

Supporting Information

Mechanistic insight on the hydrogenation of conjugated alkenes with H₂ catalyzed by early main-group metal catalysts

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Table S3. Electronic energies (E_{elec}), ZPE-corrected energies (E_0), Gibbs free energies G_g (333.15K and 20 bar) and free energies of solvation $\Delta G_{(s)}$ of the related species involved in the strontium-mediated hydrogenation of DPE. The E_{elec} , E_0 and G_g energies are in a.u. and $\Delta G_{(s)}$ are in kcal/mol. -----7

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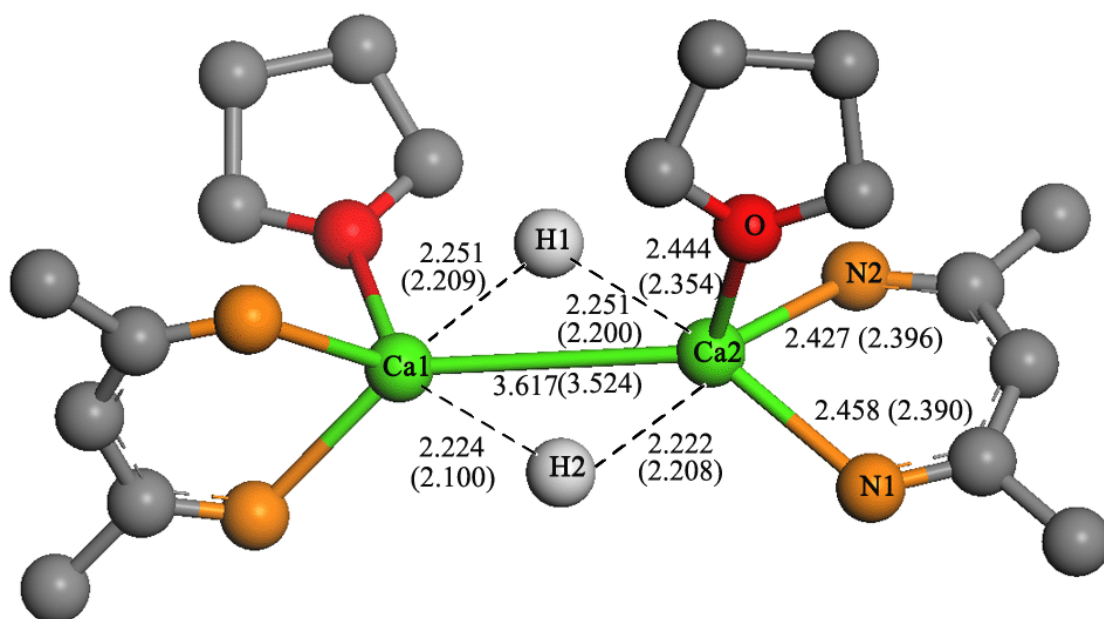


Figure S1. The optimized structure of the dimeric species. All hydrogen atoms (except two hydrides) and two 2,6-diisopropylphenyl substituents bound to the nitrogen atoms are omitted for clarity. The X-ray data are presented in parenthesis. All the distances are in Å.

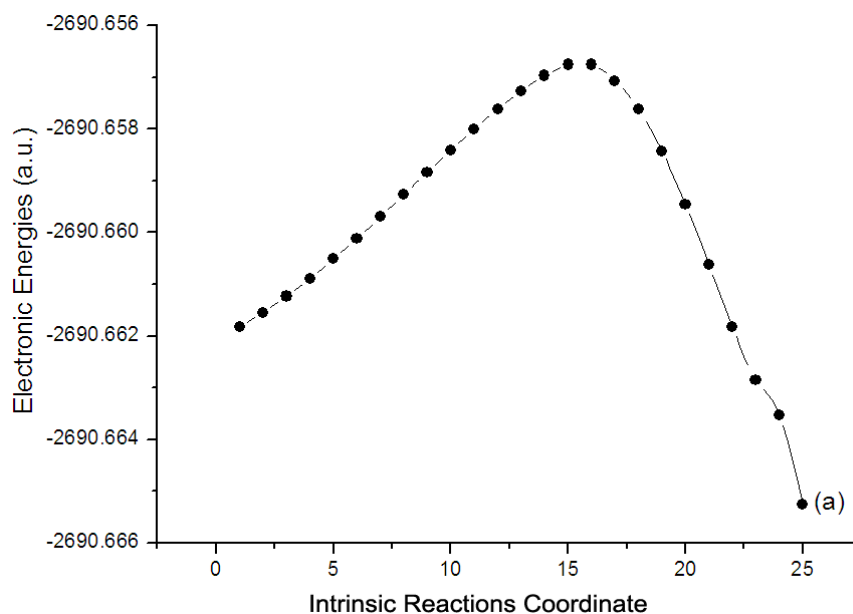


Figure S2. Intrinsic reaction coordinate calculations of TS_1 . (a) At this point, the calculation terminated abnormally.

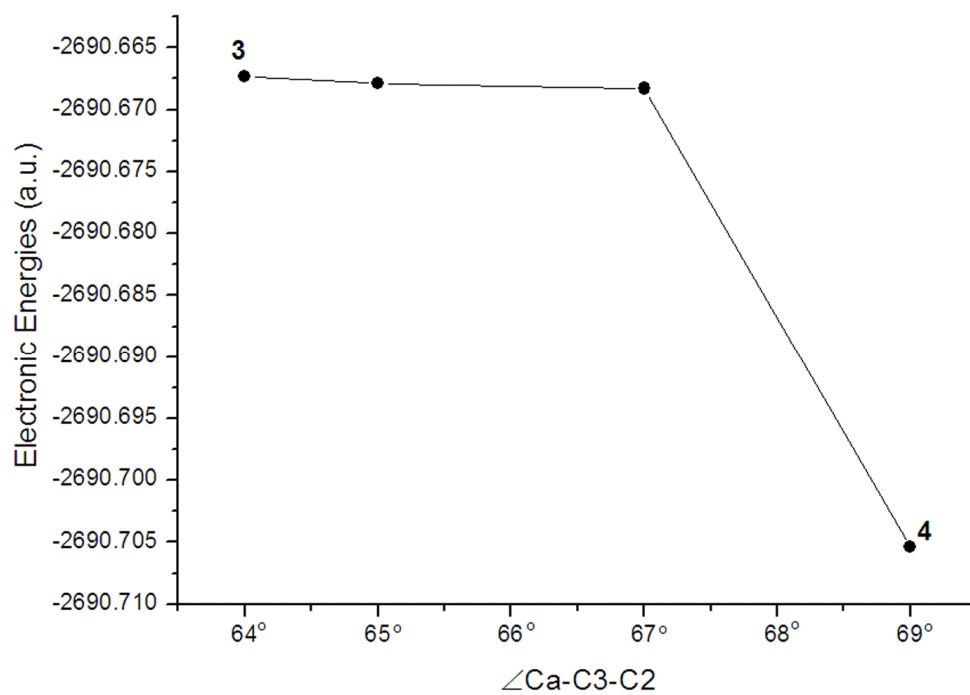


Figure S3. The relaxed potential energy scan results from **3** to **4** by fixing $\angle \text{Ca-C3-C2}$.

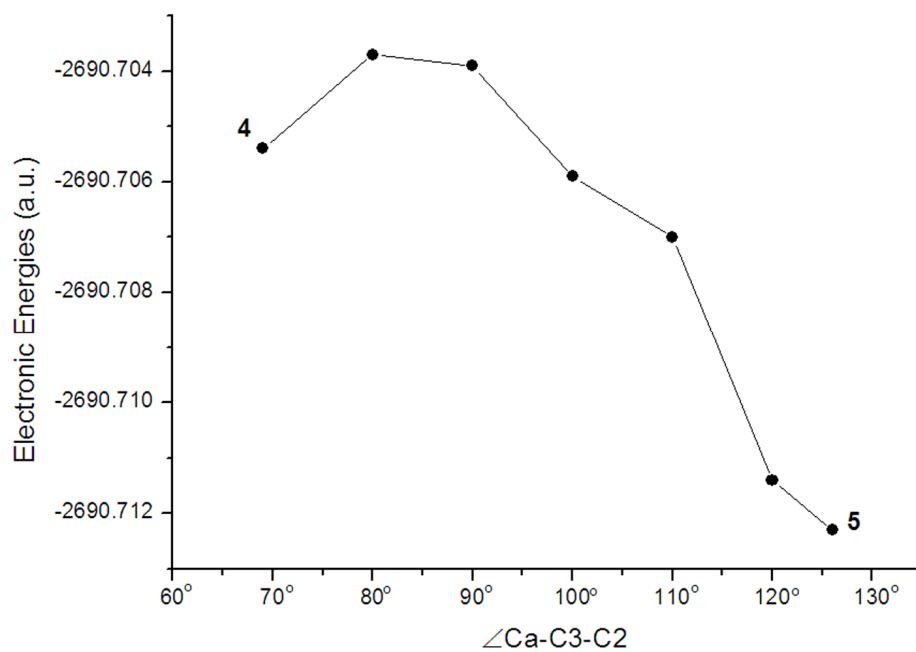


Figure S4. The relaxed potential energy scan results from **4** to **5** by fixing $\angle \text{Ca-C3-C2}$.

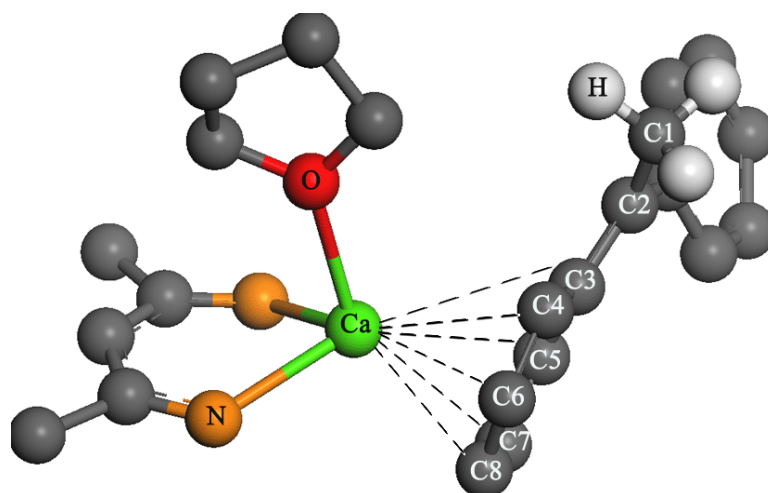


Figure S5. Comparison of the optimized structure of species **5** with the X-ray data (in parenthesis). All hydrogen atoms (except those involved in the hydrogenation reaction) and two 2,6-diisopropylphenyl substituents bound to the nitrogen atoms are omitted for clarity. All the distances are in Å. Ca-C₄: 2.837(2.838); Ca-C₅: 2.893(2.819); Ca-C₆: 2.774(2.754); Ca-C₇: 2.813(2.754); Ca-C₈: 2.763(2.752); C₂-C₃: 1.391(1.387); C₁-C₂: 1.518(1.521). The Ca...Ph distance is about 2.330 Å.

