

Supporting Information

An Active Site Tyr Residue Guides the Regioselectivity of Lysine Hydroxylation by the Nonheme Iron Lysine-4-Hydroxylase enzymes Through Proton-Coupled-Electron-Transfer.

Yuanxin Cao,^{§,&} Sam Hay,^{§,&} and Sam P. de Visser^{*§,⊥}

[§] Manchester Institute of Biotechnology, The University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom

[&] Department of Chemistry, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

[⊥] Department of Chemical Engineering, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

Email: sam.devisser@manchester.ac.uk

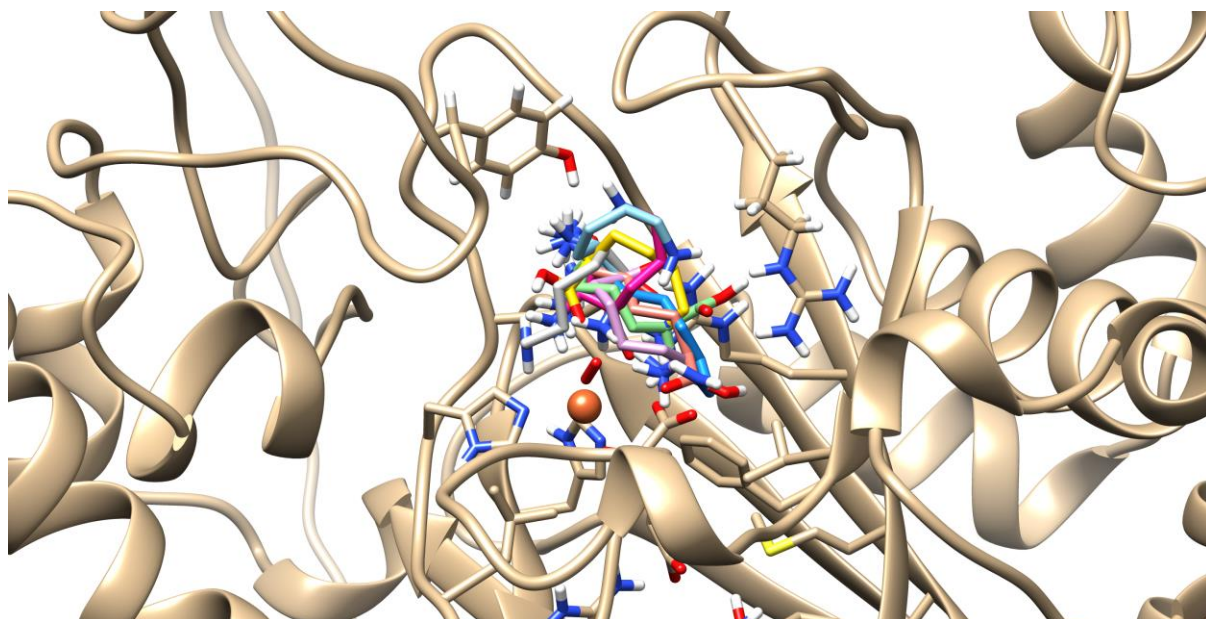


Figure S1: Overlay of the docked substrate positions in the active site of KDO5. The light-blue structure/position was selected as starting point for the MD simulation.

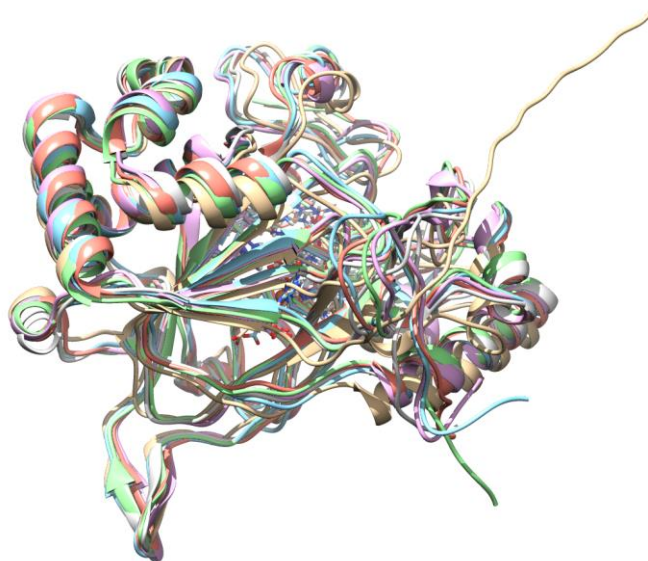


Figure S2: Overlay of the MD frames after 0 ns (starting point, yellow), 10 ns, 20 ns, 30 ns, 40 ns and 50 ns (other colors).

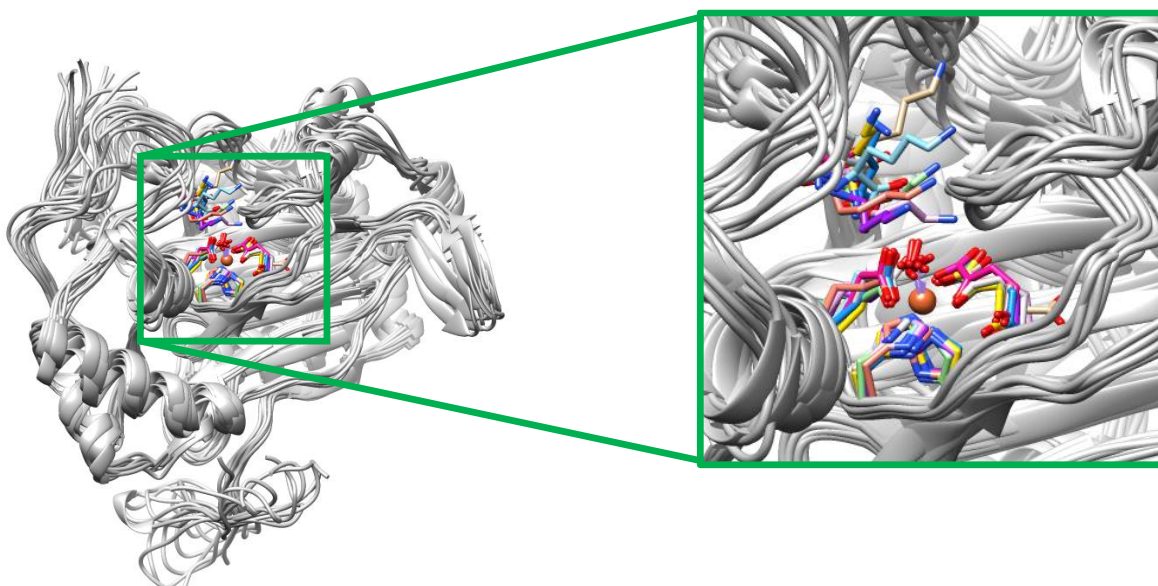
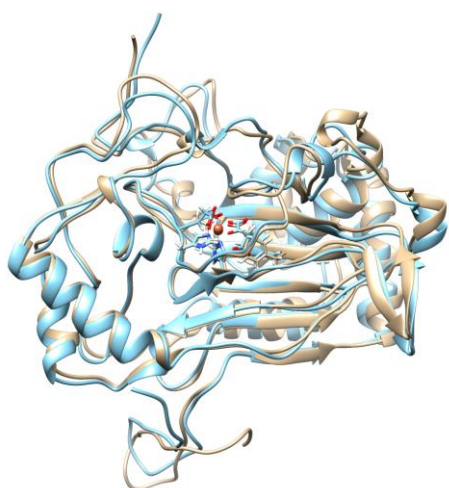


Figure S3: Overlay of the MD frames after 20, 40, 60, 80, 100, 120, 140, 160, 180, and 200 ns. As can be seen the protein chains are highly similar throughout the MD simulation and also the metal with its first coordination appears rigid during the full MD simulation. Even the α KG is in similar positions throughout the MD simulation.



Overlay Sn_{50} and Sn_{200}



Overlay 6EUR pdb and Sn_{200}

Figure S4: Overlay of the MD frames after 50 ns and 200 ns (left-hand-side) and an overlay of the MD frame after 200 ns with the original 6EUR pdb file. As can be seen, both MD frames have almost identical fold and metal first-coordination sphere. The overlay of the last frame from the MD with the crystal structure coordinates also shows similar fold.

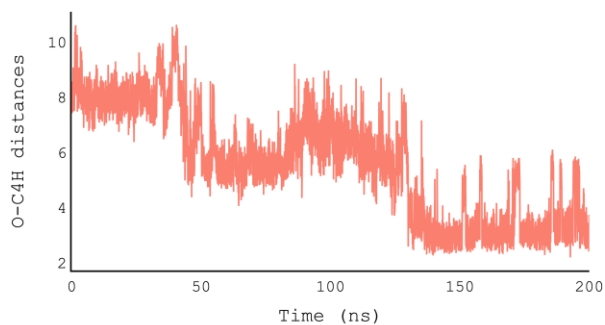
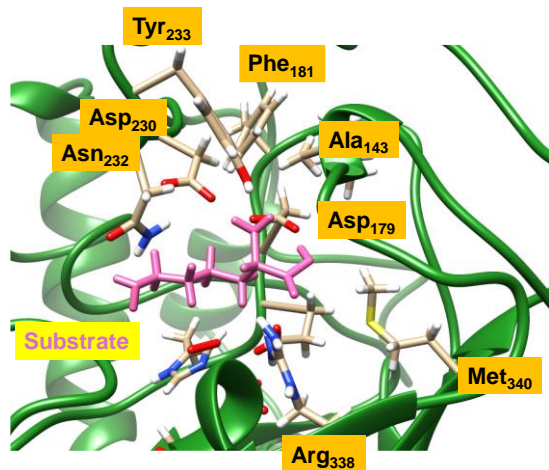


Figure S5: Left: Substrate positioning in the active site in the snapshot after 200 ns from the MD simulation. Right O-HC₄ distance measured along the 200 ns MD simulation.

Table S1: Docking results given by Autodock vina on L-Lys docking into the 6EUR pdb file (chain A).

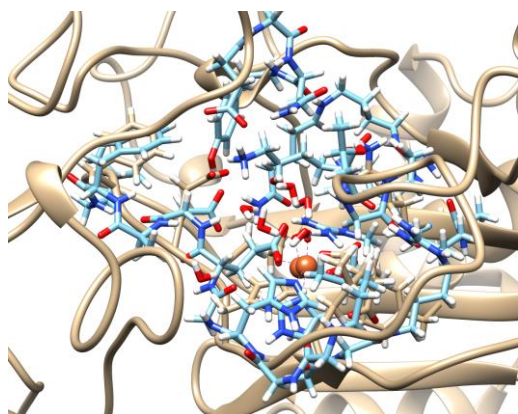
Position	Score	RMSD Å	BFE kcal/mol
1	-4.816	0.000	-6.878
2	-4.798	3.191	-6.854
3	-4.751	3.565	-6.788
4	-4.746	1.881	-6.782
5	-4.715	2.599	-6.738
6	-4.712	2.694	-6.735
7	-4.578	2.469	-6.550
8	-4.556	3.407	-6.519
9	-4.527	4.241	-6.479

Table S2: Atoms selected in the measurement of residue-substrate distances in the MD structural analysis.

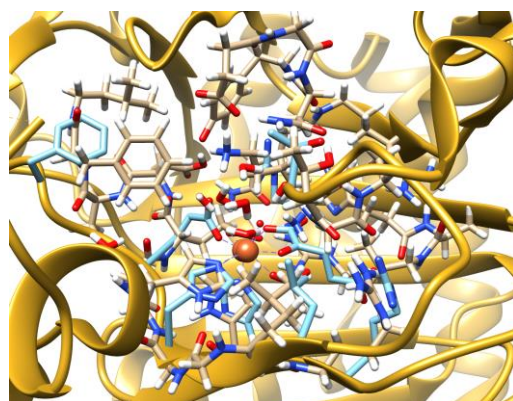
atom1		atom2	
ALA143	HB2	L-LYS	HC
ARG145	2HH1	L-LYS	H22
ASP179	OD2	L-LYS	H15
ASP230	OD1	L-LYS	HC4
ASN232	OD1	L-LYS	HC7
ARG338	2HH2	L-LYS	O1

Table S3: Atomic names and coordinates of L-Lysine used as a substrate in MD simulations.

C3	28.39	34.07	59.40
HC2	28.22	34.59	60.35
HC3	28.95	33.16	59.63
C1	29.13	34.93	58.34
HC	28.45	35.64	57.88
C2	30.15	35.94	59.04
O1	29.83	36.53	60.02
O2	31.30	36.28	58.42
H15	31.27	35.93	57.52
N1	29.75	34.08	57.22
2HN1	30.15	33.28	57.73
3HN1	30.42	34.53	56.58
1HN1	28.96	33.73	56.66
C4	26.95	33.62	58.89
HC4	26.45	32.97	59.62
HC5	27.05	33.10	57.93
C5	25.88	34.74	58.62
HC6	24.96	34.19	58.38
HC7	26.06	35.37	57.74
C6	25.73	35.68	59.84
HC8	24.83	36.28	59.65
HC9	25.59	35.22	60.82
N2	26.76	36.71	59.86
H21	26.44	37.39	60.55
H22	27.57	36.27	60.30

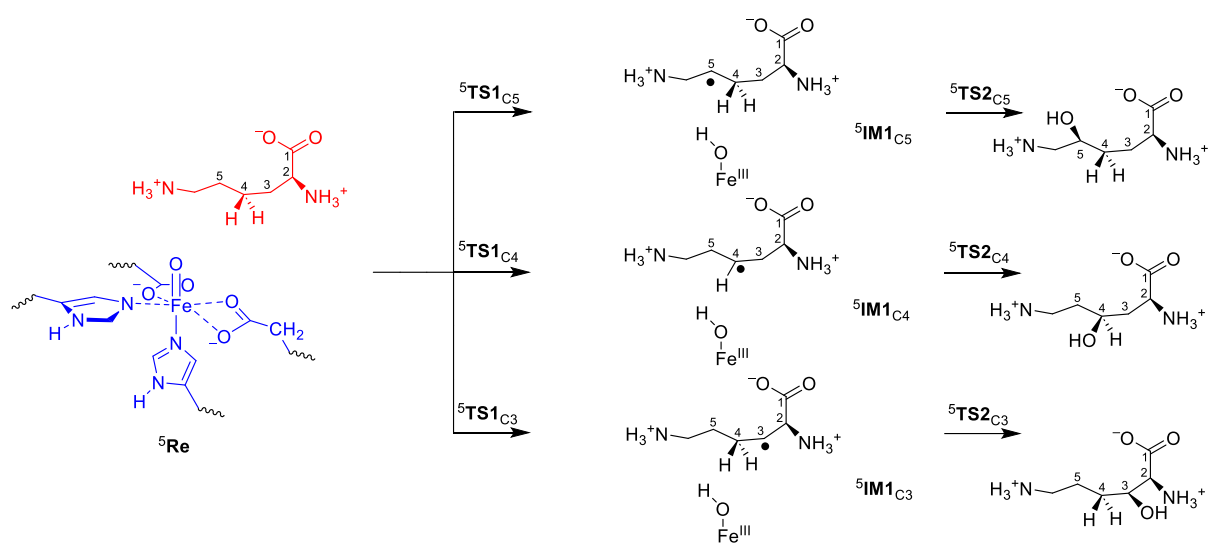


Overlay $^5\text{Re}_c$ and Sn_{200}



Overlay $^5\text{Re}_c$ and 6EUR pdb

Figure S6: Overlay of the optimized reactant spin structure ($^5\text{Re}_c$) with the last snapshot of the MD simulation (left-hand-side) and with the crystal structure coordinates of the 6EUR pdb (right-hand-side).



Scheme S1: Reaction scheme calculated with DFT methods in this work with definition of the nomenclature of the structures of local minima and transition states.

Table S4: Absolute (in au) energies and free energies of UB3LYP/BS1 optimized geometries along the reaction mechanisms calculated for KDO5 in Gaussian-09. Gc is the free energy correction at 298 K.

Model 1	E [BS1, au]	ZPE [au]	G [au]	E [BS2, au]	Gc [au]
⁵ Re _A	-7650.646028	2.507816	-7648.378123	-7652.729653	2.267905
⁵ TS1 _{A,C5}	-7650.610004	2.498905	-7648.353059	-7652.697867	2.256945
⁵ IM1 _{A,C5}	-7650.641737	2.504120	-7648.375615	-7652.728843	2.266114
⁵ TS2 _{A,C5}	-7650.621548	2.503945	-7648.356197	-7652.707399	2.265456
⁵ Pr _{A,C5}	-7650.729836	2.509469	-7648.456352	-7652.813251	2.273280
⁵ TS1 _{A,C4}	-7650.605494	2.499527	-7648.343429	-7652.694329	2.262057
⁵ IM1 _{A,C4}	-7650.642883	2.503369	-7648.377702	-7652.730585	2.265126
⁵ TS2 _{A,C4}	-7650.625957	2.501926	-7648.362692	-7652.715353	2.262899
⁵ Pr _{A,C4}	-7650.735192	2.508804	-7648.464784	-7652.822205	2.270259
⁵ TS1 _{A,C3}	-7650.607613	2.498632	-7648.353178	-7652.692831	2.254407
⁵ IM1 _{A,C3}	-7650.641982	2.503959	-7648.376087	-7652.730180	2.265909
⁵ TS2 _{A,C3}	-7650.637967	2.502395	-7648.374000	-7652.722477	2.263792
⁵ Pr _{A,C3}	-7650.719555	2.508531	-7648.447306	-7652.802216	2.272007
Model 2					
⁵ Re _B	-8063.345994	2.635052	-8060.956658	-8065.676410	2.389239
⁵ TS1 _{B,C5}	-8063.314679	2.628298	-8060.923727	-8065.648193	2.390679
⁵ IM1 _{B,C5}	-8063.350480	2.631786	-8060.965946	-8065.687672	2.384390
⁵ TS2 _{B,C5}	-8063.337647	2.631481	-8060.946380	-8065.667092	2.391106
⁵ Pr _{B,C5}	-8063.430289	2.636468	-8061.039137	-8065.754705	2.391144
⁵ TS1 _{B,C4}	-8063.310985	2.630503	-8060.920033	-8065.633251	2.390936
⁵ IM1 _{B,C4}	-8063.354446	2.633997	-8060.964838	-8065.683408	2.389364
⁵ TS2 _{B,C4}	-8063.334099	2.633260	-8060.943995	-8065.662965	2.389808
⁵ Pr _{B,C4}	-8063.442634	2.640735	-8061.039116	-8065.748459	2.403373
⁵ TS1 _{B,C3}	-8063.307444	2.628488	-8060.919484	-8065.630661	2.387755
⁵ IM1 _{B,C3}	-8063.364949	2.631786	-8060.975699	-8065.688797	2.389035
⁵ TS2 _{B,C3}	-8063.344781	2.633608	-8060.943012	-8065.652929	2.401419
⁵ Pr _{B,C3}	-8063.430289	2.637738	-8061.031498	-8065.732990	2.399506
Model 3					
¹ Re _C	-11045.049473	3.468631	-11041.848519	-11056.082383	3.201001
³ Re _C	-11045.076807	3.469389	-11041.876789	-11056.110260	3.199625
⁵ Re _C	-11045.085570	3.468591	-11041.888015	-11056.117861	3.197507
⁵ TS1 _{C,C5}	-11045.040713	3.461841	-11041.848896	-11056.068558	3.191272
⁵ IM1 _{C,C5}	-11045.046489	3.463608	-11041.846505	-11056.078657	3.199610
⁵ Pr _{C,C5}	-11045.134049	3.469995	-11041.930091	-11056.156385	3.203388
⁵ TS1 _{C,C4}	-11045.043038	3.462502	-11041.851395	-11056.072437	3.191642
⁵ IM1 _{C,C4}	-11045.047015	3.464278	-11041.849144	-11056.078397	3.197707
⁵ Pr _{C,C4}	-11045.132566	3.469799	-11041.927643	-11056.154066	3.204616
⁵ TS1 _{C,C3}	-11045.041669	3.466475	-11041.842899	-11056.073214	3.198467
⁵ IM1 _{C,C3}	-11045.046998	3.462083	-11041.859441	-11056.085439	3.187202
⁵ TS2 _{C,C3}	-11045.043761	3.463368	-11041.853183	-11056.085486	3.190121

⁵ Pr _{C,C3}	-11045.085273	3.467007	-11041.891361	-11056.123567	3.193559
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Table S5: Relative (in kcal mol⁻¹) energies and free energies of UB3LYP/BS1 optimized geometries along the reaction mechanisms calculated for KDO5 in Gaussian-09.

Model 1	ΔE [BS1]	$\Delta E+ZPE$	ΔG [BS1]	ΔE [BS2]	$\Delta E+ZPE$	ΔG [BS2]
⁵ Re _A	0.00	0.00	0.00	0.00	0.00	0.00
⁵ TS1 _{A,C5}	22.61	17.01	15.73	19.95	14.35	13.07
⁵ IM1 _{A,C5}	2.69	0.37	1.57	0.51	-1.81	-0.62
⁵ TS2 _{A,C5}	15.36	12.93	13.76	13.96	11.54	12.43
⁵ Pr _{A,C5}	-52.59	-51.55	-49.09	-52.46	-51.42	-49.09
⁵ TS1 _{A,C4}	25.44	20.23	21.77	22.17	16.96	18.50
⁵ IM1 _{A,C4}	1.97	-0.82	0.26	-0.58	-3.38	-2.33
⁵ TS2 _{A,C4}	12.59	8.90	9.68	8.97	5.28	5.83
⁵ Pr _{A,C4}	-55.95	-55.33	-54.38	-58.08	-57.46	-56.60
⁵ TS1 _{A,C3}	24.11	18.34	15.65	23.11	17.34	14.64
⁵ IM1 _{A,C3}	2.54	0.12	1.28	-0.33	-2.75	-1.58
⁵ TS2 _{A,C3}	5.06	1.66	2.59	4.50	1.10	1.92
⁵ Pr _{A,C3}	-46.14	-45.69	-43.41	-45.53	-45.09	-42.96
Model 2						
⁵ Re _B	0.00	0.00	0.00	0.00	0.00	0.00
⁵ TS1 _{B,C5}	19.65	15.41	20.66	17.71	13.47	18.61
⁵ IM1 _{B,C5}	-2.82	-4.86	-5.83	-7.07	-9.12	-10.11
⁵ TS2 _{B,C5}	5.24	3.00	6.45	5.85	3.61	7.02
⁵ Pr _{B,C5}	-52.90	-52.01	-51.76	-49.13	-48.24	-47.94
⁵ TS1 _{B,C4}	21.97	19.11	22.98	27.08	24.23	28.15
⁵ IM1 _{B,C4}	-5.30	-5.97	-5.13	-4.39	-5.05	-4.31
⁵ TS2 _{B,C4}	7.46	6.34	7.95	8.44	7.31	8.79
⁵ Pr _{B,C4}	-60.64	-57.08	-51.74	-45.21	-41.65	-36.34
⁵ TS1 _{B,C3}	24.19	20.07	23.33	28.71	24.59	27.78
⁵ IM1 _{B,C3}	-11.89	-13.94	-11.95	-7.77	-9.82	-7.90
⁵ TS2 _{B,C3}	0.76	-0.14	8.56	14.73	13.83	22.38
⁵ Pr _{B,C3}	-52.90	-51.21	-46.96	-35.50	-33.82	-29.06
Model 3						
¹ Re _C	22.65	22.68	24.78	22.26	22.29	24.46
³ Re _C	5.50	6.00	7.04	4.77	5.27	6.10
⁵ Re _C	0.00	0.00	0.00	0.00	0.00	0.00
⁵ TS1 _{C,C5}	28.15	23.91	24.55	30.94	26.70	27.03
⁵ IM1 _{C,C5}	24.52	21.40	26.05	24.60	21.47	25.92
⁵ Pr _{C,C5}	-30.42	-29.54	-26.40	-24.17	-23.29	-20.48
⁵ TS1 _{C,C4}	26.69	22.87	22.98	28.50	24.68	24.82
⁵ IM1 _{C,C4}	24.19	21.49	24.39	24.76	22.06	24.89
⁵ Pr _{C,C4}	-29.49	-28.73	-24.87	-22.72	-21.96	-18.26
⁵ TS1 _{C,C3}	27.55	26.22	28.31	28.02	26.69	28.62
⁵ IM1 _{C,C3}	24.20	20.12	17.93	20.35	16.26	13.88

⁵ TS _{C,C3}	26.23	22.96	21.86	20.32	17.04	15.68
⁵ Pr _{C,C3}	0.19	-0.81	-2.10	-3.58	-4.58	-6.06

Table S6: Group charges and group spin densities of UB3LYP/BS1 optimized geometries along the reaction mechanisms calculated for KDO5 in Gaussian-09.

Charge	Fe	O	Succ	SubH	Prot	Wat	Total
Model 1							
⁵ Re _A	0.71	-0.40	-0.34	0.71	-1.68	0.00	-1.00
⁵ TS _{1,A,C5}	0.80	-0.61	-0.38	0.95	-1.77	0.00	-1.00
⁵ IM _{1,A,C5}	0.81	-0.81	-0.41	1.20	-1.80	0.00	-1.00
⁵ TS _{2,A,C5}	0.61	-0.77	-0.48	1.49	-1.85	0.00	-1.00
⁵ Pr _{A,C5}	0.58	-0.69	-0.49	1.50	-1.90	0.00	-1.00
⁵ TS _{1,A,C4}	0.80	-0.60	-0.36	0.91	-1.75	0.00	-1.00
⁵ IM _{1,A,C4}	0.81	-0.81	-0.40	1.19	-1.80	0.00	-1.00
⁵ TS _{2,A,C4}	0.81	-0.78	-0.36	1.17	-1.83	0.00	-1.00
⁵ Pr _{A,C4}	0.56	-0.67	-0.55	1.47	-1.81	0.00	-1.00
⁵ TS _{1,A,C3}	0.80	-0.63	-0.36	0.97	-1.79	0.00	-1.00
⁵ IM _{1,A,C3}	0.81	-0.81	-0.40	1.18	-1.79	0.00	-1.00
⁵ TS _{2,A,C3}	0.63	-0.74	-0.47	1.51	-1.94	0.00	-1.00
⁵ Pr _{A,C3}	0.62	-0.68	-0.47	1.49	-1.96	0.00	-1.00
Model 2							
⁵ Re _B	0.83	-0.50	-0.42	0.72	-0.64	0.00	0.00
⁵ TS _{1,B,C5}	0.84	-0.62	-0.35	0.91	-0.78	0.00	0.00
⁵ IM _{1,B,C5}	0.87	-0.81	-0.36	1.12	-0.82	0.00	0.00
⁵ TS _{2,B,C5}	0.61	-0.77	-0.49	1.62	-0.97	0.00	0.00
⁵ Pr _{B,C5}	0.80	-0.72	-0.54	1.39	-0.94	0.00	0.00
⁵ TS _{1,B,C4}	0.70	-0.70	-0.36	1.09	-0.73	0.00	0.00
⁵ IM _{1,B,C4}	0.79	-0.80	-0.47	1.13	-0.66	0.00	0.00
⁵ TS _{2,B,C4}	0.83	-0.78	-0.51	1.32	-0.86	0.00	0.00
⁵ Pr _{B,C4}	0.72	-0.69	-0.52	1.40	-0.91	0.00	0.00
⁵ TS _{1,B,C3}	0.80	-0.65	-0.37	1.03	-0.81	0.00	0.00
⁵ IM _{1,B,C3}	0.85	-0.81	-0.37	1.12	-0.79	0.00	0.00
⁵ TS _{2,B,C3}	0.74	-0.73	-0.42	1.30	-0.89	0.00	0.00
⁵ Pr _{B,C3}	0.65	-0.66	-0.46	1.44	-0.98	0.00	0.00
Model 3							
⁵ Re _C	0.89	-0.72	-0.48	0.06	1.94	0.30	2.00
¹ Re _C	0.76	-1.06	-0.55	0.12	2.76	-0.02	2.00
³ Re _C	0.96	-1.05	-0.54	0.11	2.51	0.01	2.00
⁷ Re _C	1.08	-1.06	-0.59	0.10	2.47	0.00	2.00
⁵ TS _{1,C,C5}	0.75	-0.62	-0.52	0.20	1.84	0.35	2.00
⁵ IM _{1,C,C5}	0.89	-0.53	-0.44	0.27	1.21	0.59	2.00
⁵ Pr _{C,C5}	0.81	-0.43	-0.48	0.56	1.22	0.32	2.00
⁵ TS _{1,C,C4}	0.75	-0.65	-0.49	0.01	2.00	0.38	2.00
⁵ IM _{1,C,C4}	0.89	-0.54	-0.44	0.19	1.57	0.34	2.00

⁵ Pr _{C,C4}	0.85	-0.44	-0.52	0.48	1.27	0.36	2.00
⁵ TS1 _{C,C3}	0.74	-0.63	-0.50	-0.03	2.06	0.36	2.00
⁵ IM1 _{C,C3}	0.81	-0.58	-0.53	0.13	1.96	0.21	2.00
⁵ Pr _{C,C3}	0.75	-0.49	-0.54	0.59	1.37	0.33	2.00
⁵ Re _{C,PBE0}	0.99	-1.05	-0.57	0.04	2.58	0.01	2.00
³ Re _{C,PBE0}	0.82	-1.02	-0.50	0.05	2.63	0.02	2.00
⁵ TS1 _{C,C3,PBE0}	0.73	-0.93	-0.56	0.05	2.69	0.03	2.00
⁵ TS1 _{C,C4,PBE0}	0.93	-1.04	-0.63	-0.05	2.72	0.07	2.00
⁵ TS1 _{C,C5,PBE0}	0.88	-0.98	-0.65	0.25	2.43	0.07	2.00
⁵ Re _{C,Solv}	1.13	-1.07	-0.59	0.11	2.43	0.00	2.00
⁵ TS1 _{C,C3,Solv}	0.87	-0.97	-0.58	0.12	2.55	0.01	2.00
⁵ TS1 _{C,C4,Solv}	1.10	-1.07	-0.65	0.02	2.56	0.05	2.00
⁵ TS1 _{C,C5,Solv}	1.05	-1.02	-0.67	0.31	2.28	0.05	2.00
Spin density	Fe	O	Succ	SubH	Prot	Wat	Total
Model 1							
⁵ Re _A	3.00	0.67	0.14	0.00	0.19	0.00	4.00
⁵ TS1 _{A,C5}	3.89	0.01	0.20	-0.36	0.26	0.00	4.00
⁵ IM1 _{A,C5}	4.05	0.44	0.19	-0.99	0.31	0.00	4.00
⁵ TS2 _{A,C5}	3.73	-0.06	0.08	0.14	0.12	0.00	4.00
⁵ Pr _{A,C5}	3.75	0.02	0.08	0.00	0.14	0.00	4.00
⁵ TS1 _{A,C4}	3.81	0.06	0.19	-0.31	0.25	0.00	4.00
⁵ IM1 _{A,C4}	4.05	0.44	0.19	-0.99	0.31	0.00	4.00
⁵ TS2 _{A,C4}	4.06	0.42	0.21	-0.99	0.31	0.00	4.00
⁵ Pr _{A,C4}	3.76	0.02	0.07	0.00	0.15	0.00	4.00
⁵ TS1 _{A,C3}	3.82	0.13	0.17	-0.39	0.26	0.00	4.00
⁵ IM1 _{A,C3}	4.05	0.43	0.19	-0.99	0.31	0.00	4.00
⁵ TS2 _{A,C3}	3.71	-0.15	0.07	0.26	0.12	0.00	4.00
⁵ Pr _{A,C3}	3.77	0.01	0.08	0.01	0.14	0.00	4.00
Model 2							
⁵ Re _B	2.98	0.68	0.14	0.00	0.19	0.00	4.00
⁵ TS1 _{B,C5}	3.77	0.02	0.18	-0.25	0.28	0.00	4.00
⁵ IM1 _{B,C5}	4.07	0.31	0.23	-0.99	0.38	0.00	4.00
⁵ TS2 _{B,C5}	3.74	0.00	0.07	0.04	0.15	0.00	4.00
⁵ Pr _{B,C5}	3.69	0.00	0.11	0.00	0.20	0.00	4.00
⁵ TS1 _{B,C4}	2.83	0.37	0.07	0.64	0.10	0.00	4.00
⁵ IM1 _{B,C4}	2.75	0.07	0.02	0.99	0.16	0.00	4.00
⁵ TS2 _{B,C4}	3.94	0.38	0.14	-0.72	0.25	0.00	4.00
⁵ Pr _{B,C4}	3.74	0.00	0.09	0.00	0.16	0.00	4.00
⁵ TS1 _{B,C3}	3.95	0.09	0.16	-0.49	0.29	0.00	4.00
⁵ IM1 _{B,C3}	4.08	0.35	0.18	-0.99	0.39	0.00	4.00
⁵ TS2 _{B,C3}	3.93	0.36	0.11	-0.63	0.22	0.00	4.00
⁵ Pr _{B,C3}	3.76	0.01	0.07	0.00	0.15	0.00	4.00
Model 3							

⁵ Re _C	4.14	0.51	0.11	0.00	-0.78	0.01	4.00
¹ Re _C	0.93	0.11	-0.01	0.00	-1.03	0.00	0.00
³ Re _C	2.75	0.23	-0.03	0.00	-0.96	0.01	2.00
⁷ Re _C	4.14	0.51	0.11	0.00	1.22	0.02	6.00
⁵ TS1 _{C,C5}	3.61	-0.40	0.00	-0.32	1.10	0.01	4.00
⁵ IM1 _{C,C5}	4.25	0.21	0.15	-0.95	0.36	-0.03	4.00
⁵ Pr _{C,C5}	3.78	0.00	0.06	0.00	0.16	0.00	4.00
⁵ TS1 _{C,C4}	4.11	0.44	0.09	0.14	-0.79	0.01	4.00
⁵ IM1 _{C,C4}	4.26	0.19	0.14	-0.96	0.38	0.00	4.00
⁵ Pr _{C,C4}	3.80	0.00	0.05	0.00	0.12	0.02	4.00
⁵ TS1 _{C,C3}	2.87	0.13	-0.03	-0.02	1.04	0.01	4.00
⁵ IM1 _{C,C3}	3.81	0.03	0.05	-1.04	1.15	0.00	4.00
⁵ Pr _{C,C3}	3.80	0.02	0.05	0.01	0.12	0.00	4.00
⁵ Re _{C,PBE0}	4.23	0.47	0.09	0.00	-0.82	0.02	4.00
³ Re _{C,PBE0}	2.85	0.17	-0.04	0.00	-0.98	0.01	2.00
⁵ TS1 _{C,C3,PBE0}	2.99	0.04	-0.03	-0.04	1.01	0.02	4.00
⁵ TS1 _{C,C4,PBE0}	4.20	0.41	0.07	0.13	-0.83	0.01	4.00
⁵ TS1 _{C,C5,PBE0}	3.71	-0.45	0.00	-0.35	1.08	0.01	4.00
⁵ Re _{C,Solv}	4.15	0.50	0.11	0.00	-0.78	0.02	4.00
⁵ TS1 _{C,C3,Solv}	2.85	0.14	-0.02	-0.01	1.04	0.02	4.00
⁵ TS1 _{C,C4,Solv}	4.12	0.43	0.09	0.13	-0.79	0.01	4.00
⁵ TS1 _{C,C5,Solv}	3.58	-0.38	0.00	-0.32	1.10	0.01	4.00

Table S7: UPBE0/BS2 single-point calculations on the optimized UB3LYP/BS1 geometries for model C. ZPE, thermal and entropic corrections taken from the UB3LYP/BS1 frequency calculations.

	E [BS2, au]	$\Delta E + ZPE$ [kcal mol ⁻¹]	ΔG [kcal mol ⁻¹]
³ Re _{C,PBE0}	-11044.291712	8.93	9.76
⁵ Re _{C,PBE0}	-11044.305142	0.00	0.00
⁵ TS1 _{C,C3,PBE0}	-11044.256874	28.96	30.89
⁵ TS1 _{C,C4,PBE0}	-11044.262420	22.99	23.13
⁵ TS1 _{C,C5,PBE0}	-11044.255177	27.12	27.44

Table S8: UB3LYP/BS2(solvent) single-point calculations on the optimized UB3LYP/BS1 geometries for model C. Self-consistent reaction field model with dielectric constant for chlorobenzene used. ZPE, thermal and entropic corrections taken from the UB3LYP/BS1 frequency calculations.

	E [BS2, au]	$\Delta E + ZPE$ [kcal mol ⁻¹]	ΔG [kcal mol ⁻¹]
⁵ Re _{C,Solv}	-11056.298612	0.00	0.00
⁵ TS1 _{C,C3,Solv}	-11056.251448	28.27	30.20
⁵ TS1 _{C,C4,Solv}	-11056.251355	25.83	25.97
⁵ TS1 _{C,C5,Solv}	-11056.248900	26.96	27.28

Table S9: UB3LYP/BS2 calculated triplet-quintet energies for model A and B. Triplet and quintet spin geometry optimizations done.

	E [BS2, au]	ΔE [kcal mol ⁻¹]
⁵ Re _A	-7650.646028	0.00
³ Re _A	-7650.639200	4.28
⁵ Re _B	-9198.999783	0.00
³ Re _B	-9198.984363	9.68

Table S10: Absolute (in au) energies of UB3LYP/6-311+G* calculated diabatic BDE values for an isolated lysine molecule for the C-H bond strength for the C₃, C₄ and C₅ position under an applied electric field ranging from -200 au to 200 au along the X, Y or Z axis.

Field direction and strength	E [6-311+G*, au]			
	Reactant	C ₃ -radical	C ₄ -radical	C ₅ -radical
X-200	-497.687	-497.037	-497.040	-497.030
X-150	-497.636	-496.987	-496.989	-496.982
X-100	-497.588	-496.940	-496.941	-496.937
X-50	-497.542	-496.896	-496.895	-496.895
X-0	-497.500	-496.854	-496.853	-496.855
X+50	-497.460	-496.816	-496.813	-496.819
X+100	-497.423	-496.781	-496.777	-496.789
X+150	-497.395	-496.764	-496.754	-496.771
X+200	-497.388	-496.772	-496.758	-496.773
Y-200	-497.492	-496.857	-496.852	-496.850
Y-150	-497.490	-496.852	-496.849	-496.848
Y-100	-497.491	-496.851	-496.848	-496.848
Y-50	-497.494	-496.852	-496.849	-496.851
Y-0	-497.500	-496.854	-496.853	-496.855
Y+50	-497.507	-496.860	-496.859	-496.862
Y+100	-497.516	-496.867	-496.866	-496.871
Y+150	-497.528	-496.877	-496.876	-496.883
Y+200	-497.542	-496.889	-496.888	-496.896
Z-200	-497.510	-496.872	-496.869	-496.862
Z-150	-497.505	-496.865	-496.862	-496.857
Z-100	-497.501	-496.859	-496.857	-496.854
Z-50	-497.499	-496.856	-496.854	-496.854
Z-0	-497.500	-496.854	-496.853	-496.855
Z+50	-497.502	-496.855	-496.854	-496.859
Z+100	-497.506	-496.858	-496.856	-496.864
Z+150	-497.512	-496.862	-496.861	-496.871
Z+200	-497.520	-496.869	-496.868	-496.881

Table S11: Relative (in kcal/mol) energies of UB3LYP/6-311+G* calculated diabatic BDE values for an isolated lysine molecule for the C-H bond strength for the C₃, C₄ and C₅ position under an applied electric field ranging from -200 au to 200 au along the X, Y or Z axis.

Electric Field Strength [in au]	BDE [6-311+G*, kcal/mol]		
	C ₃	C ₄	C ₅
X-200	93.15	91.25	97.56
X-150	92.63	91.44	95.81
X-100	92.04	91.57	94.01
X-50	91.37	91.62	92.12
X-0	90.60	91.60	90.10
X+50	89.71	91.47	87.76
X+100	88.24	91.17	83.72
X+150	81.99	87.71	77.56
X+200	72.49	81.10	71.62
Y-200	84.34	87.06	88.41
Y-150	86.10	88.24	89.04
Y-100	87.70	89.39	89.48
Y-50	89.19	90.51	89.82
Y-0	90.60	91.60	90.10
Y+50	91.93	92.67	90.35
Y+100	93.20	93.71	90.56
Y+150	94.40	94.74	90.76
Y+200	95.54	95.75	90.95
Z-200	86.40	88.04	92.87
Z-150	87.51	88.96	92.22
Z-100	88.58	89.86	91.55
Z-50	89.61	90.74	90.84
Z-0	90.60	91.60	90.10
Z+50	91.55	92.45	89.34
Z+100	92.45	93.28	88.55
Z+150	93.30	94.10	87.72
Z+200	94.11	94.90	86.86

Table S12: Absolute (in au) energies and unpaired spin contribution on Tyr₂₃₃ of UB3LYP/BS1 geometries for the reactant cluster model C and model C2.

	E [BS1, au]	spin on Tyr
⁵ Re _C	-11045.086	-0.97
⁵ Re _{C2}	-11517.444	-0.97

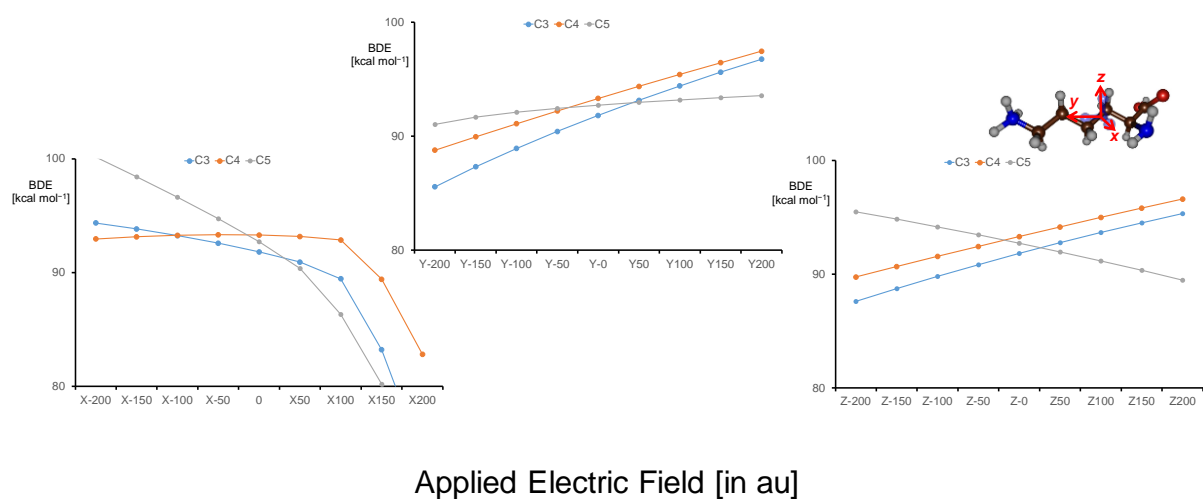


Figure S7: Electric field effects on the BDE values for the C₃-H, C₄-H and C₅-H bonds of an isolated substrate molecule with an electric field applied along the x-, y- or z-direction (directions defined as in Gaussian).

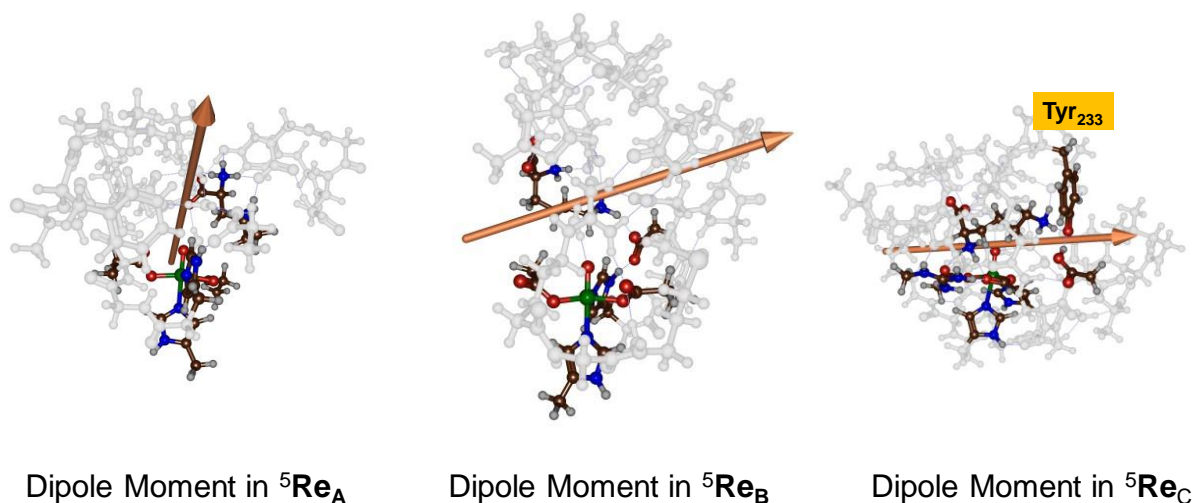


Figure S8: Electric dipole moment vectors in ⁵Re_A, ⁵Re_B and ⁵Re_C.

