

Ruffling Drives Coproheme Decarboxylation by Facilitating PCET: A

Theoretical Investigation of ChdC

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Supplementary Information

Supplementary Figure

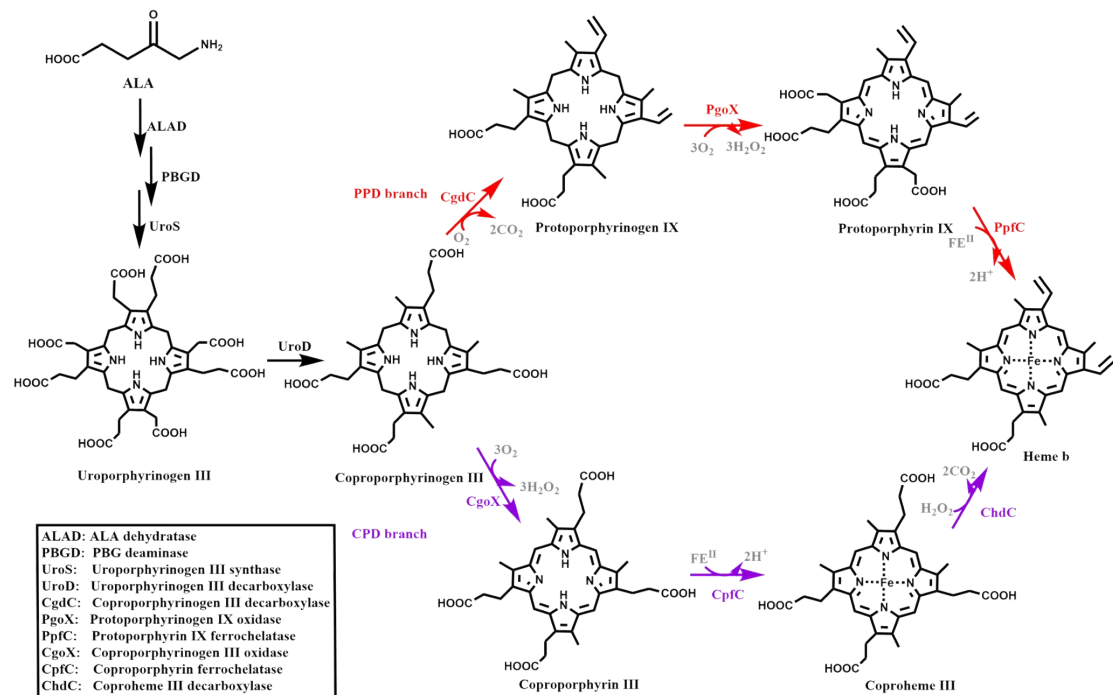


Fig.S1 Heme b biosynthesis pathways (red: PPD branch; magenta: CPD branch)

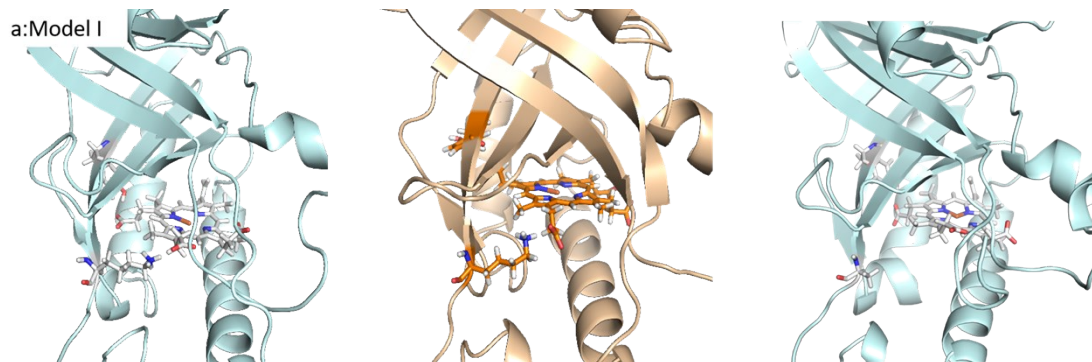


Fig.S2 Three ChdC-hardroheme complex models for MD simulation (a: the hardroheme is rotated for 90° so that its p4 propionate is placed in the vicinity of Tyr145; b: the hardroheme maintains its orientation as that of coproheme in the crystal structure, c: mutation Lys149 of Model I to an alanine)

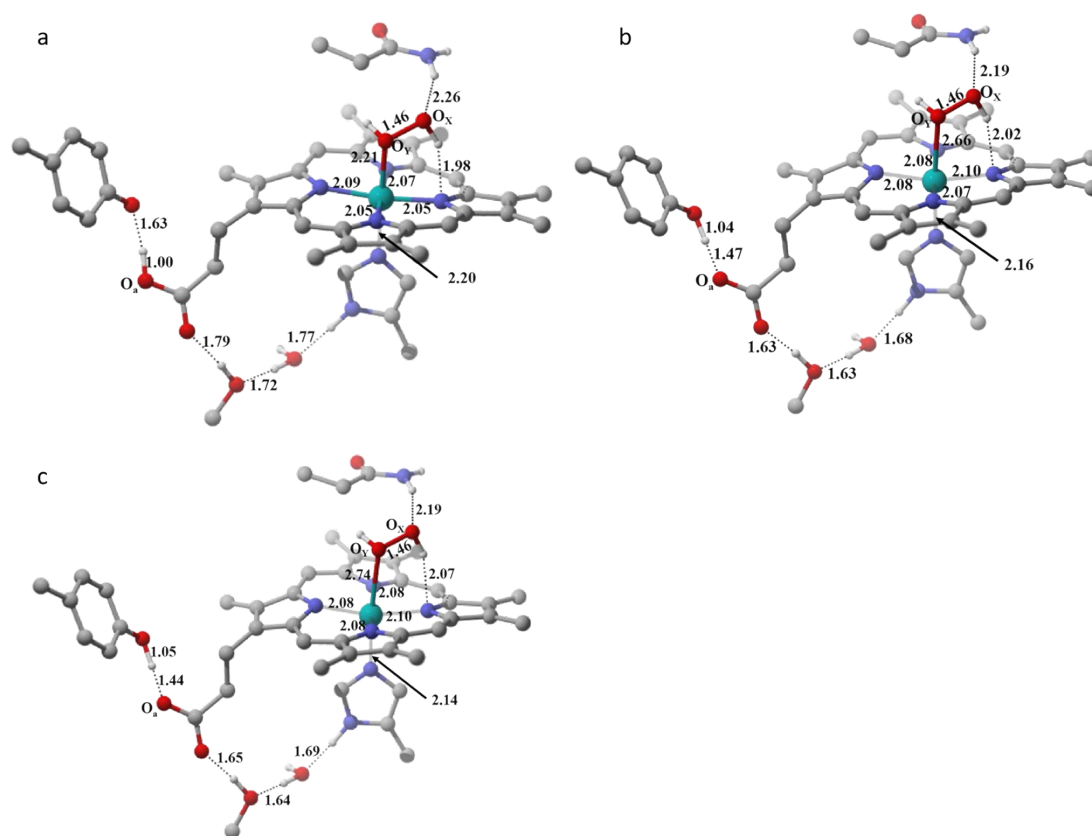


Fig.S3 The optimized geometry structures of RE in different spin states, distances are labelled in Å (a: doublet, b: quartet, c: sextet)

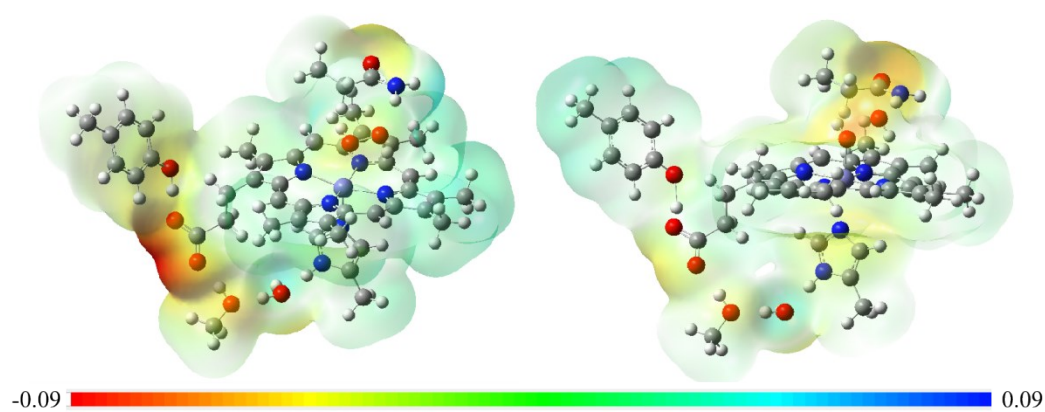


Fig.S4 Electrostatic potential diagrams of ${}^6\text{RE}$ and ${}^6\text{TS1}$.