Table S1. Electronic energies (E_{elec}), ZPE-corrected energies (E_0), Gibbs free energies G_g (333.15K and 20 bar), and free energies of solvation $\Delta G_{(s)}$ of the related species involved in the calcium-mediated hydrogenation of DPE and myrcene. The E_{elec} , E_0 and G_g energies are in a.u. and $\Delta G_{(s)}$ are in kcal/mol.

Species	$E_{\text{elec}}(\text{a.u.})$	$E_0(\text{a.u.})$	$G_g(\text{a.u.})$	$\Delta G_{(s)}$ (kcal/mol)	$G_s(\text{a.u.})$
1	-2149.9167	-2149.1530	-2149.2447	17.71	-2149.2165
2	-540.7498	-540.5349	-540.5757	1.51	-540.5733
TS₁	-2690.6567	-2689.6768	-2689.7880	28.09	-2689.7432
3	-2690.6673	-2689.6842	-2689.7931	26.61	-2689.7507
4	-2690.7054	-2689.7194	-2689.8269	27.47	-2689.7831
5	-2690.7123	-2689.7261	-2689.8351	26.79	-2689.7924
H₂	-1.1796	-1.1695	-1.1796	1.98	-1.1764
TS₂	-2691.8646	-2690.8653	-2690.9737	28.10	-2690.9289
6	-541.9757	-541.7375	-541.7800	1.20	-541.7781
7	-390.6366	-390.4040	-390.4466	2.18	-390.4431
TS3	-2540.5414	-2539.5442	-2539.6538	25.61	-2539.6130
8	-2540.5503	-2539.5505	-2539.6621	24.67	-2539.6228
9	-2540.6101	-2539.6056	-2539.7138	26.39	-2539.6717
10	-2540.6021	-2539.5987	-2539.7103	25.87	-2539.6691
TS4	-2541.7621	-2540.7458	-2540.8569	27.12	-2540.8137
11	-391.8685	-391.6123	-391.6556	1.42	-391.6533

Table S2. Electronic energies (E_{elec}), ZPE-corrected energies (E_0), Gibbs free energies G_g (333.15K and 20 bar) and free energies of solvation $\Delta G_{(s)}$ of the related species involved in the magnesium-mediated hydrogenation of DPE. The E_{elec} , E_0 and G_g energies are in a.u. and $\Delta G_{(s)}$ are in kcal/mol.

Species	$E_{\text{elec}}(\text{a.u.})$	$E_0(\text{a.u.})$	$G_g(\text{a.u.})$	$\Delta G_{(s)}$ kcal/mol	$G_s(\text{a.u.})$
1-Mg	-1672.4121	-1671.6451	-1671.7319	17.57	-1671.7039
2	-540.7498	-540.5349	-540.5757	1.51	-540.5733
TS₁-Mg	-2213.1402	-2212.1578	-2212.2669	27.83	-2212.2226

Table S3. Electronic energies (E_{elec}), ZPE-corrected energies (E_0), Gibbs free energies G_g (333.15K and 20 bar) and free energies of solvation $\Delta G_{(s)}$ of the related species involved in the strontium-mediated hydrogenation of DPE. The E_{elec} , E_0 and G_g energies are in a.u. and $\Delta G_{(s)}$ are in kcal/mol.

Species	$E_{\text{elec}}(\text{a.u.})$	$E_0(\text{a.u.})$	$G_g(\text{a.u.})$	$\Delta G_{(s)}$ kcal/mol	$G_s(\text{a.u.})$
1-Sr	-1502.7294	-1501.9672	-1502.0624	18.11	-1502.0335
TS₁-Sr	-2043.4754	-2042.4972	-2042.6105	29.88	-2042.5629
3-Sr	-2043.4966	-2042.5147	-2042.6246	29.10	-2042.5782
4-Sr	-2043.5324	-2042.5480	-2042.6609	27.65	-2042.6168
TS₂-Sr	-2044.6931	-2043.7046	-2043.8178	29.32	-2043.7711

Cartesian coordinates of all obtained stationary points optimized by B3LYP.

1

Ca	-0.530572	0.112403	0.201438
N	-2.878684	-0.134301	0.341014
N	-1.062470	2.404501	0.377612
O	0.576925	-0.939614	2.022246
C	-5.233200	0.489978	0.754815
C	-3.743246	0.811877	0.694776
C	-3.409614	2.154231	0.987676
C	-2.231502	2.903894	0.770079
C	-2.385038	4.410850	0.954572
C	-3.352854	-1.426611	-0.058402
C	-3.594233	-1.686640	-1.436644
C	-3.983305	-2.978390	-1.827101
C	-4.139521	-4.004442	-0.895430
C	-3.892628	-3.746113	0.452942
C	-3.495309	-2.473293	0.895769
C	-3.438984	-0.609091	-2.514803
C	-4.772053	-0.331303	-3.250031
C	-2.330369	-0.981549	-3.528831
C	-3.233115	-2.269384	2.392219
C	-2.111402	-3.207664	2.898879
C	-4.506772	-2.474191	3.247805
C	-0.007709	3.288306	-0.023764
C	1.050864	3.600576	0.872278
C	2.103521	4.416362	0.422818
C	2.136130	4.909445	-0.881026
C	1.104787	4.581498	-1.762239
C	0.026853	3.776766	-1.361151
C	1.077500	3.099523	2.320050
C	0.863360	4.250141	3.333801
C	2.389347	2.345211	2.641825
C	-1.057294	3.430141	-2.387808
C	-1.698540	4.688878	-3.017694
H	-2.102214	5.361039	-2.252418
H	-2.518989	4.400670	-3.685959
H	-0.971458	5.256061	-3.610734
C	-0.495583	2.504333	-3.494185
C	0.452919	-0.715541	3.457933
H	-0.590772	-0.881179	3.741694
H	0.717417	0.328373	3.651016
C	1.430078	-1.693410	4.126725

H	0.915259	-2.620019	4.405186
H	1.873602	-1.266007	5.030877
C	2.467974	-1.963561	3.014248
H	3.216565	-1.165491	2.966461
H	2.988839	-2.917100	3.139472
C	1.602801	-1.952511	1.757642
H	0.724688	-0.649721	-1.395009
H	-5.624988	0.344404	-0.259121
H	-5.793320	1.303247	1.221782
H	-5.427330	-0.435245	1.302576
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H	-3.267520	4.642718	1.556122
H	-2.501954	4.901133	-0.019354
H	-4.167215	-3.181839	-2.877690
H	-4.445925	-4.995031	-1.216431
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H	-3.139568	0.320774	-2.018420
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H	-5.566612	-0.050890	-2.549548
H	-4.646799	0.487736	-3.968576
H	-1.364487	-1.123433	-3.029215
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H	-2.900653	-1.233885	2.533164
H	-1.187183	-3.064170	2.329790
H	-1.902020	-3.019947	3.959800
H	-2.401838	-4.260066	2.802340
H	-4.290302	-2.282116	4.305969
H	-5.314988	-1.802864	2.941431
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H	2.958690	5.537329	-1.208853
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H	-0.082161	4.772924	3.156850
H	1.672719	4.986747	3.264405
H	3.259940	3.004432	2.558154
H	2.369953	1.962056	3.670224
H	2.554128	1.505595	1.957479
H	-1.850893	2.882302	-1.868910
H	0.308083	3.002206	-4.050387
H	-1.283742	2.236336	-4.208239

H	-0.087615	1.578457	-3.072505
H	2.128004	-1.667244	0.844324
H	1.101551	-2.914910	1.597334
H	1.122537	-5.593550	-1.511516
C	2.058620	-5.041108	-1.534715
C	2.031359	-3.641905	-1.594124
C	3.277195	-5.728785	-1.504719
C	3.223599	-2.876861	-1.621260
H	1.073337	-3.129753	-1.607669
C	4.470726	-4.991522	-1.540932
H	3.299998	-6.813206	-1.462012
C	3.173258	-1.406668	-1.710703
C	4.445320	-3.595913	-1.596375
H	5.426460	-5.508790	-1.539337
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H	5.381900	-3.049031	-1.648824
H	1.501496	-1.398586	-3.044763
H	2.080912	0.240144	-2.537564
C	4.877826	-1.027831	0.122829
C	4.388453	0.779179	-1.375193
C	5.769410	-0.212442	0.813755
H	4.734307	-2.046882	0.460354
C	5.274442	1.594469	-0.681346
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H	6.678968	1.742548	0.955195

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C	-1.280263	0.391708	-0.033087
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C	2.629825	-1.424634	0.941160
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C	3.594838	0.113454	-0.658900
H	2.276476	1.657782	-1.388979
C	3.725277	-1.002220	0.176699
H	2.722709	-2.289343	1.590920
H	4.433758	0.438108	-1.266838
H	4.666077	-1.541028	0.226354

TS₁

Ca	-0.530572	0.112403	0.201438
N	-2.878684	-0.134301	0.341014
N	-1.062470	2.404501	0.377612
O	0.576925	-0.939614	2.022246
C	-5.233200	0.489978	0.754815
C	-3.743246	0.811877	0.694776
C	-3.409614	2.154231	0.987676
C	-2.231502	2.903894	0.770079
C	-2.385038	4.410850	0.954572
C	-3.352854	-1.426611	-0.058402
C	-3.594233	-1.686640	-1.436644
C	-3.983305	-2.978390	-1.827101
C	-4.139521	-4.004442	-0.895430
C	-3.892628	-3.746113	0.452942
C	-3.495309	-2.473293	0.895769
C	-3.438984	-0.609091	-2.514803
C	-4.772053	-0.331303	-3.250031
C	-2.330369	-0.981549	-3.528831
C	-3.233115	-2.269384	2.392219
C	-2.111402	-3.207664	2.898879
C	-4.506772	-2.474191	3.247805
C	-0.007709	3.288306	-0.023764
C	1.050864	3.600576	0.872278
C	2.103521	4.416362	0.422818
C	2.136130	4.909445	-0.881026
C	1.104787	4.581498	-1.762239
C	0.026853	3.776766	-1.361151
C	1.077500	3.099523	2.320050
C	0.863360	4.250141	3.333801

C	2.389347	2.345211	2.641825
C	-1.057294	3.430141	-2.387808
C	-1.698540	4.688878	-3.017694
H	-2.102214	5.361039	-2.252418
H	-2.518989	4.400670	-3.685959
H	-0.971458	5.256061	-3.610734
C	-0.495583	2.504333	-3.494185
C	0.452919	-0.715541	3.457933
H	-0.590772	-0.881179	3.741694
H	0.717417	0.328373	3.651016
C	1.430078	-1.693410	4.126725
H	0.915259	-2.620019	4.405186
H	1.873602	-1.266007	5.030877
C	2.467974	-1.963561	3.014248
H	3.216565	-1.165491	2.966461
H	2.988839	-2.917100	3.139472
C	1.602801	-1.952511	1.757642
H	0.724688	-0.649721	-1.395009
H	-5.624988	0.344404	-0.259121
H	-5.793320	1.303247	1.221782
H	-5.427330	-0.435245	1.302576
H	-4.248391	2.749986	1.320465
H	-1.503394	4.850251	1.427799
H	-3.267520	4.642718	1.556122
H	-2.501954	4.901133	-0.019354
H	-4.167215	-3.181839	-2.877690
H	-4.445925	-4.995031	-1.216431
H	-4.013261	-4.547222	1.176158
H	-3.139568	0.320774	-2.018420
H	-5.111566	-1.213840	-3.805168
H	-5.566612	-0.050890	-2.549548
H	-4.646799	0.487736	-3.968576
H	-1.364487	-1.123433	-3.029215
H	-2.213387	-0.188631	-4.277048
H	-2.575092	-1.909730	-4.059228
H	-2.900653	-1.233885	2.533164
H	-1.187183	-3.064170	2.329790
H	-1.902020	-3.019947	3.959800
H	-2.401838	-4.260066	2.802340
H	-4.290302	-2.282116	4.305969
H	-5.314988	-1.802864	2.941431
H	-4.876406	-3.502917	3.162386
H	2.910280	4.667501	1.104281
H	2.958690	5.537329	-1.208853