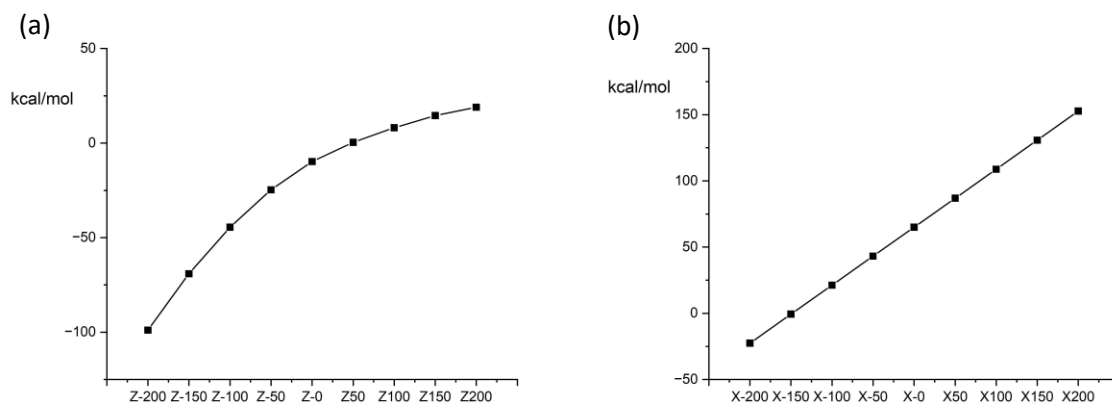


Figure S9: (a) Electric field effects on the iron(IV)-oxo reduction potential along the z-coordinate as calculated from the quintet/sextet energy gap. **(b)** Ionization potential of the p-cresol-acetate couple and its ability to perform PCET as calculated from the singlet/doublet energy gap.

Cartesian coordinates of optimized geometries:**Model 1 structures:**⁵Re_A

C	-0.29965	2.945358	-4.97702
H	-1.31963	2.565371	-5.12216
C	-0.30546	4.267329	-4.20365
H	0.712471	4.663969	-4.12657
H	-0.88654	5.021322	-4.75204
C	-0.87812	4.112208	-2.7889
H	-1.89053	3.690537	-2.82541
H	-0.26057	3.400856	-2.22159
C	-0.90951	5.422891	-2.0145
O	-0.07107	6.317318	-2.20906
N	-1.9027	5.560338	-1.10777
H	-2.54684	4.796861	-0.91057
H	-1.91493	6.396984	-0.5306
C	-5.4134	8.980307	-0.31534
H	-6.30099	8.866833	-0.94957
C	-5.20849	7.767871	0.597373
H	-5.07594	6.866644	-0.01716
H	-4.26448	7.891564	1.140952
C	-6.33297	7.529943	1.564422
N	-6.31975	6.458347	2.45006
C	-7.44764	6.5237	3.131367
H	-7.7646	5.833412	3.901334
N	-8.19541	7.587566	2.740632
H	-9.09994	7.84855	3.104808
C	-7.49706	8.238785	1.738838
H	-7.88702	9.118777	1.252231
C	3.629824	-7.30228	2.476803
C	4.66022	-6.19797	2.72417
C	2.454265	-7.00273	1.524424
O	5.231311	-6.12014	3.809324
C	1.674473	-5.76858	1.87772
C	0.87233	-5.42938	2.943849
N	1.693771	-4.65101	1.064841
C	0.92804	-3.70304	1.637685
N	0.411322	-4.13887	2.785167
H	4.176381	-8.17893	2.100515
H	2.814148	-6.89666	0.496316
H	1.790758	-7.87685	1.530653
H	0.598488	-6.01748	3.807873
H	0.750809	-2.73165	1.202335
H	2.284057	-4.58459	0.188534
N	4.941173	-5.3449	1.689602

H	4.494878	-5.43272	0.775401
C	6.007842	-4.36962	1.822577
H	6.71119	-4.72445	2.579938
C	5.616934	-2.93563	2.214957
O	6.498968	-2.07809	2.296655
N	4.29947	-2.69926	2.413999
C	3.711188	-1.3788	2.669376
C	4.401164	-0.29711	1.806851
C	3.670983	-0.99436	4.157785
O	4.80185	0.762305	2.2736
C	2.682465	0.141033	4.472788
C	1.19158	-0.16326	4.270769
O	0.39644	0.805097	4.200515
O	0.850011	-1.39718	4.210476
H	3.671631	-3.48603	2.310466
H	2.678265	-1.45406	2.309344
H	3.404457	-1.89381	4.721668
H	4.676179	-0.68897	4.46443
H	2.936217	1.031766	3.892166
H	2.79268	0.432254	5.527782
N	4.510973	-0.64211	0.489604
H	3.820181	-1.30195	0.142778
C	4.820035	0.35367	-0.53117
H	4.954196	-0.2247	-1.45595
C	3.671728	1.340623	-0.76119
H	3.477954	1.887086	0.169228
H	3.96515	2.083909	-1.5055
C	2.370547	0.657515	-1.22395
O	1.533693	1.39632	-1.81498
O	2.226946	-0.57817	-0.96685
C	6.180079	1.025866	-0.30832
O	6.446673	2.119232	-0.82022
N	7.123526	0.270089	0.319537
H	6.822805	-0.53387	0.868683
C	8.468811	0.789938	0.543149
H	8.390768	1.848845	0.815526
C	9.162789	0.02255	1.672083
H	9.203097	-1.05037	1.453667
H	8.617349	0.151904	2.611337
H	10.18245	0.398932	1.78553
C	9.341811	0.790019	-0.73398
O	10.44651	1.323216	-0.73792
N	8.783718	0.179021	-1.81614
H	7.877163	-0.24989	-1.68442
C	9.330242	0.219167	-3.15622
H	10.40286	0.415444	-3.05411
C	9.13669	-1.14291	-3.87325

H	9.771324	-1.88158	-3.37035
H	9.504466	-1.01568	-4.895
C	7.696525	-1.61806	-3.87591
C	7.208947	-2.43993	-2.8472
H	7.894644	-2.79268	-2.079
C	5.860482	-2.80541	-2.7906
H	5.493747	-3.43081	-1.98054
C	4.974032	-2.36366	-3.77691
H	3.924493	-2.64056	-3.72482
C	5.453195	-1.56699	-4.82097
H	4.773411	-1.22482	-5.59709
C	6.798637	-1.19562	-4.86899
H	7.161486	-0.56066	-5.67276
C	8.786553	1.378004	-4.03547
O	9.120965	1.434985	-5.22245
N	7.994898	2.284182	-3.41935
H	7.721222	2.144022	-2.44974
C	7.504044	3.489491	-4.07597
H	7.976585	3.527144	-5.05952
C	5.971429	3.555221	-4.17813
H	5.556881	3.492797	-3.16309
H	5.70873	4.55273	-4.56438
C	5.303363	2.48331	-5.06027
H	5.562112	1.500479	-4.6432
C	3.773809	2.626466	-5.00621
H	3.285302	1.860567	-5.62093
H	3.383852	2.523403	-3.98673
H	3.45761	3.606801	-5.38967
C	5.806901	2.523253	-6.51207
H	6.877464	2.30262	-6.57706
H	5.276583	1.783906	-7.12579
H	5.629692	3.510068	-6.96318
C	-4.66337	-2.78538	-6.06582
H	-3.86083	-3.45713	-6.38526
C	-4.22927	-2.00069	-4.81953
H	-3.36961	-1.36409	-5.06601
H	-5.03401	-1.3288	-4.50247
C	-3.83889	-2.86979	-3.61836
O	-3.89976	-4.12364	-3.74049
O	-3.48938	-2.25312	-2.5605
C	-5.96352	-3.55135	-5.84511
O	-7.0373	-2.98331	-5.63709
N	-5.86388	-4.91441	-5.91067
H	-4.93426	-5.29801	-5.80282
C	-6.99865	-5.76593	-5.60556
H	-7.8773	-5.37353	-6.12299
C	-7.40203	-5.90366	-4.12506

O	-8.41143	-6.53313	-3.8311
N	-6.5958	-5.28279	-3.22074
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C	-6.90208	-5.28775	-1.79843
H	-7.381	-6.24127	-1.55732
C	-5.6201	-5.14156	-0.9566
H	-5.94066	-5.07355	0.086815
H	-5.11135	-4.20988	-1.2281
C	-4.68666	-6.34717	-1.08074
O	-4.96968	-7.43701	-0.60819
N	-3.48581	-6.09308	-1.72332
H	-3.50611	-5.37341	-2.46095
H	-2.976	-6.9401	-1.95501
C	-7.90508	-4.19612	-1.35301
O	-8.30751	-4.18639	-0.19127
N	-8.27901	-3.27262	-2.2748
H	-7.96333	-3.36312	-3.23371
C	-9.31785	-2.30193	-1.95202
H	-9.11977	-1.92778	-0.94277
C	-9.40041	-1.14992	-2.96354
H	-9.52855	-1.56463	-3.9716
H	-10.33	-0.60607	-2.74123
C	-8.23356	-0.17969	-2.96617
C	-7.4948	0.049154	-4.13491
H	-7.72737	-0.5178	-5.03192
C	-6.4332	0.952774	-4.15835
H	-5.86272	1.12262	-5.06722
C	-6.06993	1.642921	-2.99629
O	-4.97922	2.463939	-3.05573
H	-4.70473	2.769517	-2.14316
C	-6.81087	1.443892	-1.82201
H	-6.54075	1.987902	-0.9206
C	-7.87888	0.545187	-1.81984
H	-8.43942	0.40392	-0.89781
C	4.577361	-7.04887	-2.45185
H	5.320923	-6.6368	-1.76324
C	3.735053	-5.93544	-3.07622
H	4.379006	-5.27447	-3.67235
H	2.993799	-6.34007	-3.7742
C	2.983007	-5.03908	-2.07871
O	1.976652	-4.43022	-2.50791
O	3.447052	-4.95998	-0.88449
C	0.646894	-6.54132	8.441942
C	0.656163	-5.37636	7.507636
C	-0.227	-4.95769	6.543699
N	1.677987	-4.4395	7.474046
C	1.385635	-3.52131	6.514789

N	0.23784	-3.80817	5.935188
H	0.64765	-6.22674	9.493857
H	-0.25308	-7.13986	8.276125
H	-1.16615	-5.39764	6.241266
H	2.015991	-2.68172	6.266735
H	2.517528	-4.45477	8.035355
C	-1.10978	9.402791	2.800423
H	-0.31373	10.08645	3.118116
C	-1.17532	8.199712	3.770863
H	-0.2373	7.631064	3.714717
H	-1.23751	8.594566	4.794436
C	-2.36108	7.275335	3.48256
H	-3.28952	7.865176	3.48675
H	-2.25524	6.888321	2.466265
C	-2.53607	6.084107	4.434802
H	-1.61052	5.518456	4.568105
H	-2.85105	6.406089	5.433676
N	-3.58038	5.178249	3.918806
H	-4.49242	5.62462	3.858718
C	-3.32635	4.420612	2.806316
N	-2.13501	3.886697	2.600921
H	-1.40817	3.819006	3.335142
H	-1.9977	3.323146	1.749224
N	-4.33813	4.226326	1.942093
H	-5.12197	4.878912	1.995449
H	-4.1665	3.761036	1.046306
C	-0.9155	9.00085	1.336492
O	-1.7844	8.378216	0.710932
N	0.258168	9.39437	0.786116
H	1.003569	9.735529	1.384152
C	0.726125	8.95517	-0.51909
H	0.025232	8.235534	-0.94367
C	2.128089	8.358905	-0.32726
O	2.889327	8.849657	0.512834
N	2.417571	7.30653	-1.12161
H	1.650626	6.897076	-1.65855
C	3.634327	6.517516	-0.94989
H	4.345702	7.143012	-0.40487
C	3.379132	5.19461	-0.20289
H	2.687118	4.581114	-0.79302
H	4.319993	4.634043	-0.14385
C	2.811014	5.413631	1.203082
H	3.531034	5.94972	1.830612
H	1.900916	6.02057	1.162007
S	2.424562	3.868733	2.115577
C	1.005805	3.233477	1.14773
H	0.586088	2.402509	1.719394

H	0.239801	4.004771	1.031939
H	1.302215	2.860608	0.16562
O	-2.3548	-1.86599	5.418105
C	-2.95361	-2.95849	5.20663
O	-2.42048	-3.86959	4.484832
C	-4.32012	-3.23436	5.819415
C	-4.95159	-2.03733	6.529592
H	-4.97002	-3.61436	5.021184
H	-4.19204	-4.07639	6.513867
H	-5.11659	-1.20796	5.833933
H	-5.91861	-2.31298	6.965832
O	-1.57747	-1.91047	2.214974
O	-2.1946	0.232737	3.598531
Fe	-0.6101	-2.80094	4.129663
C	-2.50142	-0.38945	-0.00734
H	-1.82747	0.135473	0.66938
H	-1.86005	-0.97397	-0.66966
C	-3.25321	0.666482	-0.83136
H	-4.33592	0.53581	-0.73828
C	-2.94184	2.127051	-0.3903
O	-3.79275	3.026893	-0.73777
O	-1.93312	2.327811	0.304203
H	-0.9825	-3.09623	-0.68137
N	-2.9529	0.468634	-2.29011
H	-1.89119	0.419581	-2.49714
H	-3.43214	1.179606	-2.86121
H	-3.2956	-0.48696	-2.55185
C	-3.46615	-1.2791	0.789483
H	-4.01373	-0.64044	1.493352
C	-2.77588	-2.39265	1.59674
C	-2.48884	-3.67785	0.814625
H	-1.79468	-4.29634	1.384684
H	-3.42544	-4.22812	0.704443
N	-1.93904	-3.54208	-0.58011
H	-1.88795	-4.49047	-0.97442
H	-2.58159	-3.03056	-1.23909
H	1.51442	-7.19664	8.290137
H	3.257819	-7.57301	3.469302
H	5.105102	-7.62112	-3.2245
H	3.954497	-7.75123	-1.88419
H	6.544845	-4.28606	0.872161
H	7.856886	4.359652	-3.50565
H	-4.30159	-1.66861	7.328614
H	-4.85084	-2.07689	-6.88127
H	-6.80749	-6.77028	-5.99543
H	-10.2931	-2.80854	-1.90738
H	-4.54315	9.106184	-0.9656

H	-5.52776	9.902581	0.267605
H	-2.05445	9.958559	2.85611
H	0.798325	9.812033	-1.20362
H	4.058264	6.301046	-1.93746
H	0.148442	3.074479	-5.96952
H	0.266194	2.17266	-4.44635
H	-2.4446	-0.31105	4.375255
H	-1.27213	0.525672	3.823915
O	-0.42669	-0.02108	-2.9026
H	-0.22062	-0.94435	-2.64455
H	0.303049	0.525646	-2.46889
O	0.026671	3.607848	4.401375
H	0.203813	2.64166	4.464477
H	0.799222	3.945774	3.903025
O	0.393854	-2.43704	-1.46374
H	0.986895	-3.14264	-1.84464
H	1.017141	-1.69313	-1.21191
H	-1.80182	-1.01655	2.635769
H	-4.21664	-1.7307	0.125984
H	-3.46555	-2.72786	2.383323

⁵TS1_{A,C3}

C	-2.05171	1.662626	-5.34794
H	-3.08995	1.306121	-5.3033
C	-1.93689	3.085955	-4.79104
H	-0.91064	3.45201	-4.90833
H	-2.57053	3.773115	-5.36534
C	-2.32651	3.160006	-3.31119
H	-3.32892	2.739004	-3.15707
H	-1.639	2.544213	-2.71533
C	-2.30608	4.577241	-2.74933
O	-1.84712	5.531451	-3.39589
N	-2.82718	4.734203	-1.51013
H	-3.14405	3.938744	-0.96078
H	-2.86021	5.671137	-1.11604
C	-6.83277	7.10689	-1.22541
H	-7.65867	6.524374	-1.65107
C	-6.26063	6.443592	0.030629
H	-5.87411	5.448231	-0.22772
H	-5.38719	7.015068	0.366497
C	-7.24653	6.302875	1.155234
N	-6.90642	5.682566	2.352396
C	-7.98962	5.706704	3.105413
H	-8.07729	5.297745	4.102798
N	-9.01886	6.317277	2.464261
H	-9.9528	6.449417	2.823695
C	-8.55991	6.701322	1.216263
H	-9.19653	7.20258	0.504469
C	4.815234	-5.59394	3.286836
C	5.599028	-4.40021	3.837171
C	3.971804	-5.34414	2.023416
O	5.733449	-4.22033	5.043658
C	3.035967	-4.17938	2.165186
C	2.47105	-3.58035	3.266502
N	2.575229	-3.46674	1.076048
C	1.762836	-2.49114	1.528448
N	1.672738	-2.52744	2.858131
H	5.529819	-6.40391	3.087603
H	4.599298	-5.19595	1.136339
H	3.407888	-6.26052	1.802269
H	2.575917	-3.83546	4.308765
H	1.27577	-1.77477	0.887266
H	2.77007	-3.75142	0.081525
N	6.161747	-3.56834	2.904116
H	5.982858	-3.73614	1.923642
C	6.963251	-2.41289	3.25891
H	7.149612	-2.48008	4.3353

C	6.337668	-1.04252	2.94995
O	7.069551	-0.08821	2.682292
N	4.987435	-0.9706	3.012619
C	4.215355	0.264174	2.816305
C	4.724472	1.048652	1.585815
C	4.152575	1.152347	4.071259
O	4.986991	2.243632	1.631894
C	2.953356	2.111657	4.074779
C	1.553491	1.480007	4.15966
O	0.549626	2.195928	4.101121
O	1.534604	0.187701	4.324594
H	4.470492	-1.80602	3.260664
H	3.201265	-0.07502	2.58627
H	4.108481	0.494192	4.945342
H	5.077444	1.733322	4.134416
H	2.98345	2.744857	3.181404
H	3.035104	2.802671	4.92446
N	4.853042	0.286389	0.457172
H	4.280254	-0.54919	0.406387
C	5.034945	0.892661	-0.86091
H	5.137863	0.041781	-1.54666
C	3.811074	1.69787	-1.31263
H	3.599676	2.491232	-0.58703
H	4.025861	2.195626	-2.26235
C	2.551859	0.826311	-1.48565
O	1.551877	1.400784	-1.99401
O	2.621334	-0.3861	-1.10267
C	6.357923	1.657668	-0.99616
O	6.546655	2.424667	-1.94666
N	7.352728	1.336706	-0.12249
H	7.119185	0.823506	0.724158
C	8.622656	2.058705	-0.14901
H	8.414503	3.113795	-0.36019
C	9.338318	1.941363	1.200123
H	9.50876	0.892839	1.467393
H	8.734044	2.394192	1.991475
H	10.30186	2.453089	1.137627
C	9.556744	1.622331	-1.29858
O	10.58114	2.25206	-1.54166
N	9.15123	0.526425	-1.99948
H	8.306143	0.064381	-1.68997
C	9.784203	0.065618	-3.21783
H	10.76657	0.549563	-3.25079
C	9.988487	-1.47037	-3.20877
H	10.77023	-1.70284	-2.47705
H	10.35831	-1.74326	-4.20121
C	8.730525	-2.24646	-2.87151

C	8.525453	-2.74866	-1.57814
H	9.303252	-2.61786	-0.82834
C	7.341109	-3.41083	-1.24398
H	7.214158	-3.80333	-0.23614
C	6.329333	-3.5784	-2.19151
H	5.395456	-4.06799	-1.92467
C	6.532008	-3.09254	-3.48751
H	5.757211	-3.22194	-4.23885
C	7.718807	-2.44022	-3.82663
H	7.869219	-2.0686	-4.83633
C	9.061838	0.518973	-4.51536
O	9.397575	0.02408	-5.59546
N	8.124015	1.483525	-4.37844
H	7.864716	1.814619	-3.45218
C	7.455097	2.103242	-5.51672
H	7.90243	1.6727	-6.41461
C	5.928297	1.931372	-5.5017
H	5.53992	2.381987	-4.57909
H	5.522286	2.524942	-6.33555
C	5.403421	0.486851	-5.6123
H	5.791067	-0.07582	-4.75082
C	3.868687	0.474825	-5.5316
H	3.479993	-0.55047	-5.54722
H	3.500243	0.954046	-4.61708
H	3.428134	1.008141	-6.38522
C	5.886744	-0.21894	-6.88957
H	6.976743	-0.32102	-6.9139
H	5.454992	-1.22516	-6.96282
H	5.575386	0.336684	-7.78556
C	-5.50073	-3.28919	-5.28815
H	-4.76073	-3.88894	-5.82801
C	-4.84431	-2.61466	-4.07279
H	-4.12812	-1.85777	-4.41395
H	-5.60468	-2.0767	-3.49419
C	-4.10706	-3.56367	-3.12149
O	-4.28003	-4.80459	-3.2448
O	-3.36232	-3.01661	-2.24205
C	-6.72292	-4.12793	-4.92862
O	-7.78548	-3.62288	-4.56363
N	-6.56911	-5.48079	-5.06905
H	-5.61425	-5.81632	-5.06963
C	-7.62009	-6.39664	-4.6681
H	-8.5725	-6.01817	-5.04647
C	-7.82041	-6.62859	-3.15933
O	-8.75994	-7.31463	-2.7739
N	-6.92307	-6.02469	-2.33216
H	-6.12448	-5.53097	-2.72734

C	-7.00972	-6.16341	-0.88531
H	-7.44253	-7.14486	-0.66844
C	-5.61383	-6.08515	-0.24204
H	-5.76105	-6.09907	0.840745
H	-5.12909	-5.14045	-0.51536
C	-4.7478	-7.28829	-0.61691
O	-4.96809	-8.40732	-0.17182
N	-3.69956	-7.00781	-1.45685
H	-3.7457	-6.18273	-2.06436
H	-3.21942	-7.82216	-1.82138
C	-7.9454	-5.14336	-0.19736
O	-8.14435	-5.22437	1.012947
N	-8.50544	-4.18286	-0.9767
H	-8.35017	-4.19665	-1.9778
C	-9.49592	-3.27515	-0.41456
H	-9.14019	-2.97034	0.574509
C	-9.76121	-2.05599	-1.30788
H	-10.1029	-2.39822	-2.29326
H	-10.6116	-1.51883	-0.86321
C	-8.59014	-1.10888	-1.48864
C	-8.11883	-0.7937	-2.77005
H	-8.56508	-1.27162	-3.63712
C	-7.05074	0.082307	-2.95583
H	-6.6856	0.318799	-3.95103
C	-6.41169	0.6526	-1.85076
O	-5.32696	1.453231	-2.08498
H	-4.89458	1.740749	-1.23371
C	-6.87834	0.364512	-0.56059
H	-6.39456	0.814942	0.30255
C	-7.95858	-0.50308	-0.39365
H	-8.30287	-0.71752	0.615815
C	3.988535	-7.36511	-2.02253
H	4.889026	-6.74758	-2.08945
C	2.779407	-6.63676	-2.60823
H	2.939868	-6.42512	-3.67477
H	1.880724	-7.26521	-2.57093
C	2.431297	-5.2975	-1.94026
O	1.315211	-4.78601	-2.25586
O	3.276393	-4.78234	-1.15158
C	2.291805	-4.66633	8.439018
C	2.028057	-3.54282	7.491642
C	1.150071	-3.40265	6.446798
N	2.722521	-2.34272	7.526348
C	2.260349	-1.55015	6.525365
N	1.307528	-2.16413	5.851668
H	2.127317	-4.37216	9.483862
H	1.618276	-5.49928	8.21948

H	0.41528	-4.10022	6.074783
H	2.622083	-0.55715	6.313424
H	3.476755	-2.1119	8.157072
C	-2.39526	9.524374	0.993997
H	-1.7015	10.37318	0.979704
C	-2.10786	8.641528	2.22981
H	-1.09545	8.222233	2.156917
H	-2.1094	9.293895	3.1141
C	-3.12586	7.510171	2.401825
H	-4.14208	7.931087	2.383672
H	-3.05933	6.851467	1.533596
C	-2.97539	6.653292	3.666018
H	-1.94892	6.307353	3.811993
H	-3.24723	7.213834	4.567805
N	-3.87205	5.488002	3.585538
H	-4.85428	5.741657	3.495115
C	-3.5594	4.418119	2.796487
N	-2.30794	4.050952	2.575284
H	-1.4999	4.443311	3.089746
H	-2.15096	3.158182	2.082871
N	-4.57758	3.720892	2.259286
H	-5.48725	4.178781	2.23531
H	-4.36066	3.037249	1.531622
C	-2.34427	8.772853	-0.33732
O	-3.09627	7.819081	-0.57681
N	-1.45381	9.256955	-1.23952
H	-0.71855	9.877733	-0.91926
C	-1.13466	8.572917	-2.48401
H	-1.78723	7.707372	-2.60279
C	0.350174	8.185944	-2.43979
O	1.164689	8.956141	-1.92184
N	0.649578	6.987705	-2.98682
H	-0.12923	6.386735	-3.26216
C	1.986378	6.409096	-2.88616
H	2.669794	7.238601	-2.68838
C	2.106433	5.338009	-1.78341
H	1.522013	4.451027	-2.05692
H	3.152858	5.012806	-1.73726
C	1.669075	5.859799	-0.41067
H	2.266491	6.731795	-0.12357
H	0.621952	6.178736	-0.43579
S	1.862597	4.66206	0.964944
C	0.57289	3.429284	0.547548
H	0.462402	2.776529	1.41688
H	-0.38323	3.928258	0.362453
H	0.858392	2.828323	-0.31901
O	-1.37117	-1.01415	5.305629

C	-1.76603	-2.2222	5.153572
O	-1.07593	-3.01876	4.454497
C	-3.0764	-2.66278	5.774028
C	-3.30552	-2.10805	7.184688
H	-3.86521	-2.29893	5.100778
H	-3.11513	-3.75647	5.756436
H	-3.26412	-1.01554	7.180432
H	-4.28514	-2.41851	7.564274
O	-0.52946	-0.79411	2.556559
O	-3.342	0.127592	3.53781
Fe	0.290886	-1.28458	3.994546
C	-2.00937	-1.26685	0.60814
H	-1.37586	-0.84895	1.625742
H	-1.16648	-1.38122	-0.08029
C	-3.02227	-0.26363	0.055216
H	-4.02913	-0.56001	0.371707
C	-2.89215	1.229272	0.476683
O	-3.73159	2.039733	-0.05535
O	-2.05323	1.528537	1.342186
H	-0.46617	-3.24915	-0.97247
N	-3.00922	-0.34996	-1.45164
H	-2.03492	-0.12417	-1.85331
H	-3.70249	0.295724	-1.85843
H	-3.23776	-1.32177	-1.77913
C	-2.65626	-2.57505	1.071011
H	-3.38901	-2.89965	0.315608
H	-3.2332	-2.33325	1.972154
C	-1.67095	-3.72126	1.381002
H	-2.04318	-4.30131	2.231371
H	-0.72524	-3.29736	1.723704
C	-1.41078	-4.72613	0.254333
H	-0.56024	-5.3623	0.516004
H	-2.27052	-5.37618	0.072504
N	-1.08547	-4.08412	-1.06184
H	-0.50809	-4.70266	-1.6585
H	-1.95957	-3.7874	-1.5652
H	3.320902	-5.03806	8.353024
H	4.182944	-5.93498	4.111487
H	4.175367	-8.30569	-2.55514
H	3.832335	-7.60178	-0.96378
H	7.927804	-2.43282	2.742916
H	7.688827	3.176822	-5.51332
H	-2.54116	-2.47057	7.882013
H	-5.85689	-2.50803	-5.96938
H	-7.44345	-7.37102	-5.13401
H	-10.4422	-3.81142	-0.24996
H	-6.05153	7.196137	-1.98548

H	-7.20406	8.116353	-1.00926
H	-3.40776	9.94037	1.082018
H	-1.29626	9.251246	-3.33267
H	2.255602	5.969376	-3.85362
H	-1.73498	1.625422	-6.39723
H	-1.43207	0.963689	-4.77501
H	-2.74394	-0.089	4.275552
H	-2.74158	0.595325	2.930319
O	-0.61584	-0.05263	-2.60314
H	-0.20019	-0.94297	-2.52358
H	0.141842	0.55308	-2.34049
O	0.061037	4.908767	3.804947
H	0.324533	3.984421	4.035347
H	0.627736	5.12087	3.035016
O	0.782268	-2.18824	-1.64541
H	1.216364	-3.00571	-2.00079
H	1.495054	-1.50017	-1.44553

⁵IM1_{A,C3}

C	-1.88626	1.964752	-4.88818
H	-2.87493	1.780951	-4.44873
C	-1.42104	3.394017	-4.59379
H	-0.49392	3.618879	-5.13208
H	-2.17187	4.108186	-4.95987
C	-1.17381	3.644354	-3.0938
H	-2.04767	3.343306	-2.50216
H	-0.32931	3.027276	-2.75898
C	-0.82286	5.102221	-2.83785
O	0.070658	5.673699	-3.47864
N	-1.55751	5.754386	-1.90498
H	-2.25125	5.27235	-1.35129
H	-1.38485	6.743473	-1.7236
C	-5.11889	8.734729	-2.17486
H	-6.02062	8.339123	-2.65731
C	-4.72937	7.908633	-0.94545
H	-4.51616	6.875435	-1.25152
H	-3.78466	8.293529	-0.54077
C	-5.77753	7.882739	0.130958
N	-5.62017	7.127663	1.287272
C	-6.71157	7.314024	2.005501
H	-6.92014	6.866357	2.967681
N	-7.57275	8.155153	1.378108
H	-8.47827	8.445147	1.717229
C	-6.99079	8.525522	0.178294
H	-7.48422	9.190239	-0.51306
C	2.680773	-6.09146	4.20553
C	4.017018	-5.34962	4.138263
C	1.591203	-5.70655	3.18368
O	4.681883	-5.17791	5.156107
C	1.296988	-4.23358	3.120265
C	0.842089	-3.33298	4.053821
N	1.497604	-3.49357	1.967532
C	1.167566	-2.21044	2.221719
N	0.768365	-2.07866	3.48638
H	2.892901	-7.16577	4.111657
H	1.874983	-6.04281	2.182655
H	0.680188	-6.25918	3.44862
H	0.558615	-3.50013	5.080891
H	1.234295	-1.4101	1.497992
H	1.907044	-3.90596	1.0973
N	4.435247	-4.90679	2.910242
H	3.90782	-5.11396	2.063956
C	5.726195	-4.2568	2.766014
H	6.366454	-4.58101	3.590971

C	5.742048	-2.71742	2.758103
O	6.783982	-2.13371	2.453242
N	4.580245	-2.09907	3.073199
C	4.354423	-0.64793	3.032669
C	5.028051	-0.02962	1.78784
C	4.72336	0.07848	4.33633
O	5.692868	0.998459	1.832109
C	4.085233	1.471927	4.464041
C	2.555678	1.55211	4.598332
O	2.013624	2.657584	4.587757
O	1.933619	0.414199	4.763556
H	3.800582	-2.68802	3.333932
H	3.275224	-0.53509	2.888001
H	4.403117	-0.55672	5.169664
H	5.812606	0.176418	4.388553
H	4.370985	2.095444	3.611654
H	4.494815	1.978588	5.348667
N	4.799276	-0.73691	0.641082
H	3.978461	-1.33238	0.626419
C	5.06244	-0.1774	-0.67903
H	4.922086	-1.01875	-1.37197
C	4.05411	0.908581	-1.06649
H	4.052012	1.694763	-0.30165
H	4.351136	1.381093	-2.0053
C	2.628701	0.34616	-1.21715
O	1.815082	1.027902	-1.8953
O	2.380807	-0.76331	-0.63792
C	6.531125	0.217511	-0.8708
O	6.869241	1.042549	-1.72557
N	7.438349	-0.53229	-0.18381
H	7.118344	-1.07182	0.618966
C	8.868095	-0.26495	-0.30017
H	9.017267	0.82049	-0.33578
C	9.621586	-0.84343	0.901304
H	9.447332	-1.92124	0.994317
H	9.283242	-0.36827	1.826698
H	10.69222	-0.66859	0.770219
C	9.481478	-0.77587	-1.62317
O	10.64031	-0.50339	-1.91925
N	8.649093	-1.51662	-2.40883
H	7.720229	-1.70372	-2.05508
C	8.971631	-1.9369	-3.75667
H	10.06208	-1.88226	-3.84277
C	8.528211	-3.4	-4.01275
H	9.117035	-4.04786	-3.35317
H	8.795552	-3.63366	-5.04675
C	7.04774	-3.6383	-3.78599

C	6.559795	-4.01849	-2.52549
H	7.263146	-4.19414	-1.71349
C	5.189018	-4.17721	-2.29826
H	4.821707	-4.46026	-1.31523
C	4.280902	-3.97154	-3.34007
H	3.215332	-4.09245	-3.16365
C	4.755019	-3.61081	-4.60428
H	4.056081	-3.45274	-5.42177
C	6.123228	-3.44162	-4.82423
H	6.486879	-3.14126	-5.80291
C	8.423857	-1.0008	-4.86651
O	8.551862	-1.33499	-6.04802
N	7.860962	0.158006	-4.45615
H	7.763812	0.351708	-3.46222
C	7.402505	1.190605	-5.37774
H	7.69047	0.868479	-6.3803
C	5.894964	1.477812	-5.28312
H	5.667609	1.778099	-4.25159
H	5.686693	2.354214	-5.91681
C	4.953848	0.328693	-5.69269
H	5.159063	-0.52434	-5.03141
C	3.487611	0.742174	-5.48589
H	2.807834	-0.07491	-5.7571
H	3.272296	1.01313	-4.44561
H	3.232015	1.605226	-6.11651
C	5.191676	-0.13379	-7.13947
H	6.197359	-0.54491	-7.27581
H	4.471716	-0.91345	-7.41912
H	5.061812	0.699693	-7.84457
C	-5.39774	-3.63787	-5.26381
H	-4.67826	-4.38374	-5.61776
C	-4.79186	-2.82922	-4.10571
H	-3.96512	-2.21463	-4.48057
H	-5.54021	-2.12931	-3.71491
C	-4.26476	-3.6625	-2.9317
O	-4.59034	-4.8773	-2.85319
O	-3.53187	-3.04763	-2.0901
C	-6.73025	-4.29218	-4.91521
O	-7.76057	-3.63881	-4.7408
N	-6.71156	-5.65832	-4.84042
H	-5.80303	-6.07655	-4.68667
C	-7.88781	-6.40028	-4.427
H	-8.74973	-6.02959	-4.98691
C	-8.28351	-6.32764	-2.94099
O	-9.33637	-6.8349	-2.5719
N	-7.42014	-5.67057	-2.11902
H	-6.53169	-5.32907	-2.48308

C	-7.70761	-5.48915	-0.70414
H	-8.27996	-6.35822	-0.36513
C	-6.40704	-5.40428	0.114527
H	-6.69318	-5.18265	1.145505
H	-5.78275	-4.58401	-0.25944
C	-5.64857	-6.73159	0.106465
O	-6.04193	-7.70569	0.734838
N	-4.491	-6.73362	-0.63179
H	-4.37152	-6.04953	-1.3873
H	-4.07923	-7.64921	-0.76899
C	-8.59826	-4.26592	-0.38339
O	-8.94977	-4.06258	0.777087
N	-8.95128	-3.46345	-1.42022
H	-8.66768	-3.70796	-2.3624
C	-9.91722	-2.3917	-1.22469
H	-9.72757	-1.95966	-0.23796
C	-9.85381	-1.32344	-2.32458
H	-10.0307	-1.79745	-3.29839
H	-10.7058	-0.64768	-2.15844
C	-8.5665	-0.52365	-2.3888
C	-7.84814	-0.42391	-3.58803
H	-8.19513	-0.96688	-4.46248
C	-6.66942	0.315797	-3.67102
H	-6.11398	0.384443	-4.60191
C	-6.1687	0.962923	-2.5373
O	-4.97658	1.626495	-2.65138
H	-4.66125	1.934871	-1.75912
C	-6.88048	0.890832	-1.33172
H	-6.50036	1.403488	-0.45183
C	-8.0665	0.158127	-1.27113
H	-8.602	0.111533	-0.32539
C	3.401165	-7.82741	-0.31177
H	4.280929	-7.27404	0.028772
C	2.571425	-6.98702	-1.2831
H	3.163431	-6.76654	-2.18282
H	1.688403	-7.53332	-1.63314
C	2.097043	-5.63143	-0.74147
O	1.097523	-5.10761	-1.31114
O	2.753915	-5.10144	0.212448
C	-0.37345	-3.32498	9.426318
C	0.086343	-2.43637	8.317672
C	-0.47997	-2.08816	7.117228
N	1.29433	-1.75456	8.341591
C	1.409122	-1.04477	7.188085
N	0.349373	-1.22477	6.425132
H	-0.48637	-2.77885	10.37207
H	-1.3468	-3.7551	9.174848

H	-1.42413	-2.40018	6.696937
H	2.255064	-0.42785	6.930005
H	1.98291	-1.78973	9.079583
C	-0.18844	9.91362	0.597548
H	0.676941	10.56945	0.750218
C	-0.27734	8.893714	1.75957
H	0.651549	8.310953	1.813438
H	-0.33968	9.462943	2.697294
C	-1.47795	7.951009	1.632339
H	-2.37814	8.543833	1.417801
H	-1.33316	7.301673	0.764834
C	-1.7656	7.061549	2.849223
H	-0.90018	6.465966	3.149419
H	-2.04875	7.663531	3.720766
N	-2.89542	6.172494	2.545866
H	-3.76113	6.659952	2.313852
C	-2.76837	5.007575	1.865092
N	-1.64522	4.291358	1.874266
H	-0.88703	4.467574	2.558705
H	-1.73251	3.324898	1.554762
N	-3.81091	4.605307	1.119235
H	-4.63937	5.1911	1.103989
H	-3.82004	3.681298	0.669531
C	-0.13136	9.252997	-0.77831
O	-1.12301	8.687221	-1.26203
N	1.059494	9.32882	-1.41517
H	1.878397	9.668366	-0.92143
C	1.382021	8.581934	-2.62239
H	0.564606	7.904155	-2.86946
C	2.699939	7.842078	-2.35649
O	3.589247	8.405663	-1.71087
N	2.775971	6.593554	-2.86411
H	1.918219	6.177903	-3.23004
C	3.906392	5.71476	-2.57425
H	4.733747	6.36027	-2.26975
C	3.601598	4.672681	-1.48087
H	2.849118	3.96366	-1.84732
H	4.514096	4.091158	-1.30337
C	3.131999	5.31118	-0.16929
H	3.891964	5.999838	0.21551
H	2.21975	5.89551	-0.33149
S	2.818731	4.126063	1.198036
C	1.33615	3.251577	0.573828
H	1.020989	2.563246	1.364327
H	0.529875	3.964298	0.373691
H	1.555858	2.672167	-0.32459
O	-1.43781	0.898296	5.312549

C	-2.26862	-0.0709	5.203892
O	-1.91478	-1.11927	4.587137
C	-3.65138	0.052717	5.809303
C	-3.62259	0.560278	7.257908
H	-4.19238	0.773316	5.183273
H	-4.14995	-0.91856	5.731733
H	-3.13495	1.537604	7.310485
H	-4.64115	0.6593	7.649368
O	-0.08632	0.565323	2.680717
O	-3.38812	2.626105	3.903241
Fe	0.12112	-0.19571	4.321196
C	-2.53565	-1.25131	0.633848
H	-1.49029	-1.03612	0.8359
C	-3.30882	-0.24702	-0.15095
H	-4.38189	-0.46538	-0.08737
C	-3.14319	1.231466	0.330398
O	-3.76614	2.118335	-0.33024
O	-2.46208	1.454056	1.360333
H	-0.84483	-3.26697	-0.44526
N	-2.9743	-0.34464	-1.62522
H	-1.93031	-0.19605	-1.85123
H	-3.53108	0.330967	-2.17087
H	-3.21381	-1.31456	-1.9471
C	-3.22125	-2.3368	1.403897
H	-3.65083	-1.89554	2.32098
C	-2.2897	-3.47727	1.859154
C	-1.98651	-4.57983	0.839991
H	-1.1985	-5.22837	1.233035
H	-2.86506	-5.19972	0.639535
N	-1.51076	-4.07838	-0.49092
H	-0.93998	-4.79178	-0.96933
H	-2.31401	-3.78849	-1.10655
H	0.321634	-4.15613	9.603253
H	2.321448	-5.93825	5.227451
H	3.74097	-8.75441	-0.78847
H	2.819277	-8.10417	0.576084
H	6.19416	-4.56999	1.82821
H	7.95155	2.116248	-5.15738
H	-3.0717	-0.1262	7.911825
H	-5.60196	-2.95407	-6.09567
H	-7.75397	-7.45444	-4.68823
H	-10.9355	-2.80734	-1.19057
H	-4.30717	8.72091	-2.90782
H	-5.30732	9.781613	-1.90747
H	-1.08516	10.54485	0.607902
H	1.529793	9.270068	-3.46622
H	4.197951	5.199847	-3.49696

H	-1.96895	1.800066	-5.96959
H	-1.19294	1.22069	-4.48014
H	-2.60913	2.386014	4.43795
H	-3.19938	2.199927	3.047524
O	-0.47651	-0.24918	-2.52538
H	-0.17233	-1.16686	-2.34121
H	0.313454	0.303106	-2.24961
O	0.563977	4.760916	3.545764
H	0.846661	3.974916	4.063865
H	1.313219	4.87043	2.924011
O	0.473257	-2.44304	-1.20151
H	0.930982	-3.30376	-1.36497
H	1.181045	-1.76784	-0.95513
H	-0.95746	0.742534	2.270139
H	-4.07379	-2.73186	0.831345
H	-1.35826	-3.04001	2.228058
H	-2.74281	-3.983	2.720024

⁵TS2_{A,C3}

C	0.120011	2.519814	-5.16298
H	-0.72463	2.671304	-5.84938
C	0.224922	3.671753	-4.15796
H	1.0882	3.49811	-3.503
H	0.397033	4.618528	-4.68165
C	-1.03499	3.82098	-3.29519
H	-1.93112	3.775041	-3.933
H	-1.12223	2.992539	-2.58487
C	-1.11152	5.152645	-2.55457
O	-0.64309	6.192314	-3.05149
N	-1.75589	5.147757	-1.36979
H	-2.09767	4.28298	-0.95049
H	-1.91105	6.035233	-0.89439
C	-5.83865	5.565504	-0.71982
H	-6.50128	4.72223	-0.94698
C	-5.32844	5.506033	0.724484
H	-4.72696	4.599011	0.865013
H	-4.6417	6.346133	0.894175
C	-6.42009	5.525533	1.758827
N	-6.17773	5.236758	3.099347
C	-7.33895	5.341795	3.716961
H	-7.51358	5.176292	4.771506
N	-8.3275	5.687088	2.852228
H	-9.30327	5.813099	3.077659
C	-7.75612	5.804171	1.597518
H	-8.33929	6.061858	0.727624
C	3.227083	-6.73187	3.219693
C	4.371704	-5.75225	3.489914
C	2.197182	-6.37006	2.12841
O	4.855156	-5.66628	4.61589
C	1.590642	-5.0043	2.285286
C	0.796985	-4.43365	3.254696
N	1.833349	-3.99292	1.373671
C	1.205848	-2.87866	1.804264
N	0.566045	-3.11127	2.947209
H	3.679147	-7.70329	2.973555
H	2.658268	-6.42926	1.138272
H	1.410628	-7.1354	2.150805
H	0.378863	-4.87926	4.144934
H	1.227895	-1.93893	1.271129
H	2.453587	-4.11641	0.536221
N	4.839745	-5.01085	2.436131
H	4.472145	-5.13169	1.492357
C	5.99155	-4.14185	2.605468
H	6.541567	-4.47787	3.488772

