	2.67562400	-0.37938800	
3.51816400			
H	1.76210500	-2.34232200	
3.61531300			
C	2.58101200	0.89038300	
2.94134100			
H	1.49894800	2.06436500	
1.48378600			
H	3.44425200	-0.59866100	
4.25424900			
H	3.26375300	1.68951800	
3.20929700			
N	0.73599600	0.15948400	
1.58069100			
C	-2.39640900	-1.47540100	
2.89189100			
C	-2.69605400	-2.68056900	
2.93829100			
C	-2.22714200	-0.06157700	
3.03144400			
C	-2.80181600	0.83714500	
2.11693000			
C	-1.44160100	0.43843700	
4.09037500			
C	-2.58338000	2.20649400	
2.25302800			
H	-3.40129200	0.45907400	
1.29847300			
C	-1.22799900	1.80733600	
4.21804700			

H	-0.98979800	-0.25756100	
4.79047100			
C	-1.79367000	2.69449900	
3.29633900			
H	-3.01964400	2.88657300	
1.52945600			
H	-0.61459000	2.18197000	
5.03285600			
H	-1.62358200	3.76364300	
3.39271800			
H	-3.39057900	-3.45611800	
3.18735800			
Fe	0.15189900	0.11181600	-
0.76972600			
CSSINT8			
Fe	-0.23750900	0.06902300	-
0.42277900			
N	-2.24343500	0.27384600	-
0.36199400			
C	1.91657900	-2.61197400	-
0.68712600			
C	-2.92529200	-2.10660700	-
0.37720900			
C	-1.37331200	-4.06382900	-
0.62083000			
C	-0.02276700	-4.20555500	-
0.68561300			
C	-1.64228800	-2.64958100	-
0.50903500			
C	0.54266600	-2.87762300	-
0.62596900			
H	0.54601500	-5.11784000	-
0.79113200			
H	-2.12637000	-4.83728100	-
0.65709700			
N	-0.03960000	2.06199800	-
0.52781800			
N	-0.46079400	-1.93517500	-
0.53478500			
N	1.74261200	-0.14344500	-
0.74866600			
C	-2.40385300	2.74068400	-
0.25313600			

C	2.41694100	2.23555900	-
0.75305400			
C	4.01523700	0.30296000	-
0.80814300			
C	-4.49922100	-0.17646200	-
0.07544400			
C	0.85078000	4.19333400	-
0.70717000			
C	3.87622600	-1.04811700	-
0.78132900			
C	-4.35202200	1.17344800	-
0.02265200			
C	-0.49205200	4.33482200	-
0.56605800			
C	2.68407600	0.86365400	-
0.79011600			
C	-3.18501500	-0.73360400	-
0.29372700			
C	1.12969100	2.77523000	-
0.66502600			
C	2.45831300	-1.32420100	-
0.75171700			
C	-2.94799600	1.45187900	-
0.21654200			
C	-1.04169300	3.00356200	-
0.43518000			
H	4.65601900	-1.79511100	-
0.77002900			
H	-5.11648700	1.91911400	
0.13835200			
H	-1.06946800	5.24752500	-
0.56621300			
H	4.93094800	0.87520900	-
0.82163400			
H	-5.40627100	-0.75213600	
0.03571000			
H	1.59097500	4.96757200	-
0.84610900			
C	1.74569300	-1.38402600	
2.59048000			
C	1.25721900	-0.12882800	
2.21631600			
C	3.18372200	0.92944400	
2.78494200			

C	3.77860200	-0.26225800	
3.20053800			
C	3.03931100	-1.44200100	
3.10123700			
H	1.14916000	-2.27731200	
2.43796400			
H	3.73220700	1.86771800	
2.82278700			
H	4.79679300	-0.26489700	
3.57578400			
H	3.47035100	-2.39671300	
3.38802900			
N	-0.04671200	-0.00772000	
1.59836900			
N	1.93579500	1.00562900	
2.30524900			
N	-1.86729500	-1.17900900	
2.59954200			
N	-0.96452800	-0.65354400	
2.16041000			
C	-4.08402200	-3.04779200	-
0.29893700			
C	-5.02500600	-3.11509300	-
1.33726000			
C	-4.25280800	-3.87870800	
0.81907300			
C	-6.10705900	-3.99339500	-
1.26120000			
H	-4.89942300	-2.47326900	-
2.20478700			
C	-5.33437500	-4.75719200	
0.89615200			
H	-3.52991900	-3.82468700	
1.62818700			
C	-6.26452400	-4.81741200	-
0.14432800			
H	-6.82490700	-4.03624600	-
2.07614700			
H	-5.45299400	-5.39111900	
1.77105300			
H	-7.10699200	-5.50133800	-
0.08480500			
C	-3.33033800	3.90450600	-
0.10441200			

C	-3.25439000	4.73665000	
1.02308300			
C	-4.28923200	4.19086600	-
1.08827800			
C	-4.11593700	5.82532000	
1.16472400			
H	-2.51278000	4.52112700	
1.78717400			
C	-5.15126100	5.27934500	-
0.94779800			
H	-4.35091000	3.55264300	-
1.96524800			
C	-5.06746500	6.09977900	
0.17961400			
H	-4.04578500	6.45708800	
2.04637300			
H	-5.88521700	5.48888400	-
1.72157100			
H	-5.73850700	6.94755500	
0.28929700			
C	3.57455900	3.17914600	-
0.73719800			
C	4.42860500	3.31199800	-
1.84178100			
C	3.83171500	3.94721500	
0.41019000			
C	5.51527000	4.18743600	-
1.79988800			
H	4.23249000	2.72369600	-
2.73379900			
C	4.91754500	4.82241900	
0.45280900			
H	3.16523600	3.84989400	
1.26282300			
C	5.76373200	4.94418300	-
0.65240800			
H	6.16487500	4.28182800	-
2.66617000			
H	5.10370700	5.40845500	
1.34921600			
H	6.60939000	5.62602300	-
0.62057400			
C	2.85588900	-3.77426400	-
0.67210700			

C	2.96126500	-4.58708100	
0.46747000			
C	3.65249000	-4.07772100	-
1.78674200			
C	3.83993300	-5.67065600	
0.49526200			
H	2.34283100	-4.36275800	
1.33233200			
C	4.53278400	-5.16045800	-
1.76100700			
H	3.57356700	-3.45628500	-
2.67417700			
C	4.63005100	-5.96002000	-
0.61973000			
H	3.90882100	-6.28767300	
1.38752600			
H	5.13905400	-5.38255500	-
2.63526200			
H	5.31472500	-6.80365800	-
0.60018200			

ossINT8

Fe	-0.26176200	0.10447200	-
0.48295600			
N	-2.27223900	0.13346200	-
0.36673800			
C	2.12068000	-2.37982300	-
0.66626300			
C	-2.75642600	-2.29331800	-
0.49405200			
C	-1.03539500	-4.10576300	-
0.71650700			
C	0.32476900	-4.13097900	-
0.72522000			
C	-1.42896100	-2.72343300	-
0.59868500			
C	0.77317600	-2.76198700	-
0.63499300			
H	0.97258800	-4.99083500	-
0.81377600			
H	-1.71676100	-4.94063000	-
0.78841700			
N	-0.22738300	2.10753900	-
0.49644200			

N	-0.31107900	-1.91159900	-
0.56937600			
N	1.73243500	0.06331200	-
0.76466300			
C	-2.63424500	2.57220100	-
0.14596300			
C	2.19774600	2.49356200	-
0.79206500			
C	3.95353500	0.70966800	-
0.85130400			
C	-4.48040100	-0.51542000	-
0.10689400			
C	0.47717500	4.30860500	-
0.62814700			
C	3.93506400	-0.64757600	-
0.78094600			
C	-4.44266900	0.83758300	
0.02110500			
C	-0.86784500	4.33061900	-
0.43534200			
C	2.57976600	1.14956500	-
0.83097500			
C	-3.12711000	-0.95163700	-
0.35156800			
C	0.87466700	2.92097500	-
0.64884000			
C	2.54822300	-1.04908200	-
0.74087500			
C	-3.06841700	1.24115500	-
0.16226900			
C	-1.30205100	2.95561700	-
0.34160000			
H	4.77838700	-1.32103900	-
0.74618900			
H	-5.26425000	1.50788800	
0.22623400			
H	-1.51762900	5.19135800	-
0.37680700			
H	4.81380700	1.36163700	-
0.88527000			
H	-5.33655400	-1.16850200	-
0.02387600			
H	1.14571500	5.14718800	-
0.75664000			

C	1.81875800	-1.48637000	
2.79360200			
C	1.30544200	-0.25359100	
2.36792700			
C	3.32264600	0.78157000	
2.57587500			
C	3.94490700	-0.38817100	
3.01355600			
C	3.16894000	-1.54276000	
3.12532500			
H	1.19151500	-2.37137600	
2.83047800			
H	3.89004700	1.70175400	
2.45442800			
H	5.00487300	-0.39467100	
3.24508700			
H	3.61171800	-2.48213100	
3.44332200			
N	-0.04782400	-0.09838300	
1.92751800			
N	2.02502900	0.85943100	
2.26352000			
N	-1.70900500	-1.67223100	
2.56986400			
N	-0.86427100	-0.96057400	
2.30671100			
C	-3.83684800	-3.32585000	-
0.47597100			
C	-4.75181400	-3.42404900	-
1.53478700			
C	-3.96132400	-4.20825800	
0.60817400			
C	-5.76461000	-4.38422400	-
1.51303800			
H	-4.66101100	-2.74151100	-
2.37520400			
C	-4.97363400	-5.16851600	
0.63047900			
H	-3.26059900	-4.12774400	
1.43426600			
C	-5.87778200	-5.25976400	-
0.43057400			
H	-6.46299100	-4.45013700	-
2.34321100			

H	-5.05949700	-5.84178700	
1.47943300			
H	-6.66635100	-6.00737300	-
0.41327200			
C	-3.64912200	3.64763100	
0.07246500			
C	-3.61516400	4.43183300	
1.23596300			
C	-4.64925400	3.89938400	-
0.87939100			
C	-4.55779400	5.43969700	
1.44374100			
H	-2.84252700	4.24253700	
1.97587200			
C	-5.59259100	4.90679900	-
0.67242000			
H	-4.67834300	3.29915700	-
1.78443400			
C	-5.54985900	5.67992000	
0.49019200			
H	-4.51902900	6.03483200	
2.35237900			
H	-6.35776900	5.09081200	-
1.42204400			
H	-6.28408000	6.46472100	
0.65152300			
C	3.27514700	3.52853100	-
0.81712900			
C	4.03684600	3.76057600	-
1.97134200			
C	3.55382800	4.27537000	
0.33865300			
C	5.05364700	4.71730600	-
1.97133800			
H	3.82505700	3.18502800	-
2.86816900			
C	4.57014300	5.23167800	
0.33922800			
H	2.96333200	4.09479900	
1.23288500			
C	5.32323900	5.45510100	-
0.81630200			
H	5.63263400	4.88865300	-
2.87507200			