H	1.138005	4.955646	-2.781089
H	0.239376	2.400898	2.442204
H	0.849237	3.860644	4.359476
H	-0.082161	4.772924	3.156850
H	1.672719	4.986747	3.264405
H	3.259940	3.004432	2.558154
H	2.369953	1.962056	3.670224
H	2.554128	1.505595	1.957479
H	-1.850893	2.882302	-1.868910
H	0.308083	3.002206	-4.050387
H	-1.283742	2.236336	-4.208239
H	-0.087615	1.578457	-3.072505
H	2.128004	-1.667244	0.844324
H	1.101551	-2.914910	1.597334
H	1.122537	-5.593550	-1.511516
C	2.058620	-5.041108	-1.534715
C	2.031359	-3.641905	-1.594124
C	3.277195	-5.728785	-1.504719
C	3.223599	-2.876861	-1.621260
H	1.073337	-3.129753	-1.607669
C	4.470726	-4.991522	-1.540932
H	3.299998	-6.813206	-1.462012
C	3.173258	-1.406668	-1.710703
C	4.445320	-3.595913	-1.596375
H	5.426460	-5.508790	-1.539337
C	2.071399	-0.820153	-2.328135
C	4.149879	-0.563975	-0.998505
H	5.381900	-3.049031	-1.648824
H	1.501496	-1.398586	-3.044763
H	2.080912	0.240144	-2.537564
C	4.877826	-1.027831	0.122829
C	4.388453	0.779179	-1.375193
C	5.769410	-0.212442	0.813755
H	4.734307	-2.046882	0.460354
C	5.274442	1.594469	-0.681346
H	3.889642	1.184046	-2.247262
C	5.978835	1.109475	0.421880
H	6.307418	-0.616369	1.666115
H	5.427757	2.615255	-1.016367
H	6.678968	1.742548	0.955195

3

Ca	0.423053	-0.225172	0.225320
N	2.740317	-0.270675	0.446775
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C	1.667158	-4.713388	0.948600
C	3.370383	0.965397	0.077436
C	3.675731	1.208173	-1.291522
C	4.216462	2.452224	-1.656597
C	4.459655	3.445646	-0.708762
C	4.153221	3.203104	0.630278
C	3.606631	1.978677	1.049086
C	3.444667	0.160168	-2.386458
C	4.768193	-0.267670	-3.065274
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C	3.293776	1.790076	2.538171
C	2.279448	2.846089	3.039555
C	4.567152	1.838926	3.417990
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C	-1.707192	-4.376159	-1.912128
C	-0.555550	-3.712503	-1.460128
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C	-1.575937	-4.220253	3.201527
C	-2.852803	-2.135953	2.528491
C	0.589305	-3.472633	-2.451409
C	1.146594	-4.792399	-3.036036
H	1.465779	-5.481481	-2.246725
H	2.011322	-4.588083	-3.678883
H	0.393933	-5.307536	-3.644198
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C	-0.578991	0.673492	3.410958
H	0.463677	0.687080	3.742667
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C	-1.441181	1.766822	4.056146
H	-0.817429	2.609902	4.373991
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C	-2.383753	2.191183	2.907877

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H	5.434754	-2.047614	1.405664
H	5.272310	-0.277817	1.480364
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H	2.467309	-5.060216	1.607188
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H	5.492103	-0.642271	-2.333414
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H	2.700152	3.856340	2.983089
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H	5.052127	2.819911	3.351229
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5

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C	4.592136	-3.564669	-1.429394
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C	0.752606	-1.083458	-2.749784
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C	1.193055	3.240740	-1.948261

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C	4.599289	-2.313413	-1.760393
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H	5.460031	1.868056	-1.504237
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H	-3.361351	-0.720115	3.586642
C	-1.910808	-1.850811	2.400163
H	-3.336172	1.482770	-2.190131
H	0.998057	4.550580	1.563182
H	2.647303	4.154449	2.096083
H	1.274747	3.826447	3.156186
H	3.074805	1.948873	2.811978
H	3.917146	-0.930369	3.070309
H	4.747023	0.597229	2.735971
H	4.865057	-0.761953	1.595639
H	-0.783324	4.954097	-2.728080
H	-2.800923	5.675012	-1.495751
H	-3.245941	4.780229	0.765645
H	1.467150	2.228203	-1.626220
H	2.158332	5.203845	-1.864358
H	2.600441	4.139531	-0.515954

H	3.287058	3.857201	-2.126067
H	0.122283	2.620446	-3.764937
H	1.882342	2.769225	-3.958331
H	0.877651	4.217567	-3.895005
H	-1.053192	2.328610	2.547351
H	-3.196702	1.470364	1.588452
H	-3.388444	1.935530	3.300185
H	-4.008195	2.989642	2.021226
H	-1.995394	3.814146	4.289132
H	-0.882802	4.755120	3.274057
H	-2.631095	4.917152	3.058891
H	3.616005	-4.920174	0.171006
H	4.999122	-4.434468	-1.823147
H	5.219458	-2.105759	-2.626310
H	1.826740	-2.309401	2.167700
H	2.609886	-4.013705	3.778939
H	4.020521	-3.202983	3.064430
H	3.560912	-4.822735	2.523603
H	1.418954	-5.143411	1.053655
H	0.530742	-4.434449	2.411296
H	0.347918	-3.759501	0.780881
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H	4.981384	-0.197950	-3.637438
H	4.051094	1.296468	-3.521021
H	3.211630	-0.264022	-3.629123
H	-1.664432	-2.920470	2.433531
H	-2.554551	-1.648516	1.542521
H	-7.027956	-2.004735	0.802268
C	-6.357532	-2.266315	-0.011890
C	-5.355801	-1.369802	-0.402287
C	-6.495116	-3.499166	-0.662972
C	-4.464566	-1.670123	-1.456134
H	-5.254584	-0.418244	0.114792
C	-5.625230	-3.814953	-1.714444
H	-7.269465	-4.197535	-0.361249
C	-3.421747	-0.673256	-1.846038
C	-4.629430	-2.911371	-2.106686
H	-5.730601	-4.759913	-2.240399
C	-3.959907	0.619075	-2.452982
C	-2.111377	-1.120994	-2.262167
H	-3.978209	-3.161899	-2.939658
H	-4.963598	0.823870	-2.076489
H	-4.027915	0.579740	-3.549272
C	-1.526806	-2.314575	-1.740609

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C	-0.177386	-2.608403	-1.898284
H	-2.157254	-3.020325	-1.214278
C	0.149829	-0.533915	-3.057247
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C	0.686917	-1.723426	-2.558611
H	0.214011	-3.541497	-1.509047
H	0.789523	0.169233	-3.579757
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6

C	-0.094428	2.538087	0.043355
C	-0.029281	1.134619	-0.590479
H	-0.139250	2.487336	1.134110
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C	-1.314998	-0.405167	0.998727
C	-3.559340	-0.341910	-0.644620
H	-2.376767	0.893844	-1.944696
C	-2.473443	-1.084285	1.370820
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C	-3.600707	-1.056229	0.550926
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H	-4.499542	-1.590105	0.838365
C	1.273457	0.390603	-0.315304
C	2.079199	0.655709	0.803032
C	1.678345	-0.623482	-1.201354
C	3.253025	-0.076518	1.034282
H	1.799406	1.438005	1.501534
C	2.849564	-1.353663	-0.977587
H	1.063786	-0.844130	-2.071215
C	3.642508	-1.083556	0.145943
H	3.860717	0.143826	1.906801
H	3.144365	-2.130399	-1.676611
H	4.551688	-1.649157	0.322923
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H	-0.994394	3.058446	-0.292334

7

C	-1.411965	1.401619	0.220608
C	-0.109112	1.477895	-0.080024
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C	0.364896	1.636998	-1.470682
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H	0.496300	1.455519	1.982163
H	1.567271	2.368263	0.909617
C	1.933674	0.229768	0.892177
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H	2.740407	0.374357	1.618597
C	1.243637	-1.094277	1.095988
C	1.496911	-2.033293	2.029855
H	0.438929	-1.296756	0.388001
C	2.571879	-1.939015	3.090532
H	2.135228	-2.048392	4.093161
H	3.299815	-2.755161	2.976785
H	3.123255	-0.996252	3.067334
C	0.693184	-3.316790	2.073160
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H	0.189320	-3.435490	3.042918
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8

Ca	0.6562	-0.10706	0.24186
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O	-0.22564	-0.85553	2.31304
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C	3.91477	1.51058	0.18982
C	3.98298	0.11195	0.01232
C	5.39197	-0.4492	-0.15701
C	0.05223	-0.58697	3.71389
C	-1.29465	-0.7364	4.46215
H	-1.60682	0.20859	4.91454

H	-1.20047	-1.4768	5.26328
C	-2.29854	-1.20208	3.37109
H	-2.88908	-0.3639	2.99116
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C	-1.39898	-1.72303	2.25242
H	-1.22734	-1.0863	-1.11308
H	2.86011	4.38302	-0.78827
H	4.30435	4.0166	0.17777
H	2.76423	4.4206	0.96468
H	4.8807	1.98849	0.27054
H	5.5166	-0.86886	-1.16141
H	6.14515	0.32841	-0.01343
H	5.58634	-1.26199	0.54784
H	0.47767	0.41827	3.7677
H	0.79741	-1.31056	4.06219
H	-1.06996	-2.75709	2.43036
H	-1.84826	-1.636	1.25566
C	-3.90792	-0.28415	-0.0325
C	-3.3247	0.97141	-0.03823
H	-2.50189	1.22313	-0.69847
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H	-2.32571	-0.43345	-2.3243
C	-5.1669	-0.48949	0.8127
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C	-6.50563	-0.2359	0.05029
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C	-8.90661	-2.26919	-0.20917
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C	0.55662	3.084	-0.19879