C	5.718634	-2.6372	2.77959
O	6.659717	-1.84498	2.703859
N	4.430631	-2.28082	2.993184
C	3.922942	-0.90424	3.052074
C	4.637296	-0.00971	2.018111
C	3.906307	-0.28937	4.460453
O	5.079465	1.099518	2.291664
C	2.956653	0.917742	4.57429
C	1.472073	0.647324	4.258513
O	0.743902	1.594087	3.896809
O	1.076464	-0.56377	4.420694
H	3.751981	-3.02928	3.04197
H	2.881839	-0.98127	2.722287
H	3.595832	-1.07519	5.156951
H	4.92172	0.01972	4.728921
H	3.304215	1.729381	3.93101
H	2.993543	1.304418	5.603353
N	4.707214	-0.56804	0.771185
H	4.008704	-1.27201	0.558809
C	5.019561	0.239042	-0.40278
H	5.096746	-0.48011	-1.23
C	3.903513	1.233112	-0.74466
H	3.731257	1.890593	0.115758
H	4.215047	1.87723	-1.56925
C	2.585138	0.539472	-1.13042
O	1.810059	1.198526	-1.8757
O	2.365672	-0.63249	-0.67544
C	6.414863	0.874814	-0.32358
O	6.712002	1.85413	-1.01445
N	7.339151	0.196822	0.413424
H	7.012882	-0.50214	1.079033
C	8.682372	0.737856	0.605265
H	8.603074	1.825172	0.721908
C	9.327663	0.138359	1.858288
H	9.369005	-0.95474	1.796136
H	8.747196	0.401234	2.747236
H	10.34462	0.525924	1.955656
C	9.604672	0.554088	-0.62027
O	10.72167	1.061107	-0.64273
N	9.0805	-0.18028	-1.64112
H	8.155235	-0.56572	-1.5061
C	9.69933	-0.32157	-2.9424
H	10.76092	-0.08874	-2.80786
C	9.570261	-1.77503	-3.46841
H	10.16035	-2.42333	-2.81042
H	10.02428	-1.79264	-4.46267
C	8.137093	-2.26491	-3.53057

C	7.535785	-2.87829	-2.41989
H	8.129576	-3.06155	-1.52638
C	6.188382	-3.25045	-2.44078
H	5.731863	-3.70761	-1.56678
C	5.421092	-3.03328	-3.5888
H	4.373191	-3.32104	-3.60196
C	6.015664	-2.44881	-4.71045
H	5.429429	-2.28216	-5.61069
C	7.35768	-2.06411	-4.68073
H	7.809131	-1.58644	-5.5459
C	9.185277	0.686206	-4.00444
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H	8.050627	1.663794	-2.59179
C	7.868244	2.735636	-4.41449
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C	6.337114	2.755825	-4.55083
H	5.904629	2.865093	-3.54749
H	6.065723	3.664839	-5.11007
C	5.703515	1.532123	-5.23936
H	5.97301	0.643121	-4.65303
C	4.171236	1.651948	-5.2326
H	3.705815	0.773754	-5.69676
H	3.767099	1.738945	-4.21711
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C	6.230456	1.326734	-6.66861
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H	6.043729	2.215722	-7.28789
C	-5.1908	-2.32913	-6.00148
H	-4.52515	-3.03654	-6.50634
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O	-5.96403	-7.59886	-1.11661
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O	-8.52106	-3.84354	-0.01956
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C	-6.21965	1.312671	-3.72806
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C	-5.58515	1.743175	-2.55827
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H	-5.71324	1.851674	-0.40524
C	-7.40596	0.814166	-1.26281
H	-7.85881	0.633886	-0.29017
C	4.734966	-7.33239	-1.27656
H	5.429683	-6.79156	-0.62735
C	4.02655	-6.3756	-2.23687
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C	0.017548	-4.17117	7.69826
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H	-9.95068	-1.58971	-1.91047
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H	-7.70036	-0.41378	0.923686
C	4.938896	-7.51567	-0.45408
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H	-3.81516	6.192181	3.484753
C	-2.66651	4.708677	2.853766
N	-1.46545	4.20531	2.652301
H	-0.61866	4.50743	3.172437
H	-1.38617	3.310893	2.144888
N	-3.76049	4.090899	2.325263
H	-4.58611	4.687495	2.24614
H	-3.57865	3.489332	1.512853
C	-0.62912	8.811994	-0.19089
O	-1.47768	7.951474	-0.46181
N	0.341795	9.190573	-1.05825
H	1.130634	9.726649	-0.71345
C	0.620216	8.487896	-2.3031
H	-0.11685	7.697971	-2.45059
C	2.054138	7.945151	-2.21854
O	2.930458	8.627233	-1.67883
N	2.236991	6.717488	-2.75048
H	1.40482	6.2004	-3.04066
C	3.48479	5.978266	-2.57656
H	4.261028	6.713742	-2.35113
C	3.391103	4.918156	-1.46258
H	2.635156	4.174079	-1.74294
H	4.345667	4.381741	-1.39888
C	3.045116	5.524186	-0.09817
H	3.833809	6.209469	0.230206
H	2.117139	6.102094	-0.15514
S	2.873285	4.292084	1.250144
C	1.344749	3.426838	0.738056
H	1.072248	2.763674	1.561602
H	0.53164	4.139858	0.573931
H	1.487502	2.824223	-0.16156
O	-2.70489	-0.42319	4.67893

C	-3.20207	-1.58701	4.613972
O	-2.47662	-2.58657	4.292301
C	-4.67955	-1.8298	4.895413
C	-5.39693	-0.67942	5.603704
H	-5.15872	-2.03539	3.927646
H	-4.75321	-2.76495	5.463452
H	-5.37828	0.21869	4.981352
H	-6.44242	-0.94485	5.80093
O	-1.30702	-0.70418	2.017005
O	-4.29874	1.116702	2.872865
Fe	-0.66999	-1.42754	4.124734
C	-1.81692	-1.04458	0.72608
H	-0.97385	-1.15065	0.028058
C	-2.74895	0.075608	0.181641
H	-3.74531	-0.03996	0.618211
C	-2.35086	1.542275	0.492475
O	-3.0818	2.451956	-0.02168
O	-1.3861	1.756115	1.258918
H	-0.83626	-3.91377	-1.52616
N	-2.87456	-0.08558	-1.30822
H	-1.91984	-0.19548	-1.80025
H	-3.39096	0.710103	-1.70775
H	-3.37373	-0.95703	-1.60347
C	-2.60289	-2.36158	0.821451
H	-3.25945	-2.28341	1.693658
C	-1.73236	-3.63154	0.93649
C	-2.0982	-4.7484	-0.0336
H	-1.50283	-5.64199	0.172941
H	-3.15558	-5.02169	0.015357
N	-1.80205	-4.346	-1.45134
H	-1.89494	-5.16212	-2.06876
H	-2.50358	-3.64418	-1.81462
H	0.294049	-5.00789	9.40291
H	2.76036	-6.57519	4.881934
H	5.532182	-8.31853	-0.90849
H	4.249024	-7.97801	0.262682
H	6.639201	-4.16088	2.146654
H	7.429648	3.403259	-4.38914
H	-4.91707	-0.44321	6.559771
H	-5.61972	-0.8007	-6.12991
H	-7.7226	-5.53902	-6.44144
H	-9.92577	-3.4324	-0.19719
H	-4.41888	7.631868	-2.04845
H	-5.51421	8.722771	-1.18853
H	-1.57801	10.14099	1.168102
H	0.556114	9.188487	-3.14648
H	3.742203	5.490393	-3.52385

H	-1.24791	1.686789	-6.27237
H	-0.87117	0.959886	-4.69479
H	-3.67127	0.653409	3.470387
H	-4.18947	2.057932	3.08926
O	-0.62398	-0.59691	-2.6517
H	-0.30381	-1.51995	-2.62139
H	0.172656	-0.04925	-2.33392
O	0.918625	4.675676	3.993792
H	0.961699	3.695336	4.148229
H	1.596747	4.834475	3.306469
O	0.640815	-3.08359	-1.676
H	1.360427	-3.77277	-1.73601
H	1.079311	-2.29575	-1.25258
H	-1.07819	0.260915	1.967837
H	-3.26087	-2.44042	-0.05073
H	-0.68376	-3.38765	0.758887
H	-1.78539	-4.02762	1.953822

⁵TS1_{A,C4}

C	-3.09533	0.249817	-5.28247
H	-3.99417	-0.34169	-5.06033
C	-3.3325	1.73854	-5.00911
H	-2.45791	2.32378	-5.31174
H	-4.17313	2.106381	-5.61354
C	-3.60644	2.013852	-3.5252
H	-4.49098	1.463556	-3.18188
H	-2.75733	1.635393	-2.93912
C	-3.75499	3.496263	-3.20751
O	-3.09584	4.355235	-3.81219
N	-4.62942	3.813813	-2.22759
H	-5.13551	3.089606	-1.7269
H	-4.69491	4.781309	-1.91427
C	-8.25142	4.752905	-0.79901
H	-9.00081	3.952837	-0.78454
C	-7.39126	4.738854	0.468846
H	-6.85731	3.781004	0.529206
H	-6.617	5.512469	0.384644
C	-8.17351	4.936032	1.736376
N	-7.57308	4.871152	2.989381
C	-8.53457	5.063837	3.873065
H	-8.41562	5.067898	4.948034
N	-9.73086	5.257021	3.261882
H	-10.6179	5.409944	3.718812
C	-9.51666	5.175545	1.897141
H	-10.3205	5.284479	1.186419
C	7.038538	-4.14104	3.01367
C	7.663711	-2.74773	3.130069
C	5.81014	-4.28189	2.096096
O	8.167231	-2.36004	4.179672
C	4.737964	-3.27968	2.406308
C	4.469617	-2.54237	3.535963
N	3.798422	-2.89006	1.473825
C	3.004105	-1.96395	2.047754
N	3.381097	-1.72415	3.303029
H	7.822311	-4.8323	2.676187
H	6.090154	-4.19744	1.038287
H	5.420558	-5.30413	2.191412
H	4.972263	-2.54948	4.490517
H	2.192843	-1.46942	1.536896
H	3.658226	-3.38639	0.553118
N	7.654203	-1.98089	1.993881
H	7.192295	-2.33106	1.166117
C	8.235842	-0.65404	1.936604
H	8.721584	-0.48736	2.903282

C	7.252561	0.495693	1.662399
O	7.634422	1.475215	1.018643
N	6.005353	0.365476	2.171115
C	4.949147	1.382219	2.044471
C	4.895023	1.942952	0.604707
C	5.043023	2.51023	3.087588
O	4.9293	3.142118	0.362707
C	3.694993	3.203511	3.34225
C	2.594569	2.347	3.993104
O	1.438427	2.763503	4.065346
O	3.007319	1.201438	4.473329
H	5.778839	-0.47363	2.692797
H	4.017716	0.8347	2.215412
H	5.420328	2.076687	4.018995
H	5.769919	3.248668	2.737091
H	3.294386	3.613484	2.409008
H	3.846665	4.069541	4.000993
N	4.814265	0.979734	-0.36558
H	4.421227	0.086999	-0.08928
C	4.497154	1.321161	-1.75134
H	4.504617	0.362007	-2.28456
C	3.099658	1.927603	-1.91209
H	2.996962	2.789754	-1.2451
H	2.978157	2.304927	-2.93035
C	1.964703	0.93237	-1.62125
O	0.811375	1.317936	-1.9701
O	2.261606	-0.16981	-1.06731
C	5.588413	2.151812	-2.44304
O	5.359138	2.698332	-3.52795
N	6.836895	2.131708	-1.90117
H	6.956614	1.825314	-0.93802
C	7.906137	2.931546	-2.49594
H	7.489881	3.900571	-2.79398
C	9.040128	3.154461	-1.49059
H	9.449165	2.201918	-1.13696
H	8.675065	3.704649	-0.61875
H	9.836491	3.724459	-1.97553
C	8.460702	2.341252	-3.81054
O	9.219381	3.000649	-4.51365
N	8.048904	1.077677	-4.11372
H	7.44416	0.611894	-3.44996
C	8.321983	0.42651	-5.37909
H	9.138113	0.994514	-5.83915
C	8.791522	-1.03605	-5.18208
H	9.790788	-1.01102	-4.73313
H	8.877547	-1.47317	-6.18087
C	7.867004	-1.86718	-4.3141

C	8.173456	-2.10668	-2.96654
H	9.104782	-1.72	-2.55733
C	7.305679	-2.83812	-2.15069
H	7.580843	-3.02818	-1.11409
C	6.104887	-3.33752	-2.65893
H	5.415651	-3.88914	-2.02366
C	5.795922	-3.10951	-4.00393
H	4.867996	-3.49735	-4.41627
C	6.66671	-2.39021	-4.82405
H	6.421627	-2.22609	-5.86958
C	7.153002	0.500214	-6.39779
O	7.205081	-0.18575	-7.42318
N	6.156534	1.367773	-6.11168
H	6.160662	1.876953	-5.23087
C	5.066102	1.655213	-7.03713
H	5.275899	1.096916	-7.95139
C	3.674774	1.32567	-6.47364
H	3.51968	1.92437	-5.56655
H	2.932082	1.673323	-7.2084
C	3.402816	-0.15489	-6.146
H	4.12416	-0.46318	-5.37541
C	1.988925	-0.31499	-5.56417
H	1.80372	-1.35072	-5.25483
H	1.824309	0.326389	-4.69051
H	1.228763	-0.05301	-6.31309
C	3.597448	-1.07306	-7.36339
H	4.629455	-1.05473	-7.72924
H	3.350495	-2.11148	-7.10815
H	2.936434	-0.77328	-8.18897
C	-5.17632	-4.07442	-4.4097
H	-4.25579	-4.44791	-4.86995
C	-4.84006	-3.30525	-3.11594
H	-4.3342	-2.36738	-3.37185
H	-5.76684	-3.02048	-2.60035
C	-3.95661	-4.05895	-2.11381
O	-3.79107	-5.3025	-2.24767
O	-3.45019	-3.37984	-1.16262
C	-6.17432	-5.20771	-4.19429
O	-7.38379	-4.99941	-4.06236
N	-5.64428	-6.46718	-4.14933
H	-4.65336	-6.49917	-3.93542
C	-6.46548	-7.59302	-3.73305
H	-7.36361	-7.63312	-4.353
C	-6.96253	-7.57435	-2.27122
O	-7.87138	-8.31708	-1.92176
N	-6.33732	-6.6806	-1.45599
H	-5.53961	-6.16042	-1.81574

C	-6.76314	-6.4161	-0.09091
H	-7.18136	-7.34359	0.314182
C	-5.56717	-5.98424	0.780002
H	-5.95971	-5.75877	1.773844
H	-5.11634	-5.07052	0.374399
C	-4.53236	-7.10146	0.915348
O	-4.71571	-8.06809	1.643387
N	-3.38187	-6.9261	0.183492
H	-3.39782	-6.32707	-0.64703
H	-2.78917	-7.74668	0.137952
C	-7.89299	-5.35848	0.02353
O	-8.27119	-4.99109	1.136622
N	-8.41212	-4.89461	-1.14057
H	-8.05101	-5.23619	-2.02537
C	-9.5977	-4.05145	-1.19245
H	-9.81455	-3.73908	-0.16851
C	-9.44834	-2.85676	-2.14207
H	-9.13774	-3.23416	-3.12552
H	-10.4527	-2.43081	-2.28589
C	-8.49962	-1.74661	-1.71955
C	-8.25288	-0.69211	-2.61476
H	-8.72911	-0.70558	-3.5935
C	-7.41444	0.370208	-2.28917
H	-7.23361	1.178258	-2.99251
C	-6.78514	0.394675	-1.03999
O	-5.93297	1.437848	-0.75978
H	-5.46952	1.269618	0.100138
C	-7.01889	-0.63986	-0.12866
H	-6.53335	-0.61816	0.842446
C	-7.868	-1.69711	-0.47064
H	-8.02204	-2.48941	0.256597
C	4.085081	-7.35738	-1.1336
H	4.82244	-6.80353	-1.72198
C	2.704654	-6.71064	-1.23945
H	2.347468	-6.73475	-2.2787
H	1.958595	-7.27307	-0.66345
C	2.63326	-5.24729	-0.77881
O	1.474528	-4.74132	-0.67044
O	3.714812	-4.63451	-0.55408
C	6.004901	-2.59843	8.673966
C	5.244923	-1.74289	7.714997
C	4.12842	-1.97653	6.95319
N	5.606623	-0.43766	7.412684
C	4.727218	0.052543	6.502096
N	3.820293	-0.85709	6.202756
H	6.044774	-2.15632	9.678059
H	5.519499	-3.57429	8.761198

H	3.517747	-2.86418	6.887761
H	4.761971	1.046779	6.085756
H	6.406076	0.05665	7.782082
C	-4.22301	8.707626	0.18307
H	-3.80613	9.698128	-0.03433
C	-3.52152	8.115204	1.427304
H	-2.45716	7.952978	1.211135
H	-3.5629	8.872613	2.222583
C	-4.16945	6.817508	1.919758
H	-5.25804	6.963768	1.962732
H	-4.00304	6.01698	1.192442
C	-3.70348	6.34787	3.30587
H	-2.6383	6.106531	3.330513
H	-3.86025	7.136729	4.0521
N	-4.48281	5.176713	3.724494
H	-5.49047	5.315652	3.644591
C	-4.13355	3.895476	3.43299
N	-2.87517	3.508353	3.274369
H	-2.04666	4.094094	3.47853
H	-2.72507	2.497871	3.170426
N	-5.13073	2.990616	3.352242
H	-6.06555	3.370631	3.223669
H	-4.92522	2.105084	2.879824
C	-4.13077	7.810335	-1.05046
O	-4.75646	6.745331	-1.12496
N	-3.32978	8.286804	-2.03655
H	-2.68969	9.041834	-1.81304
C	-2.88687	7.494636	-3.17318
H	-3.38776	6.527304	-3.17651
C	-1.36033	7.360932	-3.07691
O	-0.69403	8.312988	-2.65656
N	-0.85705	6.172465	-3.46966
H	-1.51634	5.423495	-3.68547
C	0.562596	5.857425	-3.3424
H	1.089903	6.813065	-3.28648
C	0.897413	4.98874	-2.11466
H	0.490716	3.978285	-2.24079
H	1.987298	4.876893	-2.07629
C	0.40533	5.606082	-0.80113
H	0.790136	6.62552	-0.68941
H	-0.68778	5.671953	-0.78485
S	0.951044	4.721429	0.713092
C	-0.0968	3.219159	0.678863
H	0.148082	2.665017	1.589721
H	-1.15795	3.488793	0.702055
H	0.123882	2.601975	-0.19539
O	0.852463	-0.42607	6.356865

C	0.73199	-1.69794	6.425961
O	1.411513	-2.42834	5.643195
C	-0.2555	-2.31198	7.39567
C	-0.44344	-1.51049	8.686939
H	-1.20742	-2.35079	6.849596
H	0.055833	-3.34357	7.592414
H	-0.78354	-0.49747	8.45817
H	-1.19151	-1.99008	9.32817
O	0.934005	-0.42746	3.502404
O	-2.01059	-0.39985	5.466542
Fe	2.172002	-0.54074	4.694894
C	-1.31088	-0.95067	1.293257
H	-0.92594	0.063292	1.436342
H	-0.81863	-1.32403	0.394038
C	-2.83383	-0.8448	1.077933
H	-3.33927	-1.74661	1.442112
C	-3.44812	0.341634	1.868197
O	-4.51536	0.861082	1.420554
O	-2.85851	0.685027	2.914398
H	-0.60305	-3.17024	-0.22411
N	-3.18813	-0.7413	-0.38237
H	-2.36474	-0.43864	-1.00677
H	-3.97075	-0.08803	-0.49145
H	-3.46356	-1.68173	-0.75964
C	-0.9329	-1.78964	2.517095
H	-1.6843	-1.73532	3.310361
H	-0.0332	-1.18515	3.046254
C	-0.39665	-3.20989	2.327302
H	-0.22699	-3.63642	3.322016
H	0.58238	-3.19748	1.834266
C	-1.29838	-4.17112	1.532767
H	-1.10498	-5.20949	1.809037
H	-2.35981	-3.98377	1.711854
N	-1.0678	-4.06476	0.049207
H	-0.36715	-4.75478	-0.28033
H	-1.97061	-4.10115	-0.47965
H	7.036851	-2.76805	8.340674
H	6.789328	-4.43442	4.037493
H	4.061961	-8.39334	-1.49326
H	4.437151	-7.36603	-0.09604
H	8.999996	-0.59098	1.15563
H	5.099385	2.724312	-7.28802
H	0.492333	-1.43501	9.253606
H	-5.64762	-3.37914	-5.11184
H	-5.90428	-8.51745	-3.90123
H	-10.4513	-4.65444	-1.5334
H	-7.62127	4.606723	-1.68121

H	-8.77248	5.710603	-0.91891
H	-5.28864	8.844232	0.40398
H	-3.13553	8.013659	-4.1087
H	0.89017	5.341102	-4.2521
H	-2.83821	0.076471	-6.33415
H	-2.28076	-0.13442	-4.65817
H	-1.09269	-0.09431	5.569728
H	-2.30542	-0.0016	4.628005
O	-1.21985	-0.36355	-2.15133
H	-0.71902	-1.20765	-2.11096
H	-0.4826	0.318091	-2.05143
O	-0.43995	4.875006	3.697989
H	0.203537	4.184598	3.974501
H	-0.09107	5.147575	2.825125
O	0.57307	-2.23174	-1.1899
H	1.143149	-3.03875	-1.18668
H	1.182672	-1.43691	-1.09686

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C	-2.077	1.654779	-4.69414
H	-3.05501	1.541601	-4.20969
C	-1.5624	3.089884	-4.54593
H	-0.64789	3.236427	-5.13081
H	-2.30482	3.791035	-4.95225
C	-1.25874	3.46524	-3.08244
H	-2.11815	3.235958	-2.43922
H	-0.41554	2.860588	-2.72273
C	-0.8722	4.931794	-2.96599
O	0.016023	5.42591	-3.67478
N	-1.57162	5.678799	-2.07782
H	-2.26097	5.261042	-1.46935
H	-1.37483	6.675481	-1.98471
C	-5.08252	8.725662	-2.44229
H	-6.01214	8.33232	-2.87065
C	-4.67575	7.960231	-1.17965
H	-4.50617	6.904353	-1.43079
H	-3.70585	8.336766	-0.83065
C	-5.68501	8.032902	-0.06882
N	-5.50673	7.348362	1.127758
C	-6.56596	7.612271	1.869485
H	-6.75165	7.233286	2.865273
N	-7.42594	8.4369	1.21905
H	-8.31003	8.775121	1.569859
C	-6.87778	8.713011	-0.02135
H	-7.3775	9.346868	-0.73673
C	2.633822	-5.89148	4.438553
C	3.978781	-5.16988	4.330235
C	1.538156	-5.53238	3.413839
O	4.650582	-4.96077	5.337068
C	1.254785	-4.06035	3.300439
C	0.811508	-3.12439	4.204139
N	1.446331	-3.36316	2.119374
C	1.122098	-2.06945	2.329812
N	0.73633	-1.89051	3.592777
H	2.831757	-6.97119	4.382872
H	1.811069	-5.90549	2.423079
H	0.624844	-6.06717	3.706494
H	0.539195	-3.25338	5.239724
H	1.18757	-1.2986	1.574229
H	1.847891	-3.80419	1.263567
N	4.39664	-4.79064	3.081733
H	3.859706	-5.02126	2.245848
C	5.694915	-4.16422	2.902145
H	6.335129	-4.45764	3.738723

C	5.72629	-2.62715	2.822359
O	6.763455	-2.06614	2.463876
N	4.578204	-1.98504	3.141973
C	4.362627	-0.53613	3.041227
C	4.992285	0.016685	1.744904
C	4.784105	0.248302	4.294453
O	5.650692	1.049566	1.712335
C	4.16229	1.652423	4.376773
C	2.635845	1.752046	4.53075
O	2.099619	2.858	4.463683
O	2.010363	0.628774	4.771794
H	3.80064	-2.55552	3.446065
H	3.279686	-0.42019	2.931012
H	4.488244	-0.34358	5.167794
H	5.875342	0.337405	4.304831
H	4.440412	2.237993	3.495702
H	4.590422	2.188567	5.234992
N	4.730155	-0.74943	0.643904
H	3.918794	-1.35591	0.690205
C	4.936434	-0.24961	-0.70956
H	4.786117	-1.12362	-1.35855
C	3.899109	0.804931	-1.10631
H	3.92323	1.628768	-0.38262
H	4.148903	1.232866	-2.07966
C	2.473842	0.226815	-1.16496
O	1.622359	0.876437	-1.82752
O	2.261228	-0.86068	-0.53176
C	6.390455	0.162736	-0.9666
O	6.685384	0.964529	-1.85841
N	7.333047	-0.5459	-0.28258
H	7.044166	-1.06049	0.547688
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H	8.866611	0.848899	-0.50325
C	9.543244	-0.7583	0.770747
H	9.408277	-1.83867	0.895206
H	9.202697	-0.26961	1.688243
H	10.60513	-0.55104	0.617719
C	9.357999	-0.77104	-1.75146
O	10.5044	-0.47738	-2.07442
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C	8.843099	-2.01224	-3.83914
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C	8.456776	-3.50097	-4.03176
H	9.085498	-4.09789	-3.36097
H	8.713449	-3.76257	-5.06166
C	6.992452	-3.79158	-3.76504

C	6.539698	-4.10293	-2.4727
H	7.260494	-4.18664	-1.66144
C	5.181177	-4.30824	-2.21252
H	4.842077	-4.53063	-1.204
C	4.250371	-4.22523	-3.25153
H	3.19521	-4.3886	-3.04919
C	4.690697	-3.93472	-4.54561
H	3.974823	-3.87181	-5.36133
C	6.045882	-3.71404	-4.79898
H	6.3812	-3.46634	-5.8022
C	8.230714	-1.1417	-4.968
O	8.336865	-1.51737	-6.13902
N	7.638429	0.012181	-4.5854
H	7.562946	0.240642	-3.59701
C	7.109219	0.986694	-5.53166
H	7.379047	0.635315	-6.52936
C	5.59452	1.214292	-5.39822
H	5.388459	1.554171	-4.37449
H	5.326268	2.048958	-6.06478
C	4.692752	0.006771	-5.71876
H	4.960672	-0.80454	-5.02777
C	3.217471	0.365002	-5.47632
H	2.567251	-0.49543	-5.67655
H	3.028402	0.684224	-4.44461
H	2.898631	1.179927	-6.1412
C	4.898603	-0.51259	-7.15111
H	5.916509	-0.88437	-7.30781
H	4.205905	-1.33609	-7.36643
H	4.703871	0.280245	-7.88745
C	-5.3456	-3.48981	-5.18031
H	-4.60417	-4.17655	-5.60153
C	-4.7699	-2.79799	-3.93258
H	-3.96764	-2.11244	-4.22993
H	-5.54257	-2.17552	-3.46619
C	-4.20701	-3.73447	-2.85797
O	-4.44614	-4.97067	-2.93745
O	-3.53407	-3.18574	-1.92624
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O	-7.73098	-3.60725	-4.78119
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H	-5.66776	-5.95166	-4.6935
C	-7.74476	-6.37553	-4.52249
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C	-8.14443	-6.40195	-3.03574
O	-9.17907	-6.96239	-2.6942
N	-7.29955	-5.76534	-2.17661
H	-6.41344	-5.40212	-2.52313

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C	-6.22942	-5.69519	0.043602
H	-6.48938	-5.55278	1.095378
H	-5.61778	-4.84565	-0.28383
C	-5.46754	-7.0151	-0.08106
O	-5.85044	-8.03614	0.475051
N	-4.31914	-6.95628	-0.83188
H	-4.21882	-6.22472	-1.54522
H	-3.90934	-7.85909	-1.04192
C	-8.45227	-4.55581	-0.27989
O	-8.73854	-4.44834	0.910924
N	-8.89353	-3.69352	-1.23094
H	-8.6586	-3.86327	-2.20153
C	-9.87423	-2.67003	-0.89601
H	-9.61777	-2.28757	0.096302
C	-9.93267	-1.53458	-1.92798
H	-10.178	-1.9527	-2.91269
H	-10.7845	-0.89809	-1.64808
C	-8.67356	-0.69751	-2.04029
C	-7.97547	-0.61292	-3.25224
H	-8.32142	-1.18019	-4.11142
C	-6.80867	0.141108	-3.36558
H	-6.2671	0.198131	-4.30521
C	-6.29857	0.815369	-2.25223
O	-5.10707	1.472751	-2.39616
H	-4.79643	1.844346	-1.52634
C	-6.99741	0.767939	-1.03749
H	-6.61651	1.311503	-0.17659
C	-8.17257	0.020806	-0.94586
H	-8.69906	-0.00996	0.005992
C	3.541152	-7.78515	0.193052
H	4.390788	-7.17349	0.510332
C	2.726044	-7.07387	-0.88745
H	3.346492	-6.91922	-1.78143
H	1.879693	-7.68717	-1.21733
C	2.17638	-5.69217	-0.5037
O	1.213323	-5.25493	-1.19569
O	2.738584	-5.0621	0.449777
C	-0.24553	-2.93254	9.59346
C	0.203556	-2.08862	8.446176
C	-0.3954	-1.74778	7.259479
N	1.43593	-1.45273	8.407401
C	1.532533	-0.77566	7.232824
N	0.438177	-0.93359	6.51503
H	-0.29771	-2.36118	10.52955
H	-1.24475	-3.32817	9.39164

H	-1.3664	-2.03348	6.883901
H	2.389939	-0.19731	6.927368
H	2.151322	-1.49766	9.118887
C	-0.05446	9.97041	0.07448
H	0.825714	10.61948	0.153777
C	-0.11983	9.032684	1.305298
H	0.799538	8.435588	1.365636
H	-0.13769	9.66426	2.204183
C	-1.34136	8.108895	1.283162
H	-2.23809	8.705396	1.064409
H	-1.24201	7.403244	0.454133
C	-1.59997	7.303858	2.563779
H	-0.73639	6.708404	2.869276
H	-1.83674	7.965012	3.405765
N	-2.75765	6.423159	2.358643
H	-3.62235	6.912461	2.127425
C	-2.6789	5.2108	1.759017
N	-1.57001	4.473127	1.779807
H	-0.7888	4.674718	2.430193
H	-1.68984	3.489419	1.531402
N	-3.75635	4.779835	1.080854
H	-4.57088	5.384613	1.050469
H	-3.81045	3.82254	0.710854
C	-0.05358	9.216433	-1.25384
O	-1.07023	8.639034	-1.66683
N	1.117536	9.223738	-1.93019
H	1.95744	9.582779	-1.48816
C	1.388947	8.387722	-3.09073
H	0.555771	7.705275	-3.26029
C	2.706542	7.65056	-2.81583
O	3.624848	8.247752	-2.24544
N	2.748419	6.366398	-3.22932
H	1.872622	5.937283	-3.53164
C	3.875546	5.493263	-2.91106
H	4.720131	6.145564	-2.67639
C	3.586727	4.535419	-1.73944
H	2.802973	3.826115	-2.03228
H	4.489873	3.942022	-1.55384
C	3.17877	5.272726	-0.45951
H	3.968141	5.965809	-0.14891
H	2.275438	5.868113	-0.63077
S	2.888078	4.191758	0.996194
C	1.366865	3.310289	0.485247
H	1.064371	2.689077	1.334045
H	0.5693	4.025083	0.259274
H	1.54121	2.661248	-0.37483
O	-1.30372	1.238004	5.416963

C	-2.17315	0.301732	5.354688
O	-1.8789	-0.77386	4.74978
C	-3.53257	0.48965	5.995406
C	-3.44354	1.02397	7.431824
H	-4.06317	1.218535	5.36998
H	-4.06951	-0.46303	5.951208
H	-2.91858	1.983052	7.451068
H	-4.44608	1.169077	7.849433
O	-0.05288	0.768522	2.741136
O	-3.22885	3.013641	4.02849
Fe	0.17446	0.043103	4.39264
C	-2.68572	-1.11084	1.211432
H	-2.7995	-0.71812	2.234734
H	-1.60978	-1.01684	1.006007
C	-3.46359	-0.18109	0.281028
H	-4.54031	-0.35868	0.393755
C	-3.23929	1.331	0.576657
O	-3.89178	2.15676	-0.13212
O	-2.47293	1.651654	1.519161
H	-0.81535	-3.5552	-0.43229
N	-3.15328	-0.46732	-1.16407
H	-2.11382	-0.34357	-1.42949
H	-3.7023	0.155959	-1.77587
H	-3.38852	-1.45549	-1.428
C	-3.1131	-2.54339	1.165116
C	-2.26492	-3.609	1.786596
C	-1.97047	-4.81107	0.871748
H	-1.18646	-5.43495	1.3098
H	-2.85195	-5.43437	0.702848
N	-1.49266	-4.36159	-0.47323
H	-0.94367	-5.09144	-0.94638
H	-2.30007	-4.04583	-1.07336
H	0.422559	-3.78716	9.762458
H	2.287006	-5.69536	5.457422
H	3.927656	-8.74236	-0.17644
H	2.933201	-7.9935	1.08201
H	6.154436	-4.52597	1.97781
H	7.625126	1.942431	-5.36677
H	-2.90031	0.329935	8.084157
H	-5.55829	-2.72407	-5.93436
H	-7.58049	-7.40954	-4.84157
H	-10.8723	-3.12436	-0.80657
H	-4.29758	8.643042	-3.19949
H	-5.22942	9.791872	-2.23118
H	-0.94044	10.61664	0.070859
H	1.515195	9.011088	-3.98676
H	4.132822	4.910249	-3.80296

H	-2.19878	1.395646	-5.75321
H	-1.39267	0.930016	-4.23913
H	-2.44423	2.760209	4.548558
H	-3.09026	2.537718	3.189789
O	-0.70964	-0.40888	-2.19197
H	-0.37394	-1.32818	-2.10037
H	0.104259	0.146863	-2.00072
O	0.700016	4.980183	3.363124
H	0.97498	4.208821	3.906368
H	1.437678	5.049017	2.722429
O	0.443746	-2.64251	-1.09999
H	0.947272	-3.47856	-1.26823
H	1.113104	-1.93398	-0.84511
H	-0.92917	0.954028	2.345585
H	-4.1233	-2.79372	0.848004
H	-1.31746	-3.17201	2.11596
H	-2.74323	-4.01468	2.693507

⁵TS2_{A,C4}

C	-1.76896	2.008027	-4.89478
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H	-0.57504	3.782417	-4.51052
H	-2.2901	4.101258	-4.69429
C	-1.72496	3.362616	-2.73944
H	-2.65752	2.858084	-2.45963
H	-0.90026	2.781357	-2.30198
C	-1.69992	4.753541	-2.12133
O	-0.98453	5.6581	-2.57746
N	-2.51049	4.947137	-1.05466
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H	-2.51998	5.86019	-0.60753
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H	-7.27308	7.650739	-1.1776
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H	-5.69758	6.12398	0.072666
H	-5.00786	7.49671	0.900302
C	-6.97235	6.95056	1.560086
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C	-7.85368	6.16996	3.383435
H	-8.03182	5.623818	4.299821
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H	-9.67188	7.243737	3.220224
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C	4.811209	-6.52659	3.066607
C	5.736221	-5.3112	3.170815
C	3.572721	-6.42476	2.151453
O	6.334547	-5.08223	4.219595
C	2.716618	-5.21757	2.408384
C	1.961696	-4.8068	3.48217
N	2.604345	-4.20557	1.471718
C	1.814335	-3.24571	1.979135
N	1.404179	-3.57488	3.206003
H	5.424171	-7.37823	2.738853
H	3.877648	-6.40555	1.10098
H	2.981929	-7.33947	2.287361
H	1.781548	-5.30406	4.423253
H	1.549691	-2.33937	1.455475
H	3.130671	-4.21303	0.552945
N	5.885297	-4.52526	2.058559
H	5.425742	-4.74695	1.172822
C	6.837536	-3.42928	2.061424
H	7.576851	-3.62021	2.844197

C	6.284684	-2.01314	2.295331
O	7.023711	-1.04379	2.114728
N	4.988875	-1.92657	2.679614
C	4.225137	-0.68035	2.815761
C	4.62235	0.330051	1.716585
C	4.268019	-0.05784	4.221716
O	4.919889	1.491434	1.966346
C	3.120383	0.941987	4.473513
C	1.709622	0.348819	4.371761
O	0.764541	1.019542	3.915568
O	1.592815	-0.87255	4.797358
H	4.485313	-2.79841	2.777813
H	3.188531	-0.96792	2.606929
H	4.215002	-0.87319	4.949989
H	5.226043	0.454435	4.352175
H	3.193491	1.786823	3.785492
H	3.223107	1.347342	5.490427
N	4.603388	-0.1993	0.456874
H	4.000054	-1.00261	0.306779
C	4.629592	0.658123	-0.72337
H	4.760797	-0.02788	-1.57177
C	3.315467	1.415669	-0.91834
H	3.136196	2.048429	-0.04159
H	3.400124	2.088751	-1.7736
C	2.095228	0.503868	-1.13854
O	1.107064	1.062886	-1.69507
O	2.154772	-0.70539	-0.75177
C	5.864197	1.569158	-0.76619
O	5.859672	2.623901	-1.41058
N	7.001503	1.067865	-0.20777
H	6.917163	0.305152	0.462529
C	8.221474	1.871277	-0.16639
H	7.948981	2.908304	0.061819
C	9.172583	1.34566	0.913086
H	9.431061	0.296106	0.73311
H	8.703578	1.410994	1.898967
H	10.08888	1.940961	0.901633
C	8.945996	1.955454	-1.52874
O	9.898185	2.713017	-1.68467
N	8.445346	1.145817	-2.50269
H	7.671566	0.545146	-2.25041
C	8.867527	1.16812	-3.88721
H	9.860886	1.628986	-3.90448
C	8.972099	-0.27113	-4.45695
H	9.793876	-0.77889	-3.93892
H	9.240332	-0.17526	-5.51235
C	7.690077	-1.06551	-4.30089

C	7.443912	-1.81391	-3.13874
H	8.216524	-1.8801	-2.37507
C	6.222452	-2.46543	-2.94421
H	6.038628	-3.02217	-2.02887
C	5.22812	-2.39746	-3.92437
H	4.27944	-2.90351	-3.76702
C	5.47292	-1.67838	-5.09778
H	4.709297	-1.62502	-5.86969
C	6.688041	-1.01546	-5.2827
H	6.863289	-0.43635	-6.18532
C	7.986926	2.052185	-4.81002
O	8.200646	2.046803	-6.02564
N	7.045564	2.809259	-4.20208
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H	6.570886	3.782951	-5.95041
C	4.714047	3.488554	-4.82614
H	4.428523	3.478183	-3.76562
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H	4.745514	1.348513	-4.99833
C	2.718671	2.003024	-5.26077
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C	4.565856	2.130527	-6.98686
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O	-4.24335	-8.35113	-1.48829
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H	-10.4289	-1.888	-1.11029
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C	-7.0668	0.210318	-3.15633
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H	-6.51337	0.830887	0.141871
C	-7.93862	-0.59248	-0.64285
H	-8.27563	-0.88859	0.348736
C	5.819402	-6.75818	-1.64216
H	6.474536	-6.10443	-1.05844
C	4.82507	-5.94355	-2.47046
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H	6.140136	-6.91257	0.36379
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H	3.087718	-2.83569	1.332686
N	5.565188	-2.79818	1.290629
H	6.548036	-3.00365	1.119958
H	5.135665	-2.06507	0.72078
C	4.411309	-7.61697	-2.40709
O	4.892078	-6.47607	-2.43996
N	3.618827	-8.11356	-3.38966
H	3.078162	-8.95152	-3.20677
C	3.083725	-7.29796	-4.47096
H	3.530244	-6.30419	-4.43255
C	1.55591	-7.2653	-4.32313
O	0.957721	-8.291	-3.98494
N	0.97574	-6.07123	-4.57337
H	1.590343	-5.27116	-4.72993
C	-0.44397	-5.8369	-4.32168
H	-0.93161	-6.81439	-4.35444
C	-0.72181	-5.14603	-2.97097
H	-0.35919	-4.11104	-2.99307
H	-1.80863	-5.08624	-2.83575
C	-0.09744	-5.90124	-1.79284
H	-0.45357	-6.93652	-1.76935
H	0.992192	-5.93755	-1.89524
S	-0.49079	-5.21674	-0.13831
C	0.410312	-3.62232	-0.18382
H	0.410044	-3.24104	0.84054
H	1.447622	-3.7808	-0.49566
H	-0.07582	-2.89778	-0.84167
O	3.141007	-0.66612	6.007201

C	2.732663	0.506117	5.842955
O	1.646088	0.847086	5.247212
C	3.558154	1.675948	6.391184
C	4.888684	1.272815	7.024588
H	3.711311	2.382697	5.565284
H	2.925235	2.20917	7.113863
H	5.528922	0.76183	6.298287
H	5.425728	2.152465	7.399894
O	0.818964	0.253203	2.356858
O	1.811698	-1.86701	3.973715
Fe	0.236977	-0.41291	4.480538
C	1.356838	1.221883	0.186687
H	0.677725	0.406531	-0.07858
H	0.978573	2.104959	-0.32645
C	2.758449	0.944212	-0.36531
H	3.483558	1.622975	0.103249
C	3.275659	-0.48992	-0.07528
O	4.33298	-0.88182	-0.67609
O	2.660102	-1.1415	0.793401
H	-0.74309	3.638197	0.162481
N	2.777975	1.289903	-1.82487
H	1.909941	0.914647	-2.34275
H	3.648564	0.983855	-2.28216
H	2.683763	2.331217	-1.90751
C	1.335989	1.426791	1.720688
C	0.487687	2.608757	2.203186
C	0.810433	3.985251	1.614454
H	0.467454	4.755873	2.308359
H	1.881864	4.140295	1.454799
N	0.116243	4.260224	0.296906
H	-0.1516	5.256552	0.252759
H	0.779443	4.131737	-0.50896
H	-0.39743	-2.20601	10.73787
H	-5.04125	1.940595	7.156819
H	-7.73341	6.031383	2.570111
H	-6.39409	5.424396	3.556366
H	-7.71698	0.585984	2.751124
H	-6.38663	-2.24898	-6.59187
H	4.731482	0.580875	7.857993
H	4.024594	5.389881	-5.54329
H	3.599253	10.16214	-3.67886
H	7.933124	7.194825	0.386323
H	7.51729	-4.76114	-3.72694
H	8.901156	-5.59843	-3.0117
H	5.810534	-8.75852	-1.29472
H	3.333529	-7.75781	-5.43637
H	-0.84941	-5.22687	-5.13695

H	2.593719	0.32611	-6.98231
H	1.794789	0.415175	-5.39552
H	2.37816	-1.71545	4.772384
H	1.291723	-2.70757	4.052319
O	0.554169	0.63241	-3.12121
H	-0.12169	1.321972	-3.00192
H	0.063411	-0.17525	-2.71398
O	1.545514	-5.62713	2.451656
H	0.922631	-5.0959	3.002789
H	1.022224	-5.81129	1.644068
O	-1.99852	2.519664	0.128816
H	-2.86578	2.997128	0.253832
H	-2.10177	1.861383	-0.59832
H	1.402614	-0.48561	2.073079
H	2.366275	1.591653	2.075391
H	-0.56286	2.399345	2.005758
H	0.611355	2.665655	3.289386

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C	-2.11915	1.28553	-5.27841
H	-3.09666	0.787304	-5.3345
C	-2.27008	2.731913	-4.79433
H	-1.29606	3.233877	-4.80571
H	-2.91153	3.297491	-5.48161
C	-2.85535	2.811422	-3.38051
H	-3.78959	2.237923	-3.31949
H	-2.16165	2.349665	-2.66367
C	-3.1303	4.238017	-2.91638
O	-2.71539	5.224139	-3.54469
N	-3.86145	4.363164	-1.78573
H	-4.15253	3.548394	-1.24851
H	-4.05759	5.298165	-1.43832
C	-8.26427	6.688214	-1.27348
H	-9.10684	6.102018	-1.65963
C	-7.5573	5.971318	-0.11952
H	-7.1636	5.009	-0.47437
H	-6.67585	6.554227	0.172611
C	-8.4323	5.722573	1.076114
N	-7.96481	5.044532	2.196019
C	-8.97597	4.978232	3.040729
H	-8.95972	4.505635	4.013446
N	-10.0798	5.584398	2.532707
H	-10.9812	5.658068	2.98112
C	-9.74823	6.062787	1.276986
H	-10.4633	6.580895	0.657763
C	6.443876	-4.25762	4.082069
C	6.876139	-2.80096	4.264867
C	5.537208	-4.57427	2.880796
O	7.039161	-2.31767	5.38057
C	4.284713	-3.74851	2.854421
C	3.597012	-3.08359	3.843942
N	3.571953	-3.53341	1.69378
C	2.50046	-2.7796	1.997338
N	2.477682	-2.48269	3.298817
H	7.356158	-4.8657	4.015236
H	6.077268	-4.44762	1.932794
H	5.287786	-5.64382	2.912864
H	3.818893	-3.00994	4.896879
H	1.78604	-2.43494	1.265403
H	3.774742	-3.98072	0.750671
N	7.10775	-2.09017	3.115409
H	6.931036	-2.52512	2.220742
C	7.624625	-0.73594	3.1179
H	7.88672	-0.50195	4.154404