H	4.77554300	5.80047200	
1.24243800			
H	6.11456400	6.19998900	-
0.81684800			
C	3.15419600	-3.45727600	-
0.61731700			
C	3.28479900	-4.26014700	
0.52700000			
C	4.01219900	-3.69367900	-
1.70243200			
C	4.24890700	-5.26682400	
0.58860800			
H	2.62014100	-4.08565000	
1.36787900			
C	4.97804500	-4.69933600	-
1.64235900			
H	3.91258800	-3.08236900	-
2.59479700			
C	5.10050300	-5.48849200	-
0.49626800			
H	4.33622900	-5.87703800	
1.48397300			
H	5.63098900	-4.87043400	-
2.49417600			
H	5.85177700	-6.27229700	-
0.45018300			
³INT8			
Fe	-0.27103600	0.11222100	-
0.52107800			
N	-2.27637500	0.08490400	-
0.38293700			
C	2.18468000	-2.30528600	-
0.69279700			
C	-2.69188600	-2.35561300	-
0.48579500			
C	-0.92247300	-4.11569900	-
0.70588700			
C	0.43739300	-4.10265300	-
0.72802800			
C	-1.35343700	-2.74554400	-
0.59040000			
C	0.84891100	-2.72224200	-
0.64513300			

H	1.10788900	-4.94438500	-
0.82043100			
H	-1.58123300	-4.96918600	-
0.76776500			
N	-0.28946700	2.11303400	-
0.49413200			
N	-0.25809400	-1.90113700	-
0.57027200			
N	1.72551400	0.12720700	-
0.76311500			
C	-2.71167100	2.51305400	-
0.17103900			
C	2.12761600	2.56980100	-
0.75859500			
C	3.92810300	0.83590500	-
0.84855900			
C	-4.46416300	-0.62676800	-
0.11252300			
C	0.35885100	4.33368900	-
0.59118300			
C	3.94650200	-0.52217100	-
0.80066800			
C	-4.46602200	0.72802500	-
0.00117500			
C	-0.98929000	4.31777800	-
0.42131300			
C	2.54416400	1.23773100	-
0.81519000			
C	-3.09983100	-1.02494400	-
0.35441600			
C	0.79289400	2.95833600	-
0.62211300			
C	2.57255200	-0.96264300	-
0.75809800			
C	-3.10501900	1.17010200	-
0.18605500			
C	-1.38864000	2.93182800	-
0.34779600			
H	4.80780900	-1.17283300	-
0.77778700			
H	-5.30609500	1.37644700	-
0.20160300			
H	-1.66273300	5.16011900	-
0.36333100			

H	4.76984100	1.51190700	-
0.87375100			
H	-5.29992900	-1.30457600	-
0.02110400			
H	1.00762600	5.19056200	-
0.69798900			
C	1.89628000	-1.50219200	
2.78276600			
C	1.30087000	-0.27559600	
2.45270800			
C	3.29131200	0.83072500	
2.53878900			
C	3.99175200	-0.32903200	
2.87265500			
C	3.27072600	-1.51717700	
2.99726600			
H	1.30782700	-2.41236500	
2.84127800			
H	3.81324500	1.77668400	
2.41047300			
H	5.06697700	-0.30181500	
3.01487100			
H	3.77307900	-2.44991800	
3.23635500			
N	-0.08631000	-0.14597400	
2.15229900			
N	1.97099700	0.86923100	
2.33576100			
N	-1.60568800	-1.91389400	
2.60227700			
N	-0.82147700	-1.11099100	
2.41885800			
C	-3.74083200	-3.41983400	-
0.45369300			
C	-4.65077500	-3.56125300	-
1.51176900			
C	-3.83881800	-4.28894700	
0.64381900			
C	-5.63373200	-4.55160700	-
1.47642400			
H	-4.57977500	-2.88892300	-
2.36229800			
C	-4.82156000	-5.27911000	
0.67938300			

H	-3.14207500	-4.17358300	
1.46900600			
C	-5.72117200	-5.41380700	-
0.38094700			
H	-6.32880100	-4.65135700	-
2.30599100			
H	-4.88800300	-5.94194400	
1.53822900			
H	-6.48652700	-6.18486200	-
0.35303900			
C	-3.76018900	3.55804100	
0.03497700			
C	-3.76621800	4.34046000	
1.20012800			
C	-4.75448300	3.78010700	-
0.93021300			
C	-4.74205700	5.31867500	
1.39596000			
H	-2.99910100	4.17273200	
1.95087500			
C	-5.73091200	4.75793300	-
0.73505900			
H	-4.75311000	3.18028900	-
1.83601700			
C	-5.72764800	5.53011200	
0.42894800			
H	-4.73436000	5.91286100	
2.30598600			
H	-6.49120300	4.91949700	-
1.49474200			
H	-6.48771100	6.29177900	
0.58115100			
C	3.17667200	3.63403400	-
0.75973800			
C	3.93047200	3.91469200	-
1.90814600			
C	3.43447800	4.36037300	
0.41372600			
C	4.92032900	4.89905400	-
1.88494400			
H	3.73414000	3.35535700	-
2.81865700			
C	4.42391100	5.34424500	
0.43735800			

H	2.84922600	4.14266600	
1.30317700			
C	5.16991900	5.61596600	-
0.71239100			
H	5.49385900	5.10815200	-
2.78418100			
H	4.61372400	5.89682500	
1.35390100			
H	5.94030000	6.38227700	-
0.69493000			
C	3.24850900	-3.35338100	-
0.66662800			
C	3.40981300	-4.17096700	
0.46343900			
C	4.10636700	-3.54684500	-
1.76041300			
C	4.40379400	-5.14925900	
0.50298100			
H	2.74477500	-4.03098800	
1.31020900			
C	5.10221300	-4.52388800	-
1.72221900			
H	3.98308200	-2.92479700	-
2.64233200			
C	5.25534500	-5.32742900	-
0.58993300			
H	4.51428700	-5.77125500	
1.38758900			
H	5.75457700	-4.66153800	-
2.58050100			
H	6.03004000	-6.08890500	-
0.56086300			
⁵INT8			
Fe	0.26639000	0.10295500	-
0.41558300			
N	2.33143800	-0.21153000	-
0.36242500			
C	-1.77074300	2.85978000	-
0.67314500			
C	3.06332500	2.14937100	-
0.21507700			
C	1.58320200	4.19763300	-
0.43196300			

C	0.23832200	4.39244100	-
0.55071600			
C	1.80343200	2.77005700	-
0.35452400			
C	-0.38389900	3.08752100	-
0.55662800			
H	-0.28522900	5.33275900	-
0.64566800			
H	2.35755300	4.95063300	-
0.41115100			
N	-0.03221600	-1.94783200	-
0.56934600			
N	0.59301500	2.12498300	-
0.45106300			
N	-1.76690900	0.38271500	-
0.77209400			
C	2.34020600	-2.68848700	-
0.42907800			
C	-2.50991500	-1.97587400	-
0.77034800			
C	-4.04308700	0.05010900	-
0.81058300			
C	4.58346800	0.12246100	-
0.02750600			
C	-1.00710600	-4.01590900	-
0.80404800			
C	-3.83279200	1.39543800	-
0.79684000			
C	4.38293900	-1.22273900	-
0.09528300			
C	0.34134100	-4.21151000	-
0.72548600			
C	-2.73941500	-0.58548100	-
0.80003100			
C	3.29175500	0.75705500	-
0.21003700			
C	-1.24065900	-2.59291100	-
0.70363700			
C	-2.39863700	1.60267600	-
0.76736500			
C	2.96507000	-1.43057800	-
0.31500600			
C	0.95335200	-2.91260100	-
0.56695400			

H	-4.57744000	2.17796700	-
0.78485800			
H	5.11988800	-2.00587100	
0.00764400			
H	0.87489300	-5.14897200	-
0.78423800			
H	-4.99130000	-0.46721800	-
0.80815800			
H	5.51577900	0.64139700	
0.14159100			
H	-1.77246400	-4.76538500	-
0.94486100			
C	-2.01482200	-1.37634400	
2.74659400			
C	-1.33542000	-0.20209700	
2.39712300			
C	-3.21201000	1.07344700	
2.58036700			
C	-3.99288400	-0.02491100	
2.94298500			
C	-3.37396000	-1.27248200	
3.02862100			
H	-1.50655700	-2.33517400	
2.76302000			
H	-3.65345800	2.06240700	
2.48073800			
H	-5.05377600	0.09394400	
3.13645200			
H	-3.94467700	-2.15937600	
3.28763000			
N	0.04408300	-0.19785000	
2.00944400			
N	-1.90377500	0.99685100	
2.31680200			
N	1.47110100	-1.99306400	
2.63556200			
N	0.73468100	-1.16984800	
2.37297200			
C	-2.66010100	4.06133900	-
0.63602300			
C	-3.41053300	4.44919300	-
1.75577600			
C	-2.76782800	4.81589200	
0.54321100			

C	-4.24883700	5.56399500	-
1.69892800			
H	-3.32983700	3.86971300	-
2.67121300			
C	-3.60597400	5.93023700	
0.60076900			
H	-2.18790700	4.51529600	
1.41160300			
C	-4.34919800	6.30744600	-
0.52057000			
H	-4.82024800	5.85407800	-
2.57681600			
H	-3.68051200	6.50225500	
1.52204400			
H	-5.00153100	7.17555000	-
0.47674700			
C	4.25306200	3.04226500	-
0.06626700			
C	4.38908200	3.87161500	
1.05834600			
C	5.25767700	3.07076100	-
1.04649500			
C	5.49877300	4.70580500	
1.19952700			
H	3.61677000	3.85331500	
1.82211800			
C	6.36805700	3.90416500	-
0.90599800			
H	5.15754600	2.43498500	-
1.92165000			
C	6.49218900	4.72452100	
0.21774000			
H	5.58924200	5.33774000	
2.07918900			
H	7.13364000	3.91616400	-
1.67739100			
H	7.35664700	5.37390500	
0.32735400			
C	3.22247700	-3.89496100	-
0.37088700			
C	3.15206500	-4.77688000	
0.71874400			
C	4.13977100	-4.16453100	-
1.39785000			

C	3.97631000	-5.90131700	
0.77832600			
H	2.45033000	-4.56606700	
1.52044800			
C	4.96439400	-5.28901100	-
1.33896400			
H	4.19859400	-3.48514000	-
2.24358200			
C	4.88453500	-6.16118500	-
0.25080600			
H	3.91282800	-6.57159700	
1.63162600			
H	5.66626100	-5.48558100	-
2.14521100			
H	5.52651600	-7.03684700	-
0.20460200			
C	-3.70487800	-2.87185100	-
0.79014800			
C	-4.58449300	-2.88689800	-
1.88420900			
C	-3.97701000	-3.71806600	
0.29741600			
C	-5.70526500	-3.71835900	-
1.88835800			
H	-4.37826200	-2.24192500	-
2.73351700			
C	-5.09615600	-4.55097300	
0.29457700			
H	-3.29945100	-3.71388900	
1.14596000			
C	-5.96577700	-4.55259700	-
0.79866500			
H	-6.37179500	-3.71908100	-
2.74682400			
H	-5.29064200	-5.19693200	
1.14700200			
H	-6.83790700	-5.20086100	-
0.80264000			
cssTS8			
Fe	-0.21856400	0.06531000	-
0.32356300			
N	-0.83201600	1.98424400	-
0.42996200			