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H	-1.13632	4.5131	-2.803
H	-1.68465	5.10788	1.40047
H	-2.32597	5.61424	-0.93424
C	3.14155	-2.08675	-0.39886
C	3.06333	-2.47962	-1.76505
C	3.34084	-3.0699	0.61039
C	3.20436	-3.83819	-2.09117
C	3.47908	-4.41542	0.2294
C	3.41724	-4.80453	-1.10838
H	3.14818	-4.1428	-3.13182
H	3.63983	-5.17004	0.99333
H	3.52845	-5.84914	-1.38132
C	2.83184	-1.47449	-2.89893
C	4.03129	-1.41858	-3.87541
C	1.5248	-1.78086	-3.66905
H	2.73046	-0.47977	-2.45045
H	4.96249	-1.16824	-3.35572
H	4.17689	-2.38143	-4.37937
H	3.85861	-0.65889	-4.6473
H	0.65571	-1.78246	-2.99975
H	1.35359	-1.02766	-4.44688
H	1.57077	-2.76158	-4.15698
C	3.40428	-2.72579	2.10282
C	2.28905	-3.45331	2.89199
C	4.78059	-3.05747	2.72986
H	3.24362	-1.64602	2.20461
H	1.29832	-3.2238	2.48572
H	2.42105	-4.54063	2.85149
H	2.31118	-3.1585	3.94869
H	5.59815	-2.54114	2.2171
H	4.80001	-2.75733	3.78473
H	4.98504	-4.13367	2.68406
C	0.88724	2.7237	-2.74246
C	-0.09504	1.86497	-3.57428
C	1.58361	3.77078	-3.64461
H	1.66711	2.05739	-2.35719
H	-0.56343	1.0836	-2.96423
H	-0.89995	2.47808	-3.99572
H	0.42919	1.3798	-4.40647

H	2.30486	4.37148	-3.07932
H	2.12191	3.27292	-4.46042
H	0.85557	4.45682	-4.09364
C	0.21106	3.43938	2.34456
C	0.70737	4.70743	3.08097
C	-1.00141	2.83979	3.09686
H	1.0253	2.70388	2.36738
H	1.58276	5.14728	2.59195
H	-0.07568	5.47405	3.11244
H	0.98152	4.46549	4.11531
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H	-0.7271	2.59196	4.13064
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TS₃

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C	3.982928	0.111213	0.012160
C	5.392434	-0.448103	-0.157890
C	0.050637	-0.588520	3.713715
C	-1.296288	-0.735612	4.462778
H	-1.608757	0.210276	4.913517
H	-1.203379	-1.474405	5.265438
C	-2.298928	-1.203167	3.371329
H	-2.891063	-0.364542	2.995001
H	-2.985075	-1.974747	3.732579
C	-1.396275	-1.723737	2.254259
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H	4.303458	4.019143	0.176558
H	2.764466	4.420964	0.966524
H	4.879671	1.990071	0.269466
H	5.515916	-0.868920	-1.162031
H	6.145836	0.329608	-0.015246
H	5.586776	-1.260478	0.547568

H	0.479226	0.415495	3.769097
H	0.794017	-1.313492	4.063538
H	-1.068114	-2.757649	2.435114
H	-1.824205	-1.641489	1.250942
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C	-3.336242	0.965759	-0.039276
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H	-3.763351	1.791827	0.518776
C	-3.398832	-1.399448	-0.759095
C	-2.370823	-1.315703	-1.678247
H	-3.740049	-2.383842	-0.449699
H	-2.048809	-2.211298	-2.197168
H	-2.236069	-0.401880	-2.244358
C	-5.169394	-0.488132	0.812249
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H	-5.147628	0.191625	1.675595
C	-6.507488	-0.237661	0.049433
H	-7.323968	-0.257902	0.781296
H	-6.468376	0.786160	-0.352464
C	-6.766581	-1.205332	-1.076433
C	-7.783615	-2.081667	-1.206347
H	-6.018333	-1.183585	-1.868190
C	-7.873965	-2.984770	-2.420137
H	-7.859578	-4.045110	-2.128071
H	-8.814862	-2.823251	-2.966408
H	-7.044067	-2.813569	-3.112991
C	-8.906772	-2.270901	-0.209697
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H	-8.864795	-1.569794	0.627110
H	-9.883418	-2.151027	-0.699816
C	0.557247	3.084289	-0.199291
C	0.188243	3.375004	-1.543601
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H	-2.326708	5.616404	-0.934647
C	3.142089	-2.085927	-0.399395
C	3.063101	-2.479029	-1.765558
C	3.340947	-3.069259	0.609518
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C	3.417137	-4.804085	-1.108771
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H	3.639795	-5.169574	0.993054
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C	2.831101	-1.474267	-2.899709
C	4.031146	-1.417882	-3.875366
C	1.524245	-1.781450	-3.669669
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H	4.962526	-1.166969	-3.355732
H	4.177273	-2.380760	-4.379445
H	3.857952	-0.658479	-4.647641
H	0.659346	-1.779005	-2.996446
H	1.355250	-1.028109	-4.448493
H	1.572710	-2.762002	-4.158648
C	3.404126	-2.725145	2.102085
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C	4.780132	-3.056886	2.729597
H	3.243323	-1.645299	2.203561
H	1.298779	-3.223393	2.483640
H	2.421325	-4.540125	2.850364
H	2.310878	-3.158100	3.948276
H	5.597614	-2.540607	2.216627
H	4.799794	-2.756924	3.784680
H	4.984590	-4.133147	2.683448
C	0.885685	2.723826	-2.743094
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H	-0.901125	2.478154	-3.997113
H	0.428765	1.380638	-4.407040
H	2.303640	4.371683	-3.079886
H	2.120273	3.272898	-4.460606
H	0.854185	4.457316	-4.094434
C	0.209832	3.439277	2.343815
C	0.705758	4.707390	3.080374
C	-1.002206	2.839354	3.096880
H	1.024059	2.703982	2.365388
H	1.582480	5.144750	2.591727
H	-0.076233	5.475327	3.109392
H	0.978227	4.466485	4.115449
H	-1.377783	1.937446	2.601130
H	-0.727838	2.589700	4.130135
H	-1.830329	3.556405	3.139560

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Ca	0.274384	0.177538	-0.631394
N	2.259312	-0.322876	0.681285
N	-0.192954	1.576179	1.250890
O	1.399710	1.888723	-1.987957
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C	2.757482	0.533185	1.566920
C	2.104391	1.690699	2.056186
C	0.755049	2.116526	2.006923
C	0.429976	3.306539	2.910148
C	2.307831	2.888478	-1.460807
C	3.157487	3.322954	-2.654032
H	3.973629	2.610844	-2.822423
H	3.591806	4.317257	-2.511631
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H	0.898394	-2.006842	-1.867558
H	4.046507	-0.416921	3.025662
H	4.565113	1.209261	2.564613
H	4.824345	-0.169633	1.466000
H	2.720715	2.287080	2.716109
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H	1.138301	3.378077	3.739550
H	0.492210	4.238766	2.334224
H	2.863083	2.433235	-0.637328
H	1.719001	3.726956	-1.064944
H	0.192266	2.201040	-3.650356
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C	-1.163585	-2.024904	-1.052555
C	0.049023	-2.686922	-1.664119
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H	-0.168236	-3.135153	-2.646161
C	-3.225214	-0.598731	-1.186533
H	-3.379302	-1.017495	-0.185026
H	-3.281571	0.494838	-1.093026
C	-4.391014	-1.063702	-2.110149
H	-5.323715	-0.635558	-1.725301

H	-4.228082	-0.623035	-3.105468
C	-4.489673	-2.561862	-2.239941
C	-5.530473	-3.362992	-1.933146
H	-3.587726	-3.036928	-2.626941
C	-5.440449	-4.862013	-2.136769
H	-5.599853	-5.400802	-1.191500
H	-6.214801	-5.215304	-2.833470
H	-4.464674	-5.158356	-2.535050
C	-6.859271	-2.891660	-1.382933
H	-6.900472	-1.812105	-1.220849
H	-7.679071	-3.160216	-2.065053
H	-7.077287	-3.384318	-0.424464
C	2.930935	-1.567110	0.452800
C	2.691815	-2.666339	1.325074
C	3.762556	-1.741286	-0.688220
C	3.280704	-3.907316	1.033493
C	4.335264	-3.001367	-0.930575
C	4.099155	-4.083365	-0.082926
H	3.094910	-4.749904	1.692830
H	4.977262	-3.135795	-1.796123
H	4.547054	-5.050450	-0.288796
C	-1.564996	1.942311	1.430665
C	-2.383895	1.130065	2.267236
C	-2.136755	3.033457	0.722673
C	-3.745214	1.446918	2.395524
C	-3.508135	3.300500	0.875684
C	-4.310886	2.523203	1.708857
H	-4.375617	0.840050	3.036568
H	-3.950519	4.132779	0.336073
H	-5.366960	2.748925	1.819730
C	-1.802661	-0.058650	3.040886
C	-1.372800	0.349984	4.472265
C	-2.759884	-1.268522	3.103415
H	-0.898699	-0.378575	2.509294
H	-0.609740	1.134032	4.454730
H	-2.232892	0.722384	5.042929
H	-0.958080	-0.513225	5.007607
H	-3.107289	-1.556729	2.105629
H	-2.243575	-2.128402	3.544823
H	-3.639727	-1.064365	3.725255
C	-1.315478	3.931672	-0.206848
C	-1.758569	3.778632	-1.681823
C	-1.374543	5.419522	0.214967
H	-0.271495	3.608343	-0.138294

H	-1.683635	2.737825	-2.015008
H	-2.799090	4.099345	-1.813848
H	-1.133167	4.398407	-2.338011
H	-1.069188	5.554373	1.257926
H	-0.712026	6.023277	-0.418337
H	-2.388925	5.821806	0.110718
C	1.793652	-2.554768	2.561747
C	0.507327	-3.399590	2.396438
C	2.532136	-2.957300	3.860526
H	1.488435	-1.508648	2.664800
H	-0.068642	-3.076753	1.522903
H	0.747391	-4.462810	2.271988
H	-0.131439	-3.302067	3.282578
H	3.451889	-2.378251	3.998797
H	1.887173	-2.785482	4.730847
H	2.804624	-4.019514	3.854035
C	4.080697	-0.594984	-1.653826
C	5.561624	-0.153481	-1.551205
C	3.738288	-0.951244	-3.120248
H	3.460959	0.259652	-1.364505
H	5.817486	0.161840	-0.534293
H	6.234548	-0.974287	-1.826831
H	5.762492	0.686329	-2.229085
H	2.692129	-1.259494	-3.226903
H	3.912412	-0.087475	-3.774564
H	4.363141	-1.773128	-3.488744

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Ca	0.36025	-0.16721	0.34452
N	0.32948	2.20997	0.16463
N	2.63918	0.12294	-0.31318
O	0.42796	-0.76073	2.68862
C	1.27513	4.4685	0.49425
C	1.42027	2.96004	0.30584
C	2.7525	2.49084	0.26062
C	3.31368	1.25293	-0.14291
C	4.80936	1.30565	-0.44552
C	1.20297	-0.09002	3.71274
C	0.47896	-0.3644	5.05323
H	0.03846	0.54856	5.46379
H	1.18599	-0.75353	5.79274
C	-0.61428	-1.41415	4.6992
H	-1.60303	-0.94863	4.65308