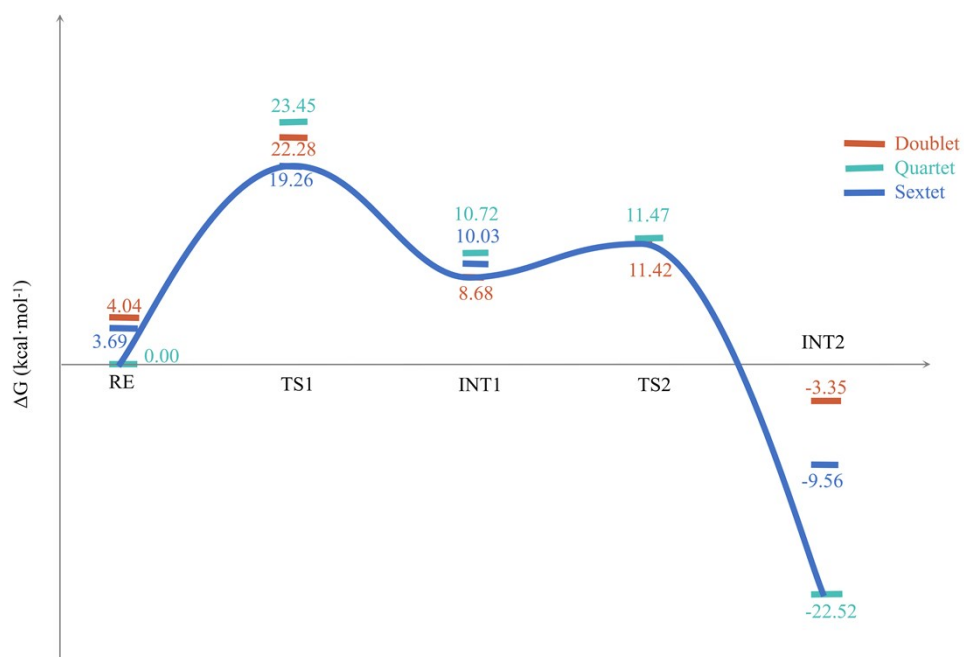


Fig.S5 Energy profile of H₂O₂ homolysis reaction in ChdC with coproheme in planar conformation.

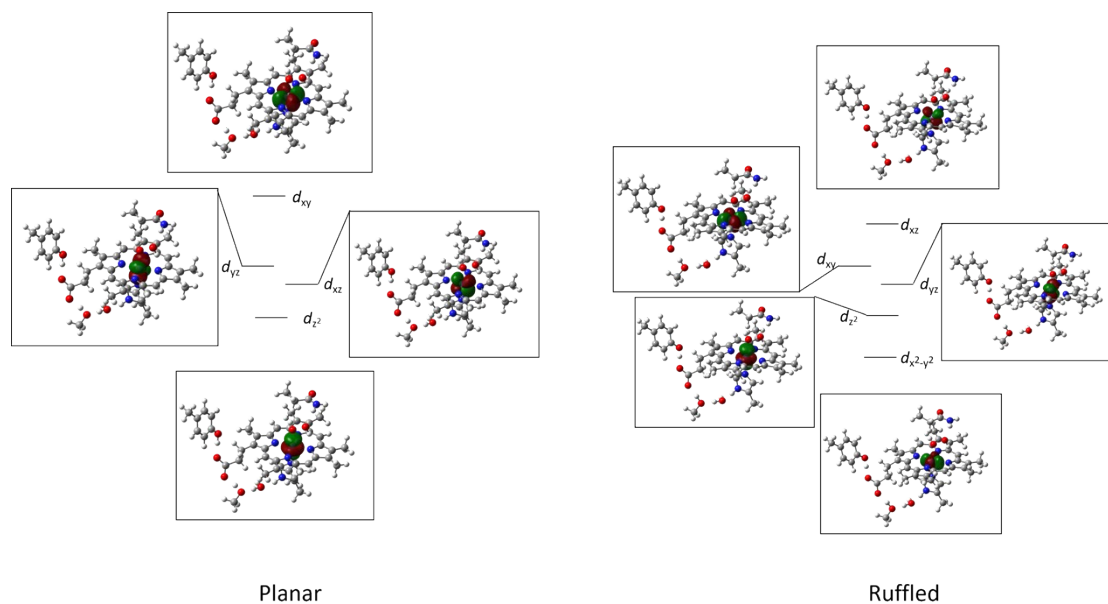


Fig.S6 The *d* orbitals of the Fe^{III} in ⁴RE_{planar} and ⁶RE_{ruffled}.

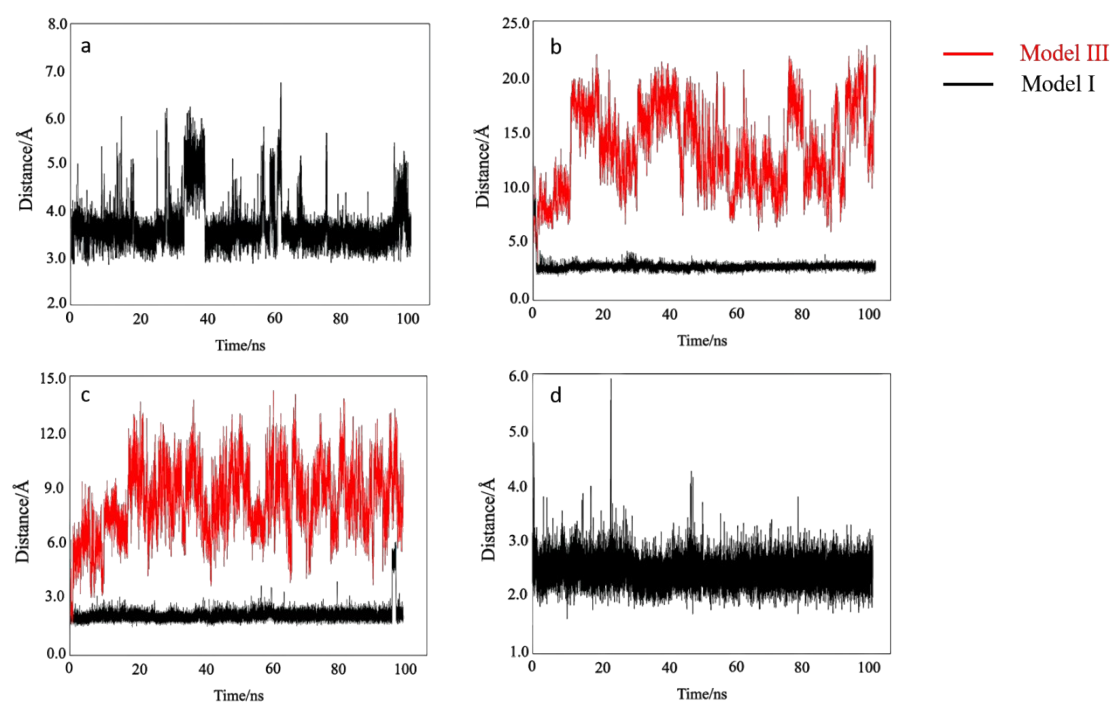


Fig.S7 Some important interatomic distances during simulation (black: model I; red: model III) :
a: the distance between ammonium N atom of Lys149 and C_{carboxyl} of p6 propionate of model I;
b: the distance between phenolic O atom of Tyr114 and C_{carboxyl} of p6 propionate;
c: the distance between hydroxyl O atom of Ser112 and C_{carboxyl} of p6 propionate;
d: the distance between phenolic O atom of Tyr145 and C_{carboxyl} of p4 propionate of model I.

Supplementary Table

Table S1. Relative free energy of the ChdC-coproheme-Fe^{III} and ChdC-coproheme-Fe^{III}-H₂O₂ complexes in different spin states (kcal·mol⁻¹).

Complexes	Doublet(s=1/2)	Quartet(s=3/2)	Sextet (s=5/2)
Coproheme-Fe ^{III}	16.15	6.04	0.00
Coproheme-Fe ^{III} -H ₂ O ₂	17.41	1.21	0.00

Table S2. The detailed Mulliken spin population of some important atoms and groups in the process of H₂O₂ homolysis .

Doublet (S =1/2)					
	RE	TS1	INT1	TS2	INT2
Fe	0.00	+0.47	+1.04	+1.03	+1.34
O _γ H	0.00	-0.01	+0.15	+0.32	+0.75
O _α H	0.00	-0.41	+0.91	+0.72	
His171	0.00	-0.01	-0.01	-0.01	-0.02
Tyr145	+0.82	+0.85	-0.85	-0.87	-0.88
Coproporphyrin III	+0.17	+0.12	-0.23	-0.19	-0.21
Quartet (S =3/2)					
	RE	TS1	INT1	TS2	INT2

Fe	+3.16	+2.76	+2.84	+2.83	+3.37
O _γ H	+0.01	-0.05	+0.43	+0.74	+0.43
O _χ H	0.00	-0.39	+0.81	+0.51	
His171	+0.09	+0.04	+0.03	+0.03	-0.02
Tyr145	-0.11	+0.74	-0.90	-0.90	-0.90
Coproporphyrin III	-0.15	+0.09	-0.22	-0.21	+0.11
Sextet (S =5/2)					
	RE	TS1	INT1	TS2	INT2
Fe	+4.23	+4.21	+4.30	+4.26	+3.38
O _γ H	+0.01	0.00	+0.41	+0.56	+0.43
O _χ H	0.00	-0.47	+0.86	+0.67	
His171	+0.11	+0.04	+0.03	+0.03	-0.02
Tyr145	+0.09	+0.85	-0.88	-0.90	-0.90
Coproporphyrin III	+0.56	+0.38	+0.29	+0.37	+0.31

Table S3. The detailed Mulliken spin population of some important atoms and groups in the process of β-hydrogen atom transfer and CO₂ release.