C	-1.82183300	-2.97287700	-
0.32362500			
C	-3.27887800	1.67581300	-
0.38212100			
C	-4.43501800	-0.53118000	-
0.65601300			
C	-4.02963500	-1.82840600	-
0.63104800			
C	-3.25517700	0.28231100	-
0.49698600			
C	-2.59769600	-1.81815000	-
0.46755200			
H	-4.63494700	-2.71784400	-
0.72610300			
H	-5.43801400	-0.14955700	-
0.77657900			
N	1.65362700	0.65438600	-
0.71541900			
N	-2.12765500	-0.51829100	-
0.43328200			
N	0.36580300	-1.84339900	-
0.54094300			
C	1.36594700	3.09994900	-
0.46936200			
C	2.79862300	-1.53283500	-
0.84980400			
C	1.68990100	-3.73497900	-
0.37994200			
C	-2.11395400	3.87753400	-
0.05945700			
C	3.92188700	0.68360900	-
1.18754200			
C	0.40237300	-4.13320600	-
0.19067100			
C	-0.81389400	4.27131700	-
0.05963100			
C	3.52417400	1.97613800	-
1.05210200			
C	1.66047000	-2.31226700	-
0.61353800			
C	-2.11982400	2.45246600	-
0.29923100			
C	2.76337600	-0.13968800	-
0.93639500			

C	-0.42380900	-2.95857800	-
0.32766300			
C	-0.01972300	3.09174800	-
0.31267200			
C	2.11707900	1.95197100	-
0.73672100			
H	0.03717100	-5.12959200	
0.01013900			
H	-0.41749200	5.26422700	
0.09386300			
H	4.11545000	2.87259200	-
1.16883500			
H	2.58334700	-4.34138600	-
0.35773300			
H	-2.99407300	4.48387700	
0.09601900			
H	4.90451100	0.31094400	-
1.43621800			
C	1.67492400	-1.38548900	
2.42916900			
C	1.20877100	-0.10625300	
2.09175700			
C	3.14475500	0.88413800	
2.79411600			
C	3.69932500	-0.33495700	
3.18861100			
C	2.93764100	-1.49032200	
3.00463200			
H	1.07857700	-2.26296400	
2.20968300			
H	3.70649700	1.80944300	
2.90901200			
H	4.69443800	-0.37401800	
3.62078000			
H	3.33101700	-2.46568300	
3.27707800			
N	-0.07053300	0.14554500	
1.49781100			
N	1.91826600	1.01042400	
2.27862200			
N	-2.18613600	-0.93345600	
2.43025800			
N	-1.08017000	-0.80971800	
2.25414500			

C	-4.60295200	2.36298200	-
0.32415000			
C	-4.98385200	3.27143800	-
1.32412700			
C	-5.49057600	2.11652700	
0.73529900			
C	-6.22046400	3.91543800	-
1.26760000			
H	-4.30209800	3.46540400	-
2.14736500			
C	-6.72659100	2.76120000	
0.79305500			
H	-5.19931800	1.41719800	
1.51387100			
C	-7.09551100	3.66233400	-
0.20861400			
H	-6.50175600	4.61181200	-
2.05317300			
H	-7.39945500	2.56282400	
1.62316900			
H	-8.05837300	4.16421100	-
0.16407900			
C	2.09616300	4.39506700	-
0.33090900			
C	2.94514400	4.59790100	
0.76790600			
C	1.95537600	5.42015300	-
1.27733700			
C	3.63790300	5.79968200	
0.91658300			
H	3.04050000	3.80540800	
1.50448200			
C	2.65052100	6.62183300	-
1.13009900			
H	1.30035700	5.26571400	-
2.13026800			
C	3.49350200	6.81443800	-
0.03309500			
H	4.28750900	5.94584300	
1.77571400			
H	2.53595000	7.40582200	-
1.87406300			
H	4.03406000	7.75023900	
0.08159700			

C	4.11712200	-2.22358300	-
0.96412200			
C	4.37099100	-3.12025100	-
2.01350200			
C	5.12448100	-1.99623800	-
0.01265300			
C	5.60114100	-3.77196700	-
2.11111900			
H	3.59580500	-3.29918600	-
2.75326100			
C	6.35386000	-2.64895500	-
0.10954700			
H	4.92882200	-1.30773900	
0.80373900			
C	6.59631700	-3.53860000	-
1.15900600			
H	5.78340000	-4.45876900	-
2.93346800			
H	7.12199800	-2.46497800	
0.63729000			
H	7.55424400	-4.04617000	-
1.23485200			
C	-2.52719600	-4.27997200	-
0.17165900			
C	-3.34240100	-4.51611500	
0.94692200			
C	-2.39755400	-5.29121700	-
1.13635700			
C	-4.00649900	-5.73369000	
1.09923800			
H	-3.44765300	-3.73549400	
1.69513400			
C	-3.06321400	-6.50835800	-
0.98542700			
H	-1.77406900	-5.11184300	-
2.00759900			
C	-3.86867300	-6.73359100	
0.13345200			
H	-4.62962200	-5.90196900	
1.97364400			
H	-2.95667600	-7.27859300	-
1.74474800			
H	-4.38681800	-7.68156000	
0.25109900			

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Fe	-0.24294800	0.05755700	-
0.33543600			
N	-1.10373400	1.85363300	-
0.48991400			
C	-1.39354100	-3.15524400	-
0.21030000			
C	-3.49271900	1.22041000	-
0.55038500			
C	-4.32190100	-1.13832000	-
0.69644300			
C	-3.74044300	-2.35785800	-
0.54817800			
C	-3.27272800	-0.15686200	-
0.58956500			
C	-2.32757300	-2.13165300	-
0.38705700			
H	-4.21107300	-3.32973500	-
0.57089800			
H	-5.36507100	-0.91310900	-
0.86066200			
N	1.52921400	0.90214000	-
0.75025800			
N	-2.04549200	-0.78233500	-
0.45036800			
N	0.58957300	-1.73734900	-
0.62685500			
C	0.92064000	3.25869800	-
0.34078700			
C	2.94814100	-1.09706300	-
1.03144600			
C	2.17560900	-3.41851300	-
0.51433500			
C	-2.64828400	3.54225400	-
0.14417200			
C	3.76426600	1.26389000	-
1.23963000			
C	0.97285400	-3.98446900	-
0.21836900			
C	-1.41375100	4.10129600	-
0.02476700			
C	3.20708100	2.47738600	-
0.98563500			

C	1.93528300	-2.02234100	-
0.76125000			
C	-2.45125100	2.14312100	-
0.42292400			
C	2.72782700	0.27991900	-
1.04172200			
C	-0.01734600	-2.94557700	-
0.32165900			
C	-0.45497000	3.05574000	-
0.26775200			
C	1.82008700	2.24306200	-
0.67177200			
H	0.76727000	-5.01330900	
0.03734900			
H	-1.16526800	5.12814000	
0.19950000			
H	3.67332100	3.45098600	-
1.02676400			
H	3.14570600	-3.89228500	-
0.54167900			
H	-3.61028400	4.01985000	-
0.03103100			
H	4.78133600	1.04225200	-
1.52688300			
C	1.79146000	-1.32232600	
2.40073400			
C	1.28396700	-0.06024800	
2.04711900			
C	3.25016500	0.96522700	
2.63127100			
C	3.84134600	-0.23728400	
3.02271800			
C	3.08411900	-1.40511600	
2.90578100			
H	1.18636600	-2.20799700	
2.24720500			
H	3.80635300	1.89938600	
2.69515500			
H	4.85860400	-0.25504100	
3.40225800			
H	3.50246500	-2.36977400	
3.18007600			
N	-0.02351200	0.10793200	
1.51151600			

N	1.99802100	1.06726600	
2.17446200			
N	-2.13594300	-0.79235500	
2.35420000			
N	-0.99061800	-0.68859300	
2.42768700			
C	-4.89471400	1.73033600	-
0.57204500			
C	-5.33752300	2.55538600	-
1.61750500			
C	-5.79010200	1.40713700	
0.46000800			
C	-6.64595600	3.04004000	-
1.63507500			
H	-4.64777600	2.81029400	-
2.41727800			
C	-7.09761100	1.89365200	
0.44324200			
H	-5.44738100	0.77748300	
1.27606900			
C	-7.52968000	2.71014800	-
0.60482500			
H	-6.97549000	3.67266700	-
2.45500200			
H	-7.77712100	1.63922100	
1.25229600			
H	-8.54834700	3.08840800	-
0.61771700			
C	1.47951800	4.60673300	-
0.03114600			
C	2.23949600	4.76934600	
1.13792800			
C	1.27438400	5.70913700	-
0.87215300			
C	2.78113100	6.01423700	
1.45884000			
H	2.37738800	3.91051200	
1.78916500			
C	1.82081600	6.95336400	-
0.55150000			
H	0.69047600	5.58269000	-
1.77970500			
C	2.57482900	7.10835800	
0.61413700			

H	3.36171300	6.13154500	
2.37016900			
H	1.66030600	7.79998300	-
1.21381600			
H	2.99893700	8.07743500	
0.86338600			
C	4.33587800	-1.60953200	-
1.23075300			
C	4.64884600	-2.40868500	-
2.34075800			
C	5.34545100	-1.31690500	-
0.30025700			
C	5.94325100	-2.89816100	-
2.52128200			
H	3.86966000	-2.63998900	-
3.06168300			
C	6.63875800	-1.80858300	-
0.48018300			
H	5.10063300	-0.71110000	
0.56688800			
C	6.94189800	-2.59915700	-
1.59145400			
H	6.17188800	-3.51044100	-
3.38955300			
H	7.40928100	-1.57778000	
0.25090000			
H	7.94966700	-2.98094100	-
1.73144600			
C	-1.90459600	-4.52569700	
0.08241700			
C	-2.62134800	-4.75984000	
1.26716500			
C	-1.69855900	-5.59216200	-
0.80624500			
C	-3.11191000	-6.03280700	
1.55928200			
H	-2.78490500	-3.93417800	
1.95417100			
C	-2.19197900	-6.86452800	-
0.51465000			
H	-1.15564500	-5.41338200	-
1.73002100			
C	-2.89821800	-7.08859700	
0.66963200			

H	-3.65958000	-6.19995200	
2.48291700			
H	-2.02989700	-7.67909100	-
1.21560300			
H	-3.28183300	-8.07969600	
0.89655100			
³TS8			
Fe	-0.20312900	0.08559900	-
0.30800400			
N	-2.03258900	0.87867900	-
0.34982900			
C	1.01147500	-3.08352100	-
0.28203800			
C	-3.42723400	-1.12994300	-
0.73542300			
C	-2.53001600	-3.47643000	-
0.73550900			
C	-1.30313000	-4.01838900	-
0.50455300			
C	-2.37175300	-2.04436700	-
0.69032500			
C	-0.37615400	-2.92121400	-
0.38004800			
H	-1.03155900	-5.06332900	-
0.46626600			
H	-3.46308900	-3.99109500	-
0.91079700			
N	0.57102800	1.88842700	-
0.54442100			
N	-1.04188600	-1.72190200	-
0.50360600			
N	1.56325300	-0.72030700	-
0.74241800			
C	-1.41140100	3.22375600	
0.09775700			
C	2.89688900	1.32570000	-
1.14576000			
C	3.85296100	-0.97547800	-
0.91835600			
C	-4.32700100	1.14957000	-
0.23192000			
C	2.00912100	3.66140500	-
0.90012700			