H	-0.65871	-2.23321	5.42334
C	-0.20086	-1.91243	3.31253
H	0.00633	-3.77001	0.69538
H	0.8329	4.92876	-0.39607
H	2.24395	4.93847	0.6782
H	0.60734	4.69793	1.32996
H	3.48984	3.26545	0.4208
H	4.96496	1.42957	-1.52453
H	5.27953	2.15405	0.05858
H	5.32044	0.38639	-0.15362
H	1.25303	0.96769	3.44058
H	2.21872	-0.50386	3.70729
H	0.54062	-2.71935	3.37958
H	-1.02394	-2.22751	2.66318
C	-2.25466	-2.11789	-0.03967
C	-1.2561	-1.58034	-0.95684
H	-0.64576	-2.34221	-1.45279
H	-1.6828	-0.91403	-1.71297
C	-2.12273	-3.28449	0.65048
C	-0.96807	-4.23375	0.47143
H	-2.92039	-3.58844	1.32315
H	-1.06388	-5.10865	1.12059
H	-0.88491	-4.60015	-0.56126
C	-3.51396	-1.27949	0.17292
H	-4.03637	-1.61754	1.07854
H	-3.23101	-0.22633	0.32938
C	-4.51389	-1.31886	-1.0225
H	-5.2958	-0.57201	-0.84216
H	-3.97506	-0.99398	-1.92553
C	-5.10548	-2.68382	-1.25887
C	-6.40629	-3.03575	-1.31221
H	-4.3647	-3.47243	-1.39314
C	-6.80955	-4.47445	-1.56476
H	-7.42131	-4.86608	-0.73895
H	-7.42	-4.56232	-2.4757
H	-5.93637	-5.1251	-1.6779
C	-7.57285	-2.0855	-1.14798
H	-8.22807	-2.41434	-0.32839
H	-7.26523	-1.05815	-0.93943
H	-8.19323	-2.0711	-2.05612
C	-0.94394	2.84229	-0.01926
C	-1.38098	3.15573	-1.33752
C	-1.807	3.08672	1.08389
C	-2.65901	3.70771	-1.51867

C	-3.0794	3.63509	0.84891
C	-3.50906	3.95014	-0.43934
H	-2.99329	3.95033	-2.52291
H	-3.74018	3.82338	1.68998
H	-4.49434	4.37602	-0.60098
C	3.29595	-1.02159	-0.87432
C	3.24911	-1.23985	-2.27871
C	3.9269	-1.97886	-0.03111
C	3.85306	-2.39192	-2.80841
C	4.51575	-3.11477	-0.6108
C	4.48871	-3.32477	-1.98932
H	3.82291	-2.55995	-3.88066
H	5.00268	-3.84609	0.02789
H	4.95153	-4.20757	-2.41902
C	2.558	-0.2671	-3.23937
C	3.56147	0.38431	-4.22078
C	1.41629	-0.96147	-4.01989
H	2.11364	0.53491	-2.64024
H	4.36679	0.90167	-3.68791
H	4.02089	-0.36757	-4.87398
H	3.05048	1.11533	-4.8592
H	0.66601	-1.38159	-3.34146
H	0.91526	-0.24538	-4.68139
H	1.80081	-1.77789	-4.6432
C	3.98599	-1.8221	1.49158
C	3.28584	-3.00452	2.20246
C	5.43457	-1.67728	2.018
H	3.44827	-0.90232	1.74887
H	2.25768	-3.13172	1.84705
H	3.81607	-3.94581	2.01693
H	3.26441	-2.84678	3.28871
H	5.94928	-0.82639	1.56059
H	5.43309	-1.52704	3.10508
H	6.02275	-2.57811	1.8065
C	-0.50668	2.9126	-2.57173
C	-1.18745	1.94411	-3.56781
C	-0.13406	4.23498	-3.28511
H	0.42422	2.44439	-2.23561
H	-1.42582	0.98684	-3.09238
H	-2.12044	2.36642	-3.96016
H	-0.52681	1.74826	-4.42055
H	0.38456	4.92558	-2.61115
H	0.5259	4.0343	-4.13801
H	-1.02768	4.7449	-3.66509

C	-1.40428	2.78127	2.52968
C	-1.43134	4.04373	3.42529
C	-2.30193	1.68118	3.14453
H	-0.37246	2.41068	2.51448
H	-0.79623	4.83928	3.02171
H	-2.4483	4.4431	3.51493
H	-1.07666	3.80455	4.43584
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H	-1.99392	1.4634	4.17448
H	-3.35009	2.00096	3.17092

TS₄

Ca	0.47576	0.02781	-0.6979
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C	3.66303	-1.77137	2.30024
C	2.68922	-0.81873	1.60608
C	3.01193	0.55444	1.75325
C	2.27077	1.73289	1.50492
C	2.88168	3.01117	2.0781
C	3.61825	0.80966	-2.02407
C	4.47096	-0.05617	-2.95391
H	4.65316	-1.03266	-2.4948
H	5.43912	0.40673	-3.16851
C	3.57928	-0.19732	-4.21945
H	3.60285	-1.21604	-4.61546
H	3.90662	0.47827	-5.01628
C	2.15921	0.18752	-3.73661
H	-1.1445	-0.02689	-3.91778
H	3.15331	-2.65507	2.69053
H	4.18589	-1.27037	3.11879
H	4.41655	-2.12335	1.5854
H	3.93173	0.72572	2.29656
H	2.12386	3.64096	2.55078
H	3.66151	2.78613	2.80951
H	3.32953	3.60517	1.27155
H	3.79395	0.65661	-0.95557
H	3.7285	1.87838	-2.25902
H	1.80717	1.11625	-4.20365
H	1.40929	-0.59352	-3.88149
C	-2.7001	-0.21558	-1.44504

C	-2.04308	0.99414	-1.26914
H	-1.7067	1.55914	-2.13489
H	-2.22215	1.58728	-0.3766
C	-2.55695	-1.02687	-2.60497
C	-2.17872	-0.4047	-3.93235
H	-3.23028	-1.87911	-2.66517
H	-2.23226	-1.14328	-4.73696
H	-2.81972	0.4427	-4.20803
C	-3.4766	-0.79804	-0.27043
H	-3.56693	-1.88552	-0.3877
H	-2.93144	-0.61122	0.66586
C	-4.90256	-0.18433	-0.11418
H	-5.34037	-0.57161	0.81298
H	-4.78335	0.90131	0.02221
H	-0.26478	-1.60421	-2.09538
H	-1.24787	-1.53005	-2.24378
C	-5.80806	-0.43767	-1.29169
C	-6.99104	-1.08473	-1.3118
H	-5.43877	-0.03817	-2.23671
C	-7.773	-1.22775	-2.60197
H	-7.93709	-2.28612	-2.85043
H	-8.76833	-0.7679	-2.515
H	-7.25462	-0.75828	-3.44412
C	-7.66488	-1.70731	-0.10871
H	-7.89408	-2.76511	-0.30086
H	-7.06164	-1.65614	0.80051
H	-8.62545	-1.21268	0.09729
C	1.32823	-2.69149	1.00753
C	0.32825	-3.1061	1.93277
C	1.92704	-3.64353	0.13926
C	-0.01901	-4.46493	1.99492
C	1.53855	-4.99043	0.23715
C	0.58161	-5.40803	1.15978
H	-0.77264	-4.79105	2.70328
H	1.99408	-5.72219	-0.42336
H	0.29967	-6.45443	1.22301
C	0.33387	2.98113	0.86469
C	-0.64865	3.12033	1.88587
C	0.44639	3.97749	-0.14211
C	-1.48601	4.24734	1.8778
C	-0.4242	5.08034	-0.11384
C	-1.3852	5.22374	0.88555
H	-2.2309	4.36149	2.65949
H	-0.34388	5.84087	-0.88524

H	-2.04725	6.08392	0.89246
C	1.4925	3.90564	-1.25765
C	0.83587	3.80061	-2.65526
C	2.46283	5.1109	-1.2217
H	2.08362	2.99882	-1.0941
H	0.1679	2.93484	-2.72258
H	0.23957	4.69353	-2.87718
H	1.60167	3.70954	-3.43659
H	2.93932	5.21439	-0.2412
H	3.25106	4.99289	-1.97647
H	1.93607	6.04842	-1.43544
C	-0.80791	2.08771	3.00639
C	-0.27463	2.62624	4.35728
C	-2.27162	1.6173	3.16629
H	-0.20358	1.21493	2.73758
H	0.78254	2.90394	4.29127
H	-0.83818	3.51314	4.67283
H	-0.37576	1.86416	5.1399
H	-2.67485	1.23541	2.22209
H	-2.33242	0.81735	3.91372
H	-2.92376	2.43131	3.50429
C	-0.35058	-2.107	2.87612
C	-1.84195	-2.42291	3.12236
C	0.39529	-2.00108	4.23006
H	-0.2919	-1.12035	2.40008
H	-2.38407	-2.56684	2.18162
H	-1.97194	-3.32634	3.73003
H	-2.31339	-1.59695	3.66698
H	1.42825	-1.66683	4.09552
H	-0.10862	-1.28352	4.88959
H	0.41279	-2.97438	4.73639
C	2.97317	-3.27012	-0.91599
C	4.31333	-4.01586	-0.7052
C	2.44519	-3.53755	-2.34692
H	3.16762	-2.19509	-0.82655
H	4.71173	-3.86443	0.30308
H	4.19036	-5.09503	-0.8544
H	5.06316	-3.66627	-1.42667
H	1.5089	-2.99923	-2.52784
H	3.18589	-3.22376	-3.0945
H	2.25489	-4.60686	-2.49948

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H	-0.851504	-0.480491	-3.660534
C	-2.571059	-0.208508	-1.354057
C	-1.862037	0.922491	-1.304116
H	-1.301612	1.297612	-2.151925
H	-1.820451	1.518832	-0.397908
C	-2.639949	-1.100795	-2.574531
C	-1.923461	-0.611304	-3.832229
H	-3.696882	-1.288226	-2.799154
H	-2.042884	-1.333670	-4.644033
H	-2.326504	0.345473	-4.176237
C	-3.369710	-0.686539	-0.147414
H	-3.476961	-1.779258	-0.189283
H	-2.813265	-0.449956	0.769250
C	-4.790666	-0.051255	-0.018422
H	-5.241121	-0.428454	0.907380
H	-4.657836	1.031744	0.116340
H	-2.239708	-2.082983	-2.286130
C	-5.702904	-0.287319	-1.196353
C	-6.746630	-1.137505	-1.281324
H	-5.478970	0.318193	-2.075799
C	-7.566921	-1.235073	-2.550967
H	-7.549309	-2.256728	-2.956851
H	-8.622093	-0.992555	-2.359786
H	-7.198358	-0.555066	-3.325827
C	-7.209468	-2.051143	-0.167683
H	-7.164487	-3.102029	-0.486883
H	-6.615204	-1.955273	0.743938
H	-8.258689	-1.848186	0.089775