C	6.675383	0.355952	2.601964
O	7.153914	1.394519	2.142948
N	5.349974	0.106811	2.71015
C	4.290455	1.084751	2.418433
C	4.594088	1.871331	1.120917
C	4.00579	2.031009	3.597687
O	4.647058	3.093614	1.089599
C	2.593	2.630224	3.559844
C	1.424609	1.64755	3.740045
O	0.258383	2.047698	3.646635
O	1.774074	0.421236	4.003312
H	5.062698	-0.76817	3.133794
H	3.395241	0.48314	2.233844
H	4.148655	1.46692	4.525362
H	4.741586	2.840366	3.577381
H	2.441301	3.167779	2.617189
H	2.488176	3.389698	4.346144
N	4.79676	1.071862	0.030301
H	4.373682	0.151	0.062843
C	4.818277	1.603761	-1.33289
H	4.949189	0.719408	-1.96761
C	3.484631	2.245569	-1.74246
H	3.235795	3.064932	-1.06064
H	3.576197	2.681116	-2.74227
C	2.332169	1.220389	-1.74331
O	1.193263	1.647034	-2.06913
O	2.634997	0.028832	-1.41573
C	6.044426	2.466912	-1.64377
O	6.125	3.05559	-2.72935
N	7.083489	2.434424	-0.76678
H	6.943225	2.055349	0.167241
C	8.274929	3.243266	-1.0069
H	7.958665	4.212566	-1.40796
C	9.055039	3.459465	0.293853
H	9.332203	2.504501	0.752633
H	8.445659	4.011478	1.015526
H	9.96264	4.027513	0.074612
C	9.199596	2.672162	-2.10353
O	10.12033	3.348587	-2.54999
N	8.915953	1.405153	-2.52275
H	8.151974	0.92241	-2.06803
C	9.552994	0.784266	-3.6673
H	10.41223	1.420689	-3.90628
C	10.07817	-0.63705	-3.34531
H	10.90088	-0.53294	-2.62896
H	10.48802	-1.0359	-4.27755
C	9.032292	-1.58141	-2.78471

C	8.947139	-1.82435	-1.40601
H	9.661626	-1.34798	-0.73751
C	7.967082	-2.67423	-0.8851
H	7.94187	-2.8637	0.187079
C	7.040362	-3.29189	-1.72694
H	6.259392	-3.93535	-1.32783
C	7.124965	-3.06203	-3.10357
H	6.415382	-3.54057	-3.77369
C	8.111151	-2.22515	-3.62821
H	8.173082	-2.05741	-4.69949
C	8.67285	0.773811	-4.94581
O	9.015903	0.084548	-5.91108
N	7.582495	1.573046	-4.9309
H	7.352785	2.111625	-4.09894
C	6.694875	1.730084	-6.0776
H	7.191549	1.262674	-6.93013
C	5.291208	1.145775	-5.84503
H	4.863667	1.635953	-4.96027
H	4.659928	1.439875	-6.69769
C	5.217689	-0.38311	-5.66819
H	5.881513	-0.65603	-4.83593
C	3.792023	-0.81061	-5.2848
H	3.727519	-1.89967	-5.16923
H	3.469642	-0.36093	-4.33856
H	3.070085	-0.51751	-6.05918
C	5.701053	-1.13643	-6.91805
H	6.754476	-0.93004	-7.13374
H	5.596455	-2.2204	-6.78188
H	5.105401	-0.85809	-7.79896
C	-4.48055	-4.77214	-4.99517
H	-3.58304	-5.29799	-5.33695
C	-4.11677	-3.78235	-3.87686
H	-3.50267	-2.97187	-4.28623
H	-5.02926	-3.31144	-3.49175
C	-3.36264	-4.38932	-2.6883
O	-3.32664	-5.64284	-2.56579
O	-2.82738	-3.56301	-1.8795
C	-5.57086	-5.76083	-4.59557
O	-6.74397	-5.41846	-4.43464
N	-5.16484	-7.05994	-4.45674
H	-4.17436	-7.19407	-4.29771
C	-6.08008	-8.08267	-3.98631
H	-7.0166	-7.99553	-4.54224
C	-6.46712	-8.0567	-2.49635
O	-7.33071	-8.8232	-2.08522
N	-5.81851	-7.14632	-1.71971
H	-5.06367	-6.58795	-2.11571

C	-6.13251	-6.99425	-0.30648
H	-6.4128	-7.97781	0.082965
C	-4.91041	-6.48356	0.476933
H	-5.24285	-6.30371	1.502381
H	-4.56293	-5.53413	0.053134
C	-3.78809	-7.52121	0.520891
O	-3.87946	-8.54346	1.187684
N	-2.67082	-7.2009	-0.21209
H	-2.76494	-6.56816	-1.01513
H	-2.003	-7.95758	-0.30593
C	-7.3465	-6.08137	-0.01386
O	-7.74242	-5.95723	1.143379
N	-7.91997	-5.44554	-1.06809
H	-7.5829	-5.62821	-2.00653
C	-9.1566	-4.69789	-0.8873
H	-9.09125	-4.19185	0.080319
C	-9.42473	-3.69834	-2.02151
H	-9.46487	-4.23857	-2.97598
H	-10.4364	-3.29941	-1.85675
C	-8.43277	-2.55705	-2.13706
C	-7.73325	-2.33773	-3.33122
H	-7.87377	-3.02014	-4.16456
C	-6.81998	-1.29195	-3.45626
H	-6.27662	-1.12917	-4.38267
C	-6.571	-0.44555	-2.37125
O	-5.61339	0.520163	-2.52023
H	-5.43497	0.993446	-1.65644
C	-7.27623	-0.63387	-1.17452
H	-7.09373	0.031058	-0.33414
C	-8.19752	-1.67692	-1.07178
H	-8.73195	-1.81087	-0.13359
C	4.324601	-7.08445	-2.30433
H	5.140203	-6.41968	-2.60495
C	3.01332	-6.31335	-2.16039
H	2.718249	-5.86287	-3.11801
H	2.188209	-6.98664	-1.8921
C	3.031971	-5.18463	-1.12098
O	1.935154	-4.57863	-0.90842
O	4.120942	-4.91584	-0.54076
C	3.267087	-3.21349	9.184155
C	2.87703	-2.3996	7.994565
C	1.981522	-2.62002	6.978641
N	3.426096	-1.15638	7.71285
C	2.864258	-0.68799	6.569352
N	1.986123	-1.55326	6.100659
H	3.045247	-2.697	10.12718
H	2.711372	-4.15513	9.183657

H	1.324609	-3.46093	6.81597
H	3.104983	0.259019	6.113186
H	4.149978	-0.69266	8.243144
C	-3.97834	9.29762	0.63675
H	-3.41661	10.23779	0.584991
C	-3.54035	8.502097	1.888738
H	-2.48646	8.209742	1.786891
H	-3.59228	9.177984	2.753642
C	-4.40273	7.259677	2.127601
H	-5.45985	7.558136	2.188298
H	-4.32175	6.614274	1.250051
C	-4.05819	6.425193	3.368614
H	-2.99014	6.204425	3.4347
H	-4.32705	6.943775	4.295667
N	-4.80476	5.154726	3.342902
H	-5.81322	5.285029	3.363976
C	-4.44466	4.177698	2.454677
N	-3.17601	3.977888	2.134815
H	-2.39086	4.310015	2.725142
H	-2.96368	3.172551	1.526077
N	-5.42054	3.42927	1.916622
H	-6.37203	3.79577	1.959977
H	-5.18969	2.749909	1.186975
C	-3.83185	8.515148	-0.66982
O	-4.49867	7.496899	-0.8975
N	-2.94589	9.035708	-1.55414
H	-2.28709	9.740698	-1.2408
C	-2.51624	8.345279	-2.76036
H	-3.01929	7.380702	-2.83587
C	-0.98886	8.20485	-2.69485
O	-0.31579	9.107638	-2.18701
N	-0.49205	7.062829	-3.2171
H	-1.15861	6.332841	-3.47515
C	0.920841	6.712947	-3.10145
H	1.458079	7.643977	-2.90471
C	1.201549	5.681457	-1.99126
H	0.746516	4.718643	-2.25339
H	2.283553	5.507327	-1.94932
C	0.703434	6.145703	-0.61867
H	1.19425	7.080548	-0.32744
H	-0.3739	6.339302	-0.64526
S	1.034106	4.968234	0.748614
C	-0.06484	3.576873	0.285378
H	-0.11743	2.912973	1.151513
H	-1.07088	3.946065	0.065512
H	0.332417	3.018714	-0.56524
O	-0.75781	-0.6187	5.400754

C	-1.14956	-1.80934	5.622082
O	-0.46542	-2.78658	5.180965
C	-2.42023	-2.07078	6.410786
C	-3.26028	-0.82343	6.691385
H	-2.99495	-2.82044	5.852646
H	-2.12055	-2.56722	7.344827
H	-3.54464	-0.32628	5.759487
H	-4.17073	-1.09351	7.23922
O	-0.03405	-1.48503	2.673974
O	-2.63925	0.877073	3.68522
Fe	0.859762	-1.30266	4.166209
C	-2.52205	-1.13361	0.891441
H	-2.48495	-0.55682	1.816652
H	-1.52153	-1.04795	0.453326
C	-3.52833	-0.47722	-0.05257
H	-4.53803	-0.8724	0.103083
C	-3.59756	1.067417	0.128798
O	-4.63251	1.663462	-0.34569
O	-2.66853	1.62493	0.739174
H	-0.17771	-2.99101	-0.27856
N	-3.17796	-0.78105	-1.48969
H	-2.19973	-0.42743	-1.75826
H	-3.87779	-0.35851	-2.12019
H	-3.15588	-1.81427	-1.66958
C	-2.85106	-2.59527	1.268203
H	-3.14188	-3.17101	0.381112
H	-3.72068	-2.58847	1.936134
C	-1.67579	-3.28327	1.974115
H	-1.91952	-3.67685	2.965151
H	-0.86854	-2.40759	2.296645
C	-0.91412	-4.34232	1.196996
H	0.03899	-4.56805	1.683399
H	-1.4931	-5.27228	1.134696
N	-0.60669	-3.9408	-0.21057
H	0.148323	-4.53689	-0.61041
H	-1.45281	-3.9503	-0.83054
H	4.337202	-3.45767	9.181147
H	5.953519	-4.54072	5.017943
H	4.232289	-7.87802	-3.05594
H	4.616094	-7.5434	-1.3539
H	8.534209	-0.66322	2.513548
H	6.602149	2.802587	-6.29127
H	-2.69884	-0.10064	7.291562
H	-4.8781	-4.20648	-5.84553
H	-5.65701	-9.06766	-4.20608
H	-10.0068	-5.39304	-0.81739
H	-7.5601	6.855024	-2.09348

H	-8.64696	7.667252	-0.9595
H	-5.03943	9.561229	0.73344
H	-2.7761	8.94049	-3.64684
H	1.267107	6.31689	-4.06339
H	-1.67394	1.253019	-6.28011
H	-1.48369	0.702067	-4.60253
H	-1.84521	0.641503	4.198448
H	-2.27535	1.217852	2.852095
O	-0.71743	-0.23525	-2.39309
H	-0.17917	-1.02834	-2.17624
H	-0.07229	0.517326	-2.23687
O	-0.83942	4.668548	3.517779
H	-0.45795	3.771591	3.669455
H	-0.2772	5.039181	2.807456
O	1.005263	-1.97676	-1.10676
H	1.580012	-2.75544	-1.27515
H	1.599841	-1.15792	-1.16272

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C	-1.9963	1.931576	-4.73679
H	-2.97716	1.830816	-4.25501
C	-1.43551	3.342892	-4.53734
H	-0.51689	3.480268	-5.11806
H	-2.15496	4.081939	-4.9171
C	-1.11897	3.656735	-3.06169
H	-1.98646	3.437321	-2.42623
H	-0.29807	3.010815	-2.72322
C	-0.67955	5.104038	-2.90047
O	0.249198	5.576519	-3.57103
N	-1.38003	5.860798	-2.02157
H	-2.09923	5.458183	-1.43695
H	-1.14837	6.847445	-1.90417
C	-4.7818	9.034853	-2.39561
H	-5.71053	8.677892	-2.85656
C	-4.405	8.199845	-1.16814
H	-4.24543	7.156205	-1.47147
H	-3.43555	8.543741	-0.78553
C	-5.43058	8.229506	-0.07033
N	-5.27733	7.487087	1.094641
C	-6.34584	7.725352	1.831762
H	-6.55041	7.301053	2.80533
N	-7.18815	8.588143	1.208219
H	-8.07439	8.918083	1.561472
C	-6.61779	8.917993	-0.0089
H	-7.10007	9.590481	-0.7006
C	2.31041	-6.05273	4.331443
C	3.682026	-5.37708	4.275653
C	1.2603	-5.63838	3.280788
O	4.33355	-5.21584	5.304273
C	1.026178	-4.15582	3.188709
C	0.604927	-3.22042	4.10352
N	1.248276	-3.44657	2.02006
C	0.96169	-2.14734	2.248073
N	0.573666	-1.97495	3.510481
H	2.472397	-7.13761	4.262735
H	1.553494	-6.00051	2.29162
H	0.321948	-6.15032	3.532711
H	0.322959	-3.35614	5.135658
H	1.059962	-1.36603	1.507094
H	1.663475	-3.8828	1.168575
N	4.144745	-4.98185	3.04806
H	3.623341	-5.17397	2.192892
C	5.464676	-4.39004	2.918241
H	6.072068	-4.71962	3.765744

C	5.540498	-2.85333	2.87416
O	6.603253	-2.31411	2.559208
N	4.401516	-2.18634	3.173939
C	4.233473	-0.72902	3.110786
C	4.91472	-0.15971	1.847749
C	4.64892	0.001407	4.398388
O	5.603881	0.853384	1.862763
C	4.077494	1.424344	4.509739
C	2.552414	1.574382	4.627492
O	2.05531	2.698326	4.557651
O	1.882966	0.471406	4.846188
H	3.60115	-2.7402	3.448326
H	3.157876	-0.57516	2.976778
H	4.306675	-0.60442	5.244608
H	5.742033	0.048454	4.43977
H	4.400505	2.027528	3.656485
H	4.50128	1.915536	5.396746
N	4.664149	-0.88833	0.719266
H	3.836767	-1.47447	0.723329
C	4.937149	-0.3681	-0.61452
H	4.78604	-1.22429	-1.28666
C	3.947485	0.724484	-1.02884
H	3.966234	1.531941	-0.28688
H	4.249414	1.16562	-1.98139
C	2.510319	0.189226	-1.15978
O	1.704359	0.883024	-1.83445
O	2.243966	-0.91119	-0.5707
C	6.411216	0.005822	-0.80936
O	6.761447	0.81505	-1.67428
N	7.307965	-0.74277	-0.10682
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H	8.884534	0.613065	-0.24841
C	9.470832	-1.03015	1.024556
H	9.300905	-2.1077	1.128513
H	9.1104	-0.54414	1.93585
H	10.54301	-0.85111	0.913398
C	9.380107	-1.00044	-1.50299
O	10.54605	-0.73568	-1.77742
N	8.560386	-1.7456	-2.29732
H	7.624342	-1.92346	-1.95821
C	8.90744	-2.18768	-3.6318
H	9.998312	-2.11983	-3.70252
C	8.487265	-3.6611	-3.86646
H	9.071821	-4.28719	-3.18247
H	8.776999	-3.91252	-4.89009
C	7.005885	-3.91352	-3.66265

C	6.493295	-4.23094	-2.39439
H	7.178382	-4.34796	-1.55678
C	5.120172	-4.39995	-2.1913
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C	4.234341	-4.27377	-3.26468
H	3.167626	-4.40881	-3.10687
C	4.733978	-3.97702	-4.53559
H	4.053211	-3.88057	-5.37767
C	6.103992	-3.79264	-4.73177
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C	8.361774	-1.27978	-4.76531
O	8.500407	-1.63709	-5.93872
N	7.789105	-0.11604	-4.38263
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C	7.322142	0.889682	-5.329
H	7.617127	0.547727	-6.32284
C	5.810854	1.159697	-5.24497
H	5.578231	1.488862	-4.22345
H	5.591223	2.01282	-5.90598
C	4.885947	-0.01476	-5.61802
H	5.102444	-0.84387	-4.93014
C	3.414059	0.385364	-5.42569
H	2.746145	-0.45192	-5.66245
H	3.195968	0.696493	-4.39725
H	3.145389	1.218461	-6.09019
C	5.130388	-0.51975	-7.04943
H	6.141628	-0.92099	-7.17307
H	4.421322	-1.31786	-7.30359
H	4.988702	0.289228	-7.78033
C	-5.47447	-3.38551	-5.29347
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C	-4.84434	-2.67234	-4.0857
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H	-5.5882	-2.01901	-3.61423
C	-4.27434	-3.59478	-3.00277
O	-4.56232	-4.82178	-3.03157
O	-3.54314	-3.04125	-2.11792
C	-6.79964	-4.06802	-4.96991
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N	-6.76504	-5.43608	-4.94672
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C	-7.92869	-6.20438	-4.54678
H	-8.80623	-5.79319	-5.05091
C	-8.27223	-6.23679	-3.04647
O	-9.30676	-6.77779	-2.67416
N	-7.38335	-5.62925	-2.21197
H	-6.50738	-5.26696	-2.58507

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C	-6.25829	-5.56906	-0.01696
H	-6.49182	-5.43674	1.042359
H	-5.6509	-4.71834	-0.34762
C	-5.50321	-6.88915	-0.17422
O	-5.87981	-7.91853	0.369807
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H	-4.28371	-6.08296	-1.64984
H	-3.96212	-7.72051	-1.17206
C	-8.46942	-4.39896	-0.29084
O	-8.74995	-4.30081	0.902
N	-8.88626	-3.50783	-1.22671
H	-8.66712	-3.67126	-2.20226
C	-9.83609	-2.46288	-0.8693
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C	-9.89877	-1.33191	-1.90527
H	-10.1646	-1.75202	-2.88375
H	-10.7394	-0.68517	-1.61502
C	-8.63526	-0.50456	-2.04373
C	-7.97399	-0.40789	-3.27543
H	-8.3473	-0.96638	-4.12889
C	-6.81098	0.347486	-3.41707
H	-6.29824	0.414089	-4.37217
C	-6.26913	1.013865	-2.31394
O	-5.08712	1.681176	-2.49028
H	-4.7377	2.027509	-1.62482
C	-6.92811	0.950347	-1.07809
H	-6.52107	1.484502	-0.22318
C	-8.09909	0.200538	-0.95748
H	-8.59526	0.159695	0.010061
C	3.331464	-7.87154	0.068452
H	4.185548	-7.28429	0.418287
C	2.558572	-7.12358	-1.01822
H	3.2045	-6.96356	-1.89295
H	1.709646	-7.71385	-1.38193
C	2.024369	-5.73963	-0.62109
O	1.094516	-5.26637	-1.33515
O	2.563618	-5.14401	0.366548
C	-0.81001	-3.09253	9.43263
C	-0.2599	-2.23905	8.337636
C	-0.75058	-1.88724	7.10534
N	0.971028	-1.60355	8.414694
C	1.172034	-0.91568	7.259779
N	0.146103	-1.06677	6.445972
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H	-1.78472	-3.48974	9.136351

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H	2.05229	-0.33364	7.037331
H	1.618704	-1.65336	9.187988
C	0.261875	10.02125	0.26595
H	1.159591	10.63966	0.384194
C	0.141123	9.047807	1.464958
H	1.04628	8.430299	1.533616
H	0.108281	9.651582	2.382304
C	-1.09688	8.150613	1.375606
H	-1.97371	8.771657	1.145271
H	-0.98346	7.467616	0.529566
C	-1.41628	7.311543	2.620103
H	-0.57633	6.688622	2.936474
H	-1.67141	7.94982	3.474217
N	-2.58263	6.462637	2.341378
H	-3.42734	6.977735	2.091625
C	-2.50359	5.269399	1.705833
N	-1.41805	4.501274	1.757437
H	-0.66069	4.662921	2.446832
H	-1.5477	3.530345	1.466915
N	-3.5531	4.89373	0.950542
H	-4.36452	5.503504	0.938262
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C	0.268119	9.307499	-1.0845
O	-0.76146	8.79097	-1.54351
N	1.458305	9.276181	-1.72562
H	2.300544	9.586382	-1.25211
C	1.724195	8.458175	-2.90027
H	0.871039	7.810411	-3.10344
C	3.008024	7.6673	-2.61633
O	3.934219	8.216146	-2.01113
N	3.014618	6.393507	-3.06331
H	2.131395	6.002514	-3.39388
C	4.107917	5.476039	-2.75179
H	4.969403	6.09449	-2.48867
C	3.772859	4.498036	-1.6096
H	2.970631	3.822468	-1.93087
H	4.653916	3.87078	-1.42872
C	3.372058	5.214264	-0.31549
H	4.178024	5.874841	0.022026
H	2.488927	5.84074	-0.48135
S	3.032745	4.103683	1.10706
C	1.502768	3.26975	0.545999
H	1.170476	2.63477	1.373221
H	0.726712	4.008509	0.323205
H	1.677468	2.63905	-0.32738
O	-1.47081	1.155432	5.287826

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O	-2.04023	-0.82161	4.518533
C	-3.74955	0.441861	5.687397
C	-3.74582	0.927694	7.143723
H	-4.22091	1.203365	5.053558
H	-4.30281	-0.49585	5.57593
H	-3.20189	1.87244	7.229266
H	-4.77059	1.083826	7.498675
O	-0.02361	0.745359	2.703069
O	-3.25155	3.037321	3.861186
Fe	0.056632	-0.04415	4.33781
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H	-1.58755	-1.22782	0.426588
C	-3.36748	-0.0723	0.076988
H	-4.44226	-0.2296	0.234324
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O	-3.7475	2.281167	-0.26983
O	-2.35544	1.707849	1.381461
H	-0.8573	-3.48421	-0.60954
N	-3.12951	-0.30016	-1.39391
H	-2.09289	-0.19214	-1.67431
H	-3.6888	0.355764	-1.96039
H	-3.38669	-1.27463	-1.68034
C	-3.30394	-2.43433	1.090232
H	-4.12327	-2.26495	1.805633
C	-2.39814	-3.50673	1.604251
C	-1.98602	-4.68037	0.780675
H	-1.14309	-5.20159	1.239852
H	-2.79602	-5.40922	0.632026
N	-1.54673	-4.28223	-0.60875
H	-1.01154	-5.0372	-1.06061
H	-2.35468	-3.98336	-1.21078
H	-0.15732	-3.94632	9.656919
H	1.939678	-5.86203	5.342928
H	3.707162	-8.82973	-0.30955
H	2.69729	-8.08315	0.938038
H	5.940255	-4.74494	1.999355
H	7.85904	1.82693	-5.12874
H	-3.26287	0.200166	7.806878
H	-5.6971	-2.63692	-6.06201
H	-7.80862	-7.23869	-4.88376
H	-10.8402	-2.89673	-0.75116
H	-3.98717	8.978552	-3.14509
H	-4.91646	10.09107	-2.13255
H	-0.60403	10.69386	0.263674
H	1.892355	9.096837	-3.77854

H	4.359303	4.908101	-3.65507
H	-2.12873	1.715841	-5.80426
H	-1.3334	1.169003	-4.3127
H	-2.51789	2.747838	4.434419
H	-3.05673	2.57744	3.024381
O	-0.64868	-0.30258	-2.35431
H	-0.34933	-1.23601	-2.28695
H	0.174916	0.215642	-2.10527
O	0.79609	4.898806	3.439761
H	1.021117	4.105338	3.974189
H	1.556882	4.95333	2.825336
O	0.410836	-2.61082	-1.30339
H	0.893262	-3.46153	-1.45168
H	1.088505	-1.93391	-0.98719
H	-0.86089	0.968965	2.247393
H	-3.76741	-2.74775	0.148718
H	-1.97595	-3.4031	2.599268

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C	2.286915	-1.85574	-5.79517
H	3.059044	-1.07768	-5.86462
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H	2.090209	-3.9157	-5.13946
H	3.687458	-3.512	-5.73599
C	3.317503	-2.87692	-3.70625
H	4.021855	-2.0368	-3.67194
H	2.463861	-2.59017	-3.07643
C	3.962578	-4.09646	-3.06038
O	3.74235	-5.24678	-3.4703
N	4.793814	-3.84523	-2.02393
H	4.859278	-2.90863	-1.62978
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C	9.435595	-4.7033	-1.37548
H	10.07125	-3.96713	-1.88233
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H	7.924154	-3.30065	-0.72895
H	7.910805	-4.81641	0.137389
C	9.379367	-3.41144	0.817767
N	8.76674	-2.71654	1.854747
C	9.737602	-2.26548	2.625541
H	9.61233	-1.67412	3.522447
N	10.95445	-2.63418	2.148619
H	11.84995	-2.40709	2.555269
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H	11.55828	-3.76804	0.415075
C	-6.16831	3.687588	4.960277
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O	-6.94017	1.496163	5.546019
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H	-7.07811	4.302662	4.906948
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H	-4.82514	5.314071	4.553882
H	-2.61111	3.51962	5.826902
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N	-6.53614	1.84084	3.334953
H	-6.31022	2.492531	2.589228
C	-7.04054	0.53232	2.9614
H	-7.74848	0.204298	3.726414
C	-6.03206	-0.61632	2.788901

O	-6.47253	-1.72849	2.485274
N	-4.72184	-0.33108	2.939136
C	-3.61834	-1.30085	2.821522
C	-3.85434	-2.26993	1.632132
C	-3.33522	-2.05012	4.136278
O	-3.82652	-3.48721	1.760609
C	-1.93819	-2.69115	4.194211
C	-0.74982	-1.71876	4.302005
O	0.373936	-2.11501	3.900362
O	-0.98122	-0.58278	4.839938
H	-4.48552	0.607793	3.234161
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H	-3.43547	-1.33317	4.956988
H	-4.09699	-2.82567	4.260735
H	-1.78066	-3.34902	3.335699
H	-1.88681	-3.33972	5.081085
N	-4.08411	-1.64108	0.44062
H	-3.83844	-0.65648	0.385927
C	-4.17242	-2.35275	-0.83551
H	-4.35799	-1.57165	-1.58252
C	-2.87356	-3.05726	-1.24781
H	-2.45403	-3.60342	-0.39797
H	-3.10914	-3.80861	-2.00797
C	-1.80359	-2.13459	-1.84406
O	-0.71366	-2.68787	-2.14773
O	-2.08093	-0.89884	-2.03672
C	-5.3805	-3.29984	-0.95724
O	-5.4505	-4.07783	-1.9184
N	-6.40229	-3.16648	-0.07446
H	-6.26926	-2.62111	0.777124
C	-7.51899	-4.11103	-0.10227
H	-7.11614	-5.10765	-0.31717
C	-8.24359	-4.13852	1.247332
H	-8.60406	-3.14276	1.523896
H	-7.5652	-4.47669	2.035788
H	-9.09343	-4.82192	1.177712
C	-8.52345	-3.86598	-1.24848
O	-9.42064	-4.67391	-1.46768
N	-8.33235	-2.73032	-1.97809
H	-7.5713	-2.12208	-1.70549
C	-9.05075	-2.43778	-3.20221
H	-9.93707	-3.08099	-3.19303
C	-9.51253	-0.95884	-3.25137
H	-10.2519	-0.81169	-2.45581
H	-10.0114	-0.81578	-4.21355
C	-8.37433	0.028373	-3.09051
C	-8.0032	0.500234	-1.82193

H	-8.58781	0.202685	-0.95338
C	-6.89496	1.335558	-1.65733
H	-6.61888	1.691721	-0.66853
C	-6.14147	1.721849	-2.76874
H	-5.26277	2.347371	-2.63721
C	-6.51946	1.285099	-4.04108
H	-5.9439	1.587047	-4.91247
C	-7.62446	0.447278	-4.20111
H	-7.90158	0.089074	-5.18855
C	-8.2785	-2.8112	-4.49623
O	-8.737	-2.46884	-5.59061
N	-7.14899	-3.53444	-4.33254
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H	-6.93472	-3.87028	-6.35378
C	-4.95993	-3.38176	-5.53666
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C	6.550936	4.412315	-3.42978
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H	4.693228	2.227834	-5.30224
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N	0.258168	9.39437	0.786116
H	1.003569	9.735529	1.384152
C	0.726125	8.95517	-0.51909
H	0.025232	8.235534	-0.94367
C	2.128089	8.358905	-0.32726
O	2.889327	8.849657	0.512834
N	2.417571	7.30653	-1.12161
H	1.650626	6.897076	-1.65855
C	3.634327	6.517516	-0.94989
H	4.345702	7.143012	-0.40487
C	3.379132	5.19461	-0.20289
H	2.687118	4.581114	-0.79302
H	4.319993	4.634043	-0.14385
C	2.811014	5.413631	1.203082
H	3.531034	5.94972	1.830612
H	1.900916	6.02057	1.162007
S	2.424562	3.868733	2.115577
C	1.005805	3.233477	1.14773
H	0.586088	2.402509	1.719394
H	0.239801	4.004771	1.031939
H	1.302215	2.860608	0.16562
O	-2.3548	-1.86599	5.418105

C	-2.95361	-2.95849	5.20663
O	-2.42048	-3.86959	4.484832
C	-4.32012	-3.23436	5.819415
C	-4.95159	-2.03733	6.529592
H	-4.97002	-3.61436	5.021184
H	-4.19204	-4.07639	6.513867
H	-5.11659	-1.20796	5.833933
H	-5.91861	-2.31298	6.965832
O	-1.57747	-1.91047	2.214974
O	-2.1946	0.232737	3.598531
Fe	-0.6101	-2.80094	4.129663
C	-2.50142	-0.38945	-0.00734
H	-1.82747	0.135473	0.66938
H	-1.86005	-0.97397	-0.66966
C	-3.25321	0.666482	-0.83136
H	-4.33592	0.53581	-0.73828
C	-2.94184	2.127051	-0.3903
O	-3.79275	3.026893	-0.73777
O	-1.93312	2.327811	0.304203
H	-0.9825	-3.09623	-0.68137
N	-2.9529	0.468634	-2.29011
H	-1.89119	0.419581	-2.49714
H	-3.43214	1.179606	-2.86121
H	-3.2956	-0.48696	-2.55185
C	-3.46615	-1.2791	0.789483
H	-4.01373	-0.64044	1.493352
C	-2.77588	-2.39265	1.59674
C	-2.48884	-3.67785	0.814625
H	-1.79468	-4.29634	1.384684
H	-3.42544	-4.22812	0.704443
N	-1.93904	-3.54208	-0.58011
H	-1.88795	-4.49047	-0.97442
H	-2.58159	-3.03056	-1.23909
H	1.51442	-7.19664	8.290137
H	3.257819	-7.57301	3.469302
H	5.105102	-7.62112	-3.2245
H	3.954497	-7.75123	-1.88419
H	6.544845	-4.28606	0.872161
H	7.856886	4.359652	-3.50565
H	-4.30159	-1.66861	7.328614
H	-4.85084	-2.07689	-6.88127
H	-6.80749	-6.77028	-5.99543
H	-10.2931	-2.80854	-1.90738
H	-4.54315	9.106184	-0.9656
H	-5.52776	9.902581	0.267605
H	-2.05445	9.958559	2.85611
H	0.798325	9.812033	-1.20362

H	4.058264	6.301046	-1.93746
H	0.148442	3.074479	-5.96952
H	0.266194	2.17266	-4.44635
H	-2.4446	-0.31105	4.375255
H	-1.27213	0.525672	3.823915
O	-0.42669	-0.02108	-2.9026
H	-0.22062	-0.94435	-2.64455
H	0.303049	0.525646	-2.46889
O	0.026671	3.607848	4.401375
H	0.203813	2.64166	4.464477
H	0.799222	3.945774	3.903025
O	0.393854	-2.43704	-1.46374
H	0.986895	-3.14264	-1.84464
H	1.017141	-1.69313	-1.21191
H	-1.80182	-1.01655	2.635769
H	-4.21664	-1.7307	0.125984
H	-3.46555	-2.72786	2.383323

Model 2 structures:

⁵Re_B

C	-2.58559	-3.25979	5.185932
H	-2.14366	-2.80753	4.289227
C	-1.47472	-3.64232	6.169501
H	-1.90848	-3.89286	7.144703
H	-0.98137	-4.54754	5.809683
C	-0.42981	-2.53403	6.351205
H	-0.88527	-1.62438	6.764461
H	0.324286	-2.86042	7.080538
C	0.299166	-2.19615	5.048072
O	0.39928	-3.0381	4.141597
N	0.834488	-0.96462	4.950951
H	0.658724	-0.27725	5.669806
H	1.182593	-0.64191	4.030268
C	-3.4122	-4.4514	4.706963
O	-3.05918	-5.62331	4.897382
N	-4.54365	-4.13569	4.02953
H	-4.76406	-3.15585	3.870711
C	-5.37489	-5.16416	3.414785
H	-6.41142	-4.8069	3.412479
C	-4.93977	-5.55327	1.991375
H	-3.86168	-5.75778	1.999445
H	-5.43409	-6.50193	1.735821
C	-5.28638	-4.51641	0.91425
H	-4.85494	-3.53594	1.148134
H	-6.37758	-4.38684	0.888607
C	-4.80629	-4.95914	-0.47943
H	-3.7562	-4.70133	-0.63218
H	-4.88596	-6.05192	-0.56477
N	-5.59606	-4.37826	-1.56608
H	-6.52651	-4.77661	-1.71388
C	-5.12198	-3.66295	-2.60428
N	-3.95221	-3.0263	-2.56445
H	-3.57788	-2.62542	-1.67946
H	-3.6318	-2.62148	-3.45135
N	-5.86662	-3.60947	-3.72707
H	-6.6859	-4.20118	-3.79082
H	-5.74242	-2.81897	-4.36689
C	0.439325	-8.17975	0.118102
H	1.46922	-8.52255	0.279081
H	0.45228	-7.50367	-0.74603
C	-0.10602	-7.49813	1.334408
N	0.464764	-6.34427	1.844042
C	-0.25529	-6.02476	2.910542
H	-0.09871	-5.15701	3.539653

N	-1.25722	-6.91063	3.118024
H	-1.98192	-6.78211	3.82471
C	-1.17945	-7.85687	2.116152
H	-1.86465	-8.6892	2.05625
C	6.037314	5.189865	-5.05979
C	5.880519	5.612637	-3.59871
C	4.937347	4.274899	-5.64726
O	6.810982	5.463478	-2.79972
C	4.686021	3.032684	-4.84316
C	5.391248	1.866234	-4.65917
N	3.582024	2.933603	-4.02206
C	3.638137	1.760218	-3.3805
N	4.724438	1.075478	-3.74241
H	6.10387	6.098182	-5.67376
H	3.994175	4.82535	-5.74462
H	5.237996	4.008444	-6.66759
H	6.324029	1.55229	-5.10287
H	2.910359	1.440198	-2.65422
H	2.880114	3.712129	-3.84163
N	4.720164	6.231325	-3.23948
H	3.853739	6.062583	-3.74562
C	4.564032	6.791665	-1.90196
H	5.539907	7.172555	-1.58728
C	4.029688	5.799858	-0.85382
O	2.96499	6.034021	-0.27549
N	4.820715	4.722513	-0.65243
C	4.49987	3.468274	0.049574
C	3.429184	3.628508	1.162522
C	5.804167	2.921494	0.658245
O	3.746296	3.867167	2.326577
C	5.727953	1.495469	1.217424
C	5.71261	0.339399	0.219494
O	5.671264	-0.83517	0.646031
O	5.811054	0.64948	-1.02883
H	5.678091	4.708416	-1.2033
H	4.115411	2.757722	-0.6926
H	6.589563	2.963468	-0.10498
H	6.085039	3.596447	1.471936
H	4.860309	1.372769	1.876478
H	6.601384	1.312858	1.856021
N	2.154285	3.377891	0.773956
H	1.922739	3.331432	-0.21908
C	1.045321	3.316715	1.722284
H	0.138825	3.280445	1.107397
C	1.089651	2.042333	2.565953
H	2.016937	2.011312	3.143432
H	0.269647	2.077159	3.292779

C	0.954881	0.753523	1.753334
O	0.38615	0.779988	0.631617
O	1.420403	-0.29756	2.310884
C	0.915388	4.56247	2.625163
O	0.458857	4.468518	3.769767
N	1.197671	5.76211	2.049999
H	1.749283	5.754767	1.19141
C	1.28843	6.971415	2.872347
H	1.767621	6.700976	3.822057
C	2.135805	8.040106	2.175563
H	3.159263	7.683387	2.032217
H	2.144895	8.939287	2.795147
H	1.722815	8.292445	1.192778
C	-0.06706	7.570041	3.304872
O	-0.08873	8.559098	4.03039
N	-1.19351	6.931488	2.875268
H	-1.08362	6.103958	2.305223
C	-2.50456	7.232679	3.421458
H	-2.4622	8.274402	3.75521
C	-3.61725	7.107185	2.353502
H	-3.41702	7.84709	1.570227
H	-4.55396	7.381448	2.8465
C	-3.73036	5.723492	1.746439
C	-3.03993	5.389557	0.571359
H	-2.45813	6.153812	0.059463
C	-3.09585	4.094297	0.049019
H	-2.55764	3.849651	-0.86316
C	-3.84993	3.110204	0.690927
H	-3.87029	2.102299	0.288826
C	-4.56195	3.437099	1.847846
H	-5.16525	2.681452	2.34449
C	-4.5024	4.730144	2.370243
H	-5.04624	4.979169	3.277084
C	-2.87274	6.425462	4.69411
O	-3.9886	6.579182	5.198215
N	-1.91256	5.616468	5.198496
H	-1.04085	5.484921	4.690028
C	-2.05484	4.925894	6.472609
H	-3.02766	5.211249	6.877201
C	-1.90743	3.400965	6.362616
H	-0.9113	3.17953	5.956122
H	-1.92858	2.991964	7.385064
C	-2.96339	2.679058	5.504766
H	-2.89434	3.078491	4.484286
C	-2.64901	1.176235	5.440902
H	-3.34466	0.648884	4.776764
H	-1.63705	0.991573	5.059524

H	-2.71857	0.719459	6.439591
C	-4.39639	2.916407	6.006199
H	-5.11844	2.35243	5.401134
H	-4.50908	2.590294	7.050261
H	-4.67539	3.973303	5.948908
C	-6.46405	1.76067	-2.88143
H	-6.09436	2.261718	-3.78403
C	-5.40309	0.744842	-2.41595
H	-5.51982	0.522137	-1.35291
H	-5.50417	-0.2025	-2.95917
C	-3.95803	1.205631	-2.66342
O	-3.70494	1.850556	-3.7336
O	-3.09766	0.879663	-1.80538
C	-7.83036	1.16451	-3.18497
O	-8.86283	1.528661	-2.6143
N	-7.85732	0.197192	-4.1564
H	-6.98806	-0.17584	-4.54369
C	-9.11045	-0.29536	-4.69788
H	-9.8005	0.541675	-4.85294
C	-9.88346	-1.31402	-3.85461
O	-10.9069	-1.83707	-4.29859
N	-9.39016	-1.56772	-2.61643
H	-8.51267	-1.13546	-2.36083
C	-10.1253	-2.32316	-1.61452
H	-11.1183	-2.49248	-2.04475
C	-9.45414	-3.6692	-1.30749
H	-10.0825	-4.21522	-0.59547
H	-8.49158	-3.50496	-0.81331
C	-9.18831	-4.54854	-2.52273
O	-8.16635	-5.25127	-2.58771
N	-10.1256	-4.58575	-3.49898
H	-10.7595	-3.80549	-3.66325
H	-9.89301	-5.15007	-4.30722
C	-10.3752	-1.53248	-0.30603
O	-10.7178	-2.14072	0.702557
N	-10.233	-0.18623	-0.39318
H	-9.97865	0.242327	-1.27893
C	-10.5374	0.713423	0.71314
H	-10.8623	0.090835	1.5495
C	-9.33927	1.602771	1.11057
H	-8.94108	2.070624	0.201495
H	-9.72887	2.416082	1.735439
C	-8.2412	0.879272	1.85997
C	-7.19094	0.23382	1.190957
H	-7.1589	0.269903	0.105909
C	-6.17327	-0.43035	1.876741
H	-5.33974	-0.8893	1.350566

C	-6.21014	-0.4617	3.2723
O	-5.19614	-1.13233	3.931568
H	-5.23249	-0.90201	4.87384
C	-7.24432	0.168258	3.967113
H	-7.26858	0.143179	5.054949
C	-8.24442	0.834531	3.259356
H	-9.0376	1.332869	3.811703
C	0.229003	5.726548	-2.12156
H	0.751835	6.367237	-1.40281
H	-0.61782	5.257682	-1.61399
C	1.220443	4.683211	-2.61812
O	1.990561	5.021003	-3.57061
O	1.254826	3.544717	-2.05407
C	10.33676	-0.62622	-5.28683
C	9.271618	-0.45006	-4.25561
C	7.914677	-0.62597	-4.29462
N	9.532071	-0.03542	-2.95582
C	8.368029	0.032739	-2.27021
N	7.365058	-0.31609	-3.06254
H	11.09027	-1.3603	-4.97455
H	9.893271	-0.98399	-6.21985
H	7.297848	-0.98164	-5.10487
H	8.313246	0.250112	-1.21278
H	10.44164	0.15976	-2.56151
C	7.559132	-6.58598	-0.97826
H	8.342815	-6.51762	-1.7431
C	6.597762	-5.38378	-1.11973
H	7.141957	-4.46048	-0.87268
H	6.285729	-5.28128	-2.1645
C	5.349274	-5.49033	-0.23165
H	4.749337	-6.35149	-0.56086
H	5.626989	-5.68232	0.811329
C	4.512531	-4.21343	-0.32398
H	5.09716	-3.36969	0.052475
H	4.264472	-4.00432	-1.36958
N	3.285335	-4.32754	0.471472
H	2.823799	-5.22917	0.499635
C	2.608678	-3.30836	1.023553
N	3.097435	-2.08295	1.117405
H	4.026951	-1.81688	0.796995
H	2.481083	-1.34525	1.511006
N	1.344626	-3.54522	1.480499
H	1.065127	-4.53492	1.483977
H	1.077833	-3.0588	2.346102
C	8.181554	-6.63224	0.410049
O	7.703653	-7.2733	1.33991
N	9.31167	-5.85677	0.555627

H	9.52355	-5.17887	-0.1673
C	9.792671	-5.49449	1.869835
H	9.180677	-6.03054	2.601333
C	9.728849	-3.97355	2.054541
O	9.797834	-3.22896	1.069882
N	9.646208	-3.54257	3.332773
H	9.531976	-4.24199	4.053844
C	9.647236	-2.13332	3.735905
H	10.09484	-1.56622	2.918068
C	8.254437	-1.56067	4.041348
H	8.379397	-0.5	4.289681
H	7.654015	-1.59574	3.127714
C	7.530987	-2.26512	5.192625
H	7.341097	-3.32007	4.956562
H	8.143874	-2.24059	6.102733
S	5.946361	-1.48503	5.689459
C	4.891909	-1.86844	4.24471
H	3.899144	-1.47087	4.471767
H	5.252998	-1.39688	3.327345
H	4.807538	-2.95031	4.099024
O	3.857671	-0.83088	-1.95557
O	8.590985	-0.67571	0.773894
Fe	5.35598	-0.52585	-2.52448
C	-2.36006	0.102942	-7.00965
H	-2.31698	0.450629	-8.0508
H	-1.94508	-0.91015	-6.99701
C	-3.8431	-0.05314	-6.63797
H	-4.39598	-0.32871	-7.54394
C	-4.23014	-1.12348	-5.57208
O	-3.35587	-1.90993	-5.18247
O	-5.46294	-1.08334	-5.23791
N	-4.48556	1.229074	-6.15257
H	-4.15863	1.505088	-5.13651
H	-5.48794	1.034017	-6.07097
H	-4.33818	2.015424	-6.78995
C	-1.48164	1.043543	-6.16334
H	-1.97804	2.019947	-6.06176
H	-0.57115	1.24454	-6.74299
C	-1.08904	0.538917	-4.76776
H	-0.37234	-0.28656	-4.84433
H	-1.96327	0.144892	-4.24866
C	-0.49656	1.68473	-3.94775
H	0.496565	1.975103	-4.29989
H	-1.15151	2.557471	-3.99713
N	-0.37164	1.333832	-2.50357
H	10.83736	-5.80885	2.010697
H	10.30064	-2.04062	4.612382