C	3.34013300	-2.19126800	-
0.58510400			
C	-3.76478000	2.34098700	
0.10904700			
C	0.83335600	4.18244700	-
0.45862400			
C	2.74725700	-0.05561700	-
0.98883000			
C	-3.24706200	0.23422300	-
0.49416200			
C	1.85837200	2.22713400	-
0.90468800			
C	1.91027700	-2.03840000	-
0.50691400			
C	-2.33716100	2.18140200	-
0.00750600			
C	-0.06431200	3.07397900	-
0.24598900			
H	3.87621200	-3.11210700	-
0.41029100			
H	-4.26544100	3.25272000	
0.39925700			
H	0.57236600	5.22202400	-
0.32488500			
H	4.88939900	-0.70806300	-
1.06137900			
H	-5.37532300	0.89181600	-
0.26436800			
H	2.90306500	4.19207600	-
1.19200500			
C	1.44643800	-1.42549300	
2.93352100			
C	1.21112300	-0.25519800	
2.18112500			
C	3.36898000	0.45467700	
2.51528400			
C	3.69702000	-0.66052100	
3.28474700			
C	2.69976000	-1.61573200	
3.49929800			
H	0.66012200	-2.16229200	
3.04676400			
H	4.11710300	1.21860600	
2.30795000			

H	4.69566300	-0.77775100	
3.69355900			
H	2.90434100	-2.51252500	
4.07843200			
N	-0.01774500	-0.00868600	
1.54376600			
N	2.15965800	0.67594000	
1.99075000			
N	-2.30090900	-0.71519600	
2.22479800			
N	-1.19195000	-0.59964300	
2.47531600			
C	-4.82060700	-1.63290300	-
0.91919800			
C	-5.54822400	-1.29855400	-
2.07090000			
C	-5.43479800	-2.42266000	
0.06511400			
C	-6.85696900	-1.75290400	-
2.24079100			
H	-5.07867100	-0.68177800	-
2.83222200			
C	-6.74347300	-2.87602100	-
0.10461600			
H	-4.87940500	-2.66648900	
0.96605100			
C	-7.45740000	-2.54403300	-
1.25874100			
H	-7.40628700	-1.49014900	-
3.14097200			
H	-7.20780400	-3.48275000	
0.66830800			
H	-8.47668600	-2.89714000	-
1.39036800			
C	-1.87941000	4.58176500	
0.50534300			
C	-1.42776300	5.14012500	
1.71108300			
C	-2.74673400	5.33130200	-
0.30407000			
C	-1.84279100	6.41342900	
2.10324900			
H	-0.75170600	4.56474400	
2.33723700			

C	-3.16051900	6.60523600	
0.08757900			
H	-3.08771800	4.91012100	-
1.24559300			
C	-2.71099000	7.14906700	
1.29318500			
H	-1.48887800	6.82969200	
3.04267000			
H	-3.82897400	7.17507300	-
0.55242900			
H	-3.03342600	8.14103800	
1.59807000			
C	4.25933700	1.85039200	-
1.45438300			
C	4.87563700	1.55601400	-
2.67995300			
C	4.96169700	2.62011000	-
0.51321200			
C	6.15950300	2.02550800	-
2.96138000			
H	4.33870400	0.95688300	-
3.41009200			
C	6.24539700	3.08885200	-
0.79391600			
H	4.48965500	2.84383300	
0.43909500			
C	6.84784200	2.79350600	-
2.01941300			
H	6.62059200	1.79334100	-
3.91772600			
H	6.77722100	3.68009900	-
0.05310500			
H	7.84777800	3.15839700	-
2.23818700			
C	1.53612300	-4.45192400	-
0.00036500			
C	1.27894600	-5.05396000	
1.24110800			
C	2.27128400	-5.16806800	-
0.95737500			
C	1.75376100	-6.33512100	
1.52335900			
H	0.70609000	-4.50510400	
1.98303000			

C	2.74603000	-6.44987700	-
0.67602400			
H	2.46134300	-4.71373800	-
1.92558300			
C	2.49014700	-7.03643600	
0.56565300			
H	1.54982700	-6.78472600	
2.49157200			
H	3.31008800	-6.99281400	-
1.42977900			
H	2.85961100	-8.03470000	
0.78426900			

⁵TS8

Fe	-0.20690100	0.09101400	-
0.11433800			
N	-2.27051800	0.29116700	-
0.33667300			
C	1.91617700	-2.58787000	-
0.68349800			
C	-2.94064300	-2.09361500	-
0.50968800			
C	-1.37582900	-4.06205400	-
0.73012000			
C	-0.02062800	-4.20184300	-
0.73905900			
C	-1.65500700	-2.64945300	-
0.60539700			
C	0.54160600	-2.87412200	-
0.64583600			
H	0.55271200	-5.11304100	-
0.83027300			
H	-2.12346400	-4.83807200	-
0.80604300			
N	-0.05088300	2.12329500	-
0.48552300			
N	-0.47265700	-1.94741300	-
0.57246100			
N	1.74595300	-0.11706900	-
0.82169900			
C	-2.42046900	2.76023700	-
0.14463700			
C	2.39086800	2.27758300	-
0.86282700			

C	4.00101000	0.34568600	-
0.92507600			
C	-4.52376100	-0.17130200	-
0.16310000			
C	0.81982300	4.24305300	-
0.71134000			
C	3.87250000	-1.00782400	-
0.83736100			
C	-4.37747800	1.17557700	-
0.01951300			
C	-0.51805200	4.37897200	-
0.49453500			
C	2.67056700	0.90236200	-
0.89950700			
C	-3.20741800	-0.72399000	-
0.36334500			
C	1.11205800	2.82885400	-
0.69247300			
C	2.46039600	-1.29711500	-
0.78082700			
C	-2.97104300	1.46788100	-
0.15369900			
C	-1.06066700	3.04850700	-
0.34790500			
H	4.66017500	-1.74579500	-
0.80181900			
H	-5.15031300	1.90830900	
0.15989700			
H	-1.09420900	5.29188000	-
0.45792000			
H	4.91434800	0.92020400	-
0.97015400			
H	-5.43685900	-0.74645500	-
0.11829900			
H	1.54502800	5.02434100	-
0.88599900			
C	1.79245800	-1.42821000	
2.97344000			
C	1.31818300	-0.25833000	
2.34117300			
C	3.37442800	0.75056200	
2.53588600			
C	3.93568500	-0.35084000	
3.17914500			

C	3.11230400	-1.45833500	
3.40324200			
H	1.13938500	-2.28370200	
3.09797000			
H	3.97606600	1.63236100	
2.32030900			
H	4.97669000	-0.34366400	
3.48567300			
H	3.50290600	-2.34909900	
3.88871700			
N	0.03058200	-0.12671700	
1.80149800			
N	2.09832200	0.81831300	
2.14312200			
N	-2.09479800	-1.22200700	
2.47545100			
N	-0.96689300	-1.09716000	
2.60392600			
C	-4.10590600	-3.03035000	-
0.51303800			
C	-4.99079000	-3.07070800	-
1.60040100			
C	-4.33524000	-3.87987100	
0.57987200			
C	-6.07920700	-3.94464400	-
1.59770300			
H	-4.81694400	-2.41359100	-
2.44801500			
C	-5.42354300	-4.75335600	
0.58262300			
H	-3.65834200	-3.83979000	
1.42837800			
C	-6.29771000	-4.78882300	-
0.50654400			
H	-6.75405300	-3.96797200	-
2.44928700			
H	-5.59154500	-5.40211400	
1.43820700			
H	-7.14516800	-5.46909700	-
0.50419700			
C	-3.34501500	3.91788200	
0.05569900			
C	-3.24776600	4.70830700	
1.21119300			

C	-4.31380200	4.24381900	-
0.90581700			
C	-4.10201700	5.79505900	
1.40288400			
H	-2.49866200	4.46055900	
1.95795200			
C	-5.16762300	5.33097200	-
0.71477800			
H	-4.38866500	3.63977600	-
1.80567100			
C	-5.06453900	6.10924200	
0.44061800			
H	-4.01727500	6.39406600	
2.30568900			
H	-5.90970100	5.57271900	-
1.47109400			
H	-5.72946900	6.95575000	
0.58955500			
C	3.54789700	3.21991800	-
0.92395400			
C	4.32774800	3.34345300	-
2.08302100			
C	3.88203200	3.98816300	
0.20308200			
C	5.41707700	4.21578400	-
2.11578100			
H	4.07199100	2.75181900	-
2.95761300			
C	4.97197800	4.85875300	
0.17057800			
H	3.27893200	3.88915600	
1.10140000			
C	5.74236200	4.97504400	-
0.98929300			
H	6.00924500	4.30470500	-
3.02274500			
H	5.22134200	5.44363700	
1.05201800			
H	6.59087100	5.65347700	-
1.01524700			
C	2.86059700	-3.74393300	-
0.61704000			
C	2.96382000	-4.49464800	
0.56409100			

C	3.65359200	-4.10188900	-
1.71731900			
C	3.84090200	-5.57682300	
0.64393200			
H	2.35633900	-4.21327000	
1.41948400			
C	4.53047500	-5.18495500	-
1.63826100			
H	3.57373200	-3.52635100	-
2.63526900			
C	4.62651800	-5.92515800	-
0.45749900			
H	3.91304700	-6.14600600	
1.56703200			
H	5.13494500	-5.45314700	-
2.50069500			
H	5.30912900	-6.76847300	-
0.39624200			
CSSINT9			
Fe	0.26693100	0.00209500	-
0.20426400			
N	2.01444200	1.01314100	-
0.22769700			
C	-0.58716300	-3.28873200	-
0.30105100			
C	3.62037400	-0.84647000	-
0.44147400			
C	2.98911100	-3.26160200	-
0.57186200			
C	1.82139300	-3.94465900	-
0.44075800			
C	2.66226700	-1.85750500	-
0.53787900			
C	0.76581200	-2.96661900	-
0.39859000			
H	1.67427900	-5.01361200	-
0.39385600			
H	3.98862800	-3.66148100	-
0.65541200			
N	-0.67795700	1.70051900	-
0.59235000			
N	1.29117700	-1.69081900	-
0.48753500			

N	-1.41618300	-0.99648900	-
0.64713700			
C	1.13188900	3.29613700	
0.00625600			
C	-2.96696600	0.87119300	-
1.05762000			
C	-3.65889400	-1.53011900	-
0.86811200			
C	4.25335300	1.52687500	
0.05745300			
C	-2.32518900	3.28216100	-
0.96602200			
C	-2.99760900	-2.68620200	-
0.59630600			
C	3.55408400	2.67550100	
0.25263000			
C	-1.19825500	3.95592400	-
0.60820100			
C	-2.67062700	-0.47912900	-
0.88644900			
C	3.28782900	0.49370600	-
0.23565100			
C	-2.01226000	1.87920500	-
0.91421200			
C	-1.60115400	-2.34838000	-
0.47372800			
C	2.16239400	2.35638500	
0.03776200			
C	-0.17588000	2.97202100	-
0.36635200			
H	-3.39969900	-3.68491200	-
0.50786700			
H	3.93541800	3.65484400	
0.50138500			
H	-1.05454800	5.02381000	-
0.53436100			
H	-4.71602700	-1.38562800	-
1.03636100			
H	5.32097100	1.37545800	
0.11998200			
H	-3.28898700	3.68874700	-
1.23472600			
N	0.10789700	-0.06163300	
1.46232500			