1-Mg

Mg	-0.00689	0.30393	-0.81424
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O	-0.17058	2.44	-0.66778
C	2.43456	-0.4712	2.81434
C	1.28765	-0.31041	1.82078
C	-0.00463	-0.36663	2.38769
C	-1.27567	-0.52298	1.78434
C	-2.39501	-0.95651	2.72416
C	2.88181	-0.45123	0.05641
C	3.28797	-1.79854	-0.14901
C	4.59053	-2.05402	-0.60589
C	5.48824	-1.01858	-0.86579
C	5.07307	0.30038	-0.69142
C	3.77743	0.60787	-0.24301
C	2.34273	-2.98665	0.05862
C	2.90972	-4.03597	1.04278
C	2.00242	-3.64918	-1.29839
C	3.38644	2.08012	-0.10035
C	3.56472	2.8398	-1.43655
C	4.17056	2.78719	1.03106
C	-2.83197	-0.65932	-0.02764
C	-3.88665	0.29202	0.03116
C	-5.13233	-0.03715	-0.5276
C	-5.35389	-1.27218	-1.13587
C	-4.31027	-2.19393	-1.20326
C	-3.04399	-1.9105	-0.66534
C	-3.71353	1.68416	0.64528
C	-4.76642	2.00004	1.73382
C	-3.75339	2.77363	-0.45419
C	-1.94418	-2.9674	-0.79651
C	-2.28458	-4.24945	0.00026
H	-2.45286	-4.0292	1.06082
H	-1.4628	-4.97249	-0.07149
H	-3.18944	-4.73049	-0.39051
C	-1.66068	-3.29935	-2.28078
C	-0.18623	3.27404	0.51967
H	0.50886	2.83862	1.24262
H	-1.19655	3.25338	0.94315
C	0.19494	4.67413	0.03383
H	1.28436	4.78493	-0.00411

H	-0.20684	5.45643	0.68494
C	-0.40979	4.69982	-1.38754
H	-1.47773	4.94069	-1.34512
H	0.07777	5.42438	-2.04634
C	-0.20208	3.26114	-1.87524
H	0.04056	0.07339	-2.53705
H	2.80257	-1.5036	2.81397
H	2.10108	-0.2341	3.82814
H	3.28215	0.16857	2.55553
H	-0.01064	-0.45876	3.46508
H	-3.21154	-0.2292	2.73693
H	-2.02391	-1.08442	3.74341
H	-2.82551	-1.90626	2.38737
H	4.90417	-3.08127	-0.76519
H	6.49425	-1.23709	-1.21032
H	5.76549	1.10828	-0.9083
H	1.40807	-2.60694	0.48302
H	3.81615	-4.50935	0.64685
H	3.16243	-3.58875	2.0106
H	2.17153	-4.82815	1.21746
H	1.55513	-2.92661	-1.98892
H	1.29535	-4.47522	-1.15438
H	2.90383	-4.05633	-1.7726
H	2.32509	2.11057	0.16118
H	3.01404	2.34759	-2.24564
H	3.20508	3.87287	-1.34515
H	4.6194	2.88527	-1.73199
H	3.85471	3.83445	1.12436
H	4.0104	2.29752	1.99792
H	5.24796	2.78069	0.8268
H	-5.94044	0.68723	-0.48665
H	-6.32563	-1.5102	-1.5573
H	-4.47765	-3.15199	-1.68577
H	-2.72593	1.71814	1.11691
H	-4.55593	2.97279	2.19561
H	-4.77405	1.24343	2.5256
H	-5.77643	2.04705	1.31059
H	-4.73349	2.79512	-0.94522
H	-3.57428	3.76769	-0.02352
H	-2.99893	2.58225	-1.22358
H	-1.02659	-2.55055	-0.36835
H	-2.54836	-3.7154	-2.77229
H	-0.85742	-4.04061	-2.35894
H	-1.35322	-2.40209	-2.82824

H	-1.00255	2.88611	-2.5177
H	0.75202	3.12601	-2.39311

TS₁-Mg

Mg	0.337770	-0.522746	0.314364
N	2.312765	-1.160133	0.467856
N	-0.488879	-2.427161	0.411362
O	-0.190124	0.618052	1.984504
C	4.019575	-2.828926	1.115779
C	2.574803	-2.380969	0.935459
C	1.599148	-3.354034	1.248653
C	0.224024	-3.425087	0.934589
C	-0.444605	-4.763409	1.223726
C	3.404575	-0.333057	0.016540
C	3.811855	-0.399501	-1.343033
C	4.850000	0.438681	-1.782015
C	5.483089	1.328969	-0.915581
C	5.070011	1.395276	0.414371
C	4.035190	0.580160	0.902997
C	3.159456	-1.342836	-2.358281
C	4.166317	-2.369947	-2.929497
C	2.493011	-0.551360	-3.508777
C	3.634601	0.721253	2.374161
C	3.138514	2.153957	2.683558
C	4.784773	0.345753	3.339901
C	-1.809920	-2.687365	-0.103191
C	-2.958102	-2.533549	0.715544
C	-4.228039	-2.742476	0.151064
C	-4.379380	-3.099692	-1.187708
C	-3.245338	-3.246858	-1.987105
C	-1.954328	-3.041687	-1.473344
C	-2.876865	-2.133690	2.190607
C	-3.500459	-3.197327	3.126184
C	-3.550492	-0.761671	2.432487
C	-0.752015	-3.237338	-2.403618
C	-0.518776	-4.734314	-2.725504
H	-0.358622	-5.322787	-1.815942
H	0.363734	-4.853987	-3.365970
H	-1.380535	-5.159033	-3.254709
C	-0.887301	-2.427798	-3.713871
C	-0.110873	0.297309	3.405061
H	0.888088	-0.099101	3.606777
H	-0.854673	-0.477946	3.615920
C	-0.419698	1.604309	4.142433

H	0.499998	2.170165	4.322890
H	-0.901798	1.417890	5.106975
C	-1.333848	2.354130	3.148283
H	-2.370641	2.013352	3.233662
H	-1.318658	3.438062	3.293252
C	-0.752776	1.965963	1.790121
H	-0.326457	0.710262	-0.993778
H	4.484819	-3.001386	0.138124
H	4.070602	-3.760343	1.684211
H	4.621139	-2.069382	1.619921
H	1.999890	-4.256988	1.687069
H	-1.118040	-4.670877	2.083595
H	0.296398	-5.532798	1.451376
H	-1.053946	-5.097548	0.379883
H	5.165398	0.392817	-2.819817
H	6.285213	1.966455	-1.273663
H	5.559078	2.092452	1.087851
H	2.375046	-1.904894	-1.840443
H	4.962651	-1.872640	-3.495991
H	4.638564	-2.958266	-2.135048
H	3.656162	-3.063975	-3.608360
H	1.747786	0.154374	-3.126433
H	1.992059	-1.234029	-4.204463
H	3.235058	0.021187	-4.077624
H	2.807346	0.027881	2.557909
H	2.313918	2.443247	2.024284
H	2.798380	2.226676	3.724117
H	3.942435	2.886707	2.548426
H	4.447268	0.419748	4.381224
H	5.140466	-0.676095	3.172505
H	5.639572	1.021209	3.217544
H	-5.110775	-2.620748	0.771332
H	-5.368858	-3.258517	-1.604639
H	-3.363784	-3.525632	-3.029390
H	-1.815550	-2.044425	2.448931
H	-3.364624	-2.908489	4.175950
H	-3.046151	-4.183188	2.982093
H	-4.576972	-3.298578	2.946230
H	-4.624671	-0.810302	2.221061
H	-3.433165	-0.452424	3.479289
H	-3.127019	0.013204	1.786178
H	0.138057	-2.873050	-1.879505
H	-1.738409	-2.769555	-4.314284
H	0.014422	-2.546351	-4.325559

H	-1.024132	-1.360156	-3.512178
H	-1.488714	1.908969	0.987750
H	0.062735	2.625739	1.478505
H	1.781727	6.924324	-1.193119
C	1.112713	6.072939	-1.268300
C	-0.262027	6.260680	-1.482907
C	1.603365	4.766666	-1.168858
C	-1.126617	5.169307	-1.582019
H	-0.660108	7.266488	-1.588518
C	0.738706	3.669188	-1.269099
H	2.665406	4.594090	-1.012813
C	-0.658026	3.832205	-1.470797
H	-2.178951	5.345352	-1.781185
H	1.155876	2.669775	-1.185359
C	-1.542195	2.669632	-1.602620
C	-0.964184	1.443820	-2.010577
C	-2.933434	2.686814	-1.132421
H	-1.636910	0.647848	-2.306650
H	-0.093866	1.500759	-2.658023
C	-3.402862	3.605865	-0.160060
C	-3.889405	1.748095	-1.595134
C	-4.713034	3.587219	0.305982
H	-2.716875	4.337000	0.249240
C	-5.196694	1.727251	-1.124252
H	-3.611125	1.035293	-2.361861
C	-5.629559	2.648611	-0.169281
H	-5.019809	4.314105	1.052123
H	-5.889532	0.991750	-1.520849
H	-6.652618	2.638955	0.189147

1-Sr

Sr	-0.003858	0.542466	-1.213671
N	1.599617	-0.506053	0.565263
N	-1.609507	-0.482190	0.573215
O	0.023500	3.072672	-0.476449
C	2.406946	-1.030682	2.840006
C	1.297776	-0.689887	1.844495
C	-0.001753	-0.637739	2.409824
C	-1.305619	-0.660856	1.852325
C	-2.417203	-0.963017	2.857566
C	2.923247	-0.772837	0.099517

C	3.273507	-2.087678	-0.319039
C	4.557270	-2.319689	-0.836947
C	5.492536	-1.290953	-0.957425
C	5.137001	0.000635	-0.570643
C	3.864560	0.283758	-0.046961
C	2.278962	-3.251165	-0.259545
C	2.796465	-4.427940	0.600101
C	1.920177	-3.743835	-1.682647
C	3.537029	1.727730	0.344642
C	3.644400	2.682333	-0.869431
C	4.427361	2.236517	1.503685
C	-2.941277	-0.718990	0.114750
C	-3.850394	0.362958	-0.048517
C	-5.129563	0.111259	-0.571551
C	-5.523071	-1.174684	-0.940172
C	-4.620071	-2.229541	-0.800726
C	-3.330647	-2.028813	-0.283537
C	-3.478578	1.800761	0.324473
C	-4.364969	2.357811	1.463944
C	-3.536233	2.739312	-0.905450
C	-2.372171	-3.221099	-0.203489
C	-2.926396	-4.366528	0.675178
H	-3.166290	-4.017275	1.685516
H	-2.187558	-5.172583	0.760810
H	-3.839037	-4.796655	0.245054
C	-2.027848	-3.748018	-1.617886
C	-0.002121	3.635620	0.860754
H	0.688818	3.059545	1.483697
H	-1.017025	3.524780	1.263689
C	0.380766	5.109072	0.696240
H	1.470526	5.227245	0.707205
H	-0.039599	5.732697	1.490868
C	-0.190073	5.435872	-0.700828
H	-1.264805	5.643522	-0.640263
H	0.296619	6.293643	-1.174165
C	0.065417	4.137635	-1.473574
H	-0.038683	0.934182	-3.526639
H	2.702011	-2.081437	2.731239
H	2.071840	-0.880572	3.869446
H	3.303771	-0.430247	2.664370
H	0.000044	-0.749182	3.485799
H	-3.305008	-0.352535	2.671030
H	-2.076541	-0.795296	3.882527
H	-2.728513	-2.011371	2.773249