H	-0.16598	-9.05244	-0.14701
H	7.019851	-7.52574	-1.13117
H	-5.32355	-6.04294	4.062454
H	-3.24845	-2.49832	5.617221
H	10.8579	0.315043	-5.50371
H	7.005039	4.685026	-5.11264
H	-0.12029	6.352893	-2.94719
H	3.851149	7.616494	-1.94502
H	-1.28842	5.302685	7.164129
H	-6.61211	2.535602	-2.12561
H	-8.91888	-0.75346	-5.67172
H	-11.3771	1.357329	0.420343
H	9.092772	-1.51523	0.797483
H	7.658319	-0.95624	0.822449
C	4.533574	-2.91054	-3.9775
O	4.581647	-4.10397	-3.72175
O	5.480592	-2.06785	-3.55814
C	3.424693	-2.31583	-4.82677
H	3.771685	-1.44165	-5.38417
H	2.604295	-1.99908	-4.17169
H	3.041022	-3.07936	-5.50788
H	0.099316	2.120343	-2.01557
H	-1.32555	1.176428	-2.1089
H	0.209598	0.463495	-2.38797
O	1.058714	-1.03211	-2.452
H	1.993856	-0.95472	-2.17472
H	0.588102	-1.45345	-1.68556
O	-3.10488	-1.59825	-0.34009
H	-3.18745	-0.7038	-0.7383
H	-2.13104	-1.69014	-0.18506
O	-0.32296	-1.66094	-0.19426
H	0.119553	-2.32888	0.371149
H	-0.04849	-0.76781	0.187516

⁵TS1_{B,C3}

C	-5.46435	1.576448	4.879669
H	-4.57762	1.611336	4.23431
C	-5.02781	1.485396	6.347984
H	-5.82305	1.866803	6.998654
H	-4.88823	0.434485	6.610554
C	-3.73262	2.254514	6.635273
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H	-3.56016	2.303055	7.719217
C	-2.49494	1.612145	6.000888
O	-2.54829	0.498044	5.458537
N	-1.33896	2.298497	6.10108
H	-1.34077	3.255345	6.425347
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C	-6.29322	0.382373	4.399848
O	-6.49918	-0.61651	5.099793
N	-6.74564	0.480981	3.123378
H	-6.47534	1.290732	2.571568
C	-7.2481	-0.67665	2.382181
H	-7.7245	-0.29771	1.473458
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H	-5.79942	-2.15883	2.964571
H	-6.58806	-2.48567	1.425701
C	-4.93608	-1.055	1.320886
H	-4.66245	-0.13579	1.852464
H	-5.18674	-0.75268	0.298571
C	-3.67076	-1.91699	1.30018
H	-2.81172	-1.28606	1.07636
H	-3.50151	-2.35385	2.294039
N	-3.68447	-3.01253	0.322445
H	-4.3016	-3.81137	0.487003
C	-2.72339	-3.22159	-0.59296
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H	-2.24281	-1.26465	-1.02826
H	-1.17901	-2.51823	-1.64834
N	-2.56161	-4.45241	-1.10808
H	-3.20411	-5.18616	-0.82874
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C	-2.92785	-6.01233	5.532379
H	-2.11157	-6.01967	6.26458
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C	-3.59919	-4.67512	5.482667
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H	-3.58537	-1.47683	5.12995
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C	8.105048	2.104204	-3.99951
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O	8.199815	2.431845	-1.61416
C	5.942422	0.765367	-4.03851
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C	4.222841	0.408605	-2.71098
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H	7.302265	1.001883	-5.67065
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O	4.45401	3.777259	2.380691
C	3.979132	0.109375	1.698536
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O	2.082861	-0.80924	0.500773
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H	3.703006	2.045505	-0.31242
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N	2.48474	3.560575	1.242076
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C	1.412551	3.77876	3.480445
H	2.340355	3.436871	3.942585
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H	5.366613	7.342149	0.500698
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H	4.168176	7.856505	-0.70084
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H	0.366166	5.657242	-3.43803
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H	0.155536	7.829452	2.694142
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C	-2.25579	6.499749	3.7667
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C	-6.07017	-5.43122	-0.90082
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C	-8.82673	0.572186	-3.77494
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C	-6.83951	0.984399	-2.24147
H	-6.21916	0.431357	-2.94184
C	-6.25259	1.515473	-1.0928
H	-5.19139	1.382937	-0.90213
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O	-6.44835	2.715256	0.955539
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C	-8.40429	2.433548	-0.46122
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H	-10.0226	2.06983	-1.82075
C	3.767665	6.151082	-4.25039
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C	3.438019	4.664145	-4.16114
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C	9.44454	-4.89071	-1.32633
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C	7.229799	-3.63788	-1.95332
N	7.751342	-3.73701	0.165435
C	6.591043	-3.05433	0.027062
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H	9.469703	-5.83091	-0.76079
H	9.540544	-5.13781	-2.38732
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H	6.03484	-2.65452	0.86129
H	8.068261	-4.08499	1.067086
C	2.009157	-7.05568	0.871632
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C	1.36612	-5.66576	0.705403
H	1.998531	-5.02338	0.083184
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C	0.344501	-3.63148	1.840662
H	1.025018	-2.91215	1.378912
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N	-0.1263	-3.11076	3.124317
H	-0.69965	-3.73848	3.680398
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H	0.346224	0.119135	3.249058
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C	6.186704	-6.24387	5.102378
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C	5.286054	-5.20703	5.79423
H	5.725579	-4.97315	6.771511
H	5.301708	-4.28344	5.206468
C	3.845446	-5.68749	5.993167
H	3.366854	-5.91279	5.031967
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O	2.410302	-2.36269	-2.27675
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H	0.105426	-0.38409	-3.9602
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N	0.628442	2.237462	-3.42785
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H	6.11397	-3.40023	3.179737
H	4.639903	-3.23634	2.814367
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O	3.940839	-4.6373	-1.31957
O	4.477871	-4.00831	-3.35796
C	4.155571	-6.37283	-2.98386
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H	3.107548	-6.67086	-3.10889
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C	-0.72709	-6.97984	4.425804
N	-0.3548	-5.64707	4.469004
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C	5.206523	3.170746	-4.5236
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O	5.463555	0.168251	-0.57781
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H	5.72614	3.061866	1.875107
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H	5.706425	0.719668	2.216857
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H	-0.05852	3.515798	2.135824
C	1.056732	2.808244	3.79492
H	2.062474	2.872615	4.216534
H	0.355486	3.117367	4.578014
C	0.754112	1.364857	3.376561

O	-0.06593	1.207662	2.432004
O	1.34807	0.439053	4.018537
C	0.820542	5.226416	3.014709
O	0.325874	5.530274	4.106654
N	1.169916	6.160971	2.094211
H	1.665777	5.871057	1.250836
C	1.226053	7.572156	2.476042
H	1.626286	7.632115	3.494266
C	2.136775	8.361095	1.530755
H	3.163413	7.987422	1.591737
H	2.120048	9.414227	1.821465
H	1.799726	8.274173	0.492266
C	-0.15417	8.254214	2.581877
O	-0.25129	9.368002	3.085822
N	-1.21218	7.541256	2.103214
H	-1.02083	6.647366	1.669176
C	-2.59173	7.958988	2.265073
H	-2.54715	9.004858	2.589193
C	-3.38072	7.890694	0.935718
H	-2.96598	8.652242	0.265648
H	-4.41258	8.168657	1.166639
C	-3.33686	6.53591	0.257323
C	-2.34956	6.244457	-0.69635
H	-1.63053	7.01426	-0.96955
C	-2.27991	4.99016	-1.30966
H	-1.5021	4.797243	-2.0458
C	-3.21042	4.002465	-0.97658
H	-3.16624	3.02643	-1.45293
C	-4.2026	4.281012	-0.03174
H	-4.93529	3.519244	0.225774
C	-4.26582	5.533917	0.581325
H	-5.03479	5.747494	1.318446
C	-3.33369	7.2031	3.397242
O	-4.56275	7.269195	3.481179
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C	-3.07824	5.868219	5.457226
H	-4.12266	6.171789	5.553508
C	-2.93083	4.339523	5.393827
H	-1.8622	4.112089	5.282222
H	-3.24098	3.92808	6.367734
C	-3.71513	3.631387	4.273135
H	-3.4302	4.092521	3.317765
C	-3.32374	2.14722	4.209024
H	-3.90041	1.615738	3.443568
H	-2.26442	2.011954	3.964502
H	-3.51406	1.652957	5.174307

C	-5.23477	3.799311	4.431961
H	-5.76738	3.274433	3.627058
H	-5.57986	3.393139	5.395016
H	-5.53277	4.850972	4.377689
C	-5.54288	0.279676	-4.78245
H	-5.06657	0.08291	-5.7443
C	-4.54898	-0.03776	-3.65055
H	-4.96226	0.242129	-2.67769
H	-4.35313	-1.11919	-3.6185
C	-3.18841	0.662851	-3.82185
O	-2.72696	0.82446	-4.99261
O	-2.59138	1.016919	-2.76632
C	-6.84092	-0.5042	-4.6791
O	-7.79347	-0.10569	-3.98154
N	-6.89746	-1.66547	-5.37606
H	-6.04867	-2.00662	-5.84305
C	-8.13776	-2.38595	-5.62274
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C	-8.7376	-3.22427	-4.48691
O	-9.40653	-4.22892	-4.74557
N	-8.54626	-2.75576	-3.2271
H	-8.05832	-1.86774	-3.14225
C	-9.31545	-3.24047	-2.0883
H	-10.112	-3.87015	-2.50002
C	-8.46394	-4.06428	-1.11131
H	-9.09701	-4.34086	-0.26033
H	-7.65209	-3.44887	-0.71107
C	-7.82721	-5.33148	-1.66442
O	-6.78267	-5.7831	-1.16028
N	-8.45827	-5.9843	-2.66416
H	-9.08426	-5.50638	-3.31511
H	-7.99545	-6.81616	-3.00979
C	-10.0533	-2.11312	-1.3214
O	-10.5449	-2.36172	-0.22564
N	-10.1529	-0.91632	-1.95622
H	-9.67649	-0.77068	-2.83873
C	-10.8376	0.23145	-1.37566
H	-11.2952	-0.11282	-0.44578
C	-9.89394	1.426748	-1.12002
H	-9.3765	1.67504	-2.05503
H	-10.5216	2.290836	-0.86732
C	-8.88632	1.183815	-0.01845
C	-7.60295	0.694985	-0.29986
H	-7.31531	0.530096	-1.3356
C	-6.68338	0.444013	0.720195
H	-5.67865	0.09654	0.500244
C	-7.04892	0.676228	2.047099

O	-6.12429	0.383444	3.039245
H	-6.25416	0.995773	3.782066
C	-8.31804	1.171239	2.351779
H	-8.59936	1.354879	3.386248
C	-9.22112	1.423825	1.320491
H	-10.2062	1.813975	1.566281
C	0.905739	6.893404	-3.32956
H	1.122766	7.085437	-2.27139
H	-0.17132	6.98949	-3.48664
C	1.379362	5.479291	-3.6432
O	2.606671	5.355176	-3.9875
O	0.561033	4.537733	-3.5163
C	10.87671	-1.35001	-3.55858
C	9.564101	-1.02394	-2.92427
C	8.340196	-0.70235	-3.45595
N	9.377524	-0.96385	-1.55074
C	8.091481	-0.62922	-1.3069
N	7.430692	-0.45738	-2.44178
H	11.26197	-2.3237	-3.23008
H	10.76671	-1.38557	-4.64597
H	8.052303	-0.64368	-4.49535
H	7.673697	-0.54454	-0.31488
H	9.982824	-1.33448	-0.82275
C	5.46286	-6.52621	-0.73366
H	5.495274	-6.79811	-1.79823
C	4.314255	-5.52801	-0.50724
H	4.516648	-4.58543	-1.02958
H	3.41174	-5.94298	-0.97551
C	4.022143	-5.2577	0.974287
H	3.697243	-6.19211	1.455028
H	4.933042	-4.93948	1.497831
C	2.947912	-4.18041	1.148295
H	3.35348	-3.21553	0.840364
H	2.085056	-4.39994	0.499833
N	2.517633	-4.09776	2.545499
H	2.247732	-4.98009	2.966829
C	1.918437	-3.01738	3.114828
N	2.033155	-1.79221	2.582397
H	2.828774	-1.5614	1.974974
H	1.688592	-0.98421	3.156744
N	1.218504	-3.21784	4.228575
H	0.869714	-4.16835	4.422342
H	0.678977	-2.45817	4.65642
C	6.869882	-6.06955	-0.35395
O	7.641742	-6.82273	0.254452
N	7.256697	-4.83475	-0.77192
H	6.618996	-4.22079	-1.2874

C	8.664685	-4.44988	-0.76616
H	9.268821	-5.31137	-1.07676
C	9.201979	-3.94357	0.585579
O	9.596175	-2.76897	0.731267
N	9.244839	-4.86348	1.561001
H	8.848056	-5.7778	1.332054
C	9.807506	-4.59577	2.884919
H	10.62411	-3.88072	2.750762
C	8.80535	-4.03486	3.907208
H	9.361599	-3.77181	4.815134
H	8.382698	-3.10511	3.513329
C	7.687388	-5.01501	4.274937
H	7.091945	-5.28965	3.395368
H	8.111017	-5.94412	4.67573
S	6.564284	-4.41437	5.59694
C	5.614705	-3.1304	4.704189
H	4.968496	-2.65266	5.445576
H	6.262113	-2.36934	4.260623
H	4.981518	-3.57894	3.931995
O	3.443021	-1.00435	-2.04952
O	7.381718	-1.33543	1.931597
Fe	5.214868	-0.55801	-2.42904
C	-0.93162	-2.16663	-5.5273
H	-0.90693	-3.00716	-4.84181
H	3.470574	-1.35263	-1.13023
C	-2.02833	-2.20832	-6.53214
H	-1.7281	-2.75457	-7.44482
C	-3.3607	-2.89801	-6.0401
O	-3.24072	-3.83487	-5.22472
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H	-3.39569	-1.01288	-7.41369
H	-1.82362	-0.41589	-7.68288
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H	0.13996	-0.5048	-6.36749
H	1.156899	-1.76505	-5.70685
C	0.357947	-0.41067	-4.19226
H	1.258696	-0.72483	-3.65412
H	-0.49066	-0.63961	-3.53938
C	0.393488	1.102588	-4.43696
H	1.373553	1.434294	-4.79218
H	-0.36764	1.389494	-5.16446
N	0.06941	1.860026	-3.19189
H	8.790555	-3.64481	-1.49013
H	10.23752	-5.53642	3.247587
H	-0.22315	-9.05075	4.159098

H	5.286201	-7.45204	-0.17775
H	-6.79398	-4.29404	3.96901
H	-4.69203	-0.77423	5.764228
H	11.64004	-0.5977	-3.32367
H	7.637497	4.653617	-4.24209
H	1.444269	7.633015	-3.929
H	3.966086	7.443706	-1.53414
H	-2.54129	6.239594	6.339792
H	-5.81101	1.340024	-4.74611
H	-7.97892	-3.06407	-6.46255
H	-11.6405	0.545417	-2.05548
H	8.216914	-1.74821	1.633437
H	6.684536	-1.88951	1.547177
C	5.664108	-2.8391	-3.54788
O	5.755111	-2.85425	-2.2805
O	5.432411	-1.74604	-4.1538
C	5.79152	-4.11606	-4.34882
H	6.426936	-4.84051	-3.83262
H	6.18939	-3.90592	-5.34422
H	4.794834	-4.55764	-4.46948
H	0.280961	2.8842	-3.31701
H	-0.94864	1.71323	-2.99017
H	0.621059	1.502794	-2.37333
O	1.632686	0.892286	-1.07355
H	2.260421	0.222543	-1.43796
H	1.076145	0.382091	-0.42653
O	-1.98177	-1.17348	-1.1429
H	-2.25753	-0.32588	-1.55461
H	-1.25504	-0.9789	-0.50357
O	0.075414	-0.6033	0.601262
H	0.616466	-1.30022	1.016989
H	-0.08725	0.043039	1.367617

⁵TS2_{B,C3}

C	-5.41712	0.55378	5.302027
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H	-5.499	0.121514	7.425811
H	-4.55999	-1.02829	6.500211
C	-3.49747	0.786796	6.972614
H	-3.67049	1.871392	7.01047
H	-3.17059	0.496376	7.980436
C	-2.34225	0.504486	6.008023
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N	-1.1985	1.191553	6.210736
H	-1.17688	1.961684	6.864403
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C	-6.2469	-0.4934	4.556913
O	-6.54861	-1.58886	5.043471
N	-6.62416	-0.12128	3.305682
H	-6.32986	0.788267	2.973082
C	-7.43954	-0.94848	2.418402
H	-8.07755	-0.27206	1.838614
C	-6.63632	-1.84323	1.456055
H	-6.15303	-2.63943	2.038144
H	-7.3588	-2.33733	0.795324
C	-5.5843	-1.07274	0.621407
H	-5.81387	-0.00104	0.615988
H	-5.62845	-1.37075	-0.43197
C	-4.13682	-1.24422	1.11369
H	-3.5173	-0.4113	0.781615
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H	-3.8369	-3.38267	1.030673
C	-2.46031	-2.5812	-0.17172
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H	-2.55593	-0.7155	-1.07469
H	-1.1563	-1.706	-1.41539
N	-1.8499	-3.76404	-0.34489
H	-2.23643	-4.58988	0.101206
H	-1.13531	-3.8262	-1.06774
C	-2.61571	-6.61814	3.777354
H	-1.65167	-6.68011	4.294449
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C	-3.34551	-5.36681	4.154445
N	-2.70635	-4.14204	4.230635
C	-3.64644	-3.26214	4.542877
H	-3.48704	-2.20557	4.711209
N	-4.85878	-3.85303	4.670429

H	-5.7104	-3.33615	4.884865
C	-4.68414	-5.19892	4.427346
H	-5.50297	-5.90166	4.462354
C	7.798006	4.200836	-3.26345
C	7.179348	4.744327	-1.97226
C	6.843	3.43298	-4.2135
O	7.639449	4.431075	-0.86943
C	6.094471	2.335491	-3.52098
C	6.403927	1.036484	-3.18897
N	4.864726	2.583152	-2.94163
C	4.483512	1.472397	-2.29105
N	5.387349	0.504535	-2.41972
H	8.243685	5.038121	-3.81617
H	6.119975	4.120524	-4.66702
H	7.44163	3.018754	-5.03236
H	7.278332	0.454857	-3.4404
H	3.561864	1.388109	-1.7408
H	4.304007	3.463018	-3.10792
N	6.160188	5.639485	-2.10645
H	5.53484	5.6002	-2.91621
C	5.594548	6.284563	-0.92778
H	6.405169	6.439566	-0.21044
C	4.45666	5.491526	-0.2714
O	3.293193	5.904188	-0.30037
N	4.82453	4.327968	0.315673
C	3.850529	3.374314	0.845289
C	2.89601	4.082605	1.842104
C	4.593102	2.229112	1.561539
O	3.322147	4.622192	2.857127
C	3.718542	0.987569	1.863376
C	3.563924	0.052991	0.659353
O	2.431291	-0.11177	0.109817
O	4.627687	-0.52533	0.269259
H	5.808618	4.073007	0.268188
H	3.259976	2.98272	0.008202
H	5.451119	1.910214	0.957757
H	4.981091	2.637014	2.500826
H	2.737173	1.276185	2.252508
H	4.222707	0.401523	2.640532
N	1.582234	4.024815	1.499362
H	1.323729	3.525396	0.64867
C	0.5113	4.563056	2.329686
H	-0.41197	4.403384	1.760114
C	0.325262	3.78066	3.640999
H	1.275922	3.675092	4.166029
H	-0.36905	4.347941	4.269055
C	-0.28151	2.417345	3.30507

O	-1.33813	2.437314	2.609926
O	0.312876	1.37087	3.716066
C	0.553599	6.083871	2.548842
O	-0.11417	6.5935	3.455543
N	1.198904	6.830956	1.618582
H	1.843829	6.383623	0.966968
C	1.259375	8.282897	1.780501
H	1.539988	8.510757	2.814421
C	2.290089	8.896406	0.827201
H	3.288067	8.498321	1.031856
H	2.299949	9.980415	0.966551
H	2.043612	8.676634	-0.21727
C	-0.10305	8.984212	1.600176
O	-0.26644	10.12053	2.02894
N	-1.06252	8.281991	0.929132
H	-0.82218	7.367453	0.569209
C	-2.41532	8.774669	0.748504
H	-2.38734	9.823379	1.064163
C	-2.86612	8.730826	-0.73275
H	-2.23571	9.432852	-1.28984
H	-3.89269	9.106032	-0.75713
C	-2.79471	7.360764	-1.37822
C	-1.66265	6.973055	-2.10959
H	-0.83716	7.672588	-2.22525
C	-1.58172	5.714165	-2.71168
H	-0.68919	5.457693	-3.27709
C	-2.64479	4.817134	-2.58362
H	-2.6003	3.837416	-3.05535
C	-3.7807	5.185081	-1.85544
H	-4.61165	4.490135	-1.75619
C	-3.85502	6.446317	-1.26014
H	-4.73925	6.735027	-0.6991
C	-3.46441	8.095127	1.662338
O	-4.66411	8.301328	1.461843
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H	-1.9832	7.250772	2.814546
C	-3.85512	6.740016	3.685325
H	-4.80352	7.281141	3.650593
C	-4.07896	5.225403	3.526333
H	-3.10388	4.719726	3.539897
H	-4.62236	4.878879	4.420633
C	-4.84984	4.776293	2.269297
H	-4.29066	5.128664	1.392087
C	-4.89021	3.240027	2.20271
H	-5.36462	2.898796	1.273643
H	-3.88256	2.813016	2.260746
H	-5.47359	2.846619	3.051094

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H	-6.80619	4.963965	1.329218
H	-6.84637	5.104127	3.094845
H	-6.24241	6.453119	2.098756
C	-3.28016	-1.86078	-5.73499
H	-2.41021	-2.09588	-6.35959
C	-2.78874	-1.22468	-4.42219
H	-3.62855	-0.81205	-3.86063
H	-2.327	-1.99442	-3.79228
C	-1.71294	-0.14353	-4.63196
O	-0.77219	-0.3968	-5.4485
O	-1.79498	0.912564	-3.94147
C	-4.10532	-3.12805	-5.54239
O	-5.28023	-3.22662	-5.90207
N	-3.44961	-4.1768	-4.94911
H	-2.50529	-4.0537	-4.5848
C	-4.00034	-5.5177	-4.96969
H	-4.5858	-5.6471	-5.88745
C	-4.92327	-5.91037	-3.81425
O	-5.16268	-7.09918	-3.58627
N	-5.47389	-4.89112	-3.1076
H	-5.18407	-3.94772	-3.332
C	-6.47768	-5.10328	-2.07416
H	-6.81233	-6.13952	-2.19706
C	-5.92686	-4.89416	-0.65714
H	-6.75471	-5.02675	0.047962
H	-5.59729	-3.85817	-0.54301
C	-4.77274	-5.7753	-0.19894
O	-4.00627	-5.37184	0.69486
N	-4.65141	-7.01001	-0.72876
H	-5.05904	-7.26152	-1.63
H	-3.86471	-7.56054	-0.40796
C	-7.74647	-4.23313	-2.26733
O	-8.49329	-4.04292	-1.31044
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H	-7.2979	-3.96288	-4.25211
C	-9.18734	-3.03787	-3.87203
H	-9.72798	-2.88362	-2.93605
C	-8.90305	-1.69747	-4.57541
H	-8.37791	-1.8923	-5.51927
H	-9.87831	-1.27088	-4.84867
C	-8.10387	-0.71412	-3.74756
C	-6.79111	-0.3837	-4.1017
H	-6.35849	-0.82251	-4.99818
C	-6.02854	0.493432	-3.32966
H	-5.02585	0.770401	-3.63887
C	-6.55898	1.041389	-2.15369

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H	-8.30646	1.203642	-0.91458
C	-8.64181	-0.11116	-2.60009
H	-9.6677	-0.32876	-2.3092
C	2.688098	7.030858	-3.79583
H	2.721191	7.367106	-2.752
H	1.784885	7.426604	-4.26534
C	2.68164	5.505428	-3.79029
O	3.812213	4.935957	-3.61585
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C	10.49329	-3.09682	0.017739
C	9.097914	-2.56294	0.005176
C	8.363848	-1.93072	-0.96733
N	8.260162	-2.60149	1.110489
C	7.086401	-2.01767	0.775139
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H	10.52603	-4.15974	0.289689
H	10.94119	-2.99371	-0.97464
H	8.653694	-1.69658	-1.98143
H	6.256793	-1.92513	1.461531
H	8.371796	-3.1551	1.960608
C	3.475316	-6.46408	-0.30817
H	3.88116	-6.617	-1.31689
C	2.758914	-5.09916	-0.26791
H	3.471804	-4.29564	-0.4726
H	2.039713	-5.06	-1.09506
C	2.015102	-4.83953	1.047665
H	1.157053	-5.52201	1.128604
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H	0.980464	-3.10406	0.254505
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H	0.603297	-4.04213	2.964874
C	0.15638	-2.09703	2.800153
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H	-1.07319	-1.2964	4.226179
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O	2.39296	-0.26025	-0.0319
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N	-3.55149	-3.95259	-4.73998
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C	-4.12041	-5.28822	-4.71048
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N	8.060185	-3.33731	1.152594
C	6.97679	-2.61411	0.781317
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H	10.1855	-5.10562	0.377882
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H	8.72903	-2.35375	-1.86679
H	6.120992	-2.46037	1.423549
H	8.071109	-3.91769	1.991812
C	2.832119	-6.83347	-0.2627
H	3.208785	-7.06457	-1.26821
C	2.231123	-5.41323	-0.27324
H	3.004562	-4.68345	-0.53313
H	1.488516	-5.36843	-1.08184
C	1.550402	-5.02979	1.045918
H	0.663563	-5.66065	1.199901
H	2.225849	-5.22721	1.887892
C	1.141554	-3.55488	1.081595
H	2.044315	-2.93017	1.085756
H	0.565582	-3.28705	0.18952
N	0.336777	-3.29772	2.276144
H	0.223114	-4.05671	2.940593
C	-0.06298	-2.08755	2.707943
N	0.245003	-0.9596	2.044268
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N	-0.79269	-2.03373	3.830557
H	-1.37802	-2.8523	4.062593
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C	3.970715	-7.06526	0.730544
O	3.907154	-7.96235	1.585275
N	5.053515	-6.25889	0.604189
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C	5.382973	-6.61871	5.047369
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C	4.286542	-5.62493	5.475142
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C	2.915569	-5.96538	4.888383
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S	1.528873	-4.8843	5.437924
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C	1.29297	-3.01083	-3.91299
H	1.59688	-4.062	-3.85868
C	0.110694	-2.85783	-2.91014
O	0.269709	-2.1255	-1.90976
O	-0.91607	-3.53175	-3.2243
N	0.639159	-2.8275	-5.26474
H	0.125637	-1.85848	-5.3505
H	-0.10445	-3.53241	-5.31233
H	1.286376	-2.95036	-6.04772
C	2.53351	-0.72843	-4.34176
H	2.193557	-0.76515	-5.38634
H	3.571446	-0.37854	-4.37127
C	1.67735	0.262855	-3.56126
H	2.029228	0.322904	-2.52986
H	0.643272	-0.06935	-3.51548
C	1.710318	1.637701	-4.20718
H	2.71284	2.071496	-4.22505
H	1.334916	1.590479	-5.23242
N	0.835407	2.590063	-3.46139
H	7.093557	-5.98569	0.819463
H	5.188062	-7.607	5.478935
H	-3.7975	-7.16883	4.026868

H	2.066166	-7.57641	-0.02063
H	-8.24188	-0.9161	3.293618
H	-5.88675	1.948212	5.617574
H	10.93657	-3.59936	0.922088
H	8.9652	3.015469	-2.88601
H	4.276114	7.225673	-4.25284
H	5.714603	6.868412	-1.13668
H	-2.82509	7.093592	4.687803
H	-3.57049	-1.27095	-6.72746
H	-3.33543	-6.00937	-4.46691
H	-10.0227	-2.98644	-4.9362
H	6.014654	-3.59194	3.646564
H	5.872178	-2.19304	4.284392
C	5.604597	-4.14784	-2.56628
O	5.163467	-4.24964	-1.38961
O	5.732251	-3.00798	-3.12967
C	6.042128	-5.37874	-3.33953
H	5.57325	-6.28272	-2.94258
H	7.129795	-5.48458	-3.24681
H	5.813755	-5.26796	-4.40294
H	1.176854	3.57249	-3.6748
H	-0.14223	2.393263	-3.72826
H	0.91746	2.436795	-2.42845
O	1.001738	2.055546	-0.68236
H	1.519915	1.255433	-0.42375
H	0.088349	1.843661	-0.35244
O	-3.13153	1.277661	-1.7391
H	-2.63344	1.287846	-2.59491
H	-2.49895	1.531273	-1.02293
O	-1.38532	1.255085	0.335567
H	-1.22374	0.312799	0.522372
H	-1.38067	1.715676	1.24953

⁵TS1_{B,C4}

C	-3.61334	-2.5395	6.160456
H	-3.18056	-1.99238	5.312639
C	-2.48222	-3.14711	6.997092
H	-2.86833	-3.45897	7.974374
H	-2.12647	-4.05253	6.50064
C	-1.30341	-2.1892	7.20488
H	-1.63036	-1.25514	7.681778
H	-0.57885	-2.64431	7.894233
C	-0.55741	-1.85529	5.908905
O	-0.71364	-2.53168	4.878563
N	0.281725	-0.80722	5.951465
H	0.384416	-0.2523	6.788525
H	0.789391	-0.52715	5.100909
C	-4.55472	-3.58028	5.553718
O	-4.29246	-4.78964	5.536442
N	-5.68172	-3.07576	4.988283
H	-5.78646	-2.06659	4.94426
C	-6.52762	-3.87937	4.103932
H	-7.48231	-3.35388	3.999738
C	-5.87953	-4.11589	2.725347
H	-4.95594	-4.68394	2.880782
H	-6.54326	-4.75511	2.127928
C	-5.56523	-2.80035	1.99546
H	-5.26702	-2.05073	2.734059
H	-6.46348	-2.39762	1.511602
C	-4.41224	-2.85145	0.995418
H	-4.20234	-1.83341	0.661503
H	-3.50829	-3.23687	1.49069
N	-4.71439	-3.67871	-0.17554
H	-5.32115	-4.49398	-0.0723
C	-4.04766	-3.60237	-1.33651
N	-3.19442	-2.6082	-1.60494
H	-3.1736	-1.7114	-1.08226
H	-2.79109	-2.63239	-2.53958
N	-4.21832	-4.57384	-2.25588
H	-4.90257	-5.29883	-2.06916
H	-3.89137	-4.38355	-3.20388
C	-1.7582	-7.04996	0.135693
H	-0.75056	-7.46741	0.018058
H	-1.88478	-6.27334	-0.62927
C	-1.96371	-6.50318	1.514408
N	-1.13308	-5.53174	2.052005
C	-1.60337	-5.28971	3.271603
H	-1.21359	-4.56388	3.975117
N	-2.6856	-6.05318	3.546577

H	-3.28596	-5.91178	4.361102
C	-2.93314	-6.82939	2.432825
H	-3.74954	-7.53465	2.393523
C	6.713325	4.328035	-5.35761
C	6.606652	4.666879	-3.86827
C	5.427224	3.810527	-6.05181
O	7.408653	4.183452	-3.05935
C	4.758171	2.688618	-5.31395
C	4.982487	1.332162	-5.22904
N	3.744721	2.954997	-4.41861
C	3.40113	1.803215	-3.83028
N	4.120612	0.783806	-4.29825
H	7.066326	5.219561	-5.89313
H	4.705355	4.626736	-6.17122
H	5.700372	3.488626	-7.06334
H	5.707165	0.728143	-5.75405
H	2.665714	1.724005	-3.0506
H	3.293731	3.91917	-4.28657
N	5.65339	5.560191	-3.49343
H	4.816315	5.725063	-4.05523
C	5.534017	5.97996	-2.10175
H	6.542337	6.10393	-1.6958
C	4.733907	5.009238	-1.216
O	3.629405	5.325608	-0.76055
N	5.338479	3.823022	-0.9837
C	4.719757	2.706864	-0.26595
C	4.111545	3.194506	1.072672
C	5.808882	1.657826	0.016564
O	4.814485	3.666851	1.960418
C	5.291447	0.325005	0.572359
C	4.737706	-0.69266	-0.43191
O	4.461976	-1.84275	-0.00948
O	4.638	-0.31351	-1.64845
H	6.232563	3.671295	-1.44906
H	3.933907	2.266255	-0.89027
H	6.364305	1.4681	-0.90882
H	6.49944	2.103247	0.740779
H	4.513385	0.485572	1.331071
H	6.101221	-0.19419	1.099949
N	2.763854	3.045549	1.173269
H	2.26742	2.559834	0.42909
C	2.004989	3.404836	2.366783
H	0.951893	3.38752	2.061628
C	2.123718	2.359567	3.484673
H	3.159295	2.037365	3.614759
H	1.80472	2.827208	4.42339
C	1.211038	1.162866	3.202183

O	0.099082	1.411072	2.661721
O	1.616534	0.001696	3.544144
C	2.232502	4.837969	2.875656
O	1.986815	5.121924	4.053455
N	2.541143	5.789423	1.956683
H	2.866283	5.505023	1.032057
C	2.868364	7.140356	2.413973
H	3.497028	7.060439	3.307676
C	3.626894	7.918998	1.334641
H	4.57622	7.426574	1.105102
H	3.825663	8.928618	1.702641
H	3.044293	7.987355	0.409671
C	1.64869	7.952634	2.890917
O	1.813268	8.982974	3.534636
N	0.421861	7.463152	2.546868
H	0.387559	6.622064	1.985603
C	-0.81526	8.046037	3.029743
H	-0.51881	8.978436	3.523335
C	-1.79124	8.40393	1.882788
H	-1.31392	9.183108	1.278052
H	-2.67972	8.836576	2.350375
C	-2.18643	7.240052	0.995797
C	-1.4725	6.953595	-0.17714
H	-0.63188	7.58477	-0.4574
C	-1.83511	5.884484	-1.00175
H	-1.2631	5.693842	-1.90714
C	-2.92508	5.079121	-0.66329
H	-3.22287	4.249737	-1.30056
C	-3.64164	5.351382	0.505953
H	-4.49387	4.732274	0.775796
C	-3.2776	6.419617	1.326992
H	-3.83563	6.629088	2.234927
C	-1.51967	7.202687	4.120787
O	-2.67918	7.472089	4.445468
N	-0.78019	6.224663	4.696106
H	0.182724	6.077728	4.402431
C	-1.2588	5.440533	5.828154
H	-2.11008	5.976019	6.254225
C	-1.63559	3.991689	5.471881
H	-0.75795	3.505216	5.025184
H	-1.84179	3.461163	6.415324
C	-2.83743	3.815679	4.523866
H	-2.61323	4.360089	3.59645
C	-3.00034	2.331138	4.15404
H	-3.80328	2.219072	3.411329
H	-2.08117	1.917346	3.725379
H	-3.26313	1.737367	5.043811

C	-4.13971	4.38672	5.104686
H	-4.98488	4.183715	4.434677
H	-4.37271	3.928142	6.076373
H	-4.07492	5.470699	5.235451
C	-5.80722	0.629602	-4.67936
H	-5.10642	0.381801	-5.47895
C	-5.0365	0.659337	-3.34893
H	-5.63481	1.112308	-2.55369
H	-4.81188	-0.36723	-3.02277
C	-3.68129	1.384017	-3.43585
O	-3.10474	1.433146	-4.56303
O	-3.20648	1.833725	-2.35088
C	-6.95799	-0.36121	-4.6637
O	-8.10279	-0.05166	-4.31254
N	-6.63706	-1.63836	-5.03304
H	-5.67709	-1.84295	-5.33084
C	-7.66677	-2.60747	-5.36169
H	-8.45536	-2.13196	-5.95843
C	-8.39868	-3.28921	-4.2052
O	-9.21072	-4.18881	-4.43971
N	-8.13076	-2.8418	-2.95287
H	-7.42747	-2.12241	-2.85057
C	-8.95689	-3.20127	-1.80886
H	-9.8206	-3.73064	-2.22529
C	-8.21931	-4.1074	-0.812
H	-8.9221	-4.38399	-0.01847
H	-7.41683	-3.54237	-0.33208
C	-7.58993	-5.37221	-1.37655
O	-6.5418	-5.82637	-0.88037
N	-8.22903	-6.01138	-2.37954
H	-8.8772	-5.52786	-3.00301
H	-7.7667	-6.83223	-2.75073
C	-9.5345	-1.98172	-1.04877
O	-10.0282	-2.1603	0.062076
N	-9.47616	-0.78571	-1.68274
H	-9.10667	-0.71583	-2.62881
C	-10.0542	0.420976	-1.09967
H	-10.7002	0.099241	-0.28025
C	-9.01106	1.446129	-0.61475
H	-8.35249	1.695541	-1.45601
H	-9.56138	2.36881	-0.37746
C	-8.17103	1.03931	0.583468
C	-6.77583	1.142822	0.546458
H	-6.28365	1.474721	-0.36445
C	-5.98253	0.8373	1.655116
H	-4.89985	0.889253	1.569269
C	-6.59351	0.429248	2.842381

O	-5.86532	0.095896	3.97068
H	-4.98473	0.503192	3.904075
C	-7.98412	0.307183	2.904896
H	-8.44801	-0.00965	3.8343
C	-8.75644	0.607544	1.784674
H	-9.83567	0.505013	1.855137
C	1.486136	7.025459	-3.12897
H	1.866819	7.09579	-2.1025
H	0.411631	7.226532	-3.11619
C	1.779483	5.616468	-3.63043
O	2.902027	5.439252	-4.21544
O	0.941141	4.703306	-3.42645
C	8.363683	-2.77783	-6.29801
C	7.445744	-2.37552	-5.19136
C	6.148926	-1.93534	-5.18501
N	7.817571	-2.38273	-3.85406
C	6.77853	-1.95896	-3.10025
N	5.750134	-1.67451	-3.88443
H	8.715007	-3.81096	-6.18291
H	7.842148	-2.70927	-7.2564
H	5.469147	-1.80402	-6.01254
H	6.808687	-1.94398	-2.01996
H	8.707942	-2.68102	-3.48068
C	5.525972	-6.94226	0.461444
H	6.206649	-7.30467	-0.32277
C	4.624077	-5.8505	-0.1377
H	5.216303	-4.9905	-0.46941
H	4.174445	-6.26384	-1.05101
C	3.499455	-5.37971	0.795284
H	2.963112	-6.24907	1.200739
H	3.918249	-4.84115	1.655204
C	2.509118	-4.47275	0.048678
H	3.012185	-3.58556	-0.3418
H	2.105276	-5.00125	-0.82145
N	1.360701	-4.06065	0.858735
H	0.603335	-4.73013	1.022057
C	1.274542	-2.95211	1.601191
N	2.264114	-2.08997	1.783213
H	3.145649	-2.14313	1.264311
H	2.066443	-1.24662	2.345618
N	0.050119	-2.66972	2.153172
H	-0.6062	-3.44403	2.075861
H	0.038137	-2.26029	3.095143
C	6.404231	-6.59716	1.665424
O	6.502901	-7.36665	2.618386
N	7.131515	-5.4373	1.583167
H	7.056699	-4.81869	0.77426

C	8.181327	-5.18638	2.547534
H	8.02081	-5.88841	3.369497
C	8.256063	-3.74006	3.037595
O	8.110685	-2.76405	2.291549
N	8.596562	-3.59828	4.340181
H	8.645907	-4.42739	4.914325
C	8.889922	-2.29836	4.951764
H	9.556278	-1.75386	4.274972
C	7.645017	-1.4425	5.229417
H	7.973842	-0.46808	5.609818
H	7.149468	-1.25563	4.2726
C	6.665873	-2.07256	6.224309
H	6.419363	-3.10192	5.937604
H	7.103736	-2.10999	7.228908
S	5.100023	-1.1309	6.405788
C	4.301255	-1.54318	4.814742
H	3.42691	-0.89856	4.697045
H	4.973997	-1.34817	3.974339
H	3.985869	-2.59132	4.79274
O	2.252254	-0.71581	-2.74733
O	6.99251	-3.08793	-0.21047
Fe	3.888069	-1.12004	-3.30064
C	-0.28927	-1.82096	-4.72955
H	0.467247	-2.46788	-5.18121
H	-0.65224	-2.33814	-3.83604
C	-1.49403	-1.74496	-5.72327
H	-1.21293	-2.24993	-6.65386
C	-2.83558	-2.42046	-5.25366
O	-2.74475	-3.29441	-4.36383
O	-3.85121	-2.00145	-5.87064
N	-1.91929	-0.36103	-6.16815
H	-2.2864	0.284807	-5.4009
H	-2.76609	-0.5441	-6.73088
H	-1.20836	0.132618	-6.71196
C	0.358852	-0.51148	-4.34615
H	0.896938	-0.00453	-5.15388
H	1.476449	-0.76247	-3.55852
C	-0.40458	0.378753	-3.3912
H	-0.10297	0.142389	-2.36503
H	-1.47458	0.159093	-3.42418
C	-0.18703	1.866809	-3.65768
H	0.838133	2.099854	-3.93551
H	-0.85444	2.222863	-4.44322
N	-0.49447	2.669378	-2.43883
H	9.171561	-5.41244	2.117091
H	9.442343	-2.4995	5.876139
H	-2.47759	-7.84685	-0.07721

H	4.925224	-7.80107	0.776172
H	-6.71976	-4.83582	4.597117
H	-4.19273	-1.80929	6.740729
H	9.247122	-2.12917	-6.35226
H	7.498554	3.570806	-5.42367
H	2.000976	7.775165	-3.73594
H	5.011507	6.936886	-2.07517
H	-0.46258	5.422938	6.582254
H	-6.23033	1.616523	-4.88724
H	-7.22165	-3.39481	-5.97517
H	-10.6856	0.896246	-1.85945
H	7.470505	-2.82358	0.609002
H	6.067885	-2.79638	-0.05238
C	3.198122	-3.35503	-4.23492
O	3.131964	-2.22724	-4.85453
O	3.604919	-3.39664	-3.04999
C	2.826644	-4.61841	-4.98166
H	2.433635	-5.36592	-4.28879
H	3.730161	-5.0295	-5.44825
H	2.100988	-4.41448	-5.77277
H	-0.17074	3.647484	-2.61483
H	-1.51965	2.585685	-2.25717
H	0.058333	2.276878	-1.65018
O	1.30946	1.149043	-0.73698
H	1.760214	0.501769	-1.32587
H	0.698696	0.604154	-0.17318
O	-3.14138	-0.12051	-0.32406
H	-3.23587	0.633176	-0.95053
H	-2.24316	-0.03654	0.085656
O	-0.61303	-0.15446	0.731311
H	-0.47099	-1.06887	1.058232
H	-0.45675	0.413455	1.555698