C	-1.14563900	-0.11541200	
2.06813700			
C	-1.87912500	1.07054300	
2.29508500			
C	-2.72448500	-1.37754400	
3.15249600			
C	-3.07655100	0.98206600	
2.99256400			
H	-1.50273600	2.01493800	
1.92029200			
C	-3.52540300	-0.26828800	
3.42746900			
H	-3.03750400	-2.37149800	
3.46983400			
H	-3.66021900	1.87925800	
3.18473400			
H	-4.46246400	-0.38219700	
3.96293800			
N	-1.55508900	-1.32324800	
2.50748700			
C	5.06927000	-1.21153300	-
0.48719300			
C	5.86222500	-0.81772800	-
1.57528300			
C	5.66594700	-1.93095400	
0.55932600			
C	7.21904200	-1.14206200	-
1.62024100			
H	5.40580600	-0.25620300	-
2.38576300			
C	7.02267200	-2.25476800	
0.51501700			
H	5.05763900	-2.22968100	
1.40828700			
C	7.80264300	-1.86209900	-
0.57538500			
H	7.81904700	-0.83379700	-
2.47234900			
H	7.47111200	-2.80922000	
1.33510700			
H	8.85915000	-2.11416800	-
0.60960300			
C	1.44125500	4.72520200	
0.31356600			

C	0.91599500	5.32735000	
1.46685900			
C	2.24431900	5.49304700	-
0.54319800			
C	1.19190700	6.66344800	
1.76018800			
H	0.29320900	4.73708900	
2.13333500			
C	2.51994200	6.82959300	-
0.25087900			
H	2.64701900	5.03402000	-
1.44168600			
C	1.99505700	7.41819500	
0.90202400			
H	0.78209100	7.11352700	
2.66048600			
H	3.14067000	7.41201200	-
0.92657800			
H	2.20984400	8.45879700	
1.12974100			
C	-4.38826900	1.25541000	-
1.31430400			
C	-4.98052600	1.01378400	-
2.56165900			
C	-5.15730600	1.84428500	-
0.29953300			
C	-6.31289900	1.36106400	-
2.79281600			
H	-4.38894200	0.55317800	-
3.34800800			
C	-6.48911500	2.19064700	-
0.53006400			
H	-4.70149100	2.01603100	
0.67130900			
C	-7.06981000	1.95115600	-
1.77810200			
H	-6.75840700	1.17195000	-
3.76585500			
H	-7.07487100	2.64283400	
0.26601200			
H	-8.10703400	2.22086600	-
1.95796900			
C	-0.98461700	-4.69350300	
0.01251600			

C	-1.46891500	-4.98017000	
1.29808200			
C	-0.90196700	-5.72281300	-
0.93440500			
C	-1.85919200	-6.27825600	
1.62918800			
H	-1.52180100	-4.17290700	
2.02399400			
C	-1.29355400	-7.02116300	-
0.60091000			
H	-0.53463400	-5.49894800	-
1.93231400			
C	-1.77260800	-7.30119500	
0.68094300			
H	-2.22865400	-6.49208100	
2.62878300			
H	-1.22843100	-7.81191000	-
1.34369200			
H	-2.07746600	-8.31182400	
0.93944900			

ossINT9

Fe	0.28114700	-0.00522300	-
0.26509100			
N	2.05523000	0.94143500	-
0.29491500			
C	-0.69415200	-3.26086100	-
0.31491000			
C	3.60261300	-0.98705000	-
0.42495600			
C	2.88798200	-3.39053500	-
0.43596400			
C	1.69060600	-4.02275000	-
0.31766200			
C	2.61454300	-1.97333600	-
0.45598700			
C	0.67501900	-2.99990000	-
0.33342800			
H	1.49743000	-5.08358600	-
0.25328500			
H	3.87209000	-3.83193400	-
0.48799900			
N	-0.63551600	1.75100700	-
0.53159600			

N	1.25332800	-1.75203500	-
0.42715600			
N	-1.42545400	-0.93363100	-
0.71400000			
C	1.25700300	3.26155100	-
0.00446100			
C	-2.93517200	0.99790900	-
1.03613700			
C	-3.68246700	-1.38742100	-
0.96410400			
C	4.31507700	1.37906200	-
0.04380700			
C	-2.23795100	3.39367200	-
0.82568400			
C	-3.06181100	-2.56966800	-
0.70632900			
C	3.65830100	2.55482400	
0.14090600			
C	-1.08085100	4.02088400	-
0.48004900			
C	-2.66540800	-0.36701700	-
0.94290200			
C	3.31289100	0.37390000	-
0.29649900			
C	-1.96424800	1.98007200	-
0.82895300			
C	-1.65957300	-2.28244800	-
0.55113500			
C	2.25350000	2.28346100	-
0.03904400			
C	-0.08365300	2.99564900	-
0.29956200			
H	-3.49947900	-3.55460200	-
0.63393400			
H	4.07844600	3.52197600	
0.37397800			
H	-0.89997500	5.08141600	-
0.38449800			
H	-4.73355800	-1.20677200	-
1.13438100			
H	5.37725400	1.19231700	
0.01358500			
H	-3.19342400	3.83851200	-
1.06159600			

N	0.09819100	-0.08983800	
1.53516700			
C	-1.17057700	-0.10435500	
2.09009600			
C	-1.83862400	1.11353300	
2.35804100			
C	-2.88787500	-1.32011800	
3.00782400			
C	-3.07790700	1.06407800	
2.98065600			
H	-1.38102500	2.05128300	
2.06480300			
C	-3.63030300	-0.17767000	
3.31028100			
H	-3.28155900	-2.30778800	
3.24504900			
H	-3.61246100	1.98530400	
3.19996700			
H	-4.60219600	-0.26002700	
3.78610300			
N	-1.68555900	-1.30699900	
2.42517300			
C	5.03850200	-1.40033500	-
0.45714500			
C	5.84054900	-1.08252200	-
1.56345000			
C	5.61409300	-2.09412600	
0.61819700			
C	7.18504200	-1.45551700	-
1.59741400			
H	5.40065100	-0.54171400	-
2.39683400			
C	6.95850800	-2.46684900	
0.58469000			
H	4.99934600	-2.33396600	
1.48108000			
C	7.74743400	-2.14941100	-
0.52359100			
H	7.79194500	-1.20595000	-
2.46373200			
H	7.39057100	-3.00042100	
1.42711900			
H	8.79437600	-2.43950100	-
0.54936400			

C	1.63853100	4.67365200	
0.30053400			
C	1.19776800	5.28261100	
1.48523600			
C	2.42444400	5.42032700	-
0.59033400			
C	1.53926400	6.60416900	
1.77555300			
H	0.58871600	4.70895500	
2.17835500			
C	2.76584500	6.74217900	-
0.30091700			
H	2.76175000	4.95644200	-
1.51295400			
C	2.32472400	7.33755100	
0.88322900			
H	1.19448800	7.05937600	
2.70020500			
H	3.37215100	7.30818000	-
1.00314600			
H	2.59068300	8.36676600	
1.10865500			
C	-4.34654100	1.42372900	-
1.27985400			
C	-4.94341000	1.23767600	-
2.53482400			
C	-5.10181400	2.00029400	-
0.24766800			
C	-6.26588000	1.62646200	-
2.75574300			
H	-4.36270500	0.78760400	-
3.33526800			
C	-6.42376300	2.38843500	-
0.46817100			
H	-4.64350400	2.12884800	
0.72848700			
C	-7.00883100	2.20369000	-
1.72339600			
H	-6.71446200	1.48030500	-
3.73475700			
H	-6.99869400	2.83024000	
0.34152800			
H	-8.03839700	2.50592300	-
1.89535600			

C	-1.16434300	-4.64454100	-
0.00449900			
C	-1.67981500	-4.90464400	
1.27443700			
C	-1.11342400	-5.67889200	-
0.94770400			
C	-2.13422900	-6.18258700	
1.60217500			
H	-1.70545300	-4.09317800	
1.99710100			
C	-1.56950200	-6.95709500	-
0.61754800			
H	-0.71929000	-5.47520100	-
1.93971500			
C	-2.08061600	-7.21099500	
0.65729100			
H	-2.52811000	-6.37665600	
2.59648800			
H	-1.52844600	-7.75245000	-
1.35713500			
H	-2.43551500	-8.20584200	
0.91322500			

³INT9

Fe	0.26480100	0.01486200	-
0.24158600			
N	2.22522400	0.47854400	-
0.30553000			
C	-1.51762100	-2.88593400	-
0.49783100			
C	3.21585200	-1.79173000	-
0.40422800			
C	1.90997200	-3.92541900	-
0.56061900			
C	0.58736900	-4.23099300	-
0.52533400			
C	2.00886700	-2.48597100	-
0.48740000			
C	-0.12712000	-2.97919900	-
0.47549700			
H	0.12153900	-5.20489700	-
0.56412000			
H	2.74978500	-4.60058200	-
0.63000200			

N	-0.16163200	1.97337800	-
0.44855500			
N	0.75074000	-1.92126300	-
0.46937000			
N	-1.61045800	-0.42679300	-
0.76408100			
C	2.07602300	2.93222900	-
0.01196500			
C	-2.58696200	1.85128600	-
0.88984800			
C	-3.91685900	-0.25616700	-
0.91242800			
C	4.51603500	0.30171000	-
0.00390100			
C	-1.29042600	3.98381700	-
0.67248800			
C	-3.62367000	-1.57509400	-
0.76052000			
C	4.19460700	1.61351400	
0.14869100			
C	0.00465300	4.28338700	-
0.39013700			
C	-2.66868400	0.45920200	-
0.88883700			
C	3.28860600	-0.40258300	-
0.27274500			
C	-1.39279500	2.54508000	-
0.68801500			
C	-2.19314300	-1.68092000	-
0.67337400			
C	2.77287000	1.72303600	-
0.05375400			
C	0.70425700	3.02947600	-
0.25021000			
H	-4.30841000	-2.40801900	-
0.70307700			
H	4.85288900	2.43701600	
0.38207000			
H	0.46287300	5.25824300	-
0.31242800			
H	-4.88969800	0.20429100	-
0.99956200			
H	5.48794700	-0.16073500	
0.08382100			

H	-2.10639700	4.66393800	-
0.86753000			
N	0.01444500	-0.04246500	
1.47446600			
C	-1.20243300	-0.16329800	
2.10700800			
C	-1.92937500	1.00491600	
2.44090400			
C	-2.81872600	-1.50173100	
3.04219400			
C	-3.14738300	0.87050300	
3.09210400			
H	-1.52523800	1.97198100	
2.16309600			
C	-3.61380000	-0.41103400	
3.40065500			
H	-3.15109600	-2.51605000	
3.26031500			
H	-3.73166400	1.75051700	
3.34967800			
H	-4.56388200	-0.56370000	
3.90299500			
N	-1.64277300	-1.40413300	
2.41591500			
C	4.49247800	-2.56833400	-
0.40587000			
C	5.39370900	-2.45010200	-
1.47468200			
C	4.81762600	-3.41901300	
0.66169900			
C	6.58964700	-3.16936300	-
1.47896000			
H	5.14758600	-1.79086000	-
2.30247100			
C	6.01401500	-4.13737000	
0.65821400			
H	4.12595100	-3.50830300	
1.49450400			
C	6.90288800	-4.01526700	-
0.41247700			
H	7.27490200	-3.07079200	-
2.31670700			
H	6.25347900	-4.78875600	
1.49452400			

H	7.83438600	-4.57492200	-
0.41511300			
C	2.83314200	4.19135200	
0.25987100			
C	2.60607500	4.91214200	
1.44205800			
C	3.77107300	4.68231700	-
0.66107400			
C	3.30352000	6.09311900	
1.69965800			
H	1.88075300	4.53579200	
2.15790500			
C	4.46790000	5.86384700	-
0.40444800			
H	3.94655200	4.13110900	-
1.58063700			
C	4.23648300	6.57220500	
0.77707700			
H	3.12027400	6.63681700	
2.62263600			
H	5.18810100	6.23308300	-
1.12976200			
H	4.77940100	7.49202700	
0.97718400			
C	-3.84915200	2.63414200	-
1.05091200			
C	-4.53450900	2.64565900	-
2.27444800			
C	-4.37630400	3.36206700	
0.02655900			
C	-5.71772800	3.37194700	-
2.41887900			
H	-4.13117200	2.08177600	-
3.11092600			
C	-5.55919400	4.08797000	-
0.11684200			
H	-3.85161700	3.34729600	
0.97758400			
C	-6.23284800	4.09533400	-
1.34074000			
H	-6.23513100	3.37489900	-
3.37456200			
H	-5.95703900	4.64396500	
0.72803300			