Doublet (S =1/2)						
	INT2	TS3	INT3	INT4	TS4	PRO
Fe	+1.34	+1.29	+1.29	+1.02	+1.02	+1.02
O _y	+0.75	+0.80	+0.79	+0.08	+0.08	+0.07
Tyr145	-0.90	-0.28	-0.02	0.00	0.00	0.00
His171	-0.02	-0.02	-0.02	-0.01	-0.01	-0.01
β-C	0.00	-0.37	-0.64	0.00	0.00	/
Coproporphyrin III	-0.20	-0.79	-1.06	-0.08	-0.08	-0.08
Quartet (S =3/2)						
	INT2	TS3	INT3	INT4	TS4	PRO
Fe	+3.37	+3.19	+3.21	+2.83	+2.83	+2.84
O _y	+0.43	+0.54	+0.53	+0.24	+0.24	+0.24
Tyr145	-0.88	-0.29	-0.02	+0.01	+0.01	+0.01
His171	-0.02	-0.01	-0.02	+0.04	+0.03	+0.03
β-C	-0.01	-0.38	-0.67	0.00	0.00	/
Coproporphyrin III	+0.11	-0.44	-0.72	-0.12	+0.12	+0.12
Sextet (S =5/2)						
	INT2	TS3	INT3	INT4	TS4	PRO
Fe	+3.38	+3.35	+3.36	+4.30	+4.30	+4.30
O _y	+0.43	+0.45	+0.45	+0.27	+0.27	+0.26
Tyr145	+0.90	+0.29	+0.02	0.00	+0.01	+0.01
His171	-0.02	-0.02	-0.02	+0.04	+0.03	+0.03

β -C	+0.01	+0.36	+0.64	0.00	0.00	
Coproporphyrin III	+0.31	+0.92	+1.19	+0.38	+0.38	+0.40

Table S4. The occupancies (%) of the hydrogen bonds along MD simulation trajectories of complex models.

	Model I			Model III		
	P4	P6	P7	P4	P6	P7
ARG131			164.4			77.7
GLN185						
LYS149		65.4				
TYR145	92.7			96.1		
ARG218	186.7			163.7		
SER223	5.7			97.2		
TYR114		88.5				3.7
SER112		102.0				28.5
SUM	285.1	255.9	164.4	357.0	0	109.9

Cartesian coordinates of stationary points	H	-5.001533	-23.498484	55.430485			
⁶RE	H	-7.033839	-21.807156	52.602913			
C	-6.283003	-15.849998	40.663002	H	-3.734818	-24.452530	53.039299
C	-6.731866	-16.737881	41.796707	H	-6.026342	-22.232298	50.312187
C	-7.100718	-18.078636	41.574566	C	-3.632989	-26.329979	44.420998
C	-6.853057	-16.236094	43.103893	C	-2.842742	-26.682720	45.673164
C	-7.577860	-18.877300	42.602673	C	-2.949149	-28.158463	46.065392
C	-7.326449	-17.016159	44.151077	O	-3.818929	-28.902794	45.627483
C	-7.709443	-18.355919	43.910614	N	-1.990708	-28.568302	46.945652
O	-8.190586	-19.147114	44.870430	H	-3.579087	-25.256201	44.218174
H	-6.169522	-14.816259	41.004063	H	-4.682079	-26.609507	44.539467
H	-7.029708	-15.841610	39.858524	H	-1.783238	-26.422413	45.557087
H	-7.021329	-18.493227	40.571949	H	-3.242914	-26.115931	46.523388
H	-6.577910	-15.202287	43.299862	H	-1.411012	-27.886084	47.418892
H	-7.871446	-19.907518	42.426857	H	-2.087888	-29.491461	47.340725
H	-7.427551	-16.617558	45.155346	C	-9.383000	-17.372021	52.378021
H	-8.202920	-18.661823	45.805660	O	-8.434927	-18.314203	51.882328
C	-5.863011	-23.187992	54.833996	H	-10.174460	-17.891459	52.934654
C	-5.498567	-23.153921	53.380154	H	-9.846892	-16.819820	51.553844
N	-6.220682	-22.445154	52.435268	H	-8.302446	-18.183638	50.902454
C	-4.511232	-23.797434	52.675190	C	-1.018206	-28.208946	53.030575
C	-5.666507	-22.673510	51.229160	C	-1.117987	-26.892973	52.336998
N	-4.623995	-23.494461	51.329952	C	-0.224008	-25.726015	52.398991
H	-6.187707	-22.204580	55.187038	C	1.049715	-25.548849	53.155441

C	-2.176033	-26.434019	51.413006	C	-3.405996	-20.929014	48.467007
C	-3.243002	-27.334986	51.047993	N	-4.270856	-25.922266	49.272243
N	-2.005984	-25.184381	50.922791	C	-4.165991	-27.087019	49.946007
C	-0.860967	-24.739994	51.486019	C	-5.220000	-26.140026	48.332989
C	-0.263016	-23.437010	51.229988	C	-5.778995	-27.518000	48.344013
N	-4.357965	-23.225328	48.124573	C	-6.748899	-28.120220	47.386040
C	-4.392003	-21.856987	47.991001	C	-5.045004	-28.163984	49.439991
C	-5.586002	-21.422012	47.270996	C	-5.149378	-29.561056	49.951572
O	-8.179803	-17.951221	47.056248	H	-0.143126	-28.239294	53.685017
C	-7.902352	-18.402098	48.211876	H	-1.900679	-28.411421	53.649555
O	-8.220315	-17.848785	49.288498	H	1.003580	-24.684263	53.828369
C	-7.151106	-19.753702	48.302040	H	1.902615	-25.391062	52.483917
C	-6.135961	-20.039644	47.161629	H	1.270214	-26.428989	53.765339
C	-6.311984	-22.663988	46.927006	H	-3.264877	-28.312031	51.511559
C	-7.603382	-22.798376	46.192581	H	0.678330	-23.219122	51.718311
C	-5.437017	-23.750011	47.445992	H	-6.649087	-19.805428	49.273754
C	-5.748992	-25.167982	47.409008	H	-7.915045	-20.543116	48.300060
N	-2.045482	-22.493641	49.806301	H	-6.640565	-19.921997	46.199478
C	-0.865991	-22.387997	50.438019	H	-5.337756	-19.290163	47.190876
C	-0.238013	-21.044994	50.311989	H	-7.848703	-21.876753	45.656513
C	1.071519	-20.612089	50.881107	H	-8.436480	-23.011900	46.875298
C	-1.197991	-20.294016	49.510014	H	-7.568891	-23.616577	45.464272
C	-1.145882	-18.879890	49.038406	H	-6.560037	-25.481062	46.764511
C	-2.263007	-21.284981	49.266979	H	1.276353	-19.565826	50.639507

H	1.902617	-21.210262	50.488220	H	1.090714	-20.706688	51.973690
H	-1.118338	-18.817436	47.944012				
H	-0.254784	-18.374214	49.419403	6TS1			
H	-2.018310	-18.307026	49.374619	C	-6.283002	-15.850000	40.663002
H	-3.521174	-19.892513	48.180317	C	-6.724055	-16.760374	41.771770
H	-6.245326	-28.376801	46.445683	C	-6.907877	-18.148294	41.546085
H	-7.580729	-27.445093	47.159092	C	-7.016621	-16.238480	43.052608
H	-7.175671	-29.041590	47.792484	C	-7.372606	-18.977242	42.540451
H	-5.329831	-29.588411	51.032822	C	-7.479354	-17.042519	44.069870
H	-5.970443	-30.093113	49.464500	C	-7.684377	-18.455460	43.850937
Fe	-3.352523	-24.107885	49.717583	O	-8.114689	-19.224771	44.772663
O	-8.359834	-20.786045	52.803089	H	-6.177874	-14.820757	41.016163
H	-4.232931	-30.133677	49.760426	H	-7.029638	-15.842801	39.857487
H	-3.251419	-26.857357	43.571766	H	-6.682307	-18.556040	40.563786
H	-8.338794	-19.839367	52.476933	H	-6.875649	-15.175480	43.229744
H	-9.181685	-21.144442	52.448154	H	-7.521075	-20.039894	42.377956
O	-1.384223	-24.704596	47.903149	H	-7.706045	-16.638721	45.051163
H	-1.940937	-24.980190	47.155148	H	-8.258131	-18.533678	46.256428
O	-0.808478	-25.981030	48.304741	C	-5.862990	-23.187996	54.834003
H	-1.133292	-25.999386	49.226242	C	-5.486022	-23.164574	53.373360
H	-0.925372	-29.038635	52.318943	N	-6.250476	-22.518805	52.416367
H	-8.909709	-16.675350	53.037983	C	-4.461247	-23.753553	52.664948
H	-5.355939	-16.134197	40.210560	C	-5.674879	-22.735121	51.208637
H	-6.656234	-23.884270	55.009743	N	-4.586412	-23.481915	51.312965

