

SUPPORTING INFORMATION

Molecular tailoring: a possible synthetic route to hexasilabenzene

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To confirm the reliability of the chosen B97-D functional and estimate the error bar, we have carried out a benchmark study on hydrogen substituted tetrapersila compounds (**A3-A6**). CCSD(T)/cc-pVTZ, RI-B97-D/cc-pVTZ, B3LYP/cc-pVTZ and M06-2X/cc-pVTZ energies (E , in Hartree) were computed at RI-B97-D/6-31G* optimized geometries (Table S1). Since our main conclusions are drawn from the relative stability of optimized structures on a PES, Table S1 contains the relative energies (ΔE , in kJ/mol) compared to **A6**, respectively, for all computed energy results. The relative difference compared to CCSD(T)/cc-pVTZ results are also shown ($\Delta\Delta E$) in Table S1 in kJ/mol ($\Delta\Delta E = \Delta E_{\text{CCSD(T)}} - \Delta E_{\text{DFT}}$). As one can see in Table S1, $\Delta\Delta E$ clearly indicates that the relative error is reasonable for RI-B97-D method (RMS = 10 kJ/mol) similar to that of the most popular B3LYP and M06-2X DFT methods (RMS are 13 and 14 kJ/mol, respectively). The error bar is estimated by that about ± 15 kJ/mol for this small molecules. For large molecules with real substituent, the error bar is obviously greater, which is expected to be about ± 30 kJ/mol. Since our main results are based on the elimination of unwanted minima protecting only one, error bars have negligible role in this study.

Table S5. Thermal corrections to Gibbs free energy at B97-D/6-31G* level (Hartree)

Substituents	Gibbs free energy of formation								
R	Si ₂ R ₂	Si ₄ R ₄						Si ₆ R ₆	
	1	2	2-TS	3	4	5	6	7	7-TS
A	-0.011687	-	-	0.001607	0.002176	0.002286	0.003315	0.011346	0.011771
B	0.134336	-	-	0.294084	0.296674	0.29509	0.299438	0.459931	0.458618
C	0.423018	0.888938	0.889996	-	-	0.892359	-	1.364001	1.362663
D	0.627172	-	-	-	-	1.313714	-	2.000485	-

R	Si ₆ R ₆							Si ₈ R ₈	
	8	8-TS	9	9-TS	10	11	12	13	14
A	0.017058	0.015731	0.014506	0.014238	0.015906	0.015739	0.018355	0.032410	0.029911
B	0.455869	0.459353	0.458485	0.460189	0.459585	0.453025	0.455381	0.627645	0.621218
C	-	-	-	-	1.356153	-	-	-	-
D	-	-	-	-	-	-	-	-	-

We have calculated all investigated reactions using Polarizable Continuum Model (PCM) solvation model. One can easily compare the results obtained with solvation model or in gas phase (Table S5 and S6). The use of the solvation model causes only a ~10 kJ/mol shift in the energies. Considering the several hundreds kJ/mol energy gain during the reactions, the solvation effect has negligible role in this study and do not change any conclusions that we have drawn.

Table S6. Gibbs free energy of the formation of different silicon compounds from disilyne in gas phase in kJ/mol.

Substituents	Gibbs free energy of formation								
R	Si ₂ R ₂	Si ₄ R ₄						Si ₆ R ₆	
	1	2	2-TS	3	4	5	6	7	7-TS
A	0	-	-	-291	-292	-265	-311	-429	-347
B	0	-	-	-314	-303	-292	-334	-415	-383
C	0	-230	-216	-	-	-276	-	-244	-227
D	0	-	-	-	-	-11	-	+473	-

R	Si ₆ R ₆							Si ₈ R ₈	
	8	8-TS	9	9-TS	10	11	12	13	14
A	-572	-519	-524	-482	-587	-549	-581	-848	-857
B	-583	-553	-566	-516	-596	-598	-602	-886	-915
C	-	-	-	-	-555	-	-	-	-
D	-	-	-	-	-	-	-	-	-

Table S7. Gibbs free energy of the formation of different silicon compounds from disilyne in THF in kJ/mol.