H	-7.15411300	4.66055600	-
1.45317000			
C	-2.30736300	-4.13294900	-
0.27683600			
C	-2.31209200	-4.70872300	
1.00341100			
C	-3.04158100	-4.74175900	-
1.30334900			
C	-3.04267000	-5.87156600	
1.25001300			
H	-1.74568500	-4.22227200	
1.79266200			
C	-3.77115600	-5.90631900	-
1.05489500			
H	-3.03420600	-4.29933500	-
2.29578800			
C	-3.77355300	-6.47306300	
0.22176100			
H	-3.04277800	-6.30753600	
2.24568500			
H	-4.33362500	-6.37248500	-
1.85959900			
H	-4.34145500	-7.37949800	
0.41408800			

⁵INT9

Fe	0.28316100	-0.00415500	-
0.01372500			
N	2.36223600	0.12808600	-
0.21455800			
C	-2.21651200	2.31970100	-
0.75465200			
C	2.61639900	2.59422500	-
0.10098900			
C	0.79033900	4.30060000	-
0.46995100			
C	-0.55671900	4.22539300	-
0.65273200			
C	1.27107800	2.94555000	-
0.30600400			
C	-0.91085300	2.82312500	-
0.60512300			
H	-1.24707500	5.03680900	-
0.83172600			

H	1.40957400	5.18565200	-
0.46797500			
N	0.47186000	-2.03977600	-
0.49252900			
N	0.21793400	2.06759300	-
0.40902900			
N	-1.65911100	-0.09988900	-
0.80870500			
C	2.91705900	-2.29231600	-
0.25211800			
C	-1.93077200	-2.56427400	-
0.69875100			
C	-3.82101100	-0.90946100	-
0.81784600			
C	4.49114300	0.92908700	
0.17072000			
C	-0.07085100	-4.27151500	-
0.68255100			
C	-3.90077500	0.44899000	-
0.84283000			
C	4.57537200	-0.42942700	
0.11877600			
C	1.28435400	-4.19602400	-
0.58459600			
C	-2.41912400	-1.25274500	-
0.79062300			
C	3.10742400	1.27662800	-
0.05245600			
C	-0.57281000	-2.91574900	-
0.61969800			
C	-2.54759000	0.95555100	-
0.82439400			
C	3.24336900	-0.92799400	-
0.13135800			
C	1.61895400	-2.79402900	-
0.43808000			
H	-4.79296400	1.05742900	-
0.84588800			
H	5.45551000	-1.04170400	
0.24899900			
H	1.99744600	-5.00671100	-
0.61531300			
H	-4.63464100	-1.61944000	-
0.79962600			

H	5.28979400	1.63337000	
0.35111800			
H	-0.68082900	-5.15404600	-
0.81108700			
C	-2.14806100	1.10635200	
2.50138900			
C	-1.47968600	-0.12070800	
2.21387200			
C	-3.31962700	-1.32599000	
2.90209100			
C	-4.05209700	-0.16409100	
3.20062800			
C	-3.44386300	1.07639100	
2.99508300			
H	-1.62462300	2.03429500	
2.29989300			
H	-3.77801600	-2.30429600	
3.04412400			
H	-5.06744100	-0.24143700	
3.57697000			
H	-3.97833500	2.00015400	
3.20019200			
N	-0.23161900	-0.09412100	
1.70786600			
N	-2.07988600	-1.33309900	
2.42841500			
C	3.60037900	3.70897900	
0.05370200			
C	4.59502200	3.92876300	-
0.91182600			
C	3.54093100	4.56185800	
1.16665800			
C	5.50795500	4.97416400	-
0.76753700			
H	4.64330400	3.27460300	-
1.77774400			
C	4.45491900	5.60622000	
1.31239500			
H	2.77397600	4.39554300	
1.91778300			
C	5.44098000	5.81559700	
0.34548000			
H	6.26878200	5.13363800	-
1.52702700			

H	4.39857800	6.25387200	
2.18331000			
H	6.15238600	6.62926100	
0.45834800			
C	4.03503900	-3.28137300	-
0.16903900			
C	4.11617000	-4.17785100	
0.90770600			
C	5.02159100	-3.33234900	-
1.16579800			
C	5.15872800	-5.10216000	
0.98582500			
H	3.35663600	-4.14029600	
1.68337200			
C	6.06323000	-4.25775200	-
1.08875200			
H	4.96247000	-2.64208500	-
2.00261200			
C	6.13492300	-5.14514900	-
0.01235700			
H	5.20994200	-5.78607300	
1.82887500			
H	6.81633800	-4.28773800	-
1.87174700			
H	6.94638400	-5.86542200	
0.04817900			
C	-2.92701200	-3.67333500	-
0.60499500			
C	-3.72877600	-4.04205600	-
1.69382800			
C	-3.07029900	-4.35865900	
0.61214400			
C	-4.65696600	-5.07796700	-
1.57007500			
H	-3.61736300	-3.51407300	-
2.63690900			
C	-3.99969900	-5.39207000	
0.73479400			
H	-2.45292500	-4.05661100	
1.45354900			
C	-4.79467400	-5.75479200	-
0.35598800			
H	-5.26925700	-5.35829300	-
2.42317200			

H	-4.10470100	-5.91336300	
1.68283200			
H	-5.51730100	-6.56092200	-
0.26055000			
C	-3.33393800	3.30879200	-
0.81877500			
C	-3.61225100	4.13917400	
0.27862200			
C	-4.12965700	3.42594400	-
1.96890800			
C	-4.65900300	5.06013400	
0.22922300			
H	-2.99941100	4.05406600	
1.17157400			
C	-5.17617600	4.34767500	-
2.01996500			
H	-3.91775600	2.78922600	-
2.82309000			
C	-5.44473500	5.16691600	-
0.92090300			
H	-4.86263700	5.69214400	
1.08968200			
H	-5.77894800	4.42868500	-
2.92060700			
H	-6.25988700	5.88437000	-
0.96076600			

CSSTS9

Fe	-0.70976100	0.09717600	
0.60664700			
N	-2.70007000	-0.20149000	
0.42059100			
C	1.91363400	-1.87616400	
1.40248200			
C	-2.86324900	-2.59762300	
0.96985300			
C	-0.94417200	-3.98760700	
1.79119700			
C	0.39843400	-3.78467900	
1.89495800			
C	-1.52175700	-2.74710200	
1.33174800			
C	0.64433500	-2.42003800	
1.51742900			

H	2.75601500	-2.54040600	
1.55741700			
H	1.16520600	-4.48411600	
2.20376600			
H	-1.50195400	-4.88908600	
1.99748500			
N	-1.01330500	2.06708000	
0.63719100			
N	-0.53956900	-1.77804600	
1.22274900			
N	1.21817600	0.43325900	
1.08109100			
C	-3.36654300	2.09907200	-
0.15678600			
C	1.30046900	2.88638200	
1.03041800			
C	3.32237300	1.39073700	
1.15120800			
C	-4.75073300	-1.21015100	
0.04900900			
C	-0.65962200	4.35336900	
0.54619200			
C	3.51147300	0.03798100	
1.12295900			
C	-4.88182300	0.10003100	-
0.29076900			
C	-1.94644400	4.13411700	
0.16671000			
C	1.90010300	1.62708100	
1.09652500			
C	-3.39159900	-1.38904100	
0.50540500			
C	-0.06954400	3.06464400	
0.80848400			
C	2.17909500	-0.54342100	
1.15086600			
C	-3.60293000	0.72514600	-
0.04366400			
C	-2.16786200	2.71049800	
0.22034600			
H	-5.76289100	0.61034400	-
0.65157700			
H	-2.68312800	4.86406000	-
0.13452400			

H	4.08307700	2.15725700	
1.14156000			
H	-5.49956400	-1.98755900	
0.00854700			
H	-0.13700300	5.29616100	
0.61175500			
N	-0.45127400	-0.06133900	-
1.11396000			
C	0.64164100	0.57740200	-
1.70938300			
C	0.40099400	1.88522800	-
2.19762500			
C	2.81462600	0.64655400	-
2.46602200			
C	1.44021900	2.56893800	-
2.81060600			
H	-0.57823500	2.33125000	-
2.07025300			
C	2.68490100	1.94396400	-
2.95568200			
H	3.75616100	0.10593200	-
2.55711200			
H	1.27976900	3.57993300	-
3.17600000			
H	3.52162000	2.44329900	-
3.43423800			
N	1.83462200	-0.02462400	-
1.85050300			
C	3.29925500	-4.80865800	-
1.40344800			
C	4.15674700	-4.44171100	-
2.44497200			
C	3.77529700	-3.43246700	-
3.33746600			
C	2.54870200	-2.79424800	-
3.19389700			
C	1.67550600	-3.15417600	-
2.14261400			
C	2.06766900	-4.17747400	-
1.25141700			
H	3.59238900	-5.58931000	-
0.70678800			
H	5.11564500	-4.93919000	-
2.56303300			

H	4.44137200	-3.14153900	-
4.14516700			
H	2.25571400	-1.99692300	-
3.86728800			
H	1.39564300	-4.45705200	-
0.44789800			
C	0.42058900	-2.52265700	-
1.98854200			
C	-0.64890900	-1.92660200	-
1.81635500			
H	-1.71759800	-1.90132900	-
1.82250100			
C	-3.76100700	-3.78906500	
1.03711100			
C	-4.84109100	-3.82580000	
1.93199900			
C	-3.54435200	-4.89118900	
0.19505600			
C	-5.68245200	-4.93801300	
1.98568700			
H	-5.01354400	-2.97553300	
2.58583700			
C	-4.38565100	-6.00309100	
0.24787100			
H	-2.71078100	-4.86526800	-
0.50149100			
C	-5.45714800	-6.02968000	
1.14385100			
H	-6.51180400	-4.95283800	
2.68789000			
H	-4.20671200	-6.84639600	-
0.41395000			
H	-6.11262300	-6.89544500	
1.18545600			
C	-4.47623200	2.95816700	-
0.67297500			
C	-4.85420600	2.88648900	-
2.02204500			
C	-5.16559500	3.83705300	
0.17567600			
C	-5.89416700	3.67781100	-
2.51234100			
H	-4.32516700	2.20459300	-
2.68217900			

C	-6.20456100	4.62994100	-
0.31418900			
H	-4.88093000	3.89168800	
1.22277700			
C	-6.57158500	4.55263500	-
1.65977300			
H	-6.17289900	3.61275100	-
3.56081000			
H	-6.73057700	5.30397700	
0.35678000			
H	-7.38117900	5.16916500	-
2.04105800			
C	2.16889600	4.09931400	
1.11653100			
C	2.09198100	4.95629900	
2.22402900			
C	3.06779800	4.40628900	
0.08330800			
C	2.89761800	6.09379100	
2.29959400			
H	1.39595400	4.72308400	
3.02517900			
C	3.87457600	5.54235400	
0.16036200			
H	3.12336800	3.74694800	-
0.77788100			
C	3.79193600	6.38947600	
1.26820600			
H	2.82890800	6.74649500	
3.16590800			
H	4.56505600	5.76842700	-
0.64818100			
H	4.41994500	7.27444300	
1.32727800			
C	4.77587000	-0.69859300	
1.01288100			
C	5.90645800	-0.31154600	
1.75263900			
C	4.89125100	-1.77765300	
0.11547300			
C	7.11635900	-0.98856400	
1.60783000			
H	5.82144900	0.51552900	
2.45247500			