H	-6.191660	-22.201595	55.176369	C	1.048471	-25.551981	53.159748
H	-5.003911	-23.491447	55.437622	C	-2.175943	-26.434048	51.412922
H	-7.079561	-21.924063	52.585445	C	-3.243025	-27.334978	51.048031
H	-3.646539	-24.355915	53.038067	N	-2.002294	-25.190281	50.939758
H	-6.069713	-22.339893	50.284359	C	-0.861058	-24.739964	51.486073
C	-3.633000	-26.330000	44.421001	C	-0.262973	-23.437016	51.229969
C	-2.828012	-26.645315	45.670662	N	-4.357705	-23.222317	48.105709
C	-2.929230	-28.105976	46.115631	C	-4.392126	-21.856997	47.991116
O	-3.770466	-28.883324	45.670162	C	-5.585943	-21.422003	47.270950
N	-2.007584	-28.451197	47.054478	O	-8.360021	-17.936356	47.056080
H	-3.603680	-25.257504	44.202496	C	-7.931246	-18.442987	48.206863
H	-4.676149	-26.627649	44.551601	O	-8.094029	-17.807541	49.240383
H	-1.770389	-26.385590	45.544018	C	-7.280251	-19.818892	48.186192
H	-3.209196	-26.051798	46.507595	C	-6.135479	-20.032335	47.156101
H	-1.452178	-27.723652	47.506142	C	-6.312044	-22.663998	46.927052
H	-2.107991	-29.355621	47.489513	C	-7.597875	-22.813700	46.180923
C	-9.382999	-17.371990	52.377995	C	-5.436889	-23.750019	47.445862
O	-8.442206	-18.338921	51.915699	C	-5.749057	-25.167982	47.409065
H	-10.190509	-17.873287	52.926037	N	-2.046848	-22.482035	49.820896
H	-9.825716	-16.820438	51.541676	C	-0.866007	-22.387997	50.438004
H	-8.290830	-18.208530	50.957256	C	-0.237998	-21.044998	50.312004
C	-1.014049	-28.208128	53.032356	C	1.071142	-20.611120	50.881840
C	-1.118019	-26.892984	52.337025	C	-1.198004	-20.293999	49.510006
C	-0.223979	-25.726013	52.398975	C	-1.143991	-18.878731	49.040878

C	-2.263006	-21.285002	49.266987	H	1.299168	-19.579170	50.600708
C	-3.405948	-20.928995	48.466965	H	1.897171	-21.239574	50.527225
N	-4.282325	-25.927258	49.272377	H	-1.166055	-18.810396	47.946411
C	-4.166012	-27.087000	49.946011	H	-0.227448	-18.389338	49.381737
C	-5.219979	-26.140011	48.332989	H	-1.989359	-18.290552	49.419666
C	-5.778999	-27.517998	48.343998	H	-3.510845	-19.892689	48.175159
C	-6.737951	-28.127131	47.379158	H	-6.219831	-28.393019	46.449089
C	-5.044990	-28.164001	49.439991	H	-7.565555	-27.452866	47.133320
C	-5.145630	-29.564697	49.942619	H	-7.172287	-29.044538	47.787716
H	-0.155859	-28.225100	53.709812	H	-5.276389	-29.601574	51.030716
H	-1.908936	-28.426418	53.627785	H	-5.995621	-30.081045	49.488464
H	1.009880	-24.677065	53.819847	Fe	-3.153623	-24.210958	49.512535
H	1.908036	-25.414207	52.491852	O	-8.464520	-20.864981	52.883438
H	1.256101	-26.425558	53.784023	H	-4.247450	-30.148449	49.703228
H	-3.264666	-28.312712	51.510334	H	-3.251409	-26.857342	43.571766
H	0.682845	-23.222630	51.711292	H	-8.409833	-19.934809	52.550301
H	-6.910983	-20.012808	49.195660	H	-9.300406	-21.201733	52.540833
H	-8.071468	-20.551432	47.982597	O	-1.745753	-24.632269	48.149715
H	-6.519498	-19.866428	46.146118	H	-2.029168	-24.752045	47.231194
H	-5.353756	-19.284620	47.327148	O	-0.659652	-26.050570	48.140373
H	-7.854370	-21.896257	45.642208	H	-0.683260	-26.076889	49.111752
H	-8.436469	-23.053843	46.848866	H	-0.888638	-29.036203	52.323586
H	-7.540697	-23.624353	45.445084	H	-8.909712	-16.675375	53.038006
H	-6.561715	-25.481323	46.766594	H	-5.355942	-16.134195	40.210564

H	-6.656248	-23.884268	55.009739	N	-4.546762	-23.533138	51.329117
H	1.074468	-20.660690	51.978016	H	-6.198457	-22.197453	55.157658
				H	-5.010253	-23.479519	55.452290
°INT1				H	-7.081796	-22.000080	52.546577
C	-6.283009	-15.849998	40.663002	H	-3.601348	-24.344475	53.081844
C	-6.720015	-16.751762	41.779999	H	-6.049284	-22.450380	50.265327
C	-6.887299	-18.144524	41.569996	C	-3.632992	-26.329973	44.421009
C	-7.026117	-16.216255	43.052570	C	-2.751799	-26.634731	45.627682
C	-7.349876	-18.965614	42.571449	C	-2.918209	-28.062256	46.139698
C	-7.486546	-17.012115	44.076767	O	-3.845320	-28.798418	45.796452
C	-7.675270	-18.429998	43.873466	N	-1.952172	-28.462027	47.011890
O	-8.102551	-19.191359	44.802128	H	-3.629331	-25.258654	44.195824
H	-6.181454	-14.817265	41.006794	H	-4.661465	-26.654816	44.592548
H	-7.031583	-15.852773	39.859203	H	-1.694447	-26.470613	45.387192
H	-6.650518	-18.561771	40.594452	H	-2.953064	-25.954168	46.458950
H	-6.896675	-15.149807	43.216831	H	-1.298707	-27.796324	47.429413
H	-7.485933	-20.031771	42.421757	H	-2.093666	-29.355968	47.457867
H	-7.721366	-16.599953	45.052704	C	-9.383005	-17.371979	52.377975
H	-8.236790	-18.487726	46.300945	O	-8.459637	-18.356915	51.921005
C	-5.862984	-23.187994	54.834003	H	-10.189055	-17.870907	52.928196
C	-5.469430	-23.187485	53.376629	H	-9.827467	-16.824026	51.539673
N	-6.240788	-22.581745	52.399609	H	-8.169849	-18.140562	51.012344
C	-4.426043	-23.769138	52.688011	C	-1.014081	-28.209017	53.029812
C	-5.651132	-22.814476	51.200836	C	-1.118013	-26.892948	52.337017

C	-0.223991	-25.726034	52.398979	C	-1.150109	-18.876572	49.047764
C	1.051071	-25.552029	53.154720	C	-2.263024	-21.284971	49.266949
C	-2.175910	-26.434044	51.412945	C	-3.405942	-20.929020	48.466976
C	-3.243053	-27.334955	51.048027	N	-4.284734	-25.925322	49.278351
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C	-0.861073	-24.739992	51.486038	C	-5.220000	-26.140011	48.332947
C	-0.262984	-23.437006	51.229977	C	-5.778987	-27.518003	48.344032
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C	-4.392126	-21.856968	47.991138	C	-5.044998	-28.163979	49.439960
C	-5.585960	-21.422033	47.270931	C	-5.139080	-29.566454	49.937508
O	-8.308964	-17.885082	47.096432	H	-0.137524	-28.238098	53.682671
C	-7.855290	-18.397591	48.237095	H	-1.895253	-28.414103	53.650002
O	-7.955345	-17.748573	49.269203	H	1.007876	-24.690287	53.831909
C	-7.252451	-19.795116	48.198841	H	1.903605	-25.393356	52.482758
C	-6.127154	-20.031452	47.150749	H	1.271881	-26.435072	53.760738
C	-6.312009	-22.663977	46.927052	H	-3.260498	-28.314697	51.505985
C	-7.592825	-22.814098	46.172714	H	0.679060	-23.219275	51.716831
C	-5.436918	-23.750038	47.445862	H	-6.876324	-20.009377	49.201519
C	-5.749046	-25.167973	47.409084	H	-8.067802	-20.501322	47.997646
N	-2.039673	-22.492632	49.796558	H	-6.529402	-19.874319	46.145840
C	-0.865980	-22.388008	50.438030	H	-5.336406	-19.288340	47.298504
C	-0.238026	-21.044985	50.311981	H	-7.855513	-21.890663	45.647575
C	1.066670	-20.609819	50.890739	H	-8.431663	-23.072868	46.833000
C	-1.197985	-20.294022	49.510029	H	-7.523235	-23.612053	45.424324

H	-6.553949	-25.484121	46.758831	H	-5.355935	-16.134199	40.210564
H	1.281585	-19.568577	50.635120	H	-6.656251	-23.884270	55.009739
H	1.899824	-21.219465	50.520290	H	1.070751	-20.687384	51.984970
H	-1.148531	-18.804613	47.953300				
H	-0.247768	-18.377623	49.411556	6TS2			
H	-2.011546	-18.301634	49.409443	C	-6.283006	-15.850000	40.663002
H	-3.513118	-19.892191	48.178516	C	-6.720283	-16.753025	41.778622
H	-6.196291	-28.384483	46.450466	C	-6.884450	-18.146255	41.566929
H	-7.558737	-27.454639	47.124378	C	-7.029441	-16.218330	43.051182
H	-7.162567	-29.047560	47.776455	C	-7.347458	-18.968695	42.566620
H	-5.265152	-29.608667	51.025959	C	-7.490240	-17.015429	44.073822
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Fe	-3.092956	-24.246708	49.411663	O	-8.104029	-19.195911	44.795498
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H	-4.239901	-30.144762	49.689781	H	-7.031555	-15.852427	39.859180
H	-3.251411	-26.857361	43.571762	H	-6.644673	-18.562073	40.591564
H	-8.438960	-19.996078	52.467167	H	-6.901768	-15.151812	43.216042
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O	-1.870959	-24.816666	48.067890	H	-7.727310	-16.604929	45.049927
H	-1.108441	-24.251177	47.888508	H	-8.239456	-18.491692	46.303787
O	-0.221204	-26.488066	48.398472	C	-5.862984	-23.187992	54.834003
H	-0.780261	-26.392408	49.191463	C	-5.470954	-23.190132	53.377769
H	-0.920617	-29.037502	52.316990	N	-6.242893	-22.588306	52.399487
H	-8.909708	-16.675383	53.038025	C	-4.429298	-23.776239	52.690750