H	4.827045	-3.322351	-1.155400
H	6.481730	-1.491976	-1.356436
H	5.859757	0.804691	-0.675290
H	1.359704	-2.880222	0.206054
H	3.696817	-4.877675	0.164193
H	3.044030	-4.103929	1.616979
H	2.033524	-5.212749	0.670000
H	1.513984	-2.932576	-2.298850
H	1.172808	-4.544589	-1.636898
H	2.804053	-4.137165	-2.198855
H	2.499583	1.744142	0.699327
H	3.012715	2.352333	-1.703344
H	3.342909	3.699372	-0.588493
H	4.673720	2.732576	-1.242618
H	4.146592	3.259189	1.786318
H	4.332398	1.600847	2.390390
H	5.484255	2.249434	1.212327
H	-5.826800	0.935660	-0.690733
H	-6.516803	-1.351605	-1.339324
H	-4.919738	-3.228405	-1.104110
H	-2.446364	1.786088	0.693874
H	-4.050632	3.373487	1.736674
H	-4.304668	1.731128	2.360087
H	-5.416756	2.405517	1.158218
H	-4.559015	2.821898	-1.290828
H	-3.199130	3.748609	-0.637033
H	-2.908871	2.373283	-1.727579
H	-1.441996	-2.870650	0.256367
H	-2.923244	-4.121984	-2.128577
H	-1.305991	-4.571028	-1.558126
H	-1.596153	-2.959737	-2.246268
H	-0.682509	3.914256	-2.239367
H	1.057715	4.124358	-1.939162

TS₁-Sr

Sr	0.319645	0.009828	-0.263122
N	1.855438	2.144686	-0.396310
N	2.782623	-0.847744	-0.418322
O	-1.336976	0.674709	1.636297
C	3.795427	3.645032	-0.784492
C	3.149885	2.264661	-0.645442
C	4.063867	1.192013	-0.782833
C	3.923302	-0.204083	-0.646792
C	5.218738	-1.003355	-0.768885
C	1.029385	3.286237	-0.188011

C	0.194536	3.753716	-1.244904
C	-0.725076	4.783061	-0.979142
C	-0.830299	5.356737	0.289482
C	0.004603	4.908011	1.315516
C	0.940051	3.881551	1.103386
C	0.335915	3.221608	-2.676775
C	1.124760	4.223910	-3.557344
C	-1.014771	2.876700	-3.341607
C	1.844271	3.448427	2.262864
C	1.033097	2.864800	3.443939
C	2.740274	4.609767	2.755948
C	2.770297	-2.266140	-0.278708
C	2.840932	-2.849643	1.019005
C	2.678105	-4.238576	1.153526
C	2.445658	-5.053788	0.043375
C	2.390266	-4.479139	-1.228646
C	2.558888	-3.097057	-1.417646
C	3.096958	-1.998741	2.267909
C	4.375122	-2.436720	3.021372
C	1.884750	-2.009749	3.229935
C	2.537050	-2.529252	-2.842277
C	3.598921	-3.201420	-3.745561
H	4.599567	-3.141749	-3.303544
H	3.628328	-2.709253	-4.724962
H	3.370128	-4.260730	-3.912231
C	1.138312	-2.642135	-3.494776
C	-1.704324	0.027905	2.890569
H	-0.823714	0.032962	3.541998
H	-1.989448	-1.005501	2.668402
C	-2.877906	0.838566	3.451848
H	-2.514733	1.649357	4.094567
H	-3.556197	0.211785	4.038225
C	-3.536147	1.406293	2.176092
H	-4.188616	0.662705	1.706600
H	-4.122206	2.311081	2.363179
C	-2.327805	1.688559	1.283443
H	-1.347869	-0.353883	-1.975218
H	4.401975	3.866901	0.102275
H	3.055478	4.439352	-0.895644
H	4.466276	3.662127	-1.649952
H	5.075046	1.513667	-0.996932
H	5.147099	-1.750416	-1.566270
H	5.420651	-1.551299	0.158697
H	6.070368	-0.351945	-0.977888

H	-1.358782	5.149220	-1.780705
H	-1.544836	6.153211	0.472948
H	-0.065778	5.368723	2.296983
H	0.929815	2.300507	-2.631108
H	0.583279	5.174053	-3.643594
H	2.113427	4.435464	-3.137472
H	1.261941	3.818097	-4.566951
H	-1.562069	2.120804	-2.768126
H	-0.841871	2.465356	-4.343249
H	-1.650609	3.762988	-3.454793
H	2.501830	2.654512	1.893812
H	0.407248	2.028106	3.115790
H	1.706961	2.506752	4.232271
H	0.375848	3.623569	3.886743
H	3.433507	4.255858	3.528869
H	3.329292	5.035278	1.937109
H	2.139506	5.417612	3.190841
H	2.736758	-4.688987	2.140499
H	2.316988	-6.124657	0.166610
H	2.222504	-5.117058	-2.091637
H	3.249350	-0.966223	1.935244
H	4.567593	-1.765874	3.867526
H	5.251417	-2.415556	2.364618
H	4.277860	-3.454756	3.417077
H	1.700315	-3.016188	3.624425
H	2.061261	-1.340756	4.081438
H	0.962424	-1.689514	2.728506
H	2.786006	-1.464393	-2.777209
H	0.809869	-3.687650	-3.547112
H	1.160038	-2.243411	-4.516459
H	0.382479	-2.073590	-2.939134
H	-2.546935	1.583236	0.216267
H	-1.886223	2.674327	1.469833
H	-8.169950	0.986101	-1.122269
C	-7.240208	0.425951	-1.118143
C	-7.236498	-0.939763	-0.803932
C	-6.031520	1.053804	-1.441509
C	-6.039477	-1.664820	-0.804110
H	-8.170287	-1.446133	-0.576184
C	-4.833987	0.327033	-1.437518
H	-6.019599	2.109398	-1.699105
C	-4.807890	-1.045722	-1.110575
H	-6.061405	-2.731674	-0.601190
H	-3.901381	0.820911	-1.697056

C	-3.527571	-1.801646	-1.159522
C	-2.711606	-1.607207	-2.250751
C	-3.044182	-2.554371	-0.000593
H	-1.899538	-2.280473	-2.472748
H	-3.081464	-1.057077	-3.105534
C	-3.804376	-2.725217	1.183349
C	-1.731010	-3.096501	0.028811
C	-3.314256	-3.427161	2.278399
H	-4.798287	-2.304067	1.242562
C	-1.241920	-3.794978	1.131318
H	-1.098506	-3.025039	-0.847439
C	-2.029254	-3.974548	2.267668
H	-3.944822	-3.545565	3.154266
H	-0.240185	-4.208270	1.089725
H	-1.653961	-4.527708	3.120950

3-Sr

Sr	0.31889500	0.00846200	-0.26255400
N	1.85275800	2.14313400	-0.39910700
N	2.78085600	-0.84395900	-0.42033600
O	-1.33471300	0.67722500	1.63213400
C	3.79424800	3.64632900	-0.78534200
C	3.15068800	2.26495200	-0.64652200
C	4.06366600	1.19456700	-0.78404700
C	3.92317800	-0.20272300	-0.64690500
C	5.21891900	-1.00121800	-0.76837300
C	1.02856400	3.28676800	-0.18874200
C	0.19317500	3.75379600	-1.24508700
C	-0.72649400	4.78355700	-0.98071900
C	-0.83105800	5.35731200	0.28769000
C	0.00435600	4.90913200	1.31358200
C	0.94014200	3.88293600	1.10232300
C	0.33614700	3.22158100	-2.67682000
C	1.12302200	4.22344900	-3.55939100
C	-1.01420600	2.87360100	-3.34194700
C	1.84436000	3.45032700	2.26180100
C	1.03317100	2.86700600	3.44294000
C	2.73989900	4.61241600	2.75413100
C	2.77104200	-2.26613400	-0.27795200
C	2.84337900	-2.84725300	1.01966700
C	2.68117500	-4.23619700	1.15422500
C	2.44859400	-5.05162400	0.04468800
C	2.39281400	-4.47813800	-1.22740200
C	2.56037000	-3.09598500	-1.41633200
C	3.09852100	-1.99608400	2.26855900
C	4.37714000	-2.43363800	3.02168900
C	1.88622900	-2.00746800	3.23029800
C	2.53863800	-2.52844400	-2.84116100
C	3.59973800	-3.20067700	-3.74526200
H	4.59969100	-3.14025800	-3.30232100
H	3.62993200	-2.70944900	-4.72518600
H	3.37159000	-4.26011700	-3.91041400
C	1.14013400	-2.64169200	-3.49384700
C	-1.70389700	0.02599800	2.89128600
H	-0.82116400	0.03394800	3.53923000
H	-1.98940800	-1.00597200	2.66448400
C	-2.87597000	0.83917100	3.45123300
H	-2.51386100	1.64961200	4.09527800

H	-3.55474600	0.21057300	4.03468200
C	-3.53578000	1.40610900	2.17601100
H	-4.18607900	0.66130300	1.70615600
H	-4.12203600	2.31085300	2.36252500
C	-2.32798300	1.68940000	1.28395400
H	-1.79266000	-0.75949500	-2.00076000
H	4.40043400	3.86914800	0.10123800
H	3.05429100	4.44066000	-0.89656500
H	4.46544800	3.66352100	-1.65046600
H	5.07495700	1.51622400	-0.99705800
H	5.14768600	-1.74870000	-1.56525400
H	5.42075900	-1.54891200	0.15914100
H	6.07000200	-0.34923700	-0.97743300
H	-1.36027200	5.15102500	-1.78172900
H	-1.54607000	6.15306800	0.47115200
H	-0.06663900	5.36969000	2.29484400
H	0.93711600	2.30351300	-2.63028800
H	0.58093500	5.17302700	-3.64442400
H	2.11074200	4.43474400	-3.13823500
H	1.26127500	3.81847000	-4.56911500
H	-1.57619000	2.12895700	-2.76311100
H	-0.84559900	2.46026800	-4.34328800
H	-1.65312200	3.75668300	-3.45457800
H	2.50229700	2.65650800	1.89325100
H	0.40721200	2.02993100	3.11635200
H	1.70748500	2.50952700	4.23083700
H	0.37613700	3.62571000	3.88594500
H	3.43281100	4.25853900	3.52710100
H	3.32922700	5.03826200	1.93563000
H	2.13902100	5.41998300	3.18919100
H	2.73647300	-4.68574500	2.14143100
H	2.31672000	-6.12173900	0.16887700
H	2.22366900	-5.11675300	-2.08953000
H	3.25148800	-0.96318000	1.93674700
H	4.56900400	-1.76261300	3.86777900
H	5.25399400	-2.41281200	2.36543400
H	4.27964800	-3.45134000	3.41778900
H	1.70155000	-3.01334900	3.62498700
H	2.06315400	-1.33790800	4.08130300
H	0.96272000	-1.69091400	2.72898400
H	2.78977600	-1.46365700	-2.77711800
H	0.80890900	-3.68553400	-3.54535300
H	1.15748400	-2.24044400	-4.51455700
H	0.37937700	-2.08508900	-2.93006800