Substituents	Gibbs free energy of formation								
R	Si ₂ R ₂	Si ₄ R ₄						Si ₆ R ₆	
	1	2	2-TS	3	4	5	6	7	7-TS
A	0	-	-	-285	-287	-257	-303	-421	-341

B	0	-	-	-308	-301	-283	-322	-410	-370
C	0	-216	-202	-	-	-257	-	-221	-202
D	0	-	-	-	-	-1	-	+485	-
R	Si₆R₆							Si₈R₈	
	8	8-TS	9	9-TS	10	11	12	13	14
A	-560	-509	-515	-473	-575	-538	-569	-837	-841
B	-570	-540	-555	-505	-581	-589	-591	-870	-894
C	-	-	-	-	-524	-	-	-	-
D	-	-	-	-	-	-	-	-	-

Optimized geometries at B97-D/6-31G* level (coordinates given in Angstroms):

A1

Si 0.000000 0.000000 0.000000
 Si 0.000000 0.000000 2.123838
 H 1.249256 0.000000 -0.842698
 H -1.249256 0.000218 2.966536

A3

Si -0.008117 -1.306100 -0.117523
 Si -1.833132 -0.000009 0.290669
 Si -0.008135 1.306107 -0.117521
 Si 1.921246 0.000003 0.054640
 H -0.166997 2.355847 -1.187222
 H -2.998758 -0.000019 -0.682378
 H -0.166981 -2.355838 -1.187226
 H 2.326657 -0.000005 1.513107

A4

Si 0.016019 -1.228365 0.298632
 Si 1.767390 -0.000017 -0.415578
 Si 0.016052 1.228380 0.298624
 Si -1.864664 0.000002 -0.446022
 H 0.123476 2.365152 1.275072
 H 3.141178 -0.000042 0.184909
 H 0.123446 -2.365123 1.275097
 H -2.475252 0.000018 0.965745

A5

Si 0.000007 -1.182823 -0.620507
 Si -1.555203 -0.000027 0.574228
 Si -0.000005 1.182855 -0.620470
 Si 1.555245 -0.000002 0.574256
 H 0.000053 -2.425909 -1.445904
 H -0.000145 2.425951 -1.445852

H -1.576398 -0.000085 2.093301
H 1.575857 -0.000002 2.093349

A6

Si -0.002467 -1.534203 -0.417438
Si 1.534342 -0.002524 0.417363
Si 0.002492 1.534175 -0.417299
Si -1.534391 0.002432 0.417368
H 1.424781 -0.001740 1.922691
H -1.424468 0.001879 1.922684
H 0.001817 1.424622 -1.922617
H -0.001779 -1.423079 -1.922673

A7

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.546455
Si	1.933901	0.000000	1.257971
Si	-1.610016	-1.095390	1.275695
Si	-3.021517	0.724922	1.357677
Si	-3.101044	2.072006	-0.522564
H	2.468497	1.422153	1.226492
H	-0.484589	1.163704	3.367677
H	-1.805827	-2.575305	1.290726
H	-0.450132	1.099434	-0.925944
H	-3.422006	1.013323	2.780717
H	-3.643202	3.239274	0.333161

A8

Si	-0.033833	-0.029645	-0.000546
Si	-0.016468	0.153452	2.322099
Si	2.112330	-0.235735	2.799250
Si	3.126285	0.000839	0.714759
Si	1.800878	1.152104	-0.863787
Si	1.847691	-1.151700	-0.880396
H	2.058967	-2.382183	-1.716603
H	1.963845	2.401800	-1.682160
H	4.607956	-0.010205	0.526545
H	2.758462	0.145877	4.094523
H	-1.155597	-0.251756	3.204689
H	-1.290438	-0.007274	-0.807592

A7-TS

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.562687
Si	1.896439	0.000000	1.318712
Si	-1.469122	-1.299364	1.302305
Si	-3.649323	-1.001434	0.445316
Si	-3.072904	-1.290387	-1.742068
H	2.629009	1.313107	1.434975