C	-5.653431	-22.827963	51.201115	C	-1.118012	-26.892963	52.337029
N	-4.550433	-23.547371	51.331497	C	-0.223990	-25.726028	52.398972
H	-6.198551	-22.197437	55.157711	C	1.047023	-25.549318	53.161091
H	-5.010346	-23.479435	55.452557	C	-2.175942	-26.434072	51.412914
H	-7.082701	-22.005560	52.545197	C	-3.243029	-27.334963	51.048027
H	-3.604997	-24.350170	53.087868	N	-1.996527	-25.189631	50.932102
H	-6.052937	-22.467623	50.264610	C	-0.861050	-24.739946	51.486088
C	-3.632996	-26.329988	44.421001	C	-0.262982	-23.437021	51.229958
C	-2.806413	-26.717108	45.643787	N	-4.363479	-23.220797	48.118973
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O	-3.978846	-28.845703	45.671474	C	-5.585949	-21.422018	47.270947
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H	-3.562906	-25.255070	44.228149	C	-7.855092	-18.397438	48.237885
H	-4.682356	-26.603588	44.551277	O	-7.953091	-17.745369	49.267879
H	-1.736810	-26.581112	45.444263	C	-7.253120	-19.795181	48.200832
H	-3.012691	-26.061934	46.494526	C	-6.127447	-20.031290	47.153069
H	-1.477867	-28.003895	47.447285	C	-6.312032	-22.663986	46.927052
H	-2.313646	-29.541044	47.366802	C	-7.594455	-22.815145	46.175846
C	-9.383001	-17.371994	52.377995	C	-5.436890	-23.750027	47.445850
O	-8.459761	-18.356668	51.920414	C	-5.749055	-25.167978	47.409077
H	-10.188335	-17.871555	52.928627	N	-2.045175	-22.488523	49.804436
H	-9.828435	-16.824020	51.540176	C	-0.865991	-22.388002	50.438015
H	-8.167520	-18.138313	51.013229	C	-0.238012	-21.044991	50.311993
C	-1.020252	-28.203987	53.040970	C	1.069856	-20.612436	50.884811

C	-1.197992	-20.294010	49.510017	H	-7.525090	-23.611521	45.425732
C	-1.147576	-18.879177	49.041470	H	-6.554611	-25.483913	46.759373
C	-2.263018	-21.284988	49.266979	H	1.279259	-19.567514	50.639866
C	-3.405938	-20.929007	48.466957	H	1.901429	-21.214893	50.499084
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C	-4.166004	-27.087015	49.946026	H	-0.247112	-18.378403	49.407372
C	-5.219991	-26.140009	48.332973	H	-2.011080	-18.302046	49.395065
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C	-5.142329	-29.565912	49.939026	H	-7.176869	-29.041300	47.794827
H	-0.123511	-28.245724	53.665012	H	-5.270632	-29.606955	51.027302
H	-1.884726	-28.381561	53.692516	H	-5.992317	-30.081726	49.484524
H	0.990287	-24.701239	53.854427	Fe	-3.067275	-24.245876	49.382229
H	1.898968	-25.365791	52.494850	O	-8.504635	-20.945171	52.736347
H	1.278461	-26.440390	53.751156	H	-4.243575	-30.146698	49.694630
H	-3.263412	-28.313145	51.509472	H	-3.251412	-26.857349	43.571766
H	0.678823	-23.218494	51.717075	H	-8.440877	-19.997494	52.466572
H	-6.877521	-20.009398	49.203674	H	-9.308360	-21.268703	52.313793
H	-8.068521	-20.501236	47.999325	O	-1.853822	-24.706558	48.023914
H	-6.528886	-19.873383	46.147949	H	-1.010763	-25.222540	48.164394
H	-5.336650	-19.288403	47.301476	O	-0.512335	-26.674116	48.468048
H	-7.860061	-21.891369	45.652863	H	-0.821110	-26.814825	49.381718
H	-8.431069	-23.076752	46.837822	H	-0.969660	-29.042845	52.336185

H	-8.909710	-16.675371	53.038010	C	-4.402774	-23.812416	52.688595
H	-5.355938	-16.134195	40.210564	C	-5.611867	-22.853432	51.186436
H	-6.656253	-23.884270	55.009739	N	-4.513487	-23.583027	51.322212
H	1.084196	-20.703199	51.978050	H	-6.206826	-22.190720	55.124630
				H	-5.017711	-23.461407	55.470093
2INT2				H	-7.037797	-22.016134	52.518631
C	-6.283005	-15.850000	40.663002	H	-3.584378	-24.392216	53.087872
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C	-6.887400	-18.142773	41.574219	C	-3.633001	-26.329996	44.421001
C	-7.022775	-16.212261	43.054081	C	-2.852317	-26.758167	45.662777
C	-7.349221	-18.962025	42.577545	C	-3.107075	-28.218863	46.034409
C	-7.482348	-17.006298	44.080090	O	-4.056027	-28.864750	45.585716
C	-7.672520	-18.424194	43.879055	N	-2.199116	-28.754110	46.893917
O	-8.099182	-19.183916	44.809544	H	-3.526798	-25.255054	44.245880
H	-6.181998	-14.816542	41.004791	H	-4.692798	-26.572878	44.523308
H	-7.031951	-15.854783	39.859558	H	-1.775811	-26.612217	45.513088
H	-6.652179	-18.561668	40.599007	H	-3.113715	-26.136120	46.525078
H	-6.892222	-15.145686	43.216633	H	-1.524220	-28.172714	47.397984
H	-7.486162	-20.028316	42.429672	H	-2.400287	-29.682949	47.233292
H	-7.715266	-16.592472	45.055779	C	-9.383001	-17.371992	52.377991
H	-8.229704	-18.478548	46.305191	O	-8.461342	-18.360006	51.923656
C	-5.862984	-23.187992	54.834003	H	-10.191532	-17.868137	52.927135
C	-5.445819	-23.215891	53.371014	H	-9.824398	-16.824493	51.537857
N	-6.202832	-22.609716	52.380779	H	-8.165302	-18.142107	51.017227

C	-1.026334	-28.204279	53.041584	C	1.071298	-20.616928	50.884872
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C	-0.223987	-25.726027	52.398972	C	-1.150702	-18.879395	49.039814
C	1.050076	-25.546417	53.154671	C	-2.263015	-21.284992	49.266979
C	-2.175941	-26.434067	51.412914	C	-3.405940	-20.929003	48.466961
C	-3.243029	-27.334965	51.048031	N	-4.287518	-25.908745	49.290836
N	-2.013964	-25.177782	50.933590	C	-4.166006	-27.087011	49.946022
C	-0.861053	-24.739950	51.486084	C	-5.219987	-26.140009	48.332973
C	-0.262979	-23.437019	51.229961	C	-5.778989	-27.518003	48.344009
N	-4.383384	-23.223164	48.173470	C	-6.750836	-28.115217	47.385387
C	-4.392133	-21.856989	47.991131	C	-5.044997	-28.163992	49.439980
C	-5.585948	-21.422016	47.270943	C	-5.135411	-29.564594	49.943516
O	-8.299898	-17.877310	47.102299	H	-0.121720	-28.253126	53.653572
C	-7.847794	-18.394354	48.241268	H	-1.883745	-28.371536	53.705132
O	-7.947782	-17.749025	49.275845	H	0.996588	-24.696724	53.846149
C	-7.247381	-19.792837	48.198700	H	1.898569	-25.365471	52.483562
C	-6.121707	-20.029367	47.150734	H	1.282912	-26.436583	53.745476
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C	-7.584216	-22.820936	46.159611	H	0.683543	-23.222626	51.709923
C	-5.436889	-23.750025	47.445854	H	-6.872836	-20.011030	49.201111
C	-5.749057	-25.167978	47.409073	H	-8.063966	-20.496820	47.994675
N	-2.057728	-22.499313	49.811836	H	-6.522935	-19.869555	46.145866
C	-0.865995	-22.388000	50.438011	H	-5.328937	-19.289110	47.300705
C	-0.238009	-21.044992	50.311996	H	-7.857734	-21.891031	45.651890