C	6.10241500	-2.45453700	-
0.02335900			
H	4.03649200	-2.06247900	-
0.49049600			
C	7.21797600	-2.06517800	
0.72177700			
H	7.97981300	-0.68042300	
2.19181700			
H	6.16968400	-3.28126200	-
0.72490400			
H	8.16125700	-2.59386000	
0.61200300			
oss-TS9			
Fe	-0.72756600	0.10769300	
0.62092900			
N	-2.71258200	-0.17019600	
0.46415300			
C	1.87938300	-1.90458900	
1.36772700			
C	-2.90618500	-2.57510200	
0.99724900			
C	-0.98589800	-4.01131000	
1.73979900			
C	0.36044600	-3.82408100	
1.81742600			
C	-1.55852400	-2.75557000	
1.31628100			
C	0.61153900	-2.45383300	
1.46321900			
H	2.72323400	-2.57139200	
1.50024700			
H	1.12617200	-4.53610100	
2.09848600			
H	-1.54944000	-4.90970200	
1.94358500			
N	-1.00495200	2.09064300	
0.62462000			
N	-0.56918400	-1.79771800	
1.19979600			
N	1.18733400	0.42347000	
1.11760600			
C	-3.34917200	2.12861900	-
0.17959100			

C	1.30283600	2.88284200	
1.06393700			
C	3.29738600	1.36494500	
1.21327600			
C	-4.77726300	-1.15492700	
0.10923800			
C	-0.62384900	4.36978500	
0.50044100			
C	3.47699900	0.01125200	
1.15935500			
C	-4.89029100	0.15260100	-
0.24797100			
C	-1.90442400	4.15686600	
0.09523000			
C	1.88058200	1.61493600	
1.14834900			
C	-3.42002100	-1.35117100	
0.55707300			
C	-0.05674500	3.07924800	
0.80103900			
C	2.14343000	-0.56311200	
1.16516200			
C	-3.60349300	0.76316300	-
0.01782500			
C	-2.14287900	2.73704600	
0.17644800			
H	-5.76425200	0.66946000	-
0.61643800			
H	-2.62720900	4.88821000	-
0.23497700			
H	4.06427600	2.12508600	
1.22034200			
H	-5.53685100	-1.92210800	
0.07890200			
H	-0.09140100	5.30741400	
0.56143100			
N	-0.43137100	-0.03576200	-
1.15392500			
C	0.67465800	0.59144200	-
1.71923400			
C	0.48114800	1.90393700	-
2.21652900			
C	2.87110400	0.61042600	-
2.41380200			

C	1.54983900	2.56322400	-
2.80724900			
H	-0.49044200	2.37288100	-
2.11170700			
C	2.78240300	1.90923000	-
2.91520900			
H	3.80586700	0.05382100	-
2.47558100			
H	1.42317400	3.57645500	-
3.18022700			
H	3.64324100	2.38655800	-
3.37342200			
N	1.86199400	-0.03805800	-
1.82580200			
C	3.36060500	-4.84009100	-
1.45449600			
C	4.21460500	-4.42994800	-
2.48297600			
C	3.80876000	-3.41576200	-
3.35837100			
C	2.56119300	-2.81810100	-
3.21339000			
C	1.69034100	-3.22381400	-
2.17751800			
C	2.10910100	-4.24916100	-
1.30156300			
H	3.67196300	-5.62401300	-
0.76922500			
H	5.18826800	-4.89741700	-
2.60354300			
H	4.47116200	-3.08927700	-
4.15566900			
H	2.24880800	-2.01895100	-
3.87590900			
H	1.44059200	-4.56331500	-
0.50762400			
C	0.41690600	-2.62604100	-
2.02183700			
C	-0.63291200	-2.00365700	-
1.84042700			
H	-1.69703300	-1.91130100	-
1.82309600			
C	-3.82504100	-3.74955700	
1.07157000			

C	-4.88475700	-3.77537000	
1.99081500			
C	-3.64857800	-4.84564700	
0.21241900			
C	-5.74567200	-4.87207100	
2.05209700			
H	-5.02596700	-2.92934700	
2.65759600			
C	-4.50973800	-5.94182500	
0.27301000			
H	-2.83162200	-4.82699400	-
0.50372200			
C	-5.56050200	-5.95821100	
1.19347100			
H	-6.55880800	-4.87917200	
2.77309800			
H	-4.36251100	-6.78068100	-
0.40207400			
H	-6.23127800	-6.81184800	
1.24090800			
C	-4.44625800	2.98406200	-
0.72786800			
C	-4.81559400	2.87651700	-
2.07691200			
C	-5.12974500	3.89609800	
0.08981600			
C	-5.84228300	3.66573800	-
2.59756600			
H	-4.29020500	2.16921000	-
2.71272400			
C	-6.15582200	4.68638200	-
0.43058900			
H	-4.85118900	3.97863000	
1.13673800			
C	-6.51460700	4.57345800	-
1.77585900			
H	-6.11468100	3.57319100	-
3.64559400			
H	-6.67793500	5.38644100	
0.21630900			
H	-7.31395900	5.18814900	-
2.18093200			
C	2.18551000	4.08484300	
1.15942700			

C	2.09996600	4.94627000	
2.26259800			
C	3.10123900	4.37931400	
0.13747000			
C	2.91566800	6.07610400	
2.34599800			
H	1.38986400	4.72297100	
3.05418500			
C	3.91753700	5.50794300	
0.22244900			
H	3.16188200	3.71704400	-
0.72114600			
C	3.82738900	6.35934600	
1.32648800			
H	2.84073500	6.73266300	
3.20884400			
H	4.62131000	5.72488700	-
0.57702700			
H	4.46301800	7.23841000	
1.39159800			
C	4.74005300	-0.72660700	
1.03987800			
C	5.86227800	-0.36326400	
1.80395500			
C	4.86347800	-1.77713300	
0.11028800			
C	7.07320700	-1.03667700	
1.65202500			
H	5.76996400	0.44215500	
2.52774400			
C	6.07635600	-2.44973000	-
0.03597200			
H	4.01543600	-2.04302500	-
0.51391900			
C	7.18353700	-2.08480100	
0.73353200			
H	7.93026600	-0.74785000	
2.25496100			
H	6.15061000	-3.25398200	-
0.76198300			
H	8.12763100	-2.61068600	
0.61745000			

³TS9

Fe	0.57510300	0.27609500	
0.65029700			
N	-1.32806000	0.48776800	
1.23416500			
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C	-1.96964300	-1.89600900	
1.24418400			
C	-0.34961400	-3.80030700	
1.37819100			
C	1.00699900	-3.89575700	
1.39698600			
C	-0.67066000	-2.40329700	
1.24890900			
C	1.52554800	-2.56444600	
1.20438400			
H	1.60895700	-4.78590300	
1.50238300			
H	-1.07499600	-4.59575600	
1.46331900			
N	0.74400100	2.27192800	
0.61008100			
N	0.48659200	-1.65347600	
1.15815800			
N	2.56911900	0.12654400	
0.50440000			
C	-1.54283700	2.94590800	
1.26686600			
C	3.06909600	2.43502800	-
0.22508900			
C	4.72173000	0.54690600	-
0.23786900			
C	-3.55210800	-0.00160500	
1.64277300			
C	1.51747400	4.38298600	
0.05906600			
C	4.68261500	-0.75220400	
0.16214100			
C	-3.41720900	1.34807500	
1.73757400			
C	0.24625200	4.53132400	
0.52145300			
C	3.40972300	1.09938300	-
0.00199600			

C	-2.24604600	-0.53011700	
1.33295800			
C	1.82473000	2.97511800	
0.11684000			
C	3.33630900	-1.01336700	
0.61124400			
C	-2.03886400	1.65205000	
1.42986700			
C	-0.23691300	3.21432700	
0.85081700			
H	5.47913000	-1.48128200	
0.13781300			
H	-4.17333700	2.08078300	
1.97898800			
H	-0.32406900	5.44271700	
0.62572000			
H	5.55923900	1.09131500	-
0.64838400			
H	-4.43825000	-0.60111900	
1.79193200			
H	2.19810500	5.15132700	-
0.27718600			
N	0.20386900	0.03569600	-
1.06739900			
C	0.19446200	-1.19478700	-
1.70419900			
C	1.42265700	-1.73324000	-
2.15465900			
C	-0.94858300	-3.04270300	-
2.46294200			
C	1.42668500	-2.98673900	-
2.75298100			
H	2.33352200	-1.16515700	-
2.00496900			
C	0.21582200	-3.66820800	-
2.91215100			
H	-1.91700100	-3.52954100	-
2.57413600			
H	2.36083800	-3.42411800	-
3.09723000			
H	0.17199200	-4.64911000	-
3.37536300			
N	-0.97497200	-1.84605600	-
1.87048300			

C	-5.77805200	-0.23152800	-
1.82310000			
C	-5.85554500	-1.18896100	-
2.83912900			
C	-4.73780700	-1.43640600	-
3.64500500			
C	-3.55307400	-0.73652600	-
3.44051600			
C	-3.46173600	0.22712300	-
2.41062200			
C	-4.59788600	0.47446400	-
1.60927300			
H	-6.63947900	-0.04026200	-
1.18897400			
H	-6.77870500	-1.73855700	-
3.00226500			
H	-4.79108500	-2.18166200	-
4.43437400			
H	-2.67731200	-0.94010800	-
4.04629900			
H	-4.52752200	1.19950700	-
0.80674000			
C	-2.25242800	0.92235400	-
2.17757100			
C	-1.13152000	1.36584300	-
1.90722300			
H	-0.41804200	2.16022800	-
1.84713500			
C	4.09487800	3.35267900	-
0.80764800			
C	3.91695300	3.88317800	-
2.09432300			
C	5.24108600	3.71124400	-
0.08226200			
C	4.86473600	4.74695800	-
2.64498800			
H	3.02967900	3.61069700	-
2.65907400			
C	6.18940400	4.57491100	-
0.63235400			
H	5.38018400	3.30938300	
0.91745400			
C	6.00411400	5.09470200	-
1.91558900			

H	4.71406700	5.14579800	-
3.64465300			
H	7.07015600	4.84567800	-
0.05605000			
H	6.74223500	5.76753000	-
2.34380500			
C	-2.48403800	4.09520300	
1.42813200			
C	-2.37154900	4.97477900	
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C	-3.49061600	4.31605000	
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C	-3.25260800	6.04951300	
2.64885800			
H	-1.59102200	4.80856000	
3.25099800			
C	-4.37072200	5.39027600	
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H	-3.56637000	3.64270200	-
0.37444500			
C	-4.25458200	6.25895400	
1.69857900			
H	-3.15725500	6.72130100	
3.49782600			
H	-5.14350600	5.55154200	-
0.13670300			
H	-4.93996100	7.09565000	
1.80423800			
C	-3.12607100	-2.83190400	
1.12376300			
C	-3.85916600	-2.83416600	-
0.07397200			
C	-3.50951900	-3.69085000	
2.16288000			
C	-4.95338400	-3.68596100	-
0.22641700			
H	-3.55639600	-2.16981100	-
0.87664800			
C	-4.60418000	-4.54384300	
2.00639200			
H	-2.95034600	-3.68111500	
3.09466200			
C	-5.32796800	-4.54342500	
0.81135900			