H	-0.381729	1.084755	3.525057
H	-0.936509	-2.696938	1.380900
H	-0.467757	1.297130	-0.588926
H	-4.452747	-2.134612	1.038067
H	-4.419479	-1.399206	-2.468733

A8-TS

Si	-0.033102	0.077490	0.040027
Si	-0.119325	-0.100478	2.346920
Si	2.033566	0.030817	1.313039
Si	3.032305	1.989302	0.806860
Si	1.575334	3.518800	0.002329
Si	-0.330363	2.368942	0.194055
H	0.090068	-0.600326	-1.294930
H	-1.694040	2.976722	0.257290
H	1.754220	4.965086	0.349448
H	4.514518	2.161303	0.677698
H	2.883755	-1.193017	1.169350
H	-0.197259	-1.581057	2.703044

A9

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.455711
Si	2.299474	0.000000	2.815059
Si	3.386048	-1.181337	1.297961
Si	1.872179	-1.175167	-0.392504
Si	-0.310784	1.999948	1.302958
H	2.001264	-2.122818	-1.545490
H	4.861519	-1.199308	1.046178
H	-1.831753	1.931394	1.138163
H	-1.189747	-0.627211	-0.662626
H	-0.725264	-1.230836	2.922381
H	2.933277	0.696425	3.975591

A9-TS

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.249680
Si	1.681268	0.000000	3.860607
Si	2.690637	-1.374301	2.388083
Si	3.687784	-0.802197	0.300233
Si	2.130106	0.650772	-0.482804
H	-1.156373	0.753739	-0.589678
H	-1.317087	-0.327398	2.895912
H	2.391980	1.418931	-1.747389
H	4.859310	0.044497	0.757628
H	3.000920	-2.777686	2.837991
H	1.124325	-0.974864	4.880538

A10

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.255748
Si	2.033733	0.000000	3.231634
Si	3.582309	1.318793	2.256279
Si	3.582279	1.318798	0.000532
Si	1.548551	1.318837	-0.975361
H	-1.037147	-0.864507	2.907270
H	2.037727	-0.012860	4.730719
H	4.932439	1.332647	2.907865
H	4.619465	2.183251	-0.650998
H	1.544565	1.331685	-2.474446
H	-1.350108	-0.013932	-0.651632

A11

H	-2.770222	2.238822	-1.078944
Si	-1.901532	1.158948	-0.513554
Si	-2.153803	-0.995943	-0.267924
H	-2.977395	-1.988032	-1.028570
Si	-0.060975	-1.194834	0.783972
H	-0.043374	-1.958251	2.072541
Si	0.060974	1.194833	0.783977
H	0.043372	1.958248	2.072548
Si	2.153798	0.995944	-0.267927
H	2.977402	1.988033	-1.028556
Si	1.901538	-1.158948	-0.513548
H	2.770220	-2.238815	-1.078962

A12

Si	-1.196567	-0.891737	-1.043792
Si	1.196398	-0.891472	-1.044084
Si	1.196045	1.350012	-0.250433
Si	-1.196742	1.349750	-0.250035
Si	-1.195980	-0.458491	1.294234
Si	1.196816	-0.458191	1.293912
H	2.181224	-1.628298	-1.908133
H	2.180742	2.466855	-0.456573
H	-2.180686	2.467311	-0.456019
H	-2.180566	-0.837057	2.365146
H	2.181227	-0.837069	2.364888
H	-2.181532	-1.629912	-1.906535

A13

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.354663
Si	2.484670	0.000000	3.146714
Si	1.139266	1.946091	2.934175
Si	1.647272	3.481530	1.177981
Si	1.138444	1.946873	-0.578640
Si	2.484182	0.000974	-0.792269

Si	2.000906	-1.117651	1.176944
H	0.806126	2.393372	-1.968500
H	-0.726468	-1.095266	-0.71255
H	-0.725566	-1.095830	3.067300
H	2.024542	-0.896607	4.271057
H	2.023995	-0.895026	-1.917357
H	0.202461	4.010781	1.178676
H	0.806408	2.392284	4.324004
H	1.870612	-2.604888	1.176917