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C	-3.28379	-2.40628	5.699482
H	-2.77307	-2.0332	4.801688
C	-2.25826	-3.07493	6.620197
H	-2.72478	-3.31163	7.58374
H	-1.95481	-4.02875	6.182362
C	-1.01619	-2.2106	6.867671
H	-1.294	-1.24046	7.301336
H	-0.37269	-2.70271	7.610098
C	-0.16585	-1.97433	5.615318
O	-0.27485	-2.69662	4.611276
N	0.722141	-0.96791	5.680611
H	0.756082	-0.35823	6.484564
H	1.265124	-0.7091	4.845835
C	-4.38082	-3.35326	5.214618
O	-4.2714	-4.58542	5.2697
N	-5.47009	-2.74832	4.676049
H	-5.45586	-1.73977	4.549994
C	-6.4744	-3.49068	3.913783
H	-7.32911	-2.81998	3.779227
C	-5.95629	-3.98953	2.549244
H	-5.22219	-4.78303	2.726171
H	-6.79643	-4.44618	2.00836
C	-5.30363	-2.87327	1.722905
H	-4.6124	-2.3196	2.36819
H	-6.05804	-2.1478	1.391002
C	-4.47923	-3.33585	0.521712
H	-3.91372	-2.48091	0.142276
H	-3.75736	-4.10483	0.8319
N	-5.32647	-3.8558	-0.55413
H	-6.20519	-4.32226	-0.32289
C	-4.98098	-3.87562	-1.84784
N	-3.86585	-3.29439	-2.30186
H	-3.34393	-2.57805	-1.77554
H	-3.76478	-3.30391	-3.31619
N	-5.76145	-4.53566	-2.72799
H	-6.60763	-4.97236	-2.38117
H	-5.65509	-4.30434	-3.71562
C	-1.391	-7.21084	0.138314
H	-0.42283	-7.72493	0.192672
H	-1.32273	-6.46676	-0.6652
C	-1.74388	-6.57016	1.444763
N	-0.96189	-5.57564	2.008213
C	-1.55579	-5.24806	3.147584
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C	-2.81435	-6.82662	2.270414
H	-3.63119	-7.5279	2.188894
C	7.244425	4.329601	-4.99709
C	6.763805	4.773101	-3.61268
C	6.234604	3.572394	-5.89265
O	7.472491	4.5683	-2.6172
C	5.587122	2.403363	-5.2087
C	6.034967	1.165473	-4.81092
N	4.292577	2.497106	-4.74459
C	3.996124	1.370819	-4.08684
N	5.031189	0.526933	-4.10484
H	7.593667	5.220413	-5.53694
H	5.44684	4.250432	-6.23864
H	6.769865	3.240182	-6.79026
H	6.994433	0.697377	-4.97181
H	3.062298	1.192446	-3.58304
H	3.695464	3.369497	-4.8407
N	5.591825	5.452127	-3.53603
H	4.874795	5.398711	-4.26382
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C	4.398686	5.017473	-1.3575
O	3.200385	5.156288	-1.08929
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C	4.674253	2.886208	-0.10213
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O	4.22923	4.063457	1.96268
C	5.551036	0.749482	1.052153
C	5.476438	-0.3686	0.013304
O	5.32648	-1.55512	0.388912
O	5.626368	-0.01424	-1.21272
H	6.142985	4.006939	-1.20001
H	4.110046	2.214417	-0.76033
H	6.662763	2.057441	-0.25244
H	6.264729	2.775125	1.316358
H	4.603029	0.741577	1.607843
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H	2.168241	2.350806	0.255394
C	1.54718	3.266449	2.09007
H	0.545665	3.048377	1.701983
C	1.767875	2.325179	3.281725
H	2.814137	2.337381	3.594196
H	1.166422	2.681989	4.124545
C	1.318019	0.907177	2.918369

O	0.23882	0.807046	2.281959
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C	2.469571	7.876422	0.735041
H	3.443561	7.47367	0.445535
H	2.58589	8.918891	1.041311
H	1.809825	7.837125	-0.13911
C	0.623528	7.791294	2.4317
O	0.725224	8.869479	3.007386
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H	-1.63055	8.678669	3.056525
C	-2.92427	7.703545	1.625101
H	-2.63061	8.462959	0.891808
H	-3.84322	8.039128	2.112961
C	-3.14608	6.37541	0.931134
C	-2.45241	6.056437	-0.2462
H	-1.78818	6.795339	-0.68981
C	-2.60473	4.807657	-0.85347
H	-2.05619	4.577328	-1.76357
C	-3.46005	3.855008	-0.29721
H	-3.55568	2.880738	-0.76728
C	-4.16994	4.168178	0.865096
H	-4.84731	3.437452	1.299809
C	-4.01412	5.414503	1.474302
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C	-1.68397	5.452811	5.86611
H	-2.64806	5.82509	6.218371
C	-1.67147	3.918973	5.761551
H	-0.68303	3.612815	5.39364
H	-1.76426	3.512065	6.780976
C	-2.75605	3.287753	4.867682
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H	-1.5582	1.559242	4.241512
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C	-4.17514	3.579477	5.381387
H	-4.92473	3.099154	4.737275
H	-4.31243	3.200509	6.405079
H	-4.39341	4.6521	5.380881
C	-5.9501	1.020445	-4.34458
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C	-4.99049	0.754404	-3.17426
H	-5.3238	1.273845	-2.27124
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C	-3.5315	1.159101	-3.45728
O	-3.14761	1.27514	-4.65977
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C	-7.33703	0.451178	-4.10841
O	-8.12174	0.957464	-3.28457
N	-7.65969	-0.64891	-4.83365
H	-6.93709	-1.08095	-5.42219
C	-9.02029	-1.15186	-4.95445
H	-9.70163	-0.31038	-5.14229
C	-9.63125	-1.92558	-3.77914
O	-10.5188	-2.75809	-3.9876
N	-9.19821	-1.59105	-2.53691
H	-8.52958	-0.82916	-2.47909
C	-9.92303	-1.97137	-1.33022
H	-10.8776	-2.39254	-1.6636
C	-9.16764	-3.01275	-0.49218
H	-9.74236	-3.1887	0.424457
H	-8.19822	-2.60957	-0.18219
C	-8.89827	-4.35878	-1.14921
O	-7.94118	-5.06105	-0.77311
N	-9.75428	-4.79502	-2.09752
H	-10.3197	-4.15385	-2.65785
H	-9.5325	-5.69025	-2.51582
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O	-10.7567	-0.98685	0.687853
N	-10.1662	0.469221	-0.97527
H	-9.75952	0.581762	-1.89798
C	-10.5079	1.686212	-0.24967
H	-11.0053	1.37546	0.671463
C	-9.27977	2.570832	0.056254
H	-8.74637	2.767425	-0.88186
H	-9.65455	3.538373	0.414373
C	-8.33182	1.982039	1.078193
C	-7.19304	1.263965	0.689239
H	-6.97608	1.14943	-0.37014
C	-6.31675	0.720293	1.630893
H	-5.41305	0.204521	1.322887
C	-6.58656	0.878541	2.991373

O	-5.71121	0.308364	3.903848
H	-5.72809	0.833528	4.720638
C	-7.71561	1.588871	3.404459
H	-7.92461	1.713997	4.464651
C	-8.57121	2.136979	2.450047
H	-9.44104	2.698096	2.783703
C	1.2565	6.009844	-3.91045
H	1.519063	6.188777	-2.86067
H	0.173655	5.869327	-3.97541
C	1.995221	4.757139	-4.36151
O	3.143026	4.904581	-4.89989
O	1.474249	3.628497	-4.15878
C	10.19031	-2.84616	-4.60567
C	9.082869	-2.16226	-3.8746
C	7.722153	-2.22037	-4.00354
N	9.301357	-1.26466	-2.83547
C	8.111893	-0.83218	-2.37313
N	7.129868	-1.38749	-3.06777
H	10.79355	-3.47349	-3.93743
H	9.775758	-3.4929	-5.3834
H	7.116451	-2.79805	-4.68201
H	7.984611	-0.14297	-1.55667
H	10.19643	-1.03432	-2.42724
C	6.771388	-6.42683	-0.29687
H	7.61219	-6.38405	-1.00359
C	5.774938	-5.30815	-0.64645
H	6.274894	-4.33425	-0.62306
H	5.459637	-5.45899	-1.68885
C	4.53469	-5.27046	0.256158
H	4.083617	-6.27104	0.318009
H	4.822575	-4.99208	1.277597
C	3.496586	-4.27001	-0.26867
H	3.935492	-3.27455	-0.36135
H	3.162315	-4.55102	-1.27367
N	2.302794	-4.17774	0.572721
H	1.618353	-4.91985	0.50055
C	2.003096	-3.20028	1.447181
N	2.845273	-2.23008	1.773567
H	3.762123	-2.12316	1.334723
H	2.48847	-1.42965	2.334514
N	0.746722	-3.19586	1.963042
H	0.19351	-4.05845	1.840703
H	0.594762	-2.74795	2.874534
C	7.35524	-6.42527	1.116802
O	7.339973	-7.43531	1.817583
N	7.931677	-5.25856	1.540747
H	8.000822	-4.44633	0.922745

C	8.657575	-5.261	2.792776
H	8.154877	-5.96001	3.467427
C	8.80132	-3.87662	3.419571
O	8.921177	-2.838	2.761496
N	8.882371	-3.87567	4.772594
H	8.736808	-4.74565	5.264034
C	9.192773	-2.66961	5.545397
H	10.02692	-2.1617	5.050825
C	8.014812	-1.69196	5.678277
H	8.37152	-0.79014	6.190271
H	7.718168	-1.3869	4.670583
C	6.815435	-2.26565	6.437887
H	6.505026	-3.22798	6.013092
H	7.071676	-2.44092	7.489668
S	5.356549	-1.15094	6.469364
C	4.790838	-1.32549	4.741095
H	3.948285	-0.64695	4.586764
H	5.579043	-1.05487	4.032413
H	4.457945	-2.34897	4.541105
O	3.434767	-0.99734	-2.22026
O	8.005312	-2.62581	0.149503
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C	-2.04491	-1.99215	-4.97949
H	-1.9731	-3.07241	-4.77504
H	-2.51653	-1.54812	-4.09669
C	-3.01248	-1.87665	-6.1674
H	-2.64774	-2.46352	-7.01841
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O	-4.55199	-3.35569	-5.07877
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N	-3.15589	-0.45704	-6.64824
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H	-4.07923	-0.43978	-7.1153
H	-2.40078	-0.16341	-7.26976
C	-0.68471	-1.39018	-5.14695
H	-0.08529	-1.65986	-6.01612
H	2.964107	-1.75763	-2.64383
C	-0.05981	-0.60783	-4.02983
H	0.945399	-0.98914	-3.80749
H	-0.66159	-0.74616	-3.12265
C	0.025169	0.907075	-4.33504
H	0.944943	1.176838	-4.85639
H	-0.83058	1.228026	-4.92929
N	-0.03468	1.726045	-3.08378
H	9.681486	-5.65134	2.658777
H	9.538694	-3.00154	6.530485
H	-2.14477	-7.94932	-0.15216

H	6.301131	-7.40765	-0.41568
H	-6.80581	-4.34137	4.515803
H	-3.73523	-1.53	6.183133
H	10.86482	-2.12988	-5.0916
H	8.118773	3.701032	-4.80933
H	1.558671	6.880435	-4.49871
H	4.430824	6.82127	-2.4914
H	-0.92191	5.762614	6.593217
H	-6.06598	2.101117	-4.48069
H	-9.06576	-1.81203	-5.82194
H	-11.2247	2.262179	-0.84874
H	8.411213	-2.50259	1.034316
H	7.072312	-2.3536	0.270403
C	3.810743	-3.34775	-4.12477
O	4.893968	-2.67902	-3.83345
O	2.692662	-3.16894	-3.62455
C	4.030261	-4.42786	-5.17338
H	3.104942	-4.97895	-5.35035
H	4.815707	-5.11651	-4.84363
H	4.370804	-3.96925	-6.10849
H	0.319708	2.684691	-3.3222
H	-1.02674	1.733427	-2.75452
H	0.584426	1.343797	-2.32659
O	1.63219	0.718763	-1.03797
H	2.351298	0.146305	-1.40547
H	1.048025	0.100556	-0.53083
O	-2.52753	-1.12201	-1.1068
H	-2.70986	-0.21326	-1.43263
H	-1.71125	-1.0439	-0.55109
O	-0.20179	-0.87556	0.340092
H	0.035098	-1.74945	0.711594
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H	-3.5287	-0.90156	5.345525
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H	-3.57314	-2.08518	8.162429
H	-2.89424	-2.95219	6.797746
C	-1.78343	-1.1905	7.356115
H	-1.9599	-0.16934	7.720775
H	-1.17447	-1.68599	8.124895
C	-0.94524	-1.12755	6.074901
O	-1.17871	-1.86903	5.107595
N	0.064233	-0.23878	6.061082
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O	-5.13731	-3.40349	5.809764
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C	-6.52	-2.75424	2.886407
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C	-5.94139	-1.59824	2.055557
H	-5.50872	-0.86018	2.737404
H	-6.73544	-1.06936	1.514219
C	-4.81059	-1.96016	1.09471
H	-4.37952	-1.03168	0.71663
H	-4.02129	-2.50447	1.634434
N	-5.26397	-2.76225	-0.04474
H	-6.01546	-3.44182	0.085575
C	-4.5803	-2.87547	-1.19382
N	-3.54529	-2.08085	-1.48684
H	-3.37889	-1.1691	-1.02042
H	-3.13204	-2.23435	-2.40442
N	-4.92678	-3.83606	-2.07244
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H	-4.55329	-3.76288	-3.01941
C	-2.87426	-6.51105	0.732286
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H	-2.75845	-5.78512	-0.0822
C	-3.01008	-5.82957	2.058479
N	-2.01644	-5.00707	2.567175
C	-2.46565	-4.58296	3.744127
H	-1.95998	-3.89391	4.409841
N	-3.68895	-5.09015	4.020081

H	-4.2776	-4.76766	4.790781
C	-4.05419	-5.88272	2.950925
H	-4.99516	-6.41118	2.922695
C	7.488069	2.511558	-5.53452
C	7.405939	3.001393	-4.08648
C	6.151931	2.216301	-6.26003
O	8.105449	2.476651	-3.21113
C	5.246601	1.291605	-5.49995
C	5.22754	-0.07099	-5.30401
N	4.229119	1.797529	-4.71755
C	3.64674	0.773805	-4.08585
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H	8.043809	3.259005	-6.11685
H	5.61062	3.148403	-6.45804
H	6.393278	1.786207	-7.23901
H	5.875951	-0.8314	-5.71294
H	2.854767	0.879661	-3.36615
H	3.969165	2.841248	-4.66111
N	6.60605	4.068703	-3.82639
H	5.819643	4.319711	-4.42818
C	6.54795	4.642405	-2.48685
H	7.559489	4.638525	-2.07024
C	5.588934	3.910046	-1.5334
O	4.539637	4.441855	-1.15341
N	5.991945	2.676442	-1.15834
C	5.181687	1.752811	-0.36143
C	4.629856	2.466907	0.897232
C	6.075436	0.576528	0.069032
O	5.379168	2.903285	1.76528
C	5.315351	-0.61034	0.673155
C	4.6272	-1.55584	-0.31507
O	4.090618	-2.60155	0.135872
O	4.675237	-1.25125	-1.55366
H	6.853031	2.332703	-1.58179
H	4.349976	1.382178	-0.9725
H	6.643571	0.227552	-0.80046
H	6.786898	0.965208	0.805348
H	4.554409	-0.27156	1.389401
H	6.002515	-1.23376	1.259298
N	3.27425	2.552572	0.958587
H	2.721014	2.096401	0.236566
C	2.563571	3.155736	2.081848
H	1.529833	3.287828	1.740823
C	2.475475	2.225386	3.300122
H	3.432834	1.735978	3.492626
H	2.238153	2.836867	4.178377
C	1.360367	1.192788	3.112741

O	0.322985	1.580965	2.509886
O	1.535804	0.021447	3.589235
C	3.028398	4.572277	2.461277
O	2.822087	5.005719	3.600282
N	3.50813	5.365411	1.467836
H	3.792933	4.940765	0.584621
C	4.072612	6.671067	1.812663
H	4.680129	6.558519	2.717398
C	4.953985	7.206391	0.679743
H	5.799082	6.534896	0.503254
H	5.331879	8.191901	0.963064
H	4.388737	7.299247	-0.25389
C	3.019685	7.72627	2.201835
O	3.366726	8.757577	2.766514
N	1.72601	7.444007	1.870465
H	1.540214	6.580428	1.37726
C	0.615511	8.284001	2.275974
H	1.077096	9.179604	2.706959
C	-0.26077	8.728562	1.080046
H	0.361798	9.35682	0.43334
H	-1.05865	9.353204	1.490511
C	-0.85404	7.5929	0.270162
C	-0.19772	7.101253	-0.86778
H	0.741998	7.552907	-1.17833
C	-0.74067	6.05547	-1.62
H	-0.20962	5.702423	-2.50128
C	-1.95604	5.479836	-1.24256
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H	-3.56608	5.51921	0.192086
C	-2.07396	7.002868	0.641127
H	-2.58994	7.372511	1.522423
C	-0.24892	7.675591	3.407035
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H	1.209845	6.282039	3.822958
C	-0.34572	6.041458	5.252286
H	-1.09525	6.754614	5.602129
C	-0.97084	4.657537	5.003256
H	-0.1878	3.983481	4.630564
H	-1.29039	4.2574	5.978795
C	-2.16407	4.617746	4.029177
H	-1.82208	5.024116	3.067487
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C	-5.64264	1.449398	-4.70812
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O	-9.78398	-2.74287	-4.32747
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H	-10.3394	-2.10362	-2.1476
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H	-9.58453	-2.77953	0.104498
H	-7.96425	-2.18916	-0.21024
C	-8.39696	-4.01634	-1.18318
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H	-8.77964	-5.49533	-2.49376
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H	-9.17825	0.739269	-2.6853
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H	-8.12072	3.088001	-1.6955
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H	-6.09287	2.583298	-0.6292
C	-5.84218	2.039809	1.426052
H	-4.76872	1.900537	1.320317
C	-6.47984	1.82488	2.649397

O	-5.78718	1.457019	3.788907
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H	-8.35242	1.777971	3.701778
C	-8.61163	2.2914	1.61705
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C	6.637895	-3.37592	-2.82355
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H	3.056894	-5.28631	2.24327
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N	0.691211	-4.14328	1.32695
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O	3.02597	-3.80451	-3.70187
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H	2.550044	-6.45163	-3.31452
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H	-9.02686	3.556432	-2.70125
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H	-4.86024	3.164697	-0.71773
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H	-9.48795	2.506368	0.934182
C	1.883189	7.00968	-2.9844
H	2.376591	7.062443	-2.00569
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O	0.971454	4.819043	-3.29059
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N	8.532817	-1.58065	-2.52258
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H	10.44683	0.301522	-3.7212
H	9.393442	1.647263	-3.2334
H	6.770145	0.906359	-3.60605
H	7.015429	-3.08326	-2.27208
H	9.34319	-2.0916	-2.20158
C	3.961739	-7.51335	-1.38852
H	4.736594	-7.74085	-2.13463
C	3.462716	-6.07713	-1.61481
H	4.297159	-5.36996	-1.54839
H	3.090128	-6.01156	-2.64612
C	2.345739	-5.64562	-0.65498
H	1.54059	-6.39355	-0.65382
H	2.728398	-5.5957	0.372725
C	1.772633	-4.28053	-1.05717
H	2.560026	-3.52332	-1.07288
H	1.372995	-4.32317	-2.07534
N	0.693	-3.8305	-0.17635
H	-0.16939	-4.39161	-0.12785
C	0.794292	-2.91553	0.789272
N	1.926559	-2.32591	1.149341
H	2.815044	-2.56807	0.715429
H	1.93108	-1.54861	1.842206
N	-0.36639	-2.51466	1.411712
H	-1.17052	-3.08269	1.15018
H	-0.28832	-2.41713	2.437224
C	4.544412	-7.86017	-0.01862
O	4.255351	-8.90994	0.552166
N	5.439962	-6.9761	0.521625
H	5.750196	-6.14932	0.006924

C	6.153117	-7.38276	1.713552
H	5.446081	-7.889	2.378133
C	6.86303	-6.23601	2.426761
O	7.354533	-5.26286	1.8464
N	6.991267	-6.40869	3.766378
H	6.55817	-7.21904	4.185194
C	7.817013	-5.54286	4.6131
H	8.796711	-5.42869	4.136252
C	7.222126	-4.1483	4.866892
H	7.921716	-3.58906	5.500187
H	7.168929	-3.6274	3.907125
C	5.841962	-4.17581	5.526985
H	5.139557	-4.76361	4.925053
H	5.892449	-4.6366	6.521055
S	5.1201	-2.50975	5.812539
C	5.056916	-1.88011	4.094096
H	4.3395	-1.05718	4.053319
H	6.036983	-1.52424	3.767021
H	4.703123	-2.66279	3.415299
O	1.45485	-1.74432	-3.54826
O	6.408929	-4.39321	-0.6239
Fe	4.259848	-1.29636	-3.29054
C	-0.79824	-2.49066	-4.0608
H	-0.26949	-3.39536	-4.37603
H	-1.09669	-2.64798	-3.01988
C	-2.08846	-2.39396	-4.91146
H	-2.08139	-3.20156	-5.6515
C	-3.46597	-2.52727	-4.16771
O	-3.46106	-2.98725	-3.00116
O	-4.44296	-2.16019	-4.87193
N	-2.26924	-1.13909	-5.74381
H	-2.42373	-0.23898	-5.17837
H	-3.18691	-1.28419	-6.19328
H	-1.53352	-0.99633	-6.43845
C	0.219849	-1.3256	-4.11453
H	0.384884	-1.03532	-5.1707
H	1.757241	-2.57771	-4.0093
C	-0.25913	-0.11202	-3.30562
H	0.185441	-0.2164	-2.31197
H	-1.34174	-0.1313	-3.16998
C	0.1305	1.238711	-3.906
H	1.170954	1.245993	-4.22734
H	-0.51343	1.493116	-4.7491
N	-0.05386	2.319001	-2.88894
H	6.927393	-8.13276	1.475925
H	7.966378	-6.07741	5.557214
H	-3.74792	-6.79936	-1.56581

H	3.151316	-8.23125	-1.54819
H	-5.94633	-4.99143	5.110413
H	-2.43356	-3.72773	7.520665
H	10.22081	0.677028	-2.00432
H	7.355771	3.258006	-5.71061
H	2.418066	7.678369	-3.66546
H	5.59652	6.53831	-1.8862
H	0.279878	5.477585	7.12223
H	-5.94917	2.169407	-4.63248
H	-7.97601	-2.70771	-5.09144
H	-11.337	2.847512	-2.43347
H	6.917921	-4.53254	0.202573
H	5.748237	-3.70403	-0.40166
C	3.590485	-3.85459	-4.86264
O	4.323017	-2.92295	-4.34843
O	2.351256	-3.9321	-4.75736
C	4.355406	-4.91247	-5.63961
H	3.672392	-5.64039	-6.08114
H	5.056158	-5.42242	-4.96926
H	4.951394	-4.43497	-6.42462
H	0.334526	3.252577	-3.19261
H	-1.07881	2.381053	-2.68098
H	0.458283	2.051559	-2.0257
O	1.530758	1.210224	-0.72655
H	2.190679	0.514664	-0.92368
H	0.809469	0.786513	-0.18249
O	-3.11877	1.023789	0.139268
H	-3.08043	1.391166	-0.7805
H	-2.17342	0.906101	0.422739
O	-0.56073	0.295387	0.725309
H	-0.62601	-0.68186	0.812528
H	-0.22419	0.570632	1.642077

⁵TS1_{B,C5}

C	-3.98748	0.012334	5.986943
H	-3.33692	0.128002	5.111526
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H	-3.73598	-0.44691	8.087255
H	-3.04881	-1.64049	7.007158
C	-1.79878	0.090473	7.307822
H	-1.89062	1.182618	7.388167
H	-1.33525	-0.2434	8.246326
C	-0.82222	-0.23437	6.171363
O	-1.0973	-1.0677	5.294292
N	0.360853	0.406723	6.203328
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H	0.995567	0.336312	5.396863
C	-5.16715	-0.86196	5.555114
O	-5.38794	-1.98232	6.036097
N	-5.93421	-0.33001	4.572785
H	-5.65736	0.554812	4.156754
C	-6.95777	-1.08887	3.853094
H	-7.46248	-0.37429	3.196813
C	-6.40505	-2.27261	3.031512
H	-6.17278	-3.09361	3.71819
H	-7.21228	-2.62646	2.375287
C	-5.14582	-1.93587	2.222139
H	-4.40664	-1.49138	2.897804
H	-5.34979	-1.17988	1.455845
C	-4.47585	-3.15532	1.573937
H	-3.41881	-2.94873	1.396104
H	-4.52114	-4.01564	2.251514
N	-5.05581	-3.57094	0.292032
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N	-3.34791	-2.66908	-1.03136
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H	-2.7694	-2.82981	-1.86516
N	-4.80108	-4.23469	-1.91627
H	-5.47303	-4.9745	-1.75805
H	-4.46469	-4.00854	-2.85449
C	-2.46263	-6.94437	3.113917
H	-1.50435	-7.33719	3.475861
H	-2.34194	-6.72157	2.045848
C	-2.87686	-5.72833	3.88331
N	-2.10223	-4.5813	3.913135
C	-2.75178	-3.72655	4.69046
H	-2.41762	-2.72829	4.943133
N	-3.90246	-4.25852	5.164061

H	-4.58724	-3.71655	5.692136
C	-4.00259	-5.53633	4.653017
H	-4.83264	-6.1868	4.884695
C	7.521548	3.031474	-5.2796
C	7.209631	3.668462	-3.92312
C	6.335441	2.390221	-6.04463
O	7.878725	3.363999	-2.92771
C	5.484614	1.487038	-5.20082
C	5.593372	0.178279	-4.78493
N	4.357729	1.984014	-4.58152
C	3.834625	1.011986	-3.83167
N	4.546408	-0.11243	-3.92945
H	7.987228	3.789455	-5.92388
H	5.693603	3.170932	-6.47014
H	6.748089	1.836282	-6.89563
H	6.342868	-0.55858	-5.03038
H	2.970447	1.143148	-3.20812
H	3.951705	2.97382	-4.70616
N	6.22962	4.607924	-3.87057
H	5.500163	4.67278	-4.57961
C	5.907534	5.286484	-2.61988
H	6.845667	5.516455	-2.10541
C	4.989495	4.491773	-1.67321
O	3.861954	4.9053	-1.38082
N	5.52213	3.34812	-1.19175
C	4.806153	2.405416	-0.33236
C	4.153749	3.151881	0.853331
C	5.82835	1.389721	0.20455
O	4.831589	3.776499	1.663634
C	5.238096	0.221955	1.001941
C	4.657269	-0.94896	0.208146
O	4.334891	-1.98742	0.828424
O	4.580102	-0.80807	-1.06701
H	6.468187	3.120147	-1.49454
H	4.035464	1.890981	-0.91785
H	6.407147	0.993663	-0.6374
H	6.515122	1.945107	0.852642
H	4.457526	0.557197	1.698219
H	6.021704	-0.21701	1.629441
N	2.798443	3.054026	0.923756
H	2.31415	2.437017	0.276499
C	2.024451	3.630103	2.01999
H	0.973625	3.517245	1.730904
C	2.188034	2.835063	3.323574
H	3.24333	2.671595	3.551447
H	1.759084	3.423975	4.142108
C	1.437277	1.50225	3.230937

O	0.337688	1.516398	2.619077
O	1.956745	0.484081	3.800867
C	2.225054	5.141429	2.225515
O	1.900099	5.664589	3.298254
N	2.632619	5.879674	1.159686
H	2.993292	5.404999	0.331826
C	3.009239	7.280247	1.358833
H	3.482657	7.362445	2.343718
C	4.000659	7.74617	0.288696
H	4.926822	7.167775	0.355123
H	4.222532	8.803549	0.451786
H	3.588748	7.619017	-0.71769
C	1.816236	8.252076	1.445407
O	1.996694	9.417688	1.782183
N	0.591406	7.7299	1.151124
H	0.550312	6.764128	0.851669
C	-0.64424	8.4578	1.365155
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C	-1.55811	8.452637	0.117204
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H	-2.47001	8.988663	0.394046
C	-1.90016	7.072953	-0.40871
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H	-0.29361	7.032023	-1.84584
C	-1.43426	5.207831	-1.90877
H	-0.81654	4.780084	-2.69525
C	-2.51752	4.498264	-1.38596
H	-2.76149	3.507614	-1.76139
C	-3.2896	5.074603	-0.37283
H	-4.1356	4.528861	0.038133
C	-2.98452	6.347767	0.112049
H	-3.58307	6.793455	0.90148
C	-1.41474	8.006162	2.631395
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C	-1.24957	6.875552	4.818556
H	-2.17944	7.430329	4.96009
C	-1.46994	5.359498	4.939008
H	-0.50621	4.861738	4.766927
H	-1.75372	5.142531	5.981273
C	-2.52267	4.751096	3.993687
H	-2.2337	4.997754	2.962603
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H	-2.75248	2.921165	5.157206

C	-3.92709	5.328773	4.230957
H	-4.65374	4.842149	3.566428
H	-4.25382	5.162776	5.268206
H	-3.96478	6.402868	4.024117
C	-5.48867	0.293339	-4.75314
H	-4.88217	0.115557	-5.64867
C	-4.60694	0.057162	-3.51382
H	-5.04815	0.517742	-2.62742
H	-4.5082	-1.01588	-3.30984
C	-3.17638	0.587484	-3.67816
O	-2.6109	0.446495	-4.80935
O	-2.63593	1.104431	-2.66366
C	-6.72526	-0.5883	-4.81164
O	-7.8742	-0.14036	-4.79947
N	-6.48605	-1.93693	-4.88464
H	-5.53036	-2.29075	-4.83977
C	-7.55577	-2.86819	-5.19087
H	-8.1725	-2.47858	-6.00856
C	-8.53512	-3.1964	-4.0607
O	-9.46697	-3.97794	-4.26134
N	-8.31576	-2.58317	-2.87097
H	-7.48409	-2.01494	-2.77796
C	-9.25273	-2.66557	-1.76149
H	-10.1444	-3.15403	-2.16938
C	-8.6912	-3.49177	-0.59502
H	-9.46421	-3.56901	0.177279
H	-7.84666	-2.96574	-0.14065
C	-8.20554	-4.88898	-0.95907
O	-7.20513	-5.37774	-0.40839
N	-8.93182	-5.60128	-1.85262
H	-9.50088	-5.14322	-2.56279
H	-8.55482	-6.5085	-2.09864
C	-9.74046	-1.28608	-1.25398
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N	-9.56102	-0.24167	-2.10205
H	-9.15106	-0.40081	-3.01867
C	-10.1159	1.082488	-1.83931
H	-10.6595	1.015625	-0.89454
C	-9.05082	2.199113	-1.78615
H	-8.41065	2.108386	-2.6729
H	-9.58171	3.15477	-1.88516
C	-8.20871	2.224634	-0.52781
C	-6.96274	1.587495	-0.46325
H	-6.59205	1.06572	-1.34089
C	-6.16935	1.621757	0.683978
H	-5.18624	1.1569	0.698501
C	-6.64239	2.299105	1.810401

O	-5.85004	2.294483	2.944521
H	-6.13405	3.007818	3.538732
C	-7.88284	2.941005	1.779621
H	-8.24658	3.471698	2.657443
C	-8.64968	2.904459	0.615241
H	-9.60675	3.421188	0.59907
C	1.924818	6.046227	-4.1241
H	2.190471	6.322097	-3.09654
H	0.839283	6.125411	-4.2318
C	2.393212	4.613961	-4.3492
O	3.542849	4.461146	-4.88892
O	1.660339	3.663169	-3.97654
C	8.816509	-4.17662	-4.73902
C	7.797128	-3.52878	-3.86079
C	6.50808	-3.1225	-4.09007
N	8.031828	-3.20299	-2.53328
C	6.919831	-2.62445	-2.01759
N	5.975284	-2.55949	-2.94243
H	9.136621	-5.15103	-4.34815
H	8.39621	-4.34085	-5.73493
H	5.918051	-3.20807	-4.98981
H	6.858327	-2.32198	-0.98022
H	8.884912	-3.36477	-2.01643
C	4.467265	-7.68759	0.963625
H	5.198854	-8.02947	0.220637
C	3.901769	-6.31508	0.533656
H	4.710707	-5.57238	0.510647
H	3.542593	-6.39579	-0.49985
C	2.766073	-5.80553	1.430968
H	1.971205	-6.5643	1.480131
H	3.120981	-5.67301	2.459098
C	2.188587	-4.48334	0.912075
H	2.965967	-3.72204	0.841156
H	1.805656	-4.60366	-0.10802
N	1.100235	-3.99558	1.762353
H	0.271858	-4.5746	1.81669
C	1.025974	-2.83233	2.437228
N	2.023395	-1.96519	2.511793
H	2.880696	-2.06446	1.963854
H	1.889436	-1.06106	3.010633
N	-0.16753	-2.53869	3.017039
H	-0.7866	-3.33909	3.215043
H	-0.19031	-1.83342	3.762183
C	5.105611	-7.6341	2.345853
O	4.478099	-7.84355	3.378414
N	6.439497	-7.30253	2.349084
H	6.851908	-6.9222	1.505082

C	7.104828	-6.90421	3.567563
H	6.356753	-6.88408	4.366969
C	7.777495	-5.54067	3.369974
O	7.981278	-5.10316	2.231008
N	8.162654	-4.9088	4.498866
H	7.895727	-5.31856	5.383735
C	8.886127	-3.63253	4.514286
H	9.491384	-3.60024	3.604828
C	7.979563	-2.39269	4.57633
H	8.622853	-1.50517	4.536246
H	7.36476	-2.36603	3.670921
C	7.114405	-2.32552	5.839104
H	6.482287	-3.2174	5.936603
H	7.748132	-2.27853	6.733574
S	6.034771	-0.84454	5.937967
C	4.714953	-1.31391	4.764376
H	4.012432	-0.47778	4.703018
H	5.109354	-1.50128	3.761743
H	4.176937	-2.19955	5.118324
O	2.322307	-1.16866	-2.62365
O	7.111559	-2.60092	1.167321
Fe	3.956765	-1.7359	-2.68903
C	-0.13649	-2.69419	-5.55133
H	0.314619	-3.1417	-6.44596
H	0.158497	-3.31938	-4.70364
C	-1.66389	-2.8519	-5.67483
H	-1.86776	-3.71207	-6.32345
C	-2.47945	-3.11135	-4.37132
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O	-3.7433	-3.08975	-4.53961
N	-2.37275	-1.68866	-6.33722
H	-2.43532	-0.80701	-5.69936
H	-3.34561	-1.99093	-6.45408
H	-1.97247	-1.43439	-7.24337
C	0.470179	-1.28952	-5.39282
H	0.090981	-0.6319	-6.19262
H	1.544307	-1.38695	-5.59105
C	0.291042	-0.58532	-4.04333
H	1.207014	-0.92993	-3.34801
H	-0.60957	-0.8954	-3.50652
C	0.360673	0.920219	-4.2294
H	1.3286	1.247737	-4.6076
H	-0.40746	1.225972	-4.94372
N	0.083098	1.69962	-2.98477
H	7.877689	-7.6313	3.859091
H	9.56876	-3.65895	5.371914
H	-3.20826	-7.74028	3.206468

H	3.66206	-8.42776	1.007214
H	-7.69633	-1.46093	4.570952
H	-4.35336	1.01928	6.228302
H	9.713275	-3.55447	-4.85476
H	8.27757	2.271523	-5.06733
H	2.421991	6.738087	-4.809
H	5.388241	6.214778	-2.85883
H	-0.54794	7.196138	5.599527
H	-5.83043	1.33054	-4.79244
H	-7.11583	-3.81062	-5.52839
H	-10.8369	1.318148	-2.63287
H	7.452765	-3.45648	1.493282
H	6.139823	-2.65333	1.245865
C	3.242808	-4.03706	-3.40994
O	3.417706	-3.73985	-2.18438
O	3.472801	-3.1705	-4.30699
C	2.747205	-5.41797	-3.77797
H	2.768583	-5.56232	-4.85992
H	1.720563	-5.54125	-3.41458
H	3.363509	-6.17844	-3.28804
H	0.429204	2.667502	-3.15304
H	-0.94633	1.655438	-2.80228
H	0.576173	1.322185	-2.13706
O	1.386743	0.670164	-0.71968
H	1.844745	-0.07383	-1.1704
H	0.711704	0.258298	-0.12286
O	-3.16676	-0.06263	-0.08609
H	-3.03954	0.427098	-0.92896
H	-2.29203	-0.00222	0.374779
O	-0.63961	-0.24869	0.989905
H	-0.63539	-1.11036	1.448647
H	-0.34567	0.402773	1.703825

⁵IM1_{B,C5}

C	-3.36057	-0.75159	6.189462
H	-2.83925	-0.42682	5.280488
C	-2.34397	-1.23841	7.22779
H	-2.80584	-1.26341	8.221027
H	-2.05485	-2.2664	6.998949
C	-1.08374	-0.36459	7.275049
H	-1.33355	0.678671	7.509665
H	-0.42619	-0.71313	8.083461
C	-0.27779	-0.41749	5.973182
O	-0.379	-1.38603	5.202246
N	0.54566	0.614557	5.727572
H	0.591535	1.401483	6.358126
H	1.066181	0.658148	4.838374
C	-4.38089	-1.81244	5.764218
O	-4.40985	-2.95389	6.244966
N	-5.23813	-1.39831	4.802689
H	-5.09835	-0.47344	4.402375
C	-6.21475	-2.27322	4.156715
H	-6.88876	-1.62179	3.591629
C	-5.59799	-3.33525	3.22437
H	-5.15507	-4.12976	3.834688
H	-6.42233	-3.79631	2.661911
C	-4.5265	-2.7875	2.272937
H	-3.70314	-2.3764	2.868444
H	-4.91127	-1.95953	1.666793
C	-3.92945	-3.85153	1.343036
H	-2.98825	-3.49618	0.922957
H	-3.70449	-4.76322	1.912057
N	-4.80431	-4.21307	0.224049
H	-5.65411	-4.7474	0.412889
C	-4.50113	-4.0429	-1.07394
N	-3.48315	-3.27822	-1.47249
H	-3.21848	-2.42674	-0.93587
H	-3.2343	-3.33517	-2.46651
N	-5.23015	-4.69822	-2.00298
H	-5.96366	-5.31986	-1.68476
H	-5.26137	-4.30146	-2.94535
C	-1.21048	-7.33998	2.750432
H	-0.23515	-7.73602	3.060486
H	-1.10798	-6.99312	1.714466
C	-1.66244	-6.23404	3.653178
N	-0.9485	-5.05434	3.78039
C	-1.61649	-4.3209	4.660483
H	-1.33893	-3.32791	4.992668
N	-2.71919	-4.96366	5.11037

H	-3.42341	-4.5204	5.702656
C	-2.76835	-6.18598	4.471757
H	-3.55226	-6.90384	4.661575
C	6.261476	2.793011	-6.24198
C	6.151448	3.61129	-4.95528
C	5.062824	1.88047	-6.59334
O	7.015389	3.52278	-4.07707
C	4.703587	0.8849	-5.52805
C	5.277299	-0.29065	-5.10327
N	3.597709	1.069957	-4.72221
C	3.526392	0.038456	-3.86394
N	4.535104	-0.81333	-4.06273
H	6.425167	3.486569	-7.07747
H	4.176277	2.484224	-6.81641
H	5.314837	1.351232	-7.52025
H	6.167067	-0.78333	-5.46346
H	2.763157	-0.06729	-3.1077
H	2.982831	1.936383	-4.77152
N	5.113169	4.492927	-4.86285
H	4.228496	4.287315	-5.33105
C	5.009948	5.380154	-3.70813
H	6.025762	5.644418	-3.40095
C	4.249825	4.760901	-2.52767
O	3.217555	5.27897	-2.08803
N	4.777727	3.611505	-2.05041
C	4.016401	2.680719	-1.21942
C	3.499446	3.366368	0.06185
C	4.919991	1.493677	-0.85568
O	4.263404	3.775388	0.929651
C	4.183087	0.3809	-0.08682
C	4.985606	-0.91289	-0.03513
O	5.226313	-1.47743	1.051112
O	5.411182	-1.38154	-1.16587
H	5.653535	3.297906	-2.46336
H	3.158544	2.322456	-1.8046
H	5.334633	1.075874	-1.77907
H	5.751655	1.874537	-0.2518
H	3.224789	0.151001	-0.57423
H	3.965966	0.6948	0.937278
N	2.143599	3.420165	0.152401
H	1.59559	3.117643	-0.64192
C	1.423396	3.893756	1.328503
H	0.363131	3.762341	1.086306
C	1.708768	3.035884	2.566662
H	2.775214	3.046342	2.802044
H	1.188713	3.478702	3.423535
C	1.235688	1.590207	2.377571

O	0.380467	1.367332	1.488739
O	1.751551	0.715099	3.157404
C	1.603729	5.395231	1.611083
O	1.256344	5.870921	2.698762
N	2.033974	6.168335	0.581623
H	2.388596	5.725683	-0.26566
C	2.281162	7.596089	0.773423
H	2.731547	7.728275	1.763986
C	3.240561	8.132905	-0.29244
H	4.216275	7.645166	-0.20607
H	3.36077	9.209298	-0.14965
H	2.855875	7.947733	-1.30086
C	0.999095	8.456762	0.833501
O	1.070138	9.649276	1.110171
N	-0.17014	7.799639	0.595121
H	-0.11929	6.822591	0.339453
C	-1.47942	8.392979	0.782208
H	-1.32294	9.477102	0.798322
C	-2.43366	8.046971	-0.38714
H	-2.04186	8.529116	-1.29006
H	-3.39921	8.501547	-0.15101
C	-2.59591	6.558715	-0.62616
C	-1.72031	5.866828	-1.47818
H	-0.9437	6.417544	-2.0055
C	-1.83434	4.486573	-1.67136
H	-1.13155	3.97577	-2.32608
C	-2.84629	3.776164	-1.02039
H	-2.94871	2.706577	-1.18137
C	-3.73138	4.453448	-0.17671
H	-4.52505	3.906488	0.327057
C	-3.60496	5.82995	0.022968
H	-4.28689	6.352661	0.687974
C	-2.13388	8.050229	2.14573
O	-3.3156	8.344111	2.343302
N	-1.32899	7.476178	3.071563
H	-0.38046	7.208322	2.821894
C	-1.76479	7.206882	4.434784
H	-2.79366	7.56439	4.509808
C	-1.64294	5.726998	4.828149
H	-0.58515	5.439484	4.76589
H	-1.93365	5.638558	5.886664
C	-2.4686	4.736608	3.986419
H	-2.13177	4.823863	2.944755
C	-2.19459	3.297232	4.448677
H	-2.69581	2.56733	3.802967
H	-1.12368	3.063961	4.431469
H	-2.54773	3.145623	5.480493

C	-3.97391	5.04344	4.0139
H	-4.52796	4.312055	3.410191
H	-4.36605	5.007498	5.041415
H	-4.19503	6.033735	3.603301
C	-6.39975	0.484182	-3.872
H	-6.08928	0.513051	-4.92339
C	-5.2422	-0.07949	-3.0244
H	-5.3349	0.237639	-1.98327
H	-5.25083	-1.1763	-3.03063
C	-3.84668	0.317381	-3.52818
O	-3.62954	0.337042	-4.78482
O	-2.97247	0.560753	-2.65874
C	-7.70166	-0.29971	-3.7728
O	-8.76038	0.208312	-3.39297
N	-7.63722	-1.61508	-4.15428
H	-6.73628	-2.06582	-4.33322
C	-8.83538	-2.42187	-4.29264
H	-9.62278	-1.83053	-4.77291
C	-9.45923	-2.97404	-3.00719
O	-10.414	-3.75105	-3.06618
N	-8.92141	-2.5383	-1.84048
H	-8.10061	-1.95009	-1.88831
C	-9.5434	-2.77492	-0.54689
H	-10.5134	-3.23399	-0.7668
C	-8.70632	-3.71639	0.327996
H	-9.23519	-3.86873	1.27541
H	-7.75067	-3.24566	0.578256
C	-8.38373	-5.07426	-0.28344
O	-7.32035	-5.65475	-0.00995
N	-9.31156	-5.65271	-1.08068
H	-10.0109	-5.1092	-1.58452
H	-9.04902	-6.54132	-1.48909
C	-9.87743	-1.46911	0.219095
O	-10.1061	-1.5227	1.423033
N	-9.9445	-0.34502	-0.53766
H	-9.74774	-0.39135	-1.53327
C	-10.3725	0.943674	-0.00686
H	-10.637	0.784139	1.040689
C	-9.29574	2.04226	-0.14588
H	-8.93864	2.046632	-1.18333
H	-9.79011	3.007663	0.020371
C	-8.13839	1.895068	0.8171
C	-6.99608	1.151856	0.488822
H	-6.92713	0.701098	-0.49743
C	-5.93609	0.991946	1.382736
H	-5.03699	0.447531	1.103374
C	-6.02573	1.58118	2.646086