H	-2.55819300	1.58686500	0.21740000
H	-1.88729000	2.67623500	1.46701600
H	-8.17112000	0.98628400	-1.12333600
C	-7.24135300	0.42623300	-1.11738600
C	-7.23517500	-0.94062600	-0.80079800
C	-6.03148800	1.05172900	-1.44234200
C	-6.04104100	-1.66490700	-0.79972700
H	-8.16970500	-1.44737500	-0.57463800
C	-4.83512300	0.32342400	-1.44135400
H	-6.01936500	2.10825000	-1.69928700
C	-4.79985300	-1.05603800	-1.11009000
H	-6.06013700	-2.73184600	-0.59846500
H	-3.90767600	0.82850100	-1.70487600
C	-3.54051300	-1.81400000	-1.13210200
C	-2.62039600	-1.53758600	-2.24530300
C	-3.05381200	-2.54215800	-0.01709400
H	-2.03563700	-2.40571700	-2.56056600
H	-3.11710200	-1.12070500	-3.12275500
C	-3.80655800	-2.72620500	1.19439700
C	-1.71954900	-3.08567200	0.02721000
C	-3.31471500	-3.42350600	2.27692100
H	-4.80243900	-2.30929000	1.25632300
C	-1.24009100	-3.79287400	1.13479400
H	-1.09594600	-3.05699000	-0.86004300
C	-2.02023700	-3.97729700	2.27115400
H	-3.94426700	-3.54215000	3.15482100
H	-0.23977900	-4.21099600	1.08960800
H	-1.64822500	-4.53509300	3.12231800

4-Sr

Sr	0.072675	-0.209342	-0.333330
N	0.611541	2.017243	0.914289
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O	-1.297715	-1.238857	1.662400
C	1.347509	3.432894	2.811193
C	1.391778	2.149955	1.978482
C	2.306098	1.178029	2.457471
C	2.840917	-0.006579	1.892669
C	4.016868	-0.598024	2.672450
C	-0.138604	3.122419	0.406364
C	0.390844	3.857146	-0.695310
C	-0.377038	4.887092	-1.261004

C	-1.649432	5.196381	-0.775589
C	-2.169698	4.463515	0.290606
C	-1.438395	3.426418	0.895698
C	1.792285	3.566720	-1.241730
C	2.852268	4.494598	-0.597199
C	1.874663	3.655679	-2.781422
C	-2.080650	2.657242	2.053781
C	-3.321027	1.863785	1.578543
C	-2.464310	3.584727	3.231537
C	3.162161	-1.654405	0.183376
C	2.910211	-3.019913	0.487455
C	3.597981	-4.018775	-0.223696
C	4.528232	-3.698074	-1.211798
C	4.779880	-2.355235	-1.500950
C	4.110715	-1.321515	-0.826777
C	1.927386	-3.442567	1.582904
C	2.628062	-4.230171	2.716130
C	0.749208	-4.270030	1.015772
C	4.444196	0.133845	-1.171714
C	5.816298	0.551975	-0.587041
H	5.842234	0.427771	0.500465
H	6.024622	1.604959	-0.813635
H	6.624665	-0.053072	-1.016026
C	4.408197	0.409514	-2.692467
C	-0.871320	-1.193504	3.040800
H	-0.196333	-0.340263	3.154996
H	-0.320275	-2.116825	3.272191
C	-2.171455	-1.106214	3.847921
H	-2.472611	-0.061190	3.967373
H	-2.055009	-1.540544	4.845675
C	-3.197229	-1.882060	2.969736
H	-3.463451	-2.847542	3.410985
H	-4.120400	-1.312410	2.836227
C	-2.475423	-2.086827	1.617419
H	-3.128479	1.887564	-1.807537
H	1.083971	4.301134	2.202690
H	2.309141	3.618315	3.297028
H	0.588076	3.343364	3.598617
H	2.801754	1.474880	3.372928
H	3.646139	-1.323828	3.408328
H	4.561435	0.178185	3.216424
H	4.712438	-1.127264	2.017343
H	0.023958	5.454976	-2.093732
H	-2.228829	5.995953	-1.226097

H	-3.161757	4.700868	0.663284
H	2.048027	2.540924	-0.948461
H	2.638271	5.545196	-0.829759
H	2.870784	4.383608	0.491347
H	3.853045	4.258366	-0.979428
H	1.100798	3.045702	-3.261114
H	2.853052	3.301172	-3.125804
H	1.759080	4.686116	-3.137527
H	-1.342214	1.936231	2.422870
H	-3.070940	1.163976	0.773560
H	-3.755378	1.290030	2.406296
H	-4.095630	2.539230	1.196996
H	-2.845915	2.994894	4.074560
H	-1.606280	4.167528	3.581645
H	-3.250089	4.291111	2.939173
H	3.407456	-5.062825	0.008461
H	5.053614	-4.482607	-1.747121
H	5.510434	-2.105742	-2.264424
H	1.516816	-2.526798	2.022036
H	1.920597	-4.449664	3.525910
H	3.466291	-3.665085	3.136180
H	3.020529	-5.185661	2.348765
H	1.105363	-5.204320	0.565939
H	0.042229	-4.533487	1.812807
H	0.203103	-3.719645	0.241087
H	3.683391	0.765256	-0.700243
H	5.190108	-0.144845	-3.225001
H	4.574526	1.475922	-2.886115
H	3.442334	0.128916	-3.126936
H	-2.146829	-3.125713	1.485986
H	-3.067753	-1.784490	0.751561
H	-6.983844	-1.319106	0.707392
C	-6.308875	-1.667441	-0.070317
C	-5.325817	-0.804506	-0.565555
C	-6.427423	-2.973649	-0.564367
C	-4.407937	-1.206595	-1.573370
H	-5.251938	0.197393	-0.151871
C	-5.557921	-3.386610	-1.583249
H	-7.188394	-3.644765	-0.179192
C	-3.372881	-0.287979	-2.072014
C	-4.578091	-2.521707	-2.081118
H	-5.657652	-4.381253	-2.010096
C	-3.774158	1.155800	-2.312692
C	-2.086880	-0.692869	-2.443899

H	-3.957360	-2.850330	-2.908703
H	-4.795209	1.343710	-1.980619
H	-3.745422	1.410307	-3.382706
C	-1.508970	-2.010994	-2.192164
C	-1.144255	0.236728	-3.064231
C	-0.205221	-2.332744	-2.526178
H	-2.124571	-2.776539	-1.741539
C	0.154075	-0.124376	-3.398480
H	-1.483500	1.229314	-3.328376
C	0.679333	-1.397608	-3.109117
H	0.149927	-3.338616	-2.322404
H	0.782895	0.609991	-3.893819
H	1.684205	-1.677751	-3.392424

TS₂-Sr

Sr	-0.167588	-0.145598	0.085470
N	1.015001	2.179277	0.371705
N	2.397652	-0.693653	0.553964
O	-0.667476	-0.585156	2.654791
C	2.498651	3.843773	1.469976
C	2.082972	2.413791	1.113581
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C	3.166849	0.061610	1.332698
C	4.408474	-0.538429	2.001794
C	0.261994	3.233857	-0.227070
C	0.452139	3.500027	-1.614719
C	-0.361426	4.454948	-2.244176

C	-1.354197	5.139978	-1.539794
C	-1.540293	4.870385	-0.184498
C	-0.750983	3.925367	0.493592
C	1.557552	2.793700	-2.405627
C	2.880426	3.599013	-2.359781
C	1.171810	2.493647	-3.869918
C	-1.016068	3.687852	1.984401
C	-2.453027	3.170428	2.234943
C	-0.758244	4.962283	2.825337
C	2.872297	-1.949394	0.069204
C	2.550451	-3.167803	0.727605
C	2.924772	-4.387593	0.136453
C	3.623396	-4.427149	-1.069872
C	3.963432	-3.227291	-1.700313
C	3.598305	-1.984465	-1.158957
C	1.849144	-3.196126	2.089003
C	2.761891	-3.800202	3.184366
C	0.502561	-3.955765	2.049357
C	4.011925	-0.696542	-1.880519
C	5.483067	-0.322048	-1.570411
H	5.646525	-0.191253	-0.496854
H	5.752808	0.616081	-2.071133
H	6.164939	-1.104948	-1.925432
C	3.804883	-0.762768	-3.410512
C	0.168951	-0.224887	3.772789
H	0.987268	0.393156	3.391613
H	0.586497	-1.143432	4.212347
C	-0.773174	0.485643	4.757003
H	-0.782628	1.562548	4.563284
H	-0.457506	0.332166	5.793674
C	-2.167528	-0.142509	4.453233
H	-2.543775	-0.737628	5.291191
H	-2.906440	0.632657	4.233290
C	-1.922970	-1.032451	3.215404
H	-3.291420	1.557165	-2.175209
H	1.928220	4.589155	0.913969
H	3.564489	3.991255	1.266895
H	2.343755	4.021698	2.541661
H	3.706750	1.834696	2.303961
H	4.150055	-0.871896	3.015833
H	5.207435	0.202925	2.092577
H	4.789200	-1.405009	1.457977
H	-0.219191	4.668409	-3.298157
H	-1.974917	5.874386	-2.043318

H	-2.315021	5.401715	0.360057
H	1.752785	1.836373	-1.904987
H	2.748305	4.582748	-2.827123
H	3.216588	3.753893	-1.330189
H	3.673586	3.068128	-2.900871
H	0.208033	1.975909	-3.934912
H	1.935323	1.859231	-4.335582
H	1.101997	3.408361	-4.469997
H	-0.319213	2.914831	2.328996
H	-2.646713	2.244397	1.681843
H	-2.607049	2.978152	3.304930
H	-3.198689	3.911480	1.922626
H	-0.888428	4.748018	3.893682
H	0.254528	5.349174	2.674985
H	-1.463780	5.757887	2.558184
H	2.677536	-5.318917	0.638150
H	3.910444	-5.377804	-1.508222
H	4.522247	-3.260168	-2.630338
H	1.640305	-2.158654	2.367882
H	2.272975	-3.746654	4.165630
H	3.716117	-3.267404	3.246593
H	2.980682	-4.854765	2.978369
H	0.648204	-5.008582	1.778700
H	0.017959	-3.929621	3.033407
H	-0.188942	-3.519244	1.320236
H	3.380372	0.110028	-1.492159
H	4.486711	-1.478226	-3.885280
H	4.003133	0.219012	-3.857199
H	2.780833	-1.054626	-3.666753
H	-1.820272	-2.091592	3.491734
H	-2.678161	-0.928174	2.432307
H	-7.530802	-1.098504	0.986394
C	-6.888288	-1.518874	0.217631
C	-5.758936	-0.809386	-0.207256
C	-7.188430	-2.769019	-0.338231
C	-4.898456	-1.321172	-1.203128
H	-5.531240	0.155223	0.239843
C	-6.348517	-3.293812	-1.328772
H	-8.062832	-3.321776	-0.009222
C	-3.716228	-0.517645	-1.641961
C	-5.223568	-2.577837	-1.756139
H	-6.576588	-4.255642	-1.779791
C	-4.053476	0.786928	-2.354391
C	-2.495416	-1.193242	-2.025333

H	-4.594788	-2.990324	-2.540577
H	-5.000203	1.185434	-1.986119
H	-4.153991	0.667976	-3.442341
C	-2.074055	-2.394985	-1.374822
C	-1.509515	-0.564604	-2.839400
C	-0.813025	-2.943955	-1.579577
H	-2.770435	-2.904064	-0.719989
C	-0.246218	-1.127487	-3.040530
H	-1.756295	0.352687	-3.358526
C	0.122623	-2.324239	-2.421269
H	-0.550093	-3.871719	-1.083116
H	0.452007	-0.624597	-3.701338
H	1.099956	-2.760972	-2.576410
H	-2.647693	0.318763	0.365823
H	-3.150086	-0.029241	-0.430899