A14

Si	0.000000	0.000000	0.000000
Si	0.000000	0.000000	2.327349
Si	2.019597	0.000000	1.176979
Si	1.328836	1.912443	2.327378
Si	0.339119	3.530146	0.933218
Si	-1.854889	4.059014	1.554268
Si	-2.715799	2.881474	-0.062528
Si	-0.612905	2.137584	-0.774580
H	-0.759489	-0.745230	3.375395
H	-0.395278	-1.268232	-0.684649
H	3.319876	-0.729606	1.042349
H	2.037200	2.249042	3.599475
H	1.236866	4.642554	0.478261
H	-0.219049	2.447140	-2.188571
H	-2.430547	4.841455	2.692810
H	-4.106575	2.418876	-0.366969

B1

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.420487
C	1.251468	0.000000	2.090113
C	2.454603	-0.016728	1.370064
C	2.432025	-0.033673	-0.033912
C	1.203327	-0.027675	-0.716976
Si	-1.603950	0.075775	2.421875
Si	-3.297408	-1.235873	2.139045
C	-5.075999	-0.826563	2.639303
C	-5.708854	0.382100	2.243814
C	-7.036597	0.647330	2.603820
C	-7.768421	-0.295620	3.346510
C	-7.167010	-1.504272	3.733044
C	-5.834836	-1.767430	3.383265
H	-5.373545	-2.706992	3.697900
H	-7.733445	-2.238214	4.310636
H	-8.805372	-0.088875	3.620732
H	-7.503498	1.588040	2.303018
H	-5.148953	1.115422	1.660255
H	-0.950406	0.012505	-0.536994

H	1.184786	-0.041259	-1.809169
H	3.368839	-0.049186	-0.595466
H	3.408057	-0.021953	1.903008
H	1.280577	0.002967	3.182681

B3

C	0.916319	1.229162	0.955619
C	0.232209	0.036227	1.293620
C	0.980026	-1.164079	1.369183
C	2.355477	-1.174649	1.097062
C	3.015628	0.016540	0.752952
C	2.291916	1.218448	0.683843
Si	-1.611970	0.059451	1.736351
Si	-3.211754	1.229173	0.597065
C	-3.956203	2.845189	1.209487
C	-5.239550	3.254460	0.766627
C	-5.801576	4.457965	1.213898
C	-5.091191	5.276792	2.107856
C	-3.817167	4.888620	2.556604
C	-3.255383	3.684141	2.112313
Si	-4.512392	-0.316410	-0.523951
Si	-3.153676	-1.442111	0.966046
C	-3.834618	-2.864912	1.990814
C	-5.107741	-3.415055	1.695265
C	-5.621987	-4.476243	2.452798
C	-4.873454	-5.010266	3.515221
C	-3.608865	-4.479183	3.821759
C	-3.094800	-3.416069	3.067329
C	-6.347010	-0.296599	0.073378
C	-6.723576	-0.005070	1.408681
C	-8.069278	-0.011958	1.801776
C	-9.075578	-0.312992	0.867900
C	-8.727479	-0.604245	-0.459968
C	-7.378061	-0.593799	-0.850132
H	0.479947	-2.101045	1.630431
H	2.911566	-2.113752	1.149169
H	4.086618	0.008048	0.538810
H	2.798471	2.147942	0.413050
H	0.365866	2.171891	0.891006
H	-5.805602	2.616888	0.084061
H	-6.794494	4.755398	0.869306
H	-5.530165	6.214366	2.456554
H	-3.265817	5.522488	3.254869
H	-2.268735	3.383137	2.474470
H	-5.703519	-2.996607	0.881156
H	-6.607939	-4.883550	2.218129
H	-5.275554	-5.836906	4.105435
H	-3.027913	-4.891107	4.650105
H	-2.115249	-3.000430	3.318529

H	-7.124535	-0.821532	-1.890240
H	-9.504716	-0.838164	-1.191749
H	-10.124144	-0.320011	1.174596
H	-8.333613	0.215626	2.837472
H	-5.954139	0.229591	2.148245