O	-4.98282	1.368911	3.531388
H	-4.9813	2.073933	4.199483
C	-7.14698	2.334739	2.999187
H	-7.2076	2.79759	3.981884
C	-8.18745	2.489392	2.084396
H	-9.05332	3.084052	2.366348
C	0.924273	5.215248	-4.5376
H	1.367037	5.808493	-3.72947
H	-0.16393	5.268674	-4.44274
C	1.407567	3.778472	-4.37869
O	2.389447	3.408443	-5.10289
O	0.831905	3.052058	-3.52068
C	10.02871	-3.29742	-5.27598
C	8.933466	-2.97343	-4.31413
C	7.571812	-2.90513	-4.45496
N	9.159535	-2.65305	-2.98293
C	7.971302	-2.40616	-2.37886
N	6.98751	-2.54523	-3.25367
H	10.62002	-4.1624	-4.94911
H	9.603924	-3.53737	-6.25456
H	6.969394	-3.11254	-5.32689
H	7.87047	-2.19443	-1.32024
H	10.05733	-2.62226	-2.52064
C	6.817933	-6.3323	2.049914
H	7.623357	-6.5962	1.349702
C	5.782092	-5.47752	1.301686
H	6.248554	-4.56478	0.918516
H	5.46526	-6.03413	0.410344
C	4.545057	-5.11636	2.135253
H	4.098099	-6.02688	2.560018
H	4.828246	-4.48035	2.983603
C	3.505164	-4.38546	1.276377
H	3.932123	-3.46934	0.866803
H	3.226114	-5.00066	0.413407
N	2.273143	-4.05182	1.996366
H	1.62799	-4.80635	2.194942
C	1.893437	-2.84163	2.444656
N	2.680311	-1.77707	2.43325
H	3.635093	-1.79288	2.071751
H	2.275055	-0.84776	2.672694
N	0.610442	-2.70889	2.879519
H	0.103203	-3.58849	3.049505
H	0.431218	-2.00172	3.604219
C	7.478533	-5.72532	3.288656
O	7.577934	-6.3597	4.337813
N	7.998154	-4.46672	3.155243
H	7.969076	-3.96918	2.262127

C	8.795235	-3.93058	4.238365
H	8.36034	-4.27816	5.180046
C	8.919828	-2.40969	4.201198
O	8.993985	-1.75788	3.155429
N	9.035026	-1.82205	5.418017
H	8.911042	-2.39234	6.241905
C	9.271313	-0.38537	5.579649
H	10.03131	-0.09103	4.849638
C	8.013734	0.474894	5.378984
H	8.303611	1.531467	5.426551
H	7.641562	0.294873	4.366116
C	6.913255	0.202665	6.408385
H	6.681689	-0.86832	6.459845
H	7.235134	0.514911	7.409364
S	5.351922	1.113959	6.09347
C	4.738331	0.201901	4.633711
H	3.798463	0.665063	4.321726
H	5.440495	0.251644	3.796451
H	4.54559	-0.84627	4.885576
O	3.032476	-2.59485	-2.24915
O	7.825743	-2.63964	0.794428
Fe	4.85619	-2.44116	-2.69075
C	-2.32111	-2.6	-6.95233
H	-2.37245	-2.7366	-8.04102
H	-1.80707	-3.47852	-6.5497
C	-3.75297	-2.67326	-6.40731
H	-4.31268	-3.38878	-7.02183
C	-3.95303	-3.14286	-4.93501
O	-2.96703	-3.55991	-4.3079
O	-5.16476	-3.07678	-4.53935
N	-4.50321	-1.36703	-6.51725
H	-4.14675	-0.61223	-5.76904
H	-5.47745	-1.56456	-6.27241
H	-4.4658	-0.96818	-7.45849
C	-1.47649	-1.3407	-6.68373
H	-2.01046	-0.43992	-7.0324
H	-0.60473	-1.41047	-7.36088
C	-1.00845	-1.1148	-5.28348
H	2.626475	-3.23754	-2.85401
H	-1.06547	-1.91086	-4.54832
C	-0.26054	0.141687	-4.99427
H	0.810722	0.053947	-5.23632
H	-0.65158	0.966635	-5.60057
N	-0.34004	0.578793	-3.57133
H	9.822966	-4.33245	4.212659
H	9.691592	-0.23846	6.58095
H	-1.92509	-8.16899	2.757566

H	6.37115	-7.27217	2.389253
H	-6.80664	-2.77122	4.93165
H	-3.90131	0.129321	6.562309
H	10.71906	-2.4548	-5.41085
H	7.16578	2.189826	-6.12854
H	1.239466	5.634699	-5.49677
H	4.473279	6.285133	-3.99847
H	-1.15759	7.806712	5.126839
H	-6.62462	1.513054	-3.58129
H	-8.61563	-3.27341	-4.94186
H	-11.2764	1.258156	-0.54462
H	8.317111	-2.14174	1.48183
H	6.898409	-2.32355	0.883784
C	4.968568	-4.88629	-3.30888
O	5.232179	-4.52884	-2.12281
O	4.622394	-4.00662	-4.16851
C	5.099644	-6.33247	-3.72489
H	6.08764	-6.4801	-4.17777
H	4.3456	-6.58494	-4.47498
H	5.01525	-6.99229	-2.85866
H	0.134745	1.513351	-3.48635
H	-1.34152	0.660546	-3.26907
H	0.152756	-0.07613	-2.91184
O	1.107939	-0.77812	-1.6759
H	1.745718	-1.5245	-1.79647
H	0.627494	-0.91585	-0.82058
O	-3.02802	-0.86009	-0.18817
H	-3.01523	-0.25933	-0.96562
H	-2.10684	-0.83144	0.178283
O	-0.39858	-0.95858	0.623436
H	-0.19911	-1.63064	1.306136
H	-0.10998	-0.07777	1.036614

⁵TS2_{B,C5}

C	-3.70152	1.192674	5.992086
H	-3.08469	1.115176	5.088052
C	-2.855	0.837134	7.218715
H	-3.3942	1.112274	8.132462
H	-2.71425	-0.24554	7.261135
C	-1.48348	1.522869	7.221267
H	-1.58927	2.612889	7.132743
H	-0.98634	1.344567	8.184773
C	-0.53818	1.02793	6.120308
O	-0.80194	0.025024	5.438269
N	0.604658	1.719351	5.962874
H	0.763679	2.57508	6.474848
H	1.215707	1.506222	5.162656
C	-4.91413	0.28193	5.789518
O	-5.11827	-0.73145	6.472822
N	-5.73467	0.648192	4.774729
H	-5.46983	1.433024	4.186386
C	-6.82211	-0.19488	4.27634
H	-7.33421	0.392704	3.508963
C	-6.36165	-1.54817	3.695695
H	-6.12688	-2.22046	4.527618
H	-7.21491	-1.9883	3.160979
C	-5.13393	-1.44788	2.782018
H	-4.34251	-0.91402	3.319202
H	-5.34649	-0.85288	1.886698
C	-4.55275	-2.80797	2.371244
H	-3.4941	-2.70462	2.125735
H	-4.61259	-3.51368	3.207698
N	-5.20491	-3.43653	1.216842
H	-6.04635	-4.00124	1.359282
C	-4.60621	-3.57342	0.022905
N	-3.54714	-2.84357	-0.32244
H	-3.39662	-1.87396	0.018415
H	-3.00355	-3.1609	-1.13403
N	-5.08961	-4.48509	-0.84878
H	-5.75241	-5.17655	-0.52281
H	-4.74979	-4.49001	-1.81122
C	-2.20205	-6.14555	4.439287
H	-1.2275	-6.45527	4.836904
H	-2.12187	-6.14271	3.344644
C	-2.59984	-4.79995	4.962035
N	-1.84163	-3.66713	4.720691
C	-2.46884	-2.67453	5.336008
H	-2.13211	-1.64621	5.373464
N	-3.59003	-3.10429	5.960916

H	-4.25561	-2.47266	6.408459
C	-3.69298	-4.46064	5.727951
H	-4.50076	-5.05489	6.128234
C	7.099514	1.799568	-6.10429
C	6.938403	2.712712	-4.88632
C	5.831845	1.061568	-6.60759
O	7.653382	2.555845	-3.89052
C	5.093102	0.307215	-5.54169
C	5.195315	-0.96207	-5.01024
N	4.099944	0.93091	-4.81942
C	3.646699	0.057707	-3.90541
N	4.278689	-1.11005	-3.98949
H	7.507866	2.39362	-6.93293
H	5.140023	1.775151	-7.07141
H	6.143924	0.373721	-7.40173
H	5.862882	-1.76675	-5.28326
H	2.902047	0.300625	-3.16601
H	3.69784	1.887767	-5.05414
N	6.039132	3.732742	-4.9717
H	5.238128	3.676836	-5.59903
C	5.877836	4.675337	-3.86877
H	6.868846	4.878309	-3.45185
C	4.942032	4.188159	-2.75112
O	3.909861	4.804661	-2.45829
N	5.327857	3.049819	-2.13552
C	4.457754	2.337519	-1.20802
C	4.076394	3.242639	-0.01817
C	5.150077	1.047968	-0.73734
O	4.91544	3.795826	0.681455
C	4.265779	0.218582	0.213277
C	4.569667	-1.27904	0.203684
O	4.740293	-1.86415	1.311305
O	4.608738	-1.8739	-0.92205
H	6.216382	2.638874	-2.41625
H	3.538298	2.069427	-1.74391
H	5.392533	0.448343	-1.62118
H	6.091023	1.316453	-0.24244
H	3.215244	0.312886	-0.0915
H	4.343622	0.589809	1.238475
N	2.730088	3.374636	0.164472
H	2.112042	2.798003	-0.39042
C	2.125746	4.125337	1.25811
H	1.045685	4.062076	1.085803
C	2.36856	3.469843	2.622699
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H	2.032669	4.157639	3.407508
C	1.578419	2.158711	2.736481

O	0.520403	2.071479	2.059297
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C	2.43496	5.629187	1.239362
O	2.162268	6.325454	2.225174
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C	4.189832	7.854454	-1.15396
H	5.12955	7.317694	-0.99272
H	4.391004	8.927363	-1.20174
H	3.770703	7.525117	-2.11014
C	2.004842	8.53132	-0.07785
O	2.159297	9.74284	0.028815
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H	-0.90804	8.74915	-2.26004
H	-2.31398	8.924665	-1.19656
C	-1.71986	6.887279	-1.55826
C	-0.91254	6.076602	-2.37037
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C	-1.19718	4.71994	-2.55012
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C	-2.30682	4.151951	-1.92045
H	-2.5456	3.10037	-2.06317
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H	-0.24975	5.755619	3.83653
H	-1.46949	6.251779	5.009195
C	-2.28496	5.511161	3.143509
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C	-3.68414	6.126094	3.306708
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C	-5.47865	-0.8402	-4.71771
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H	-5.0989	-0.14676	-2.6915
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O	-9.79866	-4.49603	-3.14919
N	-8.47323	-2.92524	-2.15954
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C	-9.35122	-2.67389	-1.02643
H	-10.2977	-3.16486	-1.27691
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H	-9.51995	-3.06898	1.076462
H	-7.87902	-2.71974	0.563702
C	-8.44938	-4.73856	0.253936
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H	-8.98405	-6.54107	-0.46257
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C	-9.92615	1.02043	-1.93661
H	-10.4897	1.195506	-1.01765
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C	-7.95821	2.264827	-0.82176
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H	-6.38385	0.89648	-1.34587
C	-5.98052	1.812193	0.547478
H	-5.02482	1.310935	0.680834
C	-6.44074	2.716461	1.507474

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C	1.677988	5.064065	-5.21619
H	2.081405	5.592923	-4.34385
H	0.588535	5.151662	-5.20767
C	2.122918	3.611352	-5.11098
O	3.262228	3.32354	-5.60038
O	1.378785	2.779071	-4.52278
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C	4.98377	-7.16849	2.679486
H	5.64359	-7.72039	1.994713
C	4.205561	-6.11482	1.875488
H	4.902912	-5.42309	1.392188
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C	3.186287	-5.32586	2.709009
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C	2.49466	-4.24928	1.863694
H	3.22446	-3.50819	1.532915
H	2.070047	-4.68667	0.951741
N	1.414698	-3.57155	2.590868
H	0.605235	-4.13191	2.826478
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C	9.224427	-1.807	5.410785
H	9.959642	-1.88526	4.605143
C	8.282615	-0.6244	5.13142
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C	7.289894	-0.3549	6.266156
H	6.735232	-1.26504	6.526839
H	7.82029	-0.02856	7.169194
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H	4.521679	-0.77066	5.214498
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C	-0.42966	-3.9505	-4.80351
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H	-2.14539	-5.16215	-5.25347
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H	-4.03823	2.23684	6.041023
H	9.065483	-5.50608	-4.87273
H	7.85823	1.068809	-5.81395
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H	7.396653	-3.53278	1.696821
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C	2.530477	-4.9498	-3.00225
O	2.607847	-4.5468	-1.80558
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C	2.086224	-6.37926	-3.27244
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H	1.703023	-6.49387	-4.28981
H	1.337271	-6.69622	-2.54135
H	0.321595	1.816318	-3.62657
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C	-2.2341	-5.16033	4.830754
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H	5.53614	0.462384	-7.56904
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H	2.834012	-0.24171	-3.06083
H	3.301677	1.57165	-4.88548
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H	3.545225	7.765123	-2.07377
C	1.737361	8.592013	-0.00916
O	1.878362	9.796424	0.1721
N	0.532256	7.993671	-0.22856
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H	-1.21876	8.708793	-2.21908
H	-2.60571	8.906414	-1.13465
C	-1.99202	6.862883	-1.42832
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H	-0.29343	6.437384	-2.68744
C	-1.40898	4.64567	-2.27018
H	-0.72518	4.01915	-2.83808
C	-2.52827	4.099479	-1.63728
H	-2.74264	3.037091	-1.72435
C	-3.37662	4.931361	-0.90107
H	-4.25188	4.512875	-0.40965
C	-3.10833	6.297811	-0.79153
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C	-1.33219	6.275815	3.994951
H	-0.33687	5.81955	3.910133
H	-1.60269	6.247139	5.062507
C	-2.33824	5.42887	3.193526
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H	-4.10168	5.949685	4.381047
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H	-5.24272	0.053057	-2.27243
H	-4.90881	-1.56022	-2.89848
C	-3.56832	-0.08891	-3.61122
O	-3.19951	-0.36188	-4.79916
O	-2.84112	0.461031	-2.74189
C	-7.30607	-1.13306	-4.08803
O	-8.42685	-0.63434	-3.95161
N	-7.12548	-2.49174	-4.09592
H	-6.18509	-2.89096	-4.11631
C	-8.25436	-3.40113	-4.15978
H	-8.99235	-3.02766	-4.87863
C	-9.03189	-3.64091	-2.86238
O	-9.96367	-4.44745	-2.84031
N	-8.64912	-2.91095	-1.78535
H	-7.8339	-2.3203	-1.8805
C	-9.41994	-2.86176	-0.55313
H	-10.3509	-3.39731	-0.76843
C	-8.68519	-3.53932	0.610561
H	-9.32957	-3.49887	1.495623
H	-7.77957	-2.97766	0.858372
C	-8.26194	-4.9827	0.367218
O	-7.21184	-5.42775	0.858822
N	-9.09208	-5.77867	-0.34713
H	-9.74182	-5.40025	-1.03479
H	-8.75832	-6.71981	-0.51583
C	-9.85931	-1.42951	-0.15669
O	-10.2408	-1.21819	0.989925
N	-9.83529	-0.50601	-1.15047
H	-9.53292	-0.77123	-2.08401
C	-10.3578	0.845361	-0.98231
H	-10.7451	0.911465	0.036669
C	-9.30562	1.943336	-1.24973
H	-8.82073	1.729144	-2.21046
H	-9.84866	2.88843	-1.3783
C	-8.2702	2.105197	-0.15763
C	-7.05002	1.416674	-0.19184
H	-6.83821	0.764118	-1.03424
C	-6.08941	1.562066	0.809988
H	-5.1303	1.052708	0.751697
C	-6.36073	2.410619	1.885795

O	-5.40568	2.511926	2.882337
H	-5.54723	3.33275	3.381618
C	-7.5678	3.110293	1.948915
H	-7.77367	3.77212	2.787797
C	-8.50625	2.957054	0.929059
H	-9.43825	3.515247	0.9823
C	1.600295	5.042146	-4.94019
H	2.101508	5.644376	-4.17367
H	0.5239	5.21974	-4.86617
C	1.927606	3.579975	-4.66353
O	2.880143	3.060798	-5.33208
O	1.268144	2.982527	-3.7669
C	9.094524	-5.7351	-4.60111
C	8.109631	-5.02039	-3.73576
C	6.897025	-4.43961	-4.00194
N	8.30102	-4.81095	-2.3779
C	7.238766	-4.13339	-1.87732
N	6.365859	-3.89258	-2.84629
H	9.267136	-6.76447	-4.26205
H	8.721317	-5.78264	-5.62769
H	6.375077	-4.38161	-4.94654
H	7.143127	-3.8528	-0.83019
H	9.103109	-5.10442	-1.83784
C	5.67145	-6.86014	3.252457
H	6.366351	-7.4424	2.630443
C	4.784204	-6.00345	2.335137
H	5.404431	-5.32466	1.73942
H	4.295274	-6.67804	1.617661
C	3.70559	-5.2036	3.078435
H	3.053053	-5.88958	3.637548
H	4.166062	-4.5355	3.816576
C	2.861408	-4.37125	2.104265
H	3.479666	-3.61006	1.623089
H	2.473357	-5.01122	1.300985
N	1.716418	-3.72164	2.741414
H	0.961854	-4.31956	3.056244
C	1.53096	-2.40593	2.962898
N	2.457719	-1.48554	2.760732
H	3.381153	-1.68494	2.368068
H	2.191775	-0.48336	2.871705
N	0.289101	-2.02281	3.367864
H	-0.30976	-2.78146	3.719656
H	0.210688	-1.16484	3.92737
C	6.51481	-6.14022	4.307216
O	6.666934	-6.61363	5.432007
N	7.130772	-4.98015	3.933856
H	7.060238	-4.60913	2.984597

C	8.035079	-4.3555	4.876747
H	7.540699	-4.27631	5.851587
C	8.52965	-2.99355	4.397145
O	8.693016	-2.71167	3.206445
N	8.851561	-2.12776	5.389053
H	8.639357	-2.38583	6.341995
C	9.377779	-0.7876	5.121405
H	10.06897	-0.87169	4.278529
C	8.284829	0.242189	4.7908
H	8.766743	1.181807	4.495401
H	7.733832	-0.11836	3.916034
C	7.325778	0.508076	5.955728
H	6.918701	-0.43102	6.351629
H	7.852261	1.005819	6.779164
S	5.918962	1.610212	5.53983
C	4.902564	0.468783	4.538256
H	4.01121	1.014376	4.216106
H	5.433636	0.12042	3.647538
H	4.5873	-0.39356	5.135642
O	0.794334	-2.12	-3.72655
O	6.99914	-3.65265	1.226836
Fe	4.561961	-2.79827	-2.49233
C	-1.2072	-3.66327	-5.81762
H	-1.02026	-4.10522	-6.80576
H	-0.73083	-4.32736	-5.08968
C	-2.7201	-3.74812	-5.55965
H	-3.10023	-4.64833	-6.05685
C	-3.22235	-3.83882	-4.08684
O	-2.37651	-3.96602	-3.18959
O	-4.49403	-3.79409	-3.9755
N	-3.51668	-2.60284	-6.15534
H	-3.37866	-1.66829	-5.60612
H	-4.50224	-2.85039	-6.01963
H	-3.32803	-2.45512	-7.14981
C	-0.52463	-2.28157	-5.80307
H	-1.07409	-1.59381	-6.46068
H	0.468469	-2.39925	-6.25404
C	-0.32649	-1.60588	-4.43372
H	0.907135	-3.10535	-3.81416
H	-1.234	-1.72495	-3.83189
C	-0.06581	-0.11279	-4.64748
H	0.922018	0.032284	-5.09134
H	-0.83094	0.314725	-5.29527
N	-0.11782	0.65845	-3.37026
H	8.920951	-4.98967	5.044168
H	9.954057	-0.48075	6.001659
H	-2.57573	-7.24011	4.414506

H	5.069495	-7.58602	3.808409
H	-7.18486	-1.10247	5.085423
H	-4.02888	1.835947	6.196385
H	10.06571	-5.22461	-4.62382
H	7.467744	1.158251	-6.21939
H	1.965513	5.350325	-5.9234
H	5.327481	5.683753	-4.35979
H	-0.5248	8.258058	4.269155
H	-6.35972	0.746579	-4.3161
H	-7.90426	-4.37295	-4.51775
H	-11.1974	0.981495	-1.67649
H	7.716404	-3.19979	1.717875
H	6.244991	-3.01381	1.246809
C	2.484494	-4.94255	-3.2911
O	1.451376	-4.7137	-3.93767
O	3.112983	-4.05873	-2.57934
C	3.072014	-6.34684	-3.26725
H	3.089016	-6.71883	-2.23676
H	4.110427	-6.32344	-3.61649
H	2.484747	-7.02306	-3.89124
H	0.332568	1.595148	-3.51265
H	-1.12201	0.742757	-3.08743
H	0.40385	0.177997	-2.59505
O	1.269666	-0.78584	-1.41032
H	1.086383	-1.55949	-1.98933
H	0.688523	-0.84712	-0.60869
O	-3.06305	-0.39866	-0.02127
H	-3.02274	-0.00055	-0.91935
H	-2.13496	-0.35034	0.322782
O	-0.42318	-0.59072	0.764806
H	-0.34106	-1.17639	1.543934
H	-0.0582	0.299988	1.085635

Model 3 structures:

¹Re_C

C	-0.65538	-6.41822	-2.89492
H	-0.38917	-5.98349	-1.91942
C	-0.62783	-5.37169	-4.00559
H	-0.86387	-5.87026	-4.9582
H	-1.42247	-4.63488	-3.83961
C	0.69163	-4.62009	-4.14219
H	0.971848	-4.15042	-3.18521
H	1.522863	-5.29104	-4.40547
C	0.583267	-3.48951	-5.15815
O	-0.45461	-2.82401	-5.26241
N	1.671563	-3.24796	-5.90761
H	2.600378	-3.64356	-5.71106
H	1.618525	-2.48145	-6.57012
C	-1.99873	-7.1343	-2.80281
O	-2.64409	-7.42196	-3.81704
N	-2.40282	-7.47237	-1.56277
H	-1.95314	-7.07555	-0.73189
C	-3.55655	-8.32146	-1.30325
H	-3.43969	-8.69006	-0.27318
C	-4.92237	-7.64349	-1.4546
H	-5.09509	-7.44329	-2.52449
H	-5.68928	-8.37829	-1.15345
C	-5.08046	-6.36031	-0.64055
H	-4.3668	-5.59685	-0.98939
H	-4.82796	-6.53904	0.417405
C	-6.494	-5.78891	-0.73973
H	-6.78837	-5.6961	-1.80364
H	-7.21038	-6.48978	-0.27212
N	-6.56033	-4.4915	-0.08706
H	-5.66348	-4.00251	0.086414
C	-7.63443	-3.70853	-0.04718
N	-8.83126	-4.13477	-0.54676
H	-8.99553	-5.13258	-0.6073
H	-9.63018	-3.54903	-0.30119
N	-7.5369	-2.47758	0.438544
H	-6.68022	-2.26594	0.987444
H	-8.3789	-1.89579	0.474534
C	-7.46048	-2.89753	-4.48128
H	-7.82315	-3.93691	-4.46266
C	-6.16496	-2.78374	-3.64697
H	-5.88171	-1.72616	-3.56652
H	-6.31999	-3.14207	-2.61898
C	-5.06052	-3.55862	-4.28587
N	-4.37166	-3.08382	-5.38828

C	-3.56777	-4.06812	-5.77412
H	-2.84944	-4.02325	-6.59043
N	-3.71556	-5.15374	-4.97918
H	-3.18662	-6.0362	-4.95768
C	-4.65161	-4.84651	-4.02279
H	-4.93395	-5.55507	-3.25565
C	-8.52795	-1.93293	-4.01614
O	-8.50557	-0.73955	-4.32297
N	-9.48867	-2.45677	-3.21256
H	-9.34963	-3.39009	-2.83811
C	-10.525	-1.63275	-2.5948
H	-10.8037	-0.87534	-3.34194
C	-11.7444	-2.46247	-2.22824
H	-12.5178	-1.8282	-1.7733
H	-11.4971	-3.24752	-1.49848
H	-12.1618	-2.938	-3.1272
C	-9.90201	-0.91083	-1.38203
O	-9.97349	-1.38646	-0.24143
N	-9.23791	0.204589	-1.71767
H	-9.15951	0.368475	-2.7229
C	-8.43293	1.061244	-0.85979
H	-8.28351	0.575837	0.114973
C	-7.08531	1.380992	-1.53264
H	-7.30304	1.526273	-2.60744
C	-6.48148	2.681835	-1.00201
H	-7.15642	3.539037	-1.16317
H	-6.26597	2.579793	0.072422
H	-5.52922	2.890448	-1.50998
C	-6.10003	0.217153	-1.39473
H	-6.55747	-0.74058	-1.67367
H	-5.75318	0.135116	-0.35429
H	-5.22052	0.370743	-2.0399
C	-2.45346	1.472741	5.955864
H	-1.51947	2.052225	6.017303
C	-2.10791	-0.0166	5.944292
H	-1.35791	-0.1848	5.148941
C	-1.49342	-0.45259	7.2703
H	-1.27186	-1.532	7.262293
H	-2.19781	-0.27025	8.096208
H	-0.55793	0.092576	7.469508
O	-3.29041	-0.74202	5.652715
H	-3.03905	-1.64636	5.335959
C	-3.21744	1.913126	4.735394
O	-4.18179	2.698211	4.831403
N	-2.85966	1.415593	3.539663
H	-2.10784	0.727795	3.436421
C	-3.73207	1.535192	2.394087

H	-3.9147	2.583091	2.122218
H	-3.23844	1.054446	1.539568
C	-5.08593	0.831753	2.580729
O	-6.04886	1.155739	1.878167
N	-5.10136	-0.12877	3.514154
H	-4.28354	-0.27754	4.117377
C	-6.21844	-1.01263	3.770647
H	-7.05975	-0.68809	3.142187
C	-5.82385	-2.45445	3.450915
H	-5.00581	-2.78683	4.110385
H	-6.6886	-3.1149	3.628994
O	-5.44853	-2.60318	2.100088
H	-4.59157	-2.16539	1.87292
C	-1.28631	8.229368	4.67007
H	-0.60172	7.884627	5.45906
C	-2.11957	7.065681	4.130133
H	-2.94718	7.466749	3.524325
H	-2.58671	6.550915	4.988562
C	-1.35016	6.036364	3.285556
H	-1.08337	6.526909	2.332389
C	-0.04335	5.573122	3.937462
H	0.682868	6.393301	4.026282
H	0.416964	4.788524	3.323319
H	-0.22697	5.145579	4.938526
C	-2.26414	4.850659	2.979318
H	-1.77553	4.128996	2.312142
H	-3.20447	5.180724	2.51314
H	-2.53341	4.32624	3.906785
C	-0.51314	8.952967	3.58514
O	-1.02462	9.305642	2.521252
N	0.782289	9.221758	3.869689
H	1.184306	8.847892	4.71922
C	1.631477	9.922316	2.947368
H	1.151456	10.86543	2.640534
C	1.967681	9.119808	1.683484
O	1.74817	7.915651	1.580859
N	2.520749	9.871931	0.713099
H	2.764147	10.83189	0.924393
C	2.993148	9.29387	-0.52394
H	2.158282	8.852382	-1.08161
C	4.069707	8.233019	-0.2777
O	4.892448	8.336246	0.616808
N	4.026244	7.200829	-1.15531
C	4.997321	6.136146	-1.09268
C	5.023173	5.434055	-2.4454
C	4.717744	5.128881	0.071618
O	4.029681	5.398494	-3.1767

C	3.336505	4.567041	0.058915
C	2.828152	3.346755	-0.34139
N	2.231312	5.323894	0.415325
C	1.123133	4.597034	0.214506
N	1.444742	3.389908	-0.24762
H	3.217783	7.077743	-1.76857
H	5.984289	6.574635	-0.88358
H	5.466225	4.326022	0.042009
H	4.885795	5.694686	1.000278
H	3.365306	2.465172	-0.67945
H	0.112759	4.939672	0.396171
H	2.215037	6.298538	0.750655
N	6.186179	4.829904	-2.76273
H	6.900752	4.690078	-2.03212
C	6.201238	3.874552	-3.84779
H	5.703503	4.298693	-4.72963
C	5.521911	2.587888	-3.38895
O	5.774101	2.102867	-2.27864
N	4.61124	2.024121	-4.19835
C	3.943125	0.808743	-3.75881
C	4.962053	-0.34835	-3.74788
C	2.74275	0.468749	-4.64092
O	5.638189	-0.58476	-4.73685
C	1.719241	-0.41344	-3.90524
C	0.813682	0.39001	-2.99521
O	-0.40735	0.467182	-3.26727
O	1.319366	0.994045	-1.98765
H	4.507109	2.347838	-5.15304
H	3.604625	0.997976	-2.73532
H	2.25303	1.398261	-4.97692
H	3.099257	-0.05632	-5.54091
H	2.243523	-1.18752	-3.32222
H	1.0765	-0.93364	-4.62257
N	5.014131	-1.02226	-2.57829
H	4.457029	-0.68066	-1.78046
C	5.92515	-2.11513	-2.313
H	5.603605	-2.55725	-1.35832
C	5.914047	-3.21449	-3.40157
H	6.564193	-2.94618	-4.24013
H	6.302849	-4.14528	-2.95882
C	4.550504	-3.49787	-4.0054
O	3.487943	-3.51991	-3.19689
O	4.39623	-3.7034	-5.19101
C	7.372623	-1.65015	-2.08077
O	8.259648	-2.47051	-1.84289
N	7.602547	-0.32454	-2.16631
H	6.82179	0.325996	-2.22603

C	8.955707	0.212767	-2.23777
H	9.580931	-0.60691	-2.62456
C	9.029819	1.40436	-3.17991
H	10.07648	1.699467	-3.33566
H	8.506829	2.269629	-2.75565
H	8.58355	1.137537	-4.14916
C	9.490642	0.543223	-0.82842
O	9.728252	1.691763	-0.4586
N	9.67891	-0.55546	-0.06968
H	9.299415	-1.42717	-0.44725
C	10.18187	-0.53176	1.298865
H	11.17634	-0.04952	1.28178
C	9.312009	0.281108	2.277237
H	9.468747	1.342402	2.049101
H	9.712862	0.080245	3.280602
C	7.83236	-0.02298	2.242748
C	6.943192	0.882171	1.641169
H	7.334548	1.783842	1.164925
C	5.563213	0.664229	1.685516
H	4.883425	1.404944	1.256929
C	5.05622	-0.47872	2.310351
H	3.97976	-0.62041	2.393936
C	5.931396	-1.41426	2.870526
H	5.53367	-2.3138	3.346279
C	7.308396	-1.18042	2.844119
H	7.992213	-1.88491	3.317522
C	10.40171	-1.97515	1.802622
O	10.26832	-2.25555	2.983173
N	10.75341	-2.88462	0.856246
H	10.86208	-2.57526	-0.10187
C	10.70923	-4.32052	1.093805
H	10.77164	-4.46548	2.179992
C	9.440288	-4.95355	0.509163
H	9.431841	-4.77049	-0.57948
H	9.503779	-6.04854	0.643332
C	8.118849	-4.43908	1.102394
H	8.126078	-3.33722	1.034646
C	6.932679	-4.91662	0.262451
H	7.065262	-4.6295	-0.79175
H	6.819744	-6.01362	0.311296
H	6.000122	-4.46456	0.627589
C	7.940984	-4.81859	2.575969
H	8.720059	-4.36683	3.207271
H	6.962908	-4.48274	2.95537
H	7.985664	-5.9144	2.703115
C	3.113285	-5.94548	5.901788
H	3.35628	-6.12387	6.961604

C	2.844602	-4.44112	5.676476
H	1.846302	-4.1593	6.045039
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C	2.305752	-7.48669	0.621941
C	2.269779	-7.15363	-0.76224
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³Re_C

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H	6.779702	-4.81398	2.901338
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C	9.750982	-4.42709	0.297088
H	9.721057	-4.17991	-0.77843
H	9.894522	-5.52062	0.364282
C	8.400306	-4.04691	0.925098
H	8.327551	-2.9452	0.926771
C	7.244941	-4.55624	0.061081
H	7.347636	-4.19427	-0.97325
H	7.213712	-5.65949	0.04004
H	6.284165	-4.19839	0.456558
C	8.26247	-4.52845	2.37285
H	9.012522	-4.06191	3.02819
H	7.266282	-4.28719	2.775985
H	8.386177	-5.62392	2.431507
C	3.485435	-5.99961	5.751522
H	3.737238	-6.18619	6.807694
C	3.15062	-4.50532	5.551801

H	2.145036	-4.27279	5.934249
H	3.873506	-3.91341	6.133667
C	3.309549	-4.06373	4.089301
O	4.4289	-4.1663	3.579871
O	2.264846	-3.61273	3.48948
C	2.336995	-6.90422	5.34807
O	2.24714	-7.44344	4.245108
N	1.343006	-7.02933	6.275127
H	1.491849	-6.62656	7.192532
C	0.2102	-7.91676	6.088824
H	0.544165	-8.93696	5.841831
C	-0.76392	-7.52767	4.972332
O	-1.6155	-8.30525	4.586649
N	-0.57455	-6.29664	4.422426
H	0.144079	-5.69139	4.801153
C	-1.28532	-5.88368	3.235687
H	-2.36597	-6.03612	3.379272
C	-0.98967	-4.40994	2.934765
H	-1.64817	-4.08419	2.119416
H	0.056234	-4.33632	2.618507
C	-1.21171	-3.4961	4.126149
O	-2.35185	-3.18585	4.494456
N	-0.0883	-3.09296	4.738672
H	0.853451	-3.23372	4.302812
H	-0.16621	-2.42168	5.494509
C	-0.92064	-6.70745	1.9828
O	-1.60666	-6.57735	0.965702
N	0.164297	-7.49863	2.067361
H	0.696673	-7.52146	2.940222
C	0.495793	-8.49347	1.064616
H	0.032648	-8.19389	0.115103
C	2.015897	-8.67028	0.892974
H	2.454059	-8.97947	1.853805
H	2.175247	-9.48739	0.171482
C	2.671627	-7.41192	0.412236
C	2.627177	-7.05614	-0.96623
H	2.194948	-7.76203	-1.6797
C	3.103541	-5.84524	-1.4054
H	3.058839	-5.5558	-2.45517
C	3.642345	-4.89395	-0.45241
O	3.962683	-3.71178	-0.79214
H	3.919973	-3.33796	-2.34281
C	3.759839	-5.30348	0.926417
H	4.211355	-4.62795	1.659999
C	3.27084	-6.5216	1.335101
H	3.31641	-6.80093	2.389427
C	-0.01377	7.746412	-4.02624

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C	-0.52047	6.4553	-4.70573
O	0.782081	7.427021	-1.7769
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N	1.310081	4.939801	-3.806
C	1.387548	3.788144	-3.11075
N	0.179196	3.294645	-2.87141
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H	-0.22538	6.478556	-5.76844
H	-1.6204	6.424858	-4.69085
H	-1.78513	4.01395	-3.43571
H	2.329121	3.378291	-2.76394
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N	-1.39757	7.956827	-2.02739
H	-2.20543	8.052842	-2.64085
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H	-1.27507	8.768109	-0.06738
H	-1.3152	7.011605	-0.14953
C	-3.24313	7.92692	-0.48893
O	-3.94878	7.671328	-1.46212
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C	-5.72348	6.842558	1.354376
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H	-5.24977	6.509555	2.292096
C	-7.2437	6.835539	1.509889
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C	-7.78431	5.535498	2.112692
H	-8.88489	5.522222	2.087508
H	-7.43815	4.674114	1.525241
N	-7.34215	5.359842	3.497348
H	-7.58736	6.105317	4.140114
C	-6.4367	4.468063	3.933812
N	-6.13119	3.372936	3.249065
H	-6.72781	2.965613	2.538653
H	-5.38752	2.787183	3.665988
N	-5.80793	4.671666	5.102444
H	-5.81852	5.578197	5.549225
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H	-6.56755	0.03124	-5.02916
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N	-4.5098	-0.3129	-5.12478

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H	-1.93762	1.320917	-4.09109
N	-2.26688	-0.84101	-5.20704
H	-2.49443	-1.77011	-5.54304
H	-1.32929	-0.70143	-4.83262
O	-3.34614	2.196642	-1.70369
C	-2.80267	3.193192	-1.18497
O	-1.61525	3.194692	-0.70488
C	-3.52024	4.521201	-1.11096
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H	-3.52002	4.879819	-0.07317
O	-0.28755	0.897026	0.332257
O	-1.10133	-0.73918	2.291434
Fe	0.052834	2.115864	-0.92504
C	-2.72427	-1.62607	-1.58698
N	-2.12864	-0.2879	-1.35371
H	-1.56346	-0.17932	-0.4851
H	-1.47305	-0.05503	-2.13402
H	-2.80747	0.505053	-1.34446
C	-3.47573	-2.16292	-0.35374
O	-3.20132	-1.66063	0.780311
O	-4.25815	-3.09281	-0.59901
C	-1.68832	-2.65911	-2.05912
C	-0.72406	-3.18618	-0.99068
C	0.522169	-2.35083	-0.64617
C	1.055161	-2.87337	0.681233
N	2.341084	-2.32829	1.165587
H	2.290023	-1.30079	1.280803
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H	3.118797	-2.5321	0.516699
H	-9.15365	1.621132	-0.38328
H	1.682057	10.31846	3.688521
H	2.81058	10.50431	-0.82669
H	7.001117	4.196865	-3.81852
H	11.8969	-4.11083	0.439665
H	-2.75443	8.547479	5.122677
H	-5.36101	8.942736	1.783403
H	1.058712	7.884916	-4.22319
H	-2.97453	5.271968	-1.69931
H	4.364353	-6.2516	5.143444
H	0.057163	-9.46674	1.34732
H	-0.35417	-7.978	7.029953
H	-2.92595	1.551353	6.814223
H	-6.19282	-1.58357	5.047641

H	0.39497	-7.17206	-3.22209
H	-3.1276	-9.26155	-2.07232
H	-7.14266	-2.8058	-5.42859
H	-0.7819	-0.13281	1.567116
H	-1.8351	-1.23012	1.855958
H	0.319925	-2.63858	1.457915
H	1.16615	-3.96703	0.64632
H	0.297014	-1.27896	-0.54493
H	1.282145	-2.44354	-1.43966
H	-1.29445	-3.38229	-0.06892
H	-0.37429	-4.17771	-1.30997
H	-1.14713	-2.28016	-2.93883
H	-2.29453	-3.50179	-2.41916
H	-3.46245	-1.50341	-2.39119
H	-5.61534	1.104582	-4.00598
O	2.062497	0.54741	1.576475
H	1.196105	0.614946	1.091435
H	1.827971	0.225883	2.49227
O	0.213438	2.530768	2.501081
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H	1.131528	2.41685	2.199245
O	3.280607	-0.22555	-0.67176
H	2.50436	0.123866	-1.15579
H	3.205895	0.175116	0.216768
O	1.204867	-0.49716	3.851397
H	0.339248	-0.75716	3.476287
H	1.020469	0.272834	4.436554
O	0.592787	1.882148	5.057403
H	0.358629	2.196479	4.145366
H	1.361702	2.406259	5.320365
O	7.306593	3.984026	-0.46446
H	6.738533	3.285945	-0.84289
H	8.180011	3.55302	-0.34194

⁵TS1_{C,C3}

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C	3.571696	-4.21867	-3.21145
H	3.770626	-3.57857	-2.33801
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H	0.352442	-10.5761	-0.44084
C	0.116867	-8.44724	-0.07267
H	0.514533	-7.49258	-0.45209
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C	-1.21075	-6.00383	-4.15251
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H	-8.64263	-2.17222	-1.56212
C	-8.03391	-1.6344	0.427424
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C	-2.84453	-0.8841	5.511635
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C	-1.48654	-1.55318	5.306346
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H	-0.42538	-0.36178	6.781016
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H	-2.93172	-3.37749	3.604557
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H	-2.28931	-6.98492	3.574545
O	-1.34315	-5.67194	2.315362
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H	-0.32142	7.649136	0.675463
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H	-3.00746	3.626464	0.215099
H	-2.55135	6.091578	0.553048
N	1.099991	7.772436	-3.10898
H	1.722116	8.173406	-2.39412
C	1.759144	7.092419	-4.19815
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C	2.184898	5.693225	-3.76121
O	2.698956	5.497718	-2.65183
N	1.950948	4.681465	-4.60675
C	2.244743	3.315851	-4.20084
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O	4.543849	3.485142	-4.90054
C	1.469155	0.916073	-4.65855
C	0.301475	0.792554	-3.69514
O	-0.59462	-0.05815	-3.91251
O	0.287028	1.576367	-2.69039
H	1.599673	4.869872	-5.53813
H	1.757671	3.162814	-3.23272
H	0.706114	2.714248	-5.58559
H	2.357247	2.276674	-6.08186
H	2.383724	0.588642	-4.14043
H	1.297622	0.216923	-5.4876
N	4.110556	2.587391	-2.83681
H	3.403209	2.512705	-2.09281
C	5.473806	2.350518	-2.41987
H	5.414834	1.828063	-1.45159
C	6.255524	1.456532	-3.41547
H	6.506839	2.042374	-4.30623
H	7.176063	1.106336	-2.92878
C	5.387664	0.30313	-3.87799
O	5.282305	-0.76657	-3.06862
O	4.750398	0.313892	-4.90523
C	6.272025	3.640333	-2.1501
O	7.46064	3.582829	-1.83337
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H	7.323902	5.829294	-2.72443
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H	6.264659	7.865347	-3.61281
H	4.665135	7.334226	-3.07578
H	5.511304	6.429348	-4.37517
C	6.430394	6.74736	-1.02062
O	5.868277	7.801816	-0.73228
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H	7.886374	7.543646	1.126505
C	6.285295	6.523955	2.108173
H	5.667726	7.377842	1.802965
H	6.661931	6.715167	3.12269
C	5.438516	5.272782	2.100051
C	4.211735	5.260606	1.414438
H	3.904291	6.145158	0.850552
C	3.363432	4.153099	1.482851
H	2.391128	4.181357	0.989019
C	3.743585	3.027737	2.222843
H	3.044215	2.193955	2.322801
C	4.985449	3.004933	2.86804
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C	5.822814	4.122855	2.809421
H	6.774931	4.122833	3.340855
C	8.665242	5.65883	1.776858
O	8.713816	5.407848	2.970791
N	9.597139	5.236298	0.883502
H	9.479209	5.490799	-0.0897
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H	10.71105	4.1902	2.272488
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C	8.202308	1.113152	0.611956
H	8.003515	1.367541	-0.44038
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H	6.487138	-7.86661	2.16478
H	4.324192	-5.35028	7.524443
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H	1.876101	2.241248	-0.00187
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⁵IM1_{C,C3}

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C	10.09283	4.523764	2.118418
H	9.583287	5.315181	2.688454
H	11.15708	4.536836	2.385614
C	9.491393	3.176495	2.441452
C	8.121079	3.048792	2.726226
H	7.49832	3.947512	2.764796
C	7.549763	1.799319	2.983221
H	6.48775	1.691808	3.20669
C	8.353692	0.655894	2.969182
H	7.910179	-0.31608	3.190448
C	9.718202	0.766254	2.689939
H	10.35165	-0.12394	2.682392
C	10.2813	2.015069	2.420735
H	11.34129	2.104071	2.179925
C	10.88708	3.92778	-0.2113
O	11.9599	3.542501	0.237242
N	10.40252	3.58654	-1.42555
H	9.485113	3.918603	-1.71466
C	11.06946	2.64666	-2.30622
H	12.07477	2.478363	-1.89866
C	10.29215	1.332279	-2.44536
H	9.311833	1.563973	-2.89568
H	10.82595	0.687316	-3.16665
C	10.07672	0.559701	-1.13447
H	9.568433	1.236405	-0.42413
C	9.154681	-0.64186	-1.36337
H	8.187103	-0.33242	-1.79017
H	9.6102	-1.36838	-2.05795
H	8.946947	-1.16807	-0.41746
C	11.3996	0.123165	-0.49738
H	12.01029	0.988629	-0.2034
H	11.21966	-0.47821	0.407161
H	11.98655	-0.49513	-1.19838
C	6.848617	-2.51266	5.260167
H	7.48659	-2.45955	6.158667
C	5.829549	-1.35827	5.30245