H	-5.51186400	-3.67059700	-
1.15817700			
H	-4.89498700	-5.20281700	
2.82040900			
H	-6.18131300	-5.20606900	
0.69196500			
C	3.86186600	-3.40141300	
1.01883200			
C	4.84492200	-3.45189500	
2.01757200			
C	3.83690400	-4.40887300	
0.04181100			
C	5.77883300	-4.48920400	
2.04331700			
H	4.87064700	-2.67182800	
2.77345300			
C	4.76988600	-5.44602000	
0.06773600			
H	3.07895400	-4.36732200	-
0.73541900			
C	5.74345800	-5.48923000	
1.06891900			
H	6.53198800	-4.51710400	
2.82633000			
H	4.73946300	-6.21805300	-
0.69675600			
H	6.47046000	-6.29669500	
1.08895300			
⁵TS9			
Fe	0.57977700	0.24128200	
0.41101400			
N	1.04874300	2.27844500	
0.51745700			
C	-2.16987300	-1.55800500	
1.43786600			
C	-1.19495600	3.20481100	
1.01807000			
C	-3.24460800	1.87743200	
1.67091400			
C	-3.52468200	0.54572700	
1.74403400			
C	-1.85087400	1.99491000	
1.29588100			

C	-2.29768600	-0.15938400	
1.44721700			
H	-4.46469000	0.07365200	
1.99133200			
H	-3.91252900	2.70806300	
1.84912100			
N	2.64343500	-0.14876300	
0.51691200			
N	-1.29370200	0.74336300	
1.20735700			
N	0.28778600	-1.68861600	
1.17006000			
C	3.45866900	2.12469400	-
0.04858400			
C	2.56632200	-2.60452800	
0.84589300			
C	0.50477100	-3.97494500	
1.35347200			
C	0.83103700	4.56822800	
0.38157600			
C	4.60833500	-1.29328100	
0.14493400			
C	-0.82169600	-3.68680200	
1.46439100			
C	2.12750100	4.26783800	
0.08589400			
C	4.85205100	0.01984200	-
0.12101500			
C	1.19454800	-2.72348600	
1.12842900			
C	0.15957800	3.32070200	
0.66215700			
C	3.22161500	-1.39597400	
0.54456500			
C	-0.95403700	-2.25288200	
1.35845700			
C	2.26006400	2.83095400	
0.16673900			
C	3.61989400	0.73824500	
0.11985200			
H	-1.63909400	-4.37616500	
1.61780900			
H	2.92619600	4.95444300	-
0.15392700			

H	5.77722100	0.46445200	-
0.45734800			
H	0.97548100	-4.94551400	
1.40513200			
H	0.37018000	5.54465400	
0.41954500			
H	5.29713600	-2.12163800	
0.06649100			
N	0.20937500	-0.10147300	-
1.35501500			
C	0.00450300	-1.34005000	-
1.90245700			
C	1.11658300	-2.03427000	-
2.44347400			
C	-1.37252600	-3.14135400	-
2.31617300			
C	0.94667900	-3.34080900	-
2.88586500			
H	2.08115300	-1.53912500	-
2.46673700			
C	-0.32426400	-3.91797500	-
2.82342200			
H	-2.38322000	-3.54615500	-
2.26665400			
H	1.79145800	-3.89689400	-
3.28500200			
H	-0.50564300	-4.93248300	-
3.16449200			
N	-1.23181000	-1.89930300	-
1.85698900			
C	-5.78103500	0.33490100	-
1.58867600			
C	-6.05533900	-0.69493100	-
2.49330400			
C	-5.05104100	-1.14990500	-
3.35610300			
C	-3.78274400	-0.57995800	-
3.32069000			
C	-3.49524100	0.45751300	-
2.40605900			
C	-4.51496300	0.91093500	-
1.54249200			
H	-6.55367900	0.68327500	-
0.90910000			

H	-7.04479500	-1.14300300	-
2.52492100			
H	-5.25926300	-1.95377400	-
4.05703200			
H	-2.99383800	-0.94031200	-
3.97102100			
H	-4.29106800	1.69196100	-
0.82579500			
C	-2.20188900	1.02839600	-
2.34841300			
C	-1.03376300	1.39737600	-
2.24031500			
H	-0.20147800	2.06336100	-
2.30165700			
C	-2.01649700	4.45383000	
1.05376100			
C	-2.97286900	4.68867800	
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C	-1.85332400	5.40445100	
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C	-3.75120200	5.84667800	
0.07309200			
H	-3.08985700	3.95882900	-
0.74320300			
C	-2.63180600	6.56332100	
2.09101500			
H	-1.11467500	5.22586400	
2.84777000			
C	-3.58313500	6.78675500	
1.09294500			
H	-4.48535300	6.01648600	-
0.71016400			
H	-2.49744100	7.28940400	
2.88848500			
H	-4.18919100	7.68865200	
1.10916200			
C	4.65497000	2.91624500	-
0.47106100			
C	4.68671800	3.54573800	-
1.72505200			
C	5.76547200	3.04911300	
0.37675500			
C	5.80015500	4.28728200	-
2.12227600			

H	3.83046600	3.44629400	-
2.38634500			
C	6.87950300	3.79032900	-
0.01958300			
H	5.74553100	2.56775200	
1.35044900			
C	6.90024800	4.41158900	-
1.27051100			
H	5.80948500	4.76451900	-
3.09868800			
H	7.72915400	3.88639800	
0.65129800			
H	7.76751200	4.98907500	-
1.57920400			
C	3.38245400	-3.85703000	
0.81383400			
C	4.40377200	-4.07050800	
1.75212600			
C	3.14861600	-4.83852200	-
0.16223900			
C	5.17179200	-5.23536000	
1.71631700			
H	4.58897500	-3.31513400	
2.51069200			
C	3.91533500	-6.00377300	-
0.19759300			
H	2.35917200	-4.67647300	-
0.88995600			
C	4.92995700	-6.20572700	
0.74117500			
H	5.95607900	-5.38643100	
2.45340000			
H	3.72286300	-6.75255400	-
0.96172900			
H	5.52756900	-7.11295600	
0.71339800			
C	-3.43596000	-2.35229800	
1.44360500			
C	-4.21957300	-2.36644800	
0.27849000			
C	-3.86284800	-3.07690200	
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C	-5.40887900	-3.09441900	
0.23962600			

H	-3.88102000	-1.80970500	-
0.58967700			
C	-5.05359100	-3.80596300	
2.52232200			
H	-3.25941700	-3.06204400	
3.46789900			
C	-5.82893000	-3.81607600	
1.36021700			
H	-6.00485000	-3.09159300	-
0.66893200			
H	-5.37722300	-4.36126100	
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H	-6.75617600	-4.38248900	
1.32962400			
³INT10			
Fe	0.52973100	0.21731900	
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C	-2.71079200	-0.51842900	
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C	-0.95882600	-3.62066500	
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C	-1.77602600	-1.55275500	
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C	0.09711000	-2.70284400	
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H	-0.81956500	-4.66725300	
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H	-3.12204400	-3.26437700	
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N	1.58157300	1.90546300	
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C	-0.12344500	3.59149600	
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C	3.68392200	-2.60843200	
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C	-2.54637100	3.06575800	
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C	2.20897600	4.13153100	
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C	-2.35025000	0.82804900	
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C	2.86086000	2.00729200	
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C	-1.16964800	2.68320700	
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C	1.16132900	3.20386100	
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H	-2.89711300	4.08076800	
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C	-1.73196600	-2.90494700	-
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C	0.59388000	-3.26581300	-
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C	-0.71686300	-3.74626300	-
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H	-0.94992900	-4.73981400	-
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C	-3.82939300	-0.04735800	-
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C	-2.69618300	0.40693100	-
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C	-3.98435000	0.53698700	-
2.52346800			
H	-6.03733300	-0.05226900	-
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H	-5.92124600	-0.57152700	-
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H	-3.77538300	-0.27756600	-
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H	-1.75694300	0.52945200	-
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H	-4.02511800	0.75567400	-
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C	-1.62866500	1.14876000	-
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H	-0.24353000	2.12392600	-
1.27687600			

C	5.01764100	1.25171100	-
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C	5.05808300	1.78176700	-
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C	6.22655100	1.04103400	-
0.22159900			
C	6.27750300	2.08692800	-
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H	4.12456000	1.95075400	-
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C	7.44620900	1.34666000	-
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H	6.20113400	0.64031400	
0.78783400			
C	7.47515300	1.86946200	-
2.12209200			
H	6.29157100	2.49251700	-
3.81545000			
H	8.37335400	1.18176900	-
0.28447900			
H	8.42488700	2.10775100	-
2.59337600			
C	-0.40382600	5.05291600	
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C	0.11969600	5.77057700	
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C	-1.17838300	5.73317900	
0.36552700			
C	-0.12957100	7.13752400	
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H	0.72306600	5.24852600	
3.13983100			
C	-1.42914200	7.09946500	
0.49986000			
H	-1.58069900	5.18174800	-
0.47982400			
C	-0.90538500	7.80518500	
1.58572900			
H	0.28018300	7.67960700	
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H	-2.02930200	7.61298300	-
0.24656900			
H	-1.09974600	8.86925800	
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C	-4.66890200	-1.47020700	
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C	-5.01657400	-0.66589800	
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C	-6.01864400	-1.81373500	
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H	-3.99772600	-1.62116200	-
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C	-6.36591200	-1.01637400	
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H	-4.62062400	-0.22172000	
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H	-6.40389000	-2.25469400	-
0.75369800			
H	-7.02208600	-0.84373800	
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H	-7.92105500	-1.85816400	
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C	1.78845400	-4.52356700	
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C	2.71086400	-4.93837500	
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C	1.23606800	-5.48289700	
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C	3.06888100	-6.28289600	
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H	3.14334400	-4.19847700	
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C	1.59494800	-6.82664100	
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H	0.53001200	-5.16069000	-
0.21574300			
C	2.51154600	-7.23071300	
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H	3.78080800	-6.58987400	
3.25251100			
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0.02198900			
H	2.79044600	-8.27746600	
1.71603400			

⁵INT10

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C	-3.35430300	-0.48239900	
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C	-2.04675000	1.33407700	
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N	-1.23366200	0.25503000	
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C	-0.28154100	-2.55786600	
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C	1.57491900	3.10796100	
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0.87995600			
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0.15095400			
N	-0.11004700	0.03083600	-
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C	1.29558300	-3.11506500	-
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H	2.09614400	-1.22704300	-
1.87780300			
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H	-2.03969600	-3.71541800	-
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4.31912600			
C	-3.99089600	0.07157500	-
3.90337000			
C	-3.67071900	0.14223000	-
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C	-4.70493500	-0.18643800	-
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1.28508800			
H	-7.24060700	-0.93973100	-
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H	-5.47610700	-0.36209200	-
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C	-2.41397200	0.48652500	-
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C	-4.84019600	4.78659300	
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H	3.62156400	-4.13669400	-
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H	7.29570300	-5.55605600	
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C	-4.57088600	-4.16601100	
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H	-2.23923800	-4.17917500	
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H	-5.22520200	-4.14743100	-
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H	-4.05673700	-5.86066300	
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H	-5.55650800	-5.85060200	
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