B4

C	0.001338	0.208039	0.220735
C	-0.013753	-0.021862	1.620236
C	1.200057	-0.449509	2.212536
C	2.366648	-0.640904	1.452477
C	2.350871	-0.405733	0.069591
C	1.161492	0.021278	-0.544228
Si	-1.534143	0.165358	2.861202
Si	-3.205508	-0.619052	1.360688
C	-3.018420	-1.944224	0.040678
C	-3.980396	-2.118161	-0.984838
C	-3.801150	-3.093422	-1.975195
C	-2.656608	-3.908949	-1.958528
C	-1.691486	-3.746979	-0.950965
C	-1.870349	-2.775084	0.043509
Si	-4.772487	0.970750	1.392991
Si	-2.731567	1.835744	1.661397
C	-2.033486	3.269110	0.664106
C	-2.824485	3.978627	-0.273267
C	-2.270926	5.017114	-1.034424
C	-0.917990	5.362214	-0.873194
C	-0.119322	4.667161	0.049672
C	-0.671685	3.630366	0.815151
C	-6.263488	1.411292	0.344124
C	-7.069696	0.400484	-0.238291
C	-8.156261	0.735172	-1.057946
C	-8.468343	2.083254	-1.302071
C	-7.691449	3.097209	-0.716735
C	-6.603953	2.766835	0.103429
H	1.234999	-0.637986	3.290440
H	3.286138	-0.972623	1.941842
H	3.255452	-0.553055	-0.525278
H	1.135949	0.206962	-1.621122
H	-0.907108	0.537028	-0.290707
H	-3.873208	3.705984	-0.415681
H	-2.890659	5.553702	-1.756508
H	-0.486685	6.169977	-1.468833
H	0.933744	4.930171	0.170841
H	-0.041262	3.084217	1.519716
H	-4.865098	-1.477227	-1.013450
H	-4.549011	-3.214952	-2.762206
H	-2.516188	-4.667201	-2.732254
H	-0.798079	-4.375071	-0.941497

H	-1.107756	-2.642902	0.813427
H	-6.012241	3.564762	0.559103
H	-7.935074	4.146734	-0.896657
H	-9.316370	2.342134	-1.939464
H	-8.762230	-0.056569	-1.504270
H	-6.842767	-0.651791	-0.049449

B5

C	2.512057	-1.324489	2.109086
C	1.860583	-0.116313	1.761373
C	2.656068	1.025252	1.504293
C	4.053746	0.956736	1.571075
C	4.683397	-0.251715	1.912136
C	3.910496	-1.392522	2.183998
Si	-0.030808	-0.058224	1.599295
Si	-1.144129	-1.199996	-0.041082
C	-2.144741	-2.790265	-0.114038
C	-2.548083	-3.446751	1.073969
C	-3.300210	-4.628864	1.017393
C	-3.662122	-5.175197	-0.225077
C	-3.269415	-4.535246	-1.412224
C	-2.517559	-3.352816	-1.358883
Si	-1.144099	1.200016	0.041084
Si	-0.030803	0.058217	-1.599291
C	1.860589	0.116268	-1.761368
C	2.512082	1.324434	-2.109080
C	3.910524	1.392444	-2.183992
C	4.683404	0.251624	-1.912133
C	4.053733	-0.956817	-1.571074
C	2.656054	-1.025310	-1.504291
C	-2.144674	2.790309	0.114037
C	-2.547974	3.446817	-1.073972
C	-3.300073	4.628949	-1.017401
C	-3.661995	5.175279	0.225067
C	-3.269328	4.535307	1.412217
C	-2.517500	3.352859	1.358879
H	1.919604	2.222409	-2.308674
H	4.397905	2.334589	-2.446891
H	5.773451	0.304754	-1.962126
H	4.653322	-1.841075	-1.344641
H	2.176194	-1.965849	-1.221360
H	2.176224	1.965799	1.221359
H	4.653350	1.840983	1.344640
H	5.773443	-0.304864	1.962129
H	4.397862	-2.334675	2.446898
H	1.919562	-2.222453	2.308683
H	-2.268169	-3.029968	2.044807
H	-3.602452	-5.124734	1.942775
H	-4.246685	-6.096922	-0.268072