H	-8.423503	-23.108723	46.806980	H	-0.993299	-29.045408	52.338650
H	-7.494195	-23.600855	45.394444	H	-8.909710	-16.675373	53.038010
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H	1.279876	-19.571001	50.643623	H	-6.656253	-23.884270	55.009735
H	1.901706	-21.217812	50.494453	H	1.087691	-20.712250	51.977558
H	-1.136877	-18.814413	47.944996				
H	-0.253248	-18.376802	49.410576	²TS3			
H	-2.017092	-18.304201	49.388977	C	-6.283005	-15.850000	40.663002
H	-3.503699	-19.895311	48.163715	C	-6.519239	-16.748356	41.864620
H	-6.244193	-28.361826	46.444099	C	-6.496862	-18.148155	41.724380
H	-7.586760	-27.440916	47.169411	C	-6.734042	-16.230343	43.149250
H	-7.171552	-29.041189	47.788532	C	-6.707537	-18.994942	42.808590
H	-5.290915	-29.602911	51.028454	C	-6.946495	-17.063148	44.247108
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Fe	-3.135222	-24.228371	49.494774	O	-7.336371	-19.284536	45.106354
O	-8.442844	-20.954077	52.720081	H	-6.227659	-14.797014	40.949909
H	-4.222997	-30.133928	49.724503	H	-7.074301	-15.960139	39.912880
H	-3.251408	-26.857344	43.571762	H	-6.319866	-18.581980	40.742710
H	-8.403930	-20.000093	52.467075	H	-6.744055	-15.152913	43.295006
H	-9.260957	-21.280184	52.328297	H	-6.713554	-20.073252	42.682610
O	-2.123156	-24.691280	48.315128	H	-7.133361	-16.636606	45.227482
H	-0.948967	-26.124752	48.344254	H	-8.093537	-18.423498	46.249092
O	-0.497488	-26.982229	48.479271	C	-5.862984	-23.187992	54.834003
H	-0.732844	-27.204781	49.389862	C	-5.443818	-23.218107	53.372280

N	-6.199289	-22.607340	52.384464	H	-8.293276	-18.304640	51.019054
C	-4.402616	-23.816290	52.688652	C	-1.026232	-28.204679	53.040436
C	-5.610321	-22.849533	51.189968	C	-1.118014	-26.892967	52.337029
N	-4.513294	-23.582855	51.322491	C	-0.223987	-25.726027	52.398972
H	-6.209713	-22.190397	55.119522	C	1.049741	-25.545485	53.154430
H	-5.019159	-23.458292	55.473240	C	-2.175941	-26.434067	51.412914
H	-7.032394	-22.011267	52.531635	C	-3.243029	-27.334965	51.048031
H	-3.585727	-24.398998	53.086506	N	-2.014689	-25.176851	50.934601
H	-6.000602	-22.483597	50.252804	C	-0.861053	-24.739950	51.486084
C	-3.633001	-26.329996	44.421001	C	-0.262979	-23.437019	51.229961
C	-2.847402	-26.752754	45.661762	N	-4.388543	-23.210159	48.185307
C	-3.101834	-28.211344	46.041908	C	-4.392133	-21.856989	47.991131
O	-4.056514	-28.856665	45.605286	C	-5.585948	-21.422016	47.270943
N	-2.188288	-28.745584	46.896049	O	-8.349598	-17.883793	47.056355
H	-3.530738	-25.255188	44.242535	C	-8.033575	-18.534004	48.166965
H	-4.691622	-26.576733	44.526062	O	-8.232138	-18.023436	49.259972
H	-1.771541	-26.608068	45.506844	C	-7.466869	-19.942657	48.008865
H	-3.105071	-26.126959	46.522572	C	-6.131784	-20.078810	47.233337
H	-1.503840	-28.166916	47.388992	C	-6.312034	-22.663988	46.927055
H	-2.383929	-29.675884	47.234516	C	-7.564935	-22.822216	46.130661
C	-9.383001	-17.371992	52.377991	C	-5.436889	-23.750025	47.445854
O	-8.461504	-18.386271	51.978439	C	-5.749057	-25.167978	47.409073
H	-10.231761	-17.826010	52.904541	N	-2.058276	-22.499458	49.815464
H	-9.768519	-16.829527	51.508511	C	-0.865995	-22.388000	50.438011

C	-0.238009	-21.044992	50.311996	H	-7.765653	-21.926359	45.536762
C	1.071701	-20.618063	50.884033	H	-8.438851	-23.007498	46.770107
C	-1.197995	-20.294006	49.510017	H	-7.491166	-23.670921	45.442192
C	-1.151009	-18.880302	49.038246	H	-6.536487	-25.488197	46.739845
C	-2.263015	-21.284992	49.266979	H	1.281737	-19.573051	50.640942
C	-3.405940	-20.929003	48.466961	H	1.900600	-21.221245	50.494198
N	-4.288565	-25.908108	49.294163	H	-1.141591	-18.817425	47.943424
C	-4.166006	-27.087011	49.946022	H	-0.251783	-18.378307	49.404903
C	-5.219987	-26.140009	48.332973	H	-2.015775	-18.304602	49.390202
C	-5.778989	-27.518003	48.344009	H	-3.500173	-19.896624	48.158733
C	-6.750659	-28.114485	47.385117	H	-6.242925	-28.359537	46.444031
C	-5.044997	-28.163992	49.439980	H	-7.587057	-27.440575	47.170074
C	-5.134032	-29.564793	49.942642	H	-7.170517	-29.041101	47.787231
H	-0.122334	-28.253363	53.653252	H	-5.292629	-29.603695	51.027061
H	-1.884403	-28.372490	53.702679	H	-5.963203	-30.093956	49.466042
H	0.995034	-24.695616	53.845448	Fe	-3.137620	-24.224768	49.509346
H	1.897572	-25.363779	52.482819	O	-8.411553	-20.956945	52.828762
H	1.283237	-26.435293	53.745232	H	-4.219666	-30.131577	49.725658
H	-3.259306	-28.315477	51.504749	H	-3.251408	-26.857344	43.571762
H	0.684054	-23.223188	51.708893	H	-8.397310	-20.002220	52.570347
H	-7.327822	-20.332178	49.022282	H	-9.268989	-21.282213	52.532047
H	-8.237830	-20.557869	47.529617	O	-2.134896	-24.682333	48.319420
H	-6.560938	-19.680721	45.931465	H	-0.936421	-26.106493	48.331390
H	-5.418435	-19.300339	47.515038	O	-0.472847	-26.957762	48.460716

H	-0.690816	-27.183636	49.374619	C	-5.442427	-23.215881	53.372772
H	-0.991963	-29.044773	52.336468	N	-6.188438	-22.591640	52.385944
H	-8.909710	-16.675373	53.038010	C	-4.406383	-23.822285	52.688549
H	-5.355939	-16.134195	40.210564	C	-5.598612	-22.834553	51.191750
H	-6.656253	-23.884270	55.009735	N	-4.510933	-23.580770	51.323631
H	1.087446	-20.711859	51.976788	H	-6.208330	-22.190437	55.121601
				H	-5.019419	-23.459604	55.473122
2INT3				H	-7.017797	-21.991465	52.528580
C	-6.283006	-15.849997	40.663006	H	-3.596699	-24.415962	53.084946
C	-6.622902	-16.833143	41.753277	H	-5.979914	-22.456627	50.255714
C	-7.945639	-17.060759	42.153034	C	-3.633001	-26.329996	44.421005
C	-5.604271	-17.540443	42.402153	C	-2.855177	-26.762465	45.663212
C	-8.245613	-17.949917	43.180901	C	-3.114370	-28.223352	46.031063
C	-5.883224	-18.433872	43.434406	O	-4.066167	-28.864286	45.581612
C	-7.207222	-18.624994	43.821690	N	-2.207535	-28.764616	46.887878
O	-7.549679	-19.461164	44.870659	H	-3.522981	-25.255186	44.246841
H	-6.170840	-14.831463	41.055023	H	-4.693637	-26.569948	44.521057
H	-7.053759	-15.818941	39.886929	H	-1.778170	-26.618773	45.515373
H	-8.754804	-16.532686	41.655254	H	-3.116873	-26.142214	46.526703
H	-4.571415	-17.389959	42.098900	H	-1.529626	-28.187969	47.392738
H	-9.269792	-18.125187	43.494595	H	-2.410328	-29.694817	47.222488
H	-5.081354	-18.972771	43.932827	C	-9.383001	-17.371994	52.377991
H	-8.090668	-18.382345	46.148552	O	-8.443744	-18.346060	51.921478
C	-5.862984	-23.187992	54.834003	H	-10.196401	-17.867125	52.922760