H	5.123023	-1.50114	6.138395
H	6.361695	-0.41508	5.482485
C	5.024589	-1.20813	4.008101
O	5.127235	-0.165	3.352059
O	4.285932	-2.2062	3.654643
C	6.242027	-3.904	5.196618
O	6.482687	-4.70319	4.291011
N	5.398297	-4.21828	6.213268
H	5.24469	-3.53609	6.944915
C	4.768575	-5.51578	6.329943
H	5.517214	-6.31676	6.225061
C	3.680952	-5.83029	5.30019
O	3.135578	-6.91858	5.305318
N	3.415796	-4.85426	4.386202
H	3.913511	-3.95868	4.381531
C	2.552244	-5.12739	3.267534
H	1.947223	-6.00466	3.548856
C	1.62041	-3.94757	2.930975
H	0.823475	-4.29329	2.262819
H	2.202067	-3.17716	2.416119
C	0.970564	-3.32845	4.155608
O	-0.13452	-3.70902	4.557489
N	1.675119	-2.34986	4.745322
H	2.612291	-2.10534	4.403098
H	1.306246	-1.90028	5.575095
C	3.327942	-5.56249	2.009714
O	2.730903	-5.66802	0.932757
N	4.634769	-5.83985	2.174816
H	5.072375	-5.63883	3.07658
C	5.456803	-6.46473	1.156462
H	4.89131	-6.4646	0.216152
C	6.820275	-5.7685	0.9624
H	7.371692	-5.78595	1.914057
H	7.3889	-6.36131	0.228329
C	6.668211	-4.35694	0.486807
C	6.423935	-4.07022	-0.88627
H	6.444011	-4.88857	-1.61039
C	6.140271	-2.79306	-1.3042
H	5.920315	-2.56569	-2.34843
C	6.061646	-1.71748	-0.33529
O	5.613591	-0.56983	-0.63944
H	5.071273	-0.33048	-2.10523
C	6.418926	-2.0052	1.03347
H	6.402954	-1.17063	1.735134
C	6.685956	-3.29369	1.424899
H	6.880332	-3.53816	2.469877
C	-5.08431	6.166689	-4.2383

C	-5.32497	6.087781	-2.73729
C	-4.45315	4.877759	-4.80889
O	-4.56673	6.642085	-1.93719
C	-3.32578	4.355579	-3.98015
C	-3.13132	3.115508	-3.40948
N	-2.24944	5.114617	-3.55615
C	-1.47351	4.347229	-2.76426
N	-1.98056	3.127823	-2.64924
H	-6.02327	6.37903	-4.7729
H	-4.12543	5.077759	-5.84336
H	-5.20911	4.080788	-4.87546
H	-3.75273	2.22967	-3.508
H	-0.59275	4.731375	-2.2603
H	-2.09506	6.120975	-3.62539
N	-6.38614	5.362349	-2.33784
H	-6.94867	4.821488	-2.99466
C	-6.75125	5.160754	-0.95634
H	-7.13817	6.078912	-0.48506
H	-5.87642	4.868453	-0.35469
C	-7.80335	4.048119	-0.90888
O	-8.07303	3.409786	-1.92243
N	-8.36267	3.834387	0.299039
H	-8.1676	4.493057	1.062822
C	-9.40038	2.83738	0.487275
H	-9.8311	2.610802	-0.49888
C	-8.89017	1.548187	1.139763
H	-8.09076	1.117763	0.515006
H	-8.42706	1.801444	2.107946
C	-9.99555	0.513946	1.349143
H	-10.3823	0.168684	0.375679
H	-10.8557	0.977775	1.866279
C	-9.5443	-0.71515	2.141788
H	-10.3482	-1.46584	2.185708
H	-8.69127	-1.19173	1.641487
N	-9.15299	-0.37441	3.510913
H	-9.87695	0.019888	4.101631
C	-7.89546	-0.32146	3.978265
N	-6.88113	-0.90186	3.356988
H	-6.96276	-1.64239	2.666119
H	-5.95305	-0.75203	3.790206
N	-7.63108	0.338508	5.120347
H	-8.29475	0.987204	5.520356
H	-6.67325	0.320068	5.474538
C	-4.58364	-2.94698	-4.83517
H	-4.95173	-3.97757	-4.9044
H	-5.01252	-2.36393	-5.66634
N	-3.13092	-2.94028	-4.88282

H	-2.59777	-3.83963	-4.99711
C	-2.41505	-1.82694	-4.76519
N	-3.00469	-0.66183	-4.40825
H	-3.79366	-0.68409	-3.76025
H	-2.36306	0.109018	-4.23631
N	-1.10047	-1.81832	-5.00345
H	-0.58407	-2.55879	-5.47502
H	-0.57523	-0.99706	-4.70045
O	-4.15356	-0.29086	-1.83623
C	-4.27806	0.789748	-1.21316
O	-3.35476	1.311138	-0.50464
C	-5.58201	1.556561	-1.28165
H	-5.95304	1.744729	-0.26486
H	-5.40125	2.539701	-1.73967
O	-0.61266	0.601853	0.415061
O	-0.50892	-1.05294	2.417758
Fe	-1.48297	2.028863	-0.82622
C	-1.01301	-2.59164	-1.50844
N	-1.59957	-1.22505	-1.39628
H	-1.30363	-0.73435	-0.51682
H	-1.2331	-0.62117	-2.16661
H	-2.64343	-1.14347	-1.46339
C	-1.43667	-3.50701	-0.33882
O	-1.58648	-2.96901	0.802752
O	-1.53649	-4.70583	-0.63079
C	0.480063	-2.47915	-1.60669
C	1.433101	-3.31026	-0.81988
C	2.69342	-2.55581	-0.36717
C	2.314895	-1.34595	0.481865
N	3.393416	-0.8373	1.361231
H	3.015806	-0.11814	2.011966
H	3.782268	-1.54288	2.042118
H	4.175975	-0.42317	0.835595
H	-8.43187	-4.12277	-0.48545
H	-6.87064	9.388115	2.974996
H	-4.9771	10.38469	-1.03528
H	2.788888	8.052546	-2.34824
H	11.18885	3.104844	-3.30196
H	-7.87298	5.003	4.940069
H	-10.1981	3.277605	1.108683
H	-4.41427	7.023254	-4.39715
H	-6.35086	1.037664	-1.86436
H	7.517887	-2.40433	4.396125
H	5.643959	-7.51814	1.427144
H	4.324746	-5.61749	7.329633
H	-3.20976	-0.00488	6.809505
H	-4.06464	-4.68067	5.038495

H	4.552265	-5.27124	-3.58424
H	3.192339	-8.96846	-1.73865
H	-4.30238	-6.14705	-5.45954
H	-0.61059	-0.37394	1.679201
H	-0.78632	-1.88164	1.960637
H	2.020133	-0.50403	-0.1538
H	1.465881	-1.58505	1.133459
H	3.285231	-2.23044	-1.23674
H	3.322752	-3.25221	0.207389
H	0.942805	-3.74187	0.062405
H	1.741842	-4.1906	-1.40992
H	0.285132	0.466588	0.080898
H	0.869023	-1.85739	-2.42122
H	-1.41848	-3.04141	-2.42998
H	-4.96589	-2.53545	-3.88823
O	0.695337	2.479734	1.870764
H	0.094072	1.901111	1.335609
H	1.166093	1.791098	2.403305
O	-1.28669	2.385251	3.750881
H	-1.92675	1.798628	3.320573
H	-0.67025	2.660867	3.030293
O	2.453326	1.79943	-0.18722
H	1.722024	1.795426	-0.84706
H	2.061501	2.301099	0.560128
O	1.703213	0.334005	3.182624
H	0.967288	-0.30972	3.047427
H	1.561074	0.684473	4.096061
O	0.67117	1.441295	5.377733
H	-0.10346	1.788504	4.865791
H	1.030212	2.206073	5.847648
O	2.32269	7.653921	0.86254
H	2.417845	6.804204	0.37782
H	3.125163	7.77116	1.386157

⁵TS2_{C,C3}

C	2.046169	-6.68768	-1.53975
H	1.868015	-6.31552	-0.52047
C	1.728633	-5.60979	-2.564
H	2.003102	-5.95619	-3.5719
H	0.648683	-5.41574	-2.57563
C	2.431293	-4.29694	-2.25543
H	2.089779	-3.96373	-1.26252
H	3.521476	-4.41546	-2.18563
C	2.072111	-3.2176	-3.26052
O	0.901398	-3.1189	-3.68105
N	3.048542	-2.3908	-3.62354
H	3.983841	-2.33656	-3.18409
H	2.88207	-1.62214	-4.26698
C	1.231451	-7.95275	-1.7506
O	0.83166	-8.3106	-2.87129
N	0.974907	-8.65012	-0.63428
H	1.241004	-8.22769	0.264819
C	0.16324	-9.85384	-0.61372
H	0.193969	-10.2349	0.417875
C	-1.29136	-9.63105	-1.05372
H	-1.30581	-9.49794	-2.14674
H	-1.85929	-10.5518	-0.83465
C	-1.96206	-8.42614	-0.39485
H	-1.39947	-7.50817	-0.63267
H	-1.93458	-8.51376	0.704961
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H	-4.86489	-4.69392	0.150187
H	-6.29886	-4.81711	-0.87354
C	-4.82791	-5.45184	-5.13488
H	-4.89726	-6.54449	-5.02491
C	-3.7918	-4.88811	-4.14314
H	-3.80492	-3.79171	-4.22031
H	-4.10259	-5.12938	-3.11704
C	-2.42206	-5.42493	-4.40301
N	-1.63992	-4.98452	-5.45546
C	-0.54445	-5.73511	-5.44146

H	0.302911	-5.6329	-6.11665
N	-0.59292	-6.64888	-4.44898
H	0.139359	-7.3011	-4.10143
C	-1.76917	-6.45985	-3.76861
H	-2.02357	-7.05215	-2.89822
C	-6.17111	-4.78644	-4.93888
O	-6.29456	-3.56414	-4.8915
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H	-7.11798	-6.60533	-4.76385
C	-8.52419	-5.04796	-4.36421
H	-8.80042	-4.25346	-5.07534
C	-9.60238	-6.1285	-4.33906
H	-10.5715	-5.69622	-4.05243
H	-9.35162	-6.91069	-3.60593
H	-9.71027	-6.58729	-5.33298
C	-8.35124	-4.43006	-2.96602
O	-7.82605	-5.08947	-2.06217
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H	-9.12646	-2.69159	-3.62992
C	-8.69229	-2.42524	-1.56729
H	-8.35772	-3.12392	-0.78766
C	-7.70789	-1.24805	-1.67831
H	-8.08213	-0.57608	-2.47454
C	-7.72137	-0.47646	-0.35444
H	-8.74513	-0.14669	-0.1026
H	-7.32958	-1.12814	0.44354
H	-7.08723	0.419161	-0.41109
C	-6.29346	-1.70687	-2.04707
H	-6.2915	-2.29128	-2.97815
H	-5.86877	-2.31617	-1.2348
H	-5.62657	-0.84549	-2.2025
C	-3.64627	-0.20743	5.661771
H	-3.344	0.839097	5.822326
C	-2.38707	-1.0781	5.639262
H	-1.68667	-0.64246	4.907028
C	-1.6901	-1.09081	6.994485
H	-0.78685	-1.71888	6.949692
H	-2.35468	-1.50859	7.766472
H	-1.38735	-0.07464	7.291095
O	-2.76111	-2.38295	5.233691
H	-1.94676	-2.89284	4.981322
C	-4.47833	-0.28044	4.403257
O	-5.72494	-0.19943	4.455166
N	-3.84285	-0.44944	3.236758
H	-2.81816	-0.54529	3.198624
C	-4.51653	-0.89637	2.040665
H	-5.39424	-0.28028	1.805417

H	-3.81964	-0.79904	1.196865
C	-4.94975	-2.37217	2.069953
O	-5.68591	-2.79945	1.175718
N	-4.45786	-3.09836	3.082364
H	-3.82906	-2.67397	3.779421
C	-4.64529	-4.53055	3.216327
H	-5.54302	-4.81713	2.649778
C	-3.42752	-5.29532	2.698184
H	-2.52353	-5.01831	3.266139
H	-3.59564	-6.37679	2.837698
O	-3.23284	-5.05641	1.315712
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C	-6.34119	5.830365	4.631459
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C	-6.1227	6.958575	3.64227
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H	-4.70273	7.777534	4.866891
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C	-4.09111	8.634887	1.929143
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N	-3.99487	9.632258	1.027207
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C	-1.66035	9.280405	0.378118
O	-1.21368	9.787633	1.393616
N	-0.94818	8.452852	-0.42591
C	0.418516	8.129492	-0.1005
C	1.129708	7.659093	-1.36606
C	0.520034	7.083721	1.052789
O	0.507822	7.220302	-2.33529
C	-0.17631	5.793037	0.77941

C	0.307171	4.526037	0.513591
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C	-1.85946	4.394968	0.42675
N	-0.75478	3.657177	0.302124
H	-1.412	7.921848	-1.1634
H	0.905372	9.041986	0.275287
H	1.577696	6.89206	1.281471
H	0.076619	7.572173	1.93416
H	1.342578	4.214672	0.40923
H	-2.87275	4.028419	0.293739
H	-2.24534	6.418413	0.885554
N	2.475065	7.731985	-1.33205
H	2.954092	7.898522	-0.43891
C	3.260292	7.068807	-2.3458
H	2.859444	7.302758	-3.34084
C	3.276493	5.557267	-2.11442
O	3.386801	5.102577	-0.95919
N	3.146882	4.786677	-3.19312
C	3.1807	3.328077	-3.13674
C	4.646436	2.883081	-3.21777
C	2.349926	2.749045	-4.28954
O	5.350131	3.247473	-4.14358
C	1.898178	1.300153	-4.06675
C	0.881906	1.156516	-2.96824
O	-0.15152	0.442943	-3.12487
O	1.067511	1.775311	-1.86857
H	3.189073	5.221879	-4.10968
H	2.736143	3.037388	-2.18155
H	1.46753	3.393052	-4.43874
H	2.955348	2.794106	-5.20815
H	2.784031	0.678201	-3.83377
H	1.47009	0.891365	-4.992
N	5.075653	2.128717	-2.17794
H	4.468203	1.999454	-1.3709
C	6.429852	1.588826	-2.16139
H	6.561254	1.102179	-1.18049
C	6.67402	0.557503	-3.27541
H	6.794387	1.084533	-4.22785
H	7.598549	0.013737	-3.04527
C	5.482219	-0.39415	-3.37922
O	5.440386	-1.38852	-2.56526
O	4.588271	-0.12549	-4.19926
C	7.459944	2.736508	-2.22244
O	8.510395	2.643026	-2.83088
N	7.118269	3.831503	-1.48002
H	6.185349	3.836606	-1.08469
C	7.798896	5.112392	-1.60753

H	7.839747	5.405352	-2.66958
C	7.049848	6.172416	-0.7997
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H	7.054674	5.906066	0.270578
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N	-5.63466	-4.9555	-0.97249
H	-4.82338	-4.64998	-0.44593
C	-5.94244	-6.38054	-0.93656

H	-5.72102	-6.81814	-1.92456
C	-5.09798	-7.07263	0.133063
H	-5.33909	-8.14399	0.139085
H	-5.32677	-6.66069	1.129961
H	-4.02043	-6.94671	-0.05544
C	-7.42447	-6.72525	-0.70198
O	-7.80878	-7.85871	-0.93221
N	-8.19652	-5.72712	-0.21423
H	-7.76351	-4.83149	-0.01657
C	-9.62105	-5.85905	0.014717
H	-9.85913	-6.92057	-0.15396
C	-9.99607	-5.47948	1.460144
H	-9.53075	-6.21183	2.137267
H	-11.0861	-5.57595	1.544603
C	-9.56047	-4.08006	1.827171
C	-8.29361	-3.84307	2.38899
H	-7.64201	-4.69431	2.610361
C	-7.87553	-2.54562	2.700217
H	-6.90504	-2.35244	3.162013
C	-8.72451	-1.46269	2.454944
H	-8.39884	-0.46306	2.740797
C	-9.98163	-1.68435	1.8883
H	-10.65	-0.84208	1.694832
C	-10.3959	-2.98019	1.572988
H	-11.3729	-3.15404	1.120161
C	-10.4722	-5.05239	-0.99341
O	-11.6526	-4.83156	-0.75238
N	-9.83156	-4.65054	-2.11236
H	-8.84096	-4.85164	-2.2261
C	-10.4538	-3.82646	-3.13276
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C	-9.88698	-2.40182	-3.16004
H	-8.81265	-2.4654	-3.40423
H	-10.3644	-1.85739	-3.99519
C	-10.0619	-1.59839	-1.86234
H	-9.58618	-2.17124	-1.04645
C	-9.33746	-0.2526	-1.95897
H	-8.26666	-0.38147	-2.17825
H	-9.77445	0.377058	-2.75323
H	-9.40632	0.306435	-1.01245
C	-11.5372	-1.40755	-1.49631
H	-12.0352	-2.3679	-1.29999
H	-11.638	-0.78839	-0.59121
H	-12.0789	-0.89339	-2.30924
C	-6.69695	2.548767	5.217712
H	-6.78158	2.062938	6.201607
C	-5.40638	2.134278	4.499354

H	-5.22123	2.84773	3.681957
H	-4.54257	2.200671	5.180528
C	-5.35252	0.768776	3.814777
O	-6.31413	0.011117	3.816607
O	-4.22972	0.569789	3.201932
C	-6.60352	4.059565	5.306989
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N	-5.85922	4.549707	6.340931
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C	-5.36787	5.9135	6.329135
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O	-4.09115	7.37275	4.906761
N	-3.87169	5.145924	4.528041
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C	-3.10854	5.293404	3.309126
H	-2.27448	5.990128	3.476152
C	-2.55462	3.945802	2.829385
H	-1.91494	4.15591	1.962382
H	-3.37618	3.29444	2.49858
C	-1.68989	3.229715	3.849478
O	-0.67622	3.781459	4.305473
N	-2.08531	1.996507	4.186555
H	-2.89381	1.499589	3.748242
H	-1.50365	1.436376	4.802654
C	-3.91612	5.8789	2.135366
O	-3.28742	6.298264	1.155393
N	-5.25062	5.822329	2.212486
H	-5.69968	5.4961	3.071229
C	-6.1387	6.322587	1.174761
H	-5.56244	6.385746	0.242859
C	-7.37533	5.433448	0.989125
H	-7.92506	5.388883	1.941575
H	-8.03431	5.942441	0.266556
C	-7.07235	4.030397	0.513643
C	-6.72536	3.766579	-0.82017
H	-6.70143	4.586719	-1.54397
C	-6.43066	2.47337	-1.25836
H	-6.17703	2.275955	-2.30101
C	-6.47691	1.402687	-0.35187
O	-6.13813	0.13785	-0.71806
H	-5.69154	0.131854	-1.64183
C	-6.85287	1.641597	0.974949
H	-6.92761	0.804403	1.66803
C	-7.13952	2.941325	1.394892
H	-7.43366	3.123698	2.429696
C	5.802801	-6.58733	-3.72856

C	5.940409	-6.19963	-2.26069
C	5.052949	-5.52401	-4.56367
O	5.192248	-6.67056	-1.39924
C	3.84596	-4.99579	-3.86162
C	3.491845	-3.70886	-3.5241
N	2.879732	-5.79803	-3.27851
C	2.014294	-5.0189	-2.61256
N	2.354547	-3.73928	-2.73525
H	6.790816	-6.77208	-4.1773
H	4.788	-5.96374	-5.53977
H	5.710855	-4.66886	-4.778
H	3.978312	-2.77655	-3.79759
H	1.188735	-5.4249	-2.03953
H	2.840835	-6.81283	-3.20494
N	6.90357	-5.30238	-1.97403
H	7.400653	-4.81226	-2.71605
C	7.200384	-4.81884	-0.64608
H	7.770975	-5.55196	-0.05319
H	6.276177	-4.64648	-0.0737
C	7.996385	-3.5146	-0.78289
O	8.073231	-2.95231	-1.87202
N	8.58732	-3.07495	0.347209
H	8.530954	-3.66067	1.189226
C	9.51174	-1.95391	0.331346
H	9.806138	-1.78539	-0.71474
C	8.944564	-0.65831	0.918983
H	8.043609	-0.36814	0.35452
H	8.6185	-0.84304	1.95582
C	9.9694	0.477221	0.894265
H	10.24406	0.716378	-0.14715
H	10.90536	0.145981	1.380098
C	9.495873	1.771591	1.561986
H	10.26181	2.556029	1.462678
H	8.594115	2.144175	1.061092
N	9.190736	1.591223	2.980294
H	9.958912	1.304653	3.577249
C	7.957042	1.546212	3.512042
N	6.890584	2.005595	2.872866
H	6.91412	2.673783	2.110156
H	5.992096	1.881821	3.377459
N	7.770295	1.010979	4.729733
H	8.49867	0.488888	5.196492
H	6.829134	1.045449	5.130855
C	3.647226	3.975856	-6.70236
H	3.393481	4.841439	-7.3281
H	4.022488	3.191094	-7.37954
N	2.435985	3.549898	-6.02361

H	1.654344	4.255283	-5.92641
C	2.31629	2.407853	-5.36194
N	3.32112	1.499787	-5.33934
H	4.215203	1.756763	-5.73505
H	3.350969	0.819707	-4.57941
N	1.189243	2.11467	-4.70262
H	0.388807	2.758703	-4.59641
H	0.96996	1.137449	-4.5107
O	3.755864	-0.05174	-2.76615
C	3.909902	-0.74191	-1.76348
O	2.95678	-0.91988	-0.86895
C	5.20411	-1.4774	-1.48083
H	5.034196	-2.55966	-1.58401
H	5.999894	-1.20402	-2.1815
O	-0.124	0.203828	-0.00719
O	0.458803	1.070778	2.491836
Fe	1.708285	-2.4434	-1.239
C	0.407916	2.314687	-1.03305
N	1.498809	1.543761	-1.69581
H	1.89736	0.822232	-1.07161
H	1.143453	0.986879	-2.50099
H	2.255962	2.178024	-1.9703
C	1.073325	3.179942	0.065925
O	0.443076	3.393107	1.133333
O	2.197311	3.62364	-0.25124
C	-0.7117	1.327749	-0.68749
C	-1.86415	1.92726	0.110821
C	-3.16205	1.125717	0.07879
C	-2.99504	-0.32763	0.513249
N	-4.25968	-0.87114	1.067523
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H	-4.38001	-0.39172	2.049957
H	-5.07044	-0.61715	0.453744
H	8.129743	3.967185	-0.99811
H	7.701173	-8.40066	3.742755
H	5.697643	-10.2397	0.12436
H	-2.24085	-8.3323	-1.43385
H	-10.2987	-4.29881	-4.11708
H	8.303721	-3.78331	5.117076
H	10.41753	-2.24554	0.88931
H	5.2539	-7.53941	-3.74428
H	5.530597	-1.29422	-0.44879
H	-7.57472	2.268217	4.622892
H	-6.45857	7.348971	1.427394
H	-4.88309	6.133914	7.290762
H	3.476506	1.372	6.603722
H	3.710322	5.557136	4.234949

H	-4.4	6.113792	-3.37243
H	-3.28436	10.10336	-1.24791
H	3.360883	6.72263	-5.73583
H	0.314737	0.587908	1.648785
H	0.331371	2.012236	2.227258
H	-2.67861	-0.95477	-0.32991
H	-2.23656	-0.43518	1.297409
H	-3.61185	1.143283	-0.92258
H	-3.87568	1.616546	0.756145
H	-1.53394	2.047655	1.145549
H	-2.05916	2.94306	-0.26324
H	-0.22212	-0.58522	-0.57707
H	-1.10887	0.968288	-1.64749
H	0.01839	3.016305	-1.78851
H	4.443379	4.289753	-6.00554
O	-0.73116	-2.43337	2.099933
H	-0.00282	-1.90786	1.728375
H	-0.9495	-1.92481	2.92353
O	1.896282	-1.43385	1.680554
H	2.392841	-0.87161	1.058723
H	2.110588	-2.33705	1.376982
O	-2.71047	-3.36729	0.52996
H	-2.38947	-4.25441	0.281079
H	-2.00375	-3.00187	1.119642
O	-0.76054	-0.7094	4.188435
H	-0.47639	0.027864	3.60497
H	0.09435	-1.05322	4.520669
O	1.83161	-1.74324	4.445945
H	1.974332	-1.53923	3.496757
H	1.66343	-2.69563	4.459796
O	-1.70911	-7.62835	1.705287
H	-1.85554	-6.84144	1.140426
H	-2.52058	-7.76723	2.211176

⁵TS1_{C,C4}

C	1.000584	-6.02854	-3.12233
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H	-0.47261	-4.64456	-3.90033
C	1.469107	-3.96424	-4.55044
H	1.597621	-3.26105	-3.71044
H	2.477814	-4.36357	-4.73768
C	1.015588	-3.17292	-5.77038
O	-0.16172	-3.15264	-6.13958
N	1.989796	-2.49826	-6.41086
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O	-0.46084	-7.77117	-3.94987
N	0.097412	-7.82107	-1.75484
H	0.423567	-7.27219	-0.95053
C	-0.68732	-9.00446	-1.44362
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C	-2.20055	-8.75845	-1.38755
H	-2.57462	-8.66187	-2.41921
H	-2.67567	-9.66214	-0.9678
C	-2.58823	-7.52441	-0.57489
H	-2.19125	-6.61271	-1.04672
H	-2.13078	-7.55809	0.427713
C	-4.0997	-7.3778	-0.43889
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H	-3.66269	-5.44829	0.39447
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N	-5.87301	-4.37256	0.684468
H	-5.12705	-4.00487	1.307148
H	-6.83953	-4.04885	0.759655
C	-6.76309	-4.95511	-4.51178
H	-6.91417	-6.02986	-4.69952
C	-5.50606	-4.75081	-3.6379
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H	-5.61302	-5.30498	-2.69357
C	-4.25497	-5.17624	-4.3299
N	-3.74002	-4.46988	-5.40121
C	-2.66008	-5.13176	-5.79799

H	-1.97147	-4.81838	-6.58013
N	-2.46335	-6.23496	-5.03885
H	-1.64017	-6.85435	-5.00028
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H	-8.14807	-6.01669	-2.67509
C	-9.63025	-4.63044	-2.02911
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C	-10.4341	-5.77903	-1.44127
H	-11.2365	-5.39642	-0.79549
H	-9.80422	-6.43583	-0.82216
H	-10.885	-6.37677	-2.24629
C	-8.99178	-3.74066	-0.94102
O	-8.63083	-4.21328	0.145636
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H	-9.02904	-2.28065	-2.3018
C	-8.19373	-1.39569	-0.56538
H	-7.83245	-1.78394	0.396519
C	-7.04828	-0.74815	-1.36436
H	-7.38885	-0.69604	-2.41542
C	-6.78345	0.677304	-0.87904
H	-7.6661	1.323261	-1.02093
H	-6.52322	0.655004	0.190565
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C	-5.77474	-1.59725	-1.31513
H	-5.97658	-2.65017	-1.55374
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H	-5.03332	-1.23028	-2.04328
C	-2.64746	0.812417	5.976717
H	-2.03165	1.721431	6.064736
C	-1.70851	-0.38503	5.80049
H	-1.0102	-0.14879	4.984478
C	-0.88453	-0.64465	7.055038
H	-0.2154	-1.50543	6.897728
H	-1.54061	-0.88045	7.907228
H	-0.2668	0.230835	7.307486
O	-2.47683	-1.52574	5.441449
H	-1.89533	-2.1407	4.929061
C	-3.62184	0.987007	4.837887
O	-4.80492	1.324328	5.051089
N	-3.19055	0.721497	3.59645
H	-2.22931	0.403383	3.413022
C	-4.10408	0.500556	2.500428
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C	-5.07768	-0.66882	2.72702
O	-6.11682	-0.73589	2.06095
N	-4.68793	-1.55739	3.648458
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C	-5.37368	-2.7918	3.964171
H	-6.23041	-2.8925	3.283037
C	-4.41023	-3.97114	3.818766
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H	-4.94371	-4.90485	4.060705
O	-3.91438	-4.09136	2.50697
H	-3.28728	-3.37133	2.259167
C	-3.54711	7.859721	4.706815
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C	-1.7306	5.568346	4.057232
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C	-0.88386	9.522033	1.395078
O	-0.6917	8.31159	1.335676
N	-0.65766	10.37864	0.379033
H	-0.74211	11.37155	0.55873
C	-0.07441	9.953374	-0.87341
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C	1.304183	9.320249	-0.66972
O	2.09897	9.752363	0.148592
N	1.555591	8.272438	-1.49327
C	2.823152	7.586562	-1.4305
C	3.02562	6.804144	-2.72538
C	2.936044	6.660238	-0.1802
O	2.081814	6.458685	-3.44084
C	1.861715	5.630855	-0.11685

C	1.85604	4.286653	-0.42094
N	0.552378	5.937155	0.223907
C	-0.1908	4.82797	0.112767
N	0.565835	3.798606	-0.27326
H	0.794754	7.836714	-2.01783
H	3.618895	8.339964	-1.33012
H	3.92495	6.181715	-0.16666
H	2.882417	7.326124	0.694022
H	2.68467	3.653763	-0.7296
H	-1.25659	4.776606	0.3031
H	0.178967	6.85776	0.498417
N	4.310884	6.501189	-3.00915
H	5.027754	6.589119	-2.27566
C	4.611735	5.577208	-4.07764
H	4.021123	5.832982	-4.96746
C	4.338327	4.145358	-3.62867
O	4.69544	3.749521	-2.51133
N	3.673262	3.33867	-4.46803
C	3.333348	1.993158	-4.03398
C	4.610368	1.146174	-3.90961
C	2.330005	1.343147	-4.98676
O	5.425678	1.09529	-4.81268
C	1.597116	0.145137	-4.36663
C	0.580215	0.535425	-3.31343
O	-0.60407	0.139388	-3.41484
O	0.97664	1.270443	-2.35039
H	3.467016	3.640622	-5.413
H	2.87978	2.091597	-3.04425
H	1.58953	2.100019	-5.29724
H	2.863128	1.009685	-5.89121
H	2.326442	-0.53938	-3.90387
H	1.084332	-0.42265	-5.14952
N	4.705026	0.481778	-2.7249
H	4.125111	0.796309	-1.93768
C	5.848861	-0.32778	-2.36069
H	5.60007	-0.80257	-1.39884
C	6.144265	-1.43884	-3.39768
H	6.660421	-1.01921	-4.26646
H	6.783836	-2.19735	-2.92301
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O	4.117877	-2.74946	-3.03264
O	4.463888	-1.92397	-5.0456
C	7.123824	0.49586	-2.09587
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C	4.864468	2.177262	2.01494
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O	5.63608	-2.96659	3.407907
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N	1.883847	-7.66821	2.136922
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H	4.390575	-8.87472	1.884282
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C	4.283309	-7.28825	0.455871
C	3.952394	-6.86146	-0.8621
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C	4.243953	-5.58991	-1.28852
H	3.974954	-5.23877	-2.28584
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H	4.556843	-2.91864	-2.14879
C	5.250965	-5.111	0.93288
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H	5.165697	-6.72778	2.342608
C	-2.33951	7.35893	-4.13203

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O	-2.38538	-4.23278	0.010509
C	-0.25367	-2.51134	-1.33392
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H	-4.33132	8.463724	5.195499
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H	6.086825	-6.08309	4.427336
H	2.078507	-9.68296	1.599935
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H	-0.80303	0.024423	1.549643
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H	2.84729	-0.43243	0.795718
H	1.955767	-1.44981	1.942436
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H	0.227173	-0.59113	-0.14929
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H	0.09747	-2.14146	-2.31146
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H	1.674471	1.11984	2.501353
O	-0.75646	2.844001	2.40477
H	-1.37592	2.695009	1.667176
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O	3.079184	1.253438	-0.62296
H	2.260368	1.117732	-1.13521
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⁵IM1_{C,C4}

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C	4.382983	1.501555	-3.80753
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O	-9.16303	2.838965	1.995908
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H	-2.85756	1.720594	-4.90712
H	-1.70459	2.822225	-5.70228
H	-0.01838	2.275908	-3.82051
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N	-1.13875	5.242559	-2.7191
H	-1.42254	4.704027	-1.90322
C	-0.09723	6.208728	-2.42074
H	0.225054	5.961278	-1.39632
C	1.130012	6.109189	-3.32419
H	0.871039	6.336083	-4.36758
H	1.872027	6.855677	-3.00949
C	1.801884	4.730093	-3.31582
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C	-0.68028	7.616859	-2.25949
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C	-2.82224	8.85769	-2.0541

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C	-2.1595	8.857975	2.513166
H	-3.24989	8.783153	2.416995
H	-1.93129	9.315815	3.48576
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C	-1.76898	5.106865	1.90982
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C	3.016114	7.231632	0.063622
H	2.55464	7.176478	-0.93315
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H	2.594575	9.195327	2.910605
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H	4.160053	8.678003	2.220251
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N	8.360557	1.422245	1.934579
H	8.29757	2.066644	2.723511
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H	9.454239	3.871188	1.379971
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C	7.911364	3.683633	-0.10383
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H	8.502378	3.471938	-2.17152
C	6.429709	4.038453	-2.01442
H	6.274394	4.067413	-3.0953
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H	3.955247	4.603025	-2.56506
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H	4.800187	4.671052	0.914813
C	6.848597	4.041315	0.739228
H	7.027338	4.082137	1.813412
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H	2.719245	1.726404	1.174187
H	3.707784	2.096468	-0.25117
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H	-3.10352	5.074928	-1.22993
C	-2.69116	5.735677	-3.23444
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H	-2.56243	6.801015	-3.00186
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O	-4.8543	7.113768	-1.72019
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H	-5.97603	4.166625	-1.88864

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C	-6.58857	5.903807	2.778365
H	-7.46941	5.25503	2.692733
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C	-2.94374	4.753342	2.67449
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H	-0.67049	8.217747	-0.05141
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C	1.066767	4.73071	3.052907
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C	3.707427	7.1159	4.492065
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C	4.267082	1.910918	3.863649
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N	6.148035	5.810865	1.804618
H	5.694624	6.319161	2.565078
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H	6.901424	5.946399	-0.12706
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H	5.728536	8.454962	1.209069
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H	5.159159	7.607423	-2.34
C	3.110322	6.959133	-2.19009
H	2.966086	6.91077	-3.27124
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O	0.849882	6.170627	-1.75068
H	0.659123	6.165756	-2.72426
C	2.227325	6.772533	0.05504
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C	3.458566	7.165469	0.566756
H	3.582376	7.291556	1.642004

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H	-5.67119	-5.23651	-5.23719
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H	2.097904	-10.0737	2.480271
H	1.780774	-8.46043	1.826295
N	1.330783	-8.68569	3.851084
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N	2.08481	-6.51993	3.389726
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O	-1.3892	-3.01198	-1.04594
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H	-1.59968	-6.25679	-1.60776
H	-1.78836	-5.51324	0.003755
O	1.104562	-0.22095	-1.68038
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C	4.279843	-0.1651	-1.5688
N	3.92372	-1.56343	-1.96221
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H	3.92829	-1.64926	-2.99081
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O	3.992222	-1.02422	0.638406
O	5.04043	0.95248	0.351068
C	3.250891	0.893585	-1.97821
C	1.925363	0.87311	-1.22517
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H	-3.54363	-6.58976	5.967765
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H	-2.95052	-5.13059	-1.27771
H	1.914465	7.459435	3.355418
H	7.734617	6.960872	1.060402
H	5.79539	6.132635	6.910748
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H	6.077331	-3.8925	4.374701
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H	9.5508	3.594744	-2.26319
H	5.936747	-4.01038	-5.66536
H	1.223735	-1.85333	-0.97956
H	1.188675	-3.35012	-1.33436
H	1.646355	2.721114	0.709606
H	2.278304	3.865579	-0.48887
H	0.080583	1.895638	-1.19615
H	1.17971	2.611334	-2.3319
H	0.651636	-0.00845	-2.54419
H	2.101086	0.652632	-0.16289
H	3.055482	0.877725	-3.06008
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H	5.230646	0.058374	-2.07082
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H	-0.94425	0.513167	0.462145
O	-0.85088	-1.14276	2.647429
H	-0.13452	-1.75318	2.881863
H	-0.88516	-1.1745	1.67066
O	-2.02756	2.466821	-0.88841
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H	3.051993	-0.3309	1.863533
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O	0.03557	1.335185	1.862314
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⁵TS1_{C,C5}

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H	-11.374	-3.4802	-1.64836
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H	-8.23286	0.335485	0.094524
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H	-4.30508	-0.56639	4.124231
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H	-4.46714	-2.41356	1.746985
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H	-3.35315	7.432452	3.762641
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C	-0.38923	5.592568	3.880123
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H	-0.39062	5.240992	4.926168
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H	-3.70498	4.982177	2.969833
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O	1.376765	8.054413	1.481364
N	1.99252	10.05767	0.589236
H	2.164019	11.03413	0.795546
C	2.511074	9.513594	-0.64544
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C	3.654703	8.528226	-0.39129
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C	4.750537	5.711471	-2.46592
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H	5.645248	6.976968	-0.96571
H	5.321343	4.766944	0.084034
H	4.592451	6.114577	0.968405
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H	-0.06013	4.764238	0.375838
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H	6.64562	5.04394	-2.00324
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H	2.208278	-7.73026	-1.46648
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H	3.267565	-6.66599	2.593886
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⁵IM1_{C,C5}

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H	-8.99688	2.495465	0.179049
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H	-7.40812	1.752521	1.776693
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C	-5.54239	3.538632	-2.95944
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H	-3.89837	8.659447	3.479102
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H	0.018454	5.905552	3.188194
C	-1.82819	6.99822	2.899859
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C	-2.51505	10.05976	1.725804
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H	0.12036	9.905487	-0.95658
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C	0.533762	8.788838	0.845448
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H	2.342274	8.052982	-0.14945
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H	1.271426	7.978387	2.727502
H	2.157156	9.411016	2.162613
C	4.698804	5.695406	4.325436
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C	4.076359	4.327824	4.018751

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C	2.764495	4.160412	3.258324
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C	7.914829	2.849903	4.906271
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C	5.388997	0.949871	2.842591
H	5.474389	0.237897	2.010505
H	4.802938	1.814624	2.494846
C	4.654826	0.260762	3.972248
O	4.899583	-0.91823	4.284
N	3.776934	1.022241	4.650421
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O	7.781869	1.068682	1.087138
N	7.776488	3.216056	1.829903
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H	8.503241	3.07092	-0.11203
C	8.233176	5.176087	0.35231
H	8.331638	5.828838	1.234194
H	8.985204	5.513643	-0.37823
C	6.846794	5.309049	-0.22871
C	6.603491	5.209856	-1.60489
H	7.445094	5.08725	-2.29315
C	5.306497	5.281001	-2.12521
H	5.135673	5.217054	-3.2019
C	4.220228	5.456955	-1.25921
O	2.92855	5.487276	-1.68153
H	2.781827	5.359368	-2.65695
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H	5.92616	5.638645	1.684013
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O	-7.89768	-2.11853	-1.31081
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C	-4.4431	-2.20905	-3.47257
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C	-4.96136	-0.17641	-2.92892
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H	-8.63995	-3.94393	-3.82825
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H	-6.27965	-3.98221	-4.42746
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H	-2.98333	-8.62828	5.464408
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C	1.10944	-2.84376	-4.97409
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H	-0.6311	-3.18257	-3.91011
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H	0.580454	-1.24977	-3.86109
O	-1.62098	-3.99154	-2.40171
C	-2.53887	-3.87756	-1.57721
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N	2.892888	-2.62377	-1.84549
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O	5.104342	-1.08065	0.532529
C	3.394795	-0.17868	-1.72623
C	2.076403	0.241792	-1.03223
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H	-5.38996	-4.59409	6.025707
H	-6.50552	-8.00982	2.400381
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H	4.610404	6.377256	3.471044
H	9.662865	3.711891	1.06316
H	7.771154	3.628691	6.920139
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H	-0.16569	-3.28523	-1.45095
H	2.388045	2.075659	0.980325
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H	1.858647	-5.47599	-5.83875
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O	-1.15991	-0.41497	3.496519
H	-0.99066	-0.98741	2.730229
H	-1.86303	0.176119	3.176474
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H	-0.63094	3.017942	-1.46725
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⁵TS2_{C,C5}

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C	32.50411	42.01124	59.52099
H	32.84195	40.99427	59.7831
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C	27.77093	41.25546	64.6569
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H	28.02416	42.98549	65.94779
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C	30.10391	44.01075	63.85473
H	29.15517	43.53008	64.05011
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C	30.50645	44.98164	70.5925
H	31.30003	45.67216	70.91413
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H	34.54614	43.05614	69.57164
C	35.1887	41.0561	69.9967
H	35.74218	41.34108	70.90749
H	34.75822	40.05248	70.12483
H	35.9009	41.00567	69.16367
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H	32.95242	40.7014	68.41355
H	34.08032	41.74756	67.52193
C	33.72895	33.52396	68.73231
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C	32.59384	33.41819	67.71338
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C	32.19149	31.96752	67.4725
H	31.35898	31.90894	66.75247
H	31.84716	31.50399	68.40962
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O	32.77303	38.80421	69.80825
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C	30.37348	37.27839	69.46734
H	30.445	38.14638	70.13751
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H	29.3644	36.70185	67.63138
H	28.49874	37.91986	68.60628
O	30.03265	38.65443	67.48955
H	30.80619	38.40002	66.93426
C	40.18657	34.06067	71.03256
H	39.9971	33.08712	70.5566
C	38.99332	34.99851	70.84676
H	39.12492	35.87564	71.49985
H	38.08823	34.47736	71.20571
C	38.74882	35.48967	69.40972
H	39.56518	36.18977	69.15883
C	38.77903	34.36067	68.37422
H	39.78221	33.9194	68.28375
H	38.49697	34.745	67.38465
H	38.05806	33.56462	68.62815
C	37.42761	36.25732	69.3593
H	37.24735	36.68769	68.36674
H	37.41383	37.07686	70.09316
H	36.58358	35.59573	69.59857
C	41.48745	34.64962	70.52332
O	41.82676	35.81277	70.74587
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O	42.335	35.37553	67.5411
N	44.56921	35.75822	67.73702
H	45.42551	35.43914	68.17395
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H	44.04037	37.48347	66.67199
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C	39.51588	36.79185	65.5551
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H	43.18831	37.47739	64.65822
H	43.90605	35.30958	62.78477
H	41.57362	34.57586	62.44831
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H	39.1991	36.16585	62.4208
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N	42.80199	36.63254	60.86044
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C	42.29439	37.48344	59.81145
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C	36.27145	37.43463	57.17177
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H	31.55432	33.35235	65.0955
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H	27.78535	38.63974	60.41063
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H	27.27842	36.09827	58.7439
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C	29.15277	37.1134	58.55974
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H	29.21984	39.21071	57.98681
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H	33.42496	41.2882	62.58099
H	31.78245	41.44185	63.19478
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H	-0.92512	2.248768	-4.99265
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H	-1.65351	3.143692	-2.38949
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C	0.220557	5.346375	-3.39555
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H	0.818274	6.208838	-3.07638
C	1.108084	4.110188	-3.53273
O	2.35056	4.275546	-3.68881
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C	-4.09125	7.197198	-1.88766

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C	-3.57907	8.442225	2.452506
H	-4.59428	8.027559	2.494879
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C	-1.22901	7.554341	2.812518
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H	8.521929	2.613623	0.062787
C	8.381249	4.732424	0.551851
H	8.508046	5.361201	1.445631
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H	7.487842	4.078969	-1.95886
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O	3.186348	5.580837	-1.62421
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H	-7.13315	-4.42058	-4.25764
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H	-7.27382	-5.25035	-2.00717
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H	5.591046	6.75584	3.838461
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C	0.87915	0.130244	-3.44415
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O	1.24363	0.780247	-2.39799
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H	2.215532	1.636102	-5.22631
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H	1.439977	-0.87107	-5.21828
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C	6.039634	-1.5889	-2.47019
H	5.749777	-2.03219	-1.50569
C	6.070881	-2.70286	-3.54459
H	6.66155	-2.38853	-4.41061
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C	4.693711	-3.06443	-4.07581
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H	11.28599	0.831446	0.975252
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H	9.862475	0.819605	3.019693
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C	7.027758	1.397355	1.361317
H	7.355766	2.307054	0.855362
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H	-2.11194	3.98895	-3.13952
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H	-1.95995	9.002578	-2.26999
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H	-2.80804	-2.00417	-5.59635
H	-1.4885	-0.98328	-5.18866
O	-3.2115	1.717174	-1.54806
C	-2.82524	2.708924	-0.89421
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H	3.34434	-2.48954	0.422214
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H	2.423063	9.057754	4.248647
H	2.652581	10.30076	-0.42472
H	6.858699	4.399344	-4.20079
H	12.08614	-3.83836	0.268155
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H	0.838949	7.796107	-4.08072
H	-3.39287	4.726204	-1.03333
H	4.560001	-6.16793	4.58929
H	0.263075	-9.51793	1.731363
H	0.108013	-6.99807	7.521119
H	-3.64492	1.92855	5.732018
H	-6.79608	-1.98904	3.921022
H	0.717678	-7.24695	-3.04223

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H	-1.99973	-4.12813	-2.05264
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H	2.468624	0.199124	-1.31002
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H	0.161217	-0.97348	3.215154
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H	6.865778	3.438164	-1.26358
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H	-5.29221	3.133506	-1.8867
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