H	-9.818863	-16.820541	51.538242	C	-0.865988	-22.388004	50.438015
H	-8.320494	-18.257132	50.957825	C	-0.238015	-21.044989	50.311993
C	-1.026739	-28.204355	53.041496	C	1.071690	-20.617371	50.884068
C	-1.118010	-26.892960	52.337029	C	-1.197991	-20.294012	49.510021
C	-0.223992	-25.726032	52.398972	C	-1.150867	-18.879705	49.039452
C	1.050101	-25.546206	53.154484	C	-2.263018	-21.284986	49.266975
C	-2.175945	-26.434074	51.412918	C	-3.405935	-20.929007	48.466953
C	-3.243029	-27.334961	51.048027	N	-4.289013	-25.907684	49.292301
N	-2.014580	-25.178057	50.933815	C	-4.166003	-27.087015	49.946026
C	-0.861046	-24.739944	51.486088	C	-5.219992	-26.140009	48.332970
C	-0.262984	-23.437021	51.229958	C	-5.778984	-27.518005	48.344017
N	-4.387621	-23.209806	48.181347	C	-6.751010	-28.114599	47.385063
C	-4.392139	-21.856989	47.991142	C	-5.045001	-28.163986	49.439976
C	-5.585950	-21.422012	47.270943	C	-5.134350	-29.565075	49.942062
O	-8.253365	-17.821480	46.942219	H	-0.120992	-28.254185	53.651676
C	-8.055319	-18.533039	48.051147	H	-1.882968	-28.370451	53.706814
O	-8.249970	-18.029207	49.144173	H	0.995601	-24.698259	53.847977
C	-7.592240	-19.974293	47.860413	H	1.897918	-25.362492	52.483349
C	-6.148089	-20.127720	47.395905	H	1.284455	-26.437422	53.743031
C	-6.312028	-22.663990	46.927048	H	-3.259496	-28.315607	51.504551
C	-7.574586	-22.852104	46.150745	H	0.683853	-23.223097	51.709385
C	-5.436892	-23.750027	47.445854	H	-7.693779	-20.459337	48.840069
C	-5.749054	-25.167976	47.409077	H	-8.293337	-20.479971	47.186874
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H	-5.485678	-19.312939	47.679386	O	-0.505205	-26.982922	48.468182
H	-7.762957	-22.016626	45.470486	H	-0.731705	-27.203865	49.381359
H	-8.453207	-22.950661	46.803513	H	-0.996026	-29.045509	52.338551
H	-7.528947	-23.762222	45.544117	H	-8.909710	-16.675371	53.038013
H	-6.537876	-25.489258	46.742256	H	-5.355938	-16.134199	40.210560
H	1.280004	-19.571251	50.643684	H	-6.656254	-23.884270	55.009739
H	1.901548	-21.217955	50.492157	H	1.088860	-20.713976	51.976574
H	-1.136472	-18.814995	47.944592				
H	-0.253717	-18.376797	49.410282	6INT4			
H	-2.017512	-18.304661	49.388187	C	-6.283009	-15.849996	40.663010
H	-3.497383	-19.896540	48.158051	C	-6.102869	-16.114941	42.151585
H	-6.245186	-28.359751	46.442982	C	-4.820415	-16.422138	42.633938
H	-7.588009	-27.440859	47.171055	C	-7.143392	-16.084091	43.089512
H	-7.170748	-29.041349	47.787350	C	-4.578503	-16.692671	43.976051
H	-5.286288	-29.604561	51.027401	C	-6.920813	-16.352682	44.445274
H	-5.967740	-30.092058	49.470181	C	-5.630537	-16.667521	44.900269
Fe	-3.133790	-24.227016	49.506760	O	-5.327642	-16.961220	46.193085
O	-8.406547	-20.923859	52.770576	H	-6.479179	-14.794191	40.443150
H	-4.222674	-30.134043	49.719269	H	-7.094168	-16.441826	40.226341
H	-3.251407	-26.857344	43.571762	H	-3.986316	-16.455400	41.936111
H	-8.385755	-19.972996	52.501976	H	-8.154355	-15.847946	42.763786
H	-9.261613	-21.251753	52.470337	H	-3.580522	-16.932762	44.329571
O	-2.130468	-24.683731	48.317097	H	-7.743744	-16.310921	45.154873
H	-0.959525	-26.127069	48.334713	H	-1.520157	-24.063820	47.559258

C	-5.862981	-23.187988	54.834000	H	-10.148732	-17.926468	52.936520
C	-5.470564	-23.168402	53.376282	H	-9.878279	-16.807972	51.580200
N	-6.191807	-22.474136	52.421741	H	-8.474913	-18.369146	50.883236
C	-4.465160	-23.793591	52.669186	C	-1.018768	-28.205025	53.037868
C	-5.615386	-22.699171	51.217442	C	-1.118002	-26.892946	52.337032
N	-4.562238	-23.498793	51.318645	C	-0.224000	-25.726044	52.398972
H	-6.195115	-22.199987	55.167271	C	1.050079	-25.550402	53.154709
H	-5.009282	-23.485863	55.448307	C	-2.175963	-26.434084	51.412926
H	-7.007625	-21.854771	52.583363	C	-3.243028	-27.334951	51.048019
H	-3.681947	-24.435013	53.044624	N	-2.007152	-25.185390	50.947533
H	-5.984412	-22.258318	50.303604	C	-0.861029	-24.739941	51.486073
C	-3.633008	-26.329996	44.421021	C	-0.262996	-23.437017	51.229969
C	-2.848944	-26.786558	45.650703	N	-4.377913	-23.196430	48.141129
C	-3.143633	-28.239285	46.023880	C	-4.392131	-21.856991	47.991146
O	-4.117491	-28.855293	45.584923	C	-5.585958	-21.422009	47.270939
N	-2.245426	-28.801033	46.874512	O	-7.215193	-17.456747	48.069202
H	-3.512399	-25.255367	44.252159	C	-7.642616	-18.602919	48.221340
H	-4.695031	-26.563229	44.520790	O	-8.269730	-19.200232	49.094875
H	-1.770926	-26.682411	45.477608	C	-7.306745	-19.618683	46.827595
H	-3.058417	-26.157740	46.520969	C	-5.975188	-20.103500	47.023975
H	-1.529609	-28.247711	47.356312	C	-6.312024	-22.663986	46.927063
H	-2.453363	-29.735439	47.193539	C	-7.564607	-22.849539	46.142338
C	-9.382989	-17.372015	52.377995	C	-5.436894	-23.750032	47.445839
O	-8.393882	-18.262461	51.852272	C	-5.749057	-25.167974	47.409088

N	-2.041096	-22.491695	49.802921	H	-6.114959	-16.977427	46.786278
C	-0.865971	-22.388018	50.438007	H	-5.209750	-19.327841	47.048206
C	-0.238026	-21.044979	50.311989	H	-7.644969	-22.110666	45.339142
C	1.066793	-20.611277	50.889908	H	-8.455697	-22.739920	46.773758
C	-1.197983	-20.294018	49.510036	H	-7.605189	-23.844795	45.692314
C	-1.153663	-18.877325	49.047821	H	-6.542415	-25.489983	46.748898
C	-2.263035	-21.284981	49.266968	H	1.283722	-19.571831	50.630505
C	-3.405930	-20.929010	48.466953	H	1.897778	-21.224993	50.521713
N	-4.285893	-25.925348	49.284328	H	-1.163284	-18.806274	47.953747
C	-4.165989	-27.087027	49.946030	H	-0.248493	-18.378675	49.403572
C	-5.219990	-26.140005	48.332951	H	-2.013089	-18.304335	49.415962
C	-5.778983	-27.518009	48.344032	H	-3.508573	-19.892212	48.177856
C	-6.754186	-28.118015	47.391827	H	-6.243014	-28.379047	46.456650
C	-5.045009	-28.163979	49.439964	H	-7.582867	-27.438696	47.164787
C	-5.137553	-29.565933	49.938118	H	-7.184643	-29.035231	47.803917
H	-0.121193	-28.247734	53.660084	H	-5.276164	-29.607483	51.024967
H	-1.882689	-28.382837	53.689850	H	-5.979055	-30.087475	49.475082
H	0.999128	-24.696609	53.841122	Fe	-3.092763	-24.246412	49.449181
H	1.899075	-25.376213	52.482513	O	-8.417562	-20.819426	52.766827
H	1.279276	-26.438078	53.750149	H	-4.231236	-30.137772	49.701569
H	-3.259708	-28.315088	51.505005	H	-3.251399	-26.857344	43.571747
H	0.679403	-23.219730	51.715847	H	-8.325947	-19.874079	52.487583
H	-8.088873	-20.370455	46.789509	H	-9.133904	-21.156857	52.215321
H	-7.391785	-18.870764	46.039135	O	-1.890845	-24.782833	48.088215

H	-0.894573	-26.210190	48.205708	H	-1.509462	-24.064199	47.565098
O	-0.438290	-27.072466	48.357830	C	-5.862979	-23.187990	54.834003
H	-0.628981	-27.261108	49.285572	C	-5.469215	-23.170412	53.376839
H	-0.969497	-29.041929	52.330990	N	-6.191095	-22.475821	52.423046
H	-8.909718	-16.675352	53.038010	C	-4.465015	-23.796129	52.668808
H	-5.355934	-16.134199	40.210560	C	-5.615914	-22.701010	51.217785
H	-6.656260	-23.884274	55.009739	N	-4.563326	-23.500984	51.318512
H	1.068573	-20.685131	51.984280	H	-6.196643	-22.199621	55.164658
				H	-5.010107	-23.484297	55.450199
6TS4				H	-7.003959	-21.856461	52.592724
C	-6.283009	-15.849996	40.663006	H	-3.681758	-24.438232	53.042950
C	-6.098613	-16.103153	42.152554	H	-5.984862	-22.260529	50.303654
C	-4.815014	-16.408030	42.633263	C	-3.633002	-26.329994	44.421005
C	-7.136868	-16.063995	43.092339	C	-2.850792	-26.786076	45.651974
C	-4.569740	-16.669788	43.976448	C	-3.142831	-28.239780	46.022778
C	-6.910856	-16.323627	44.449146	O	-4.115463	-28.856901	45.582630
C	-5.620035	-16.637300	44.901546	N	-2.244034	-28.801443	46.872971
O	-5.314455	-16.924900	46.196644	H	-3.512155	-25.255344	44.252415
H	-6.483749	-14.796652	40.435818	H	-4.695223	-26.562735	44.520000
H	-7.092867	-16.448217	40.232731	H	-1.772596	-26.678019	45.482773
H	-3.983033	-16.447084	41.933346	H	-3.065801	-26.159065	46.522118
H	-8.148295	-15.829056	42.767410	H	-1.529735	-28.248137	47.356838
H	-3.571419	-16.909107	44.329342	H	-2.452432	-29.735655	47.192295
H	-7.732331	-16.276791	45.160210	C	-9.383001	-17.371998	52.377987

O	-8.399080	-18.282156	51.876770	C	-5.749049	-25.167976	47.409081
H	-10.165783	-17.908613	52.930210	N	-2.040980	-22.491791	49.802597
H	-9.857165	-16.808945	51.566830	C	-0.865978	-22.388008	50.438023
H	-8.476342	-18.401726	50.910694	C	-0.238023	-21.044983	50.311981
C	-1.018883	-28.204958	53.038208	C	1.066864	-20.611160	50.889915
C	-1.118003	-26.892948	52.337029	C	-1.197986	-20.294018	49.510036
C	-0.224001	-25.726042	52.398968	C	-1.153015	-18.877308	49.047539
C	1.050150	-25.550604	53.154804	C	-2.263027	-21.284979	49.266968
C	-2.175952	-26.434088	51.412918	C	-3.405918	-20.929016	48.466934
C	-3.243027	-27.334951	51.048019	N	-4.285775	-25.925423	49.283562
N	-2.007173	-25.185575	50.947273	C	-4.166000	-27.087023	49.946037
C	-0.861036	-24.739939	51.486084	C	-5.219997	-26.140007	48.332954
C	-0.262992	-23.437021	51.229958	C	-5.778976	-27.518011	48.344028
N	-4.377530	-23.198475	48.139648	C	-6.755362	-28.117516	47.392529
C	-4.392162	-21.856977	47.991184	C	-5.045008	-28.163980	49.439964
C	-5.585942	-21.422018	47.270924	C	-5.137856	-29.565788	49.938614
O	-7.224323	-17.445726	48.084034	H	-0.119894	-28.248600	53.658394
C	-7.631863	-18.589317	48.250389	H	-1.881452	-28.381559	53.692364
O	-8.238253	-19.226049	49.100826	H	0.998964	-24.697760	53.842426
C	-7.281209	-19.617090	46.778355	H	1.899046	-25.375072	52.482819
C	-5.965011	-20.100836	46.991009	H	1.279958	-26.438953	53.749084
C	-6.312026	-22.663988	46.927055	H	-3.259836	-28.315132	51.504963
C	-7.564122	-22.849726	46.141232	H	0.679354	-23.219687	51.716003
C	-5.436894	-23.750029	47.445847	H	-8.079508	-20.350889	46.741699

H	-7.368441	-18.828913	46.033417	O	-1.886736	-24.785303	48.086502
H	-6.101183	-16.934769	46.784431	H	-0.890583	-26.211378	48.215706
H	-5.189840	-19.334356	46.990719	O	-0.438016	-27.075972	48.365837
H	-7.642225	-22.112061	45.336452	H	-0.630762	-27.266388	49.292816
H	-8.456351	-22.738094	46.770683	H	-0.972315	-29.042330	52.331688
H	-7.605261	-23.845602	45.692543	H	-8.909710	-16.675367	53.038013
H	-6.543682	-25.489906	46.750309	H	-5.355935	-16.134199	40.210560
H	1.284295	-19.571968	50.629677	H	-6.656259	-23.884272	55.009739
H	1.897863	-21.225384	50.522568	H	1.068515	-20.684019	51.984379
H	-1.162344	-18.806232	47.953442				
H	-0.247623	-18.378983	49.403351	PRO			
H	-2.012087	-18.303577	49.415489	C	-6.283012	-15.849995	40.656811
H	-3.510008	-19.891855	48.179203	C	-6.137535	-15.983811	42.157452
H	-6.247429	-28.375034	46.454670	C	-4.940980	-16.461170	42.710861
H	-7.586219	-27.439199	47.170132	C	-7.170590	-15.648106	43.041012
H	-7.182817	-29.036793	47.803234	C	-4.772830	-16.607552	44.085060
H	-5.281031	-29.606833	51.024933	C	-7.021275	-15.788290	44.421509
H	-5.976656	-30.088820	49.472313	C	-5.818453	-16.273027	44.947697
Fe	-3.091348	-24.247646	49.444698	O	-5.611821	-16.449373	46.291553
O	-8.410883	-20.824282	52.852543	H	-6.530154	-14.825073	40.357456
H	-4.229761	-30.136633	49.706528	H	-7.068251	-16.504580	40.260979
H	-3.251406	-26.857346	43.571758	H	-4.119659	-16.728235	42.050274
H	-8.330500	-19.885908	52.551220	H	-8.112364	-15.271036	42.648769
H	-9.161183	-21.169437	52.353664	H	-3.843577	-16.981180	44.502712

H	-7.837893	-15.521389	45.089031	C	-9.401601	-17.347198	52.421379
H	-1.572686	-24.115982	47.470997	O	-8.437572	-18.323322	52.023022
C	-5.862976	-23.187986	54.840202	H	-10.227912	-17.795218	52.989651
C	-5.460055	-23.188150	53.388226	H	-9.824129	-16.827114	51.553867
N	-6.199670	-22.519688	52.428810	H	-8.716529	-18.694178	51.175179
C	-4.451546	-23.807465	52.683083	C	-1.013605	-28.204519	53.039471
C	-5.625181	-22.751387	51.220757	C	-1.117995	-26.892933	52.337029
N	-4.562685	-23.530943	51.331562	C	-0.224012	-25.719854	52.398968
H	-6.214116	-22.198643	55.149887	C	1.051231	-25.549686	53.156357
H	-5.013979	-23.466127	55.469879	C	-2.169761	-26.434105	51.419121
H	-6.989414	-21.898314	52.634743	C	-3.243025	-27.341141	51.048012
H	-3.656499	-24.434597	53.057865	N	-2.002152	-25.188887	50.948666
H	-5.999945	-22.337576	50.296246	C	-0.854822	-24.739927	51.492287
C	-3.626803	-26.329994	44.421009	C	-0.263003	-23.437025	51.229954
C	-2.882351	-26.820307	45.661804	N	-4.370896	-23.218359	48.152866
C	-3.174612	-28.286160	45.980526	C	-4.416952	-21.856972	48.009777
O	-4.139039	-28.892166	45.507725	C	-5.592164	-21.453022	47.270943
N	-2.283856	-28.869457	46.824936	O	-8.149247	-16.541389	47.969402
H	-3.537871	-25.244818	44.310181	C	-8.616395	-17.445015	48.543770
H	-4.682965	-26.603123	44.463486	O	-9.112151	-18.324654	49.134171
H	-1.800174	-26.696655	45.535851	C	-7.142770	-19.622585	46.528828
H	-3.135867	-26.224083	46.542679	C	-5.941410	-20.083250	46.922848
H	-1.589722	-28.319550	47.342735	C	-6.293409	-22.645388	46.914650
H	-2.504785	-29.805616	47.130108	C	-7.525232	-22.828146	46.094929

C	-5.412100	-23.768627	47.458229	H	1.007300	-24.693375	53.840500
C	-5.742844	-25.167974	47.415295	H	1.903502	-25.384464	52.485695
N	-2.044359	-22.489958	49.802639	H	1.273931	-26.436932	53.755596
C	-0.865964	-22.388012	50.438030	H	-3.257212	-28.320053	51.508675
C	-0.238035	-21.051176	50.311970	H	0.680131	-23.216291	51.714146
C	1.067983	-20.610508	50.882988	H	-8.026242	-20.248087	46.474407
C	-1.210377	-20.294027	49.503845	H	-7.246701	-18.589310	46.216824
C	-1.159611	-18.878084	49.037819	H	-6.403057	-16.179016	46.775822
C	-2.269236	-21.284966	49.266960	H	-5.132988	-19.354813	46.960751
C	-3.430714	-20.935225	48.473137	H	-7.555225	-22.110849	45.266815
N	-4.279009	-25.935116	49.282509	H	-8.440598	-22.678038	46.683517
C	-4.159796	-27.099434	49.952248	H	-7.576276	-23.835245	45.672241
C	-5.213810	-26.146206	48.339146	H	-6.548417	-25.479738	46.764893
C	-5.778965	-27.518017	48.350243	H	1.275143	-19.567316	50.628342
C	-6.758981	-28.114054	47.398727	H	1.902431	-21.213978	50.505054
C	-5.045015	-28.170170	49.446152	H	-1.153576	-18.807890	47.943184
C	-5.143239	-29.573294	49.940502	H	-0.258291	-18.378742	49.404026
H	-0.117161	-28.241646	53.664375				
H	-1.877454	-28.389250	53.690117				
H	-2.022134	-18.300261	49.392700				
H	-3.540839	-19.895901	48.195259				
H	-6.258690	-28.371902	46.456852				
H	-7.589081	-27.433044	47.180199				
H	-7.188292	-29.033209	47.808945				

H	-5.263661	-29.618078	51.029564		
H	-5.997303	-30.085747	49.489574		
Fe	-3.067407	-24.261772	49.417545		
O	-8.201240	-20.745556	53.385933		
H	-4.246277	-30.153509	49.688042		
H	-3.189405	-26.801546	43.559357		
H	-8.217190	-19.836946	53.019661		
H	-9.122797	-21.026354	53.421288		
O	-1.850769	-24.813438	48.079063		
H	-0.907994	-26.278755	48.202751		
O	-0.521411	-27.168447	48.387329		
H	-0.797512	-27.333408	49.298573		
H	-0.956327	-29.042747	52.334377		
H	-8.909709	-16.619566	53.038021		
H	-5.355932	-16.121801	40.198158		
H	-6.650062	-23.890474	55.015938		
H		1.081305		-20.690519	51.977139