H -3.547559 -4.958282 -2.380338
H -2.214169 -2.862716 -2.287372
H -2.214142 2.862743 2.287370
H -3.547480 4.958341 2.380329
H -4.246536 6.097019 0.268058
H -3.602283 5.124836 -1.942784
H -2.268052 3.030036 -2.044808

B6

Si -0.373870 -0.990591 1.207388
Si 0.373662 -1.207955 -0.990714
Si -0.373923 0.990280 -1.207776
Si 0.374164 1.207192 0.990081
C 2.259094 -1.372737 -0.984020
C 2.259390 1.372686 0.983827
C -2.259285 0.984056 -1.372473
C -2.259208 -0.983917 1.372605
C -2.873597 0.229436 -2.403424
C -4.266418 0.217744 -2.558944
C -5.076437 0.960327 -1.684732
C -4.486556 1.718276 -0.660037
C -3.093920 1.735893 -0.510472
H -2.253454 -0.363286 -3.081598
H -4.720299 -0.375722 -3.356310
H -6.162706 0.947315 -1.799917
H -5.113609 2.286282 0.030502
H -2.648697 2.319774 0.298316
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C -4.486637 -1.717827 0.660292
C -5.076328 -0.959975 1.685173
C -4.266134 -0.217580 2.559375
C -2.873335 -0.229349 2.403679
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H -5.113826 -2.285644 -0.030280
H -6.162582 -0.946868 1.800493
H -4.719860 0.375819 3.356881
H -2.253052 0.363241 3.081844
C 2.873560 2.403856 0.229406
C 4.266345 2.559589 0.217779
C 5.076499 1.685314 0.960143
C 4.486775 0.660364 1.717868
C 3.094151 0.510663 1.735534
H 2.253301 3.082066 -0.363151
H 4.720113 3.357144 -0.375516
H 6.162753 1.800642 0.947107
H 5.113940 -0.030232 2.285681
H 2.649039 -0.298316 2.319229
C 3.093847 -0.510998 -1.736014
C 4.486489 -0.660562 -1.718147

C 5.076258 -1.685045 -0.959833
C 4.266107 -2.559031 -0.217130
C 2.873292 -2.403486 -0.229037
H 2.648739 0.297648 -2.320182
H 5.113620 0.029796 -2.286294
H 6.162523 -1.800243 -0.946641
H 4.719887 -3.356228 0.376645
H 2.253060 -3.081499 0.363774

B7

C -0.009340 4.742062 1.183771
C -0.038809 3.488912 0.522911
C -0.472489 3.459769 -0.826858
C -0.863543 4.633497 -1.485131
C -0.811145 5.868579 -0.815885
C -0.378619 5.922505 0.518821
Si 0.460803 1.926884 1.519287
Si 1.651201 0.593265 0.002820
C 3.431648 1.209381 -0.084330
C 4.528191 0.338044 -0.318000
C 5.832418 0.839239 -0.427498
C 6.071505 2.219351 -0.316658
C 4.998635 3.101546 -0.098784
C 3.694964 2.603529 0.015002
Si 1.296805 -1.687770 0.068801
Si -0.687409 -2.133098 -1.016868
Si -1.980569 -3.570720 0.295424
C -3.661355 -2.622494 -0.010939
C -4.206877 -1.674702 0.889017
C -5.406380 -1.002494 0.605750
C -6.104680 -1.270266 -0.583271
C -5.601870 -2.232648 -1.474538
C -4.402649 -2.901945 -1.185968
C 2.832206 -2.790704 0.071959
C 3.270222 -3.429720 -1.110889
C 4.462588 -4.170087 -1.128434
C 5.234931 -4.285590 0.038458
C 4.808234 -3.665309 1.224927
C 3.617450 -2.925055 1.241431
Si -0.477870 -2.075625 1.571355
C -1.273811 -0.403985 2.132638
C -1.630218 0.701308 1.284917
C -2.434668 1.774082 1.766614
C -2.794218 1.831571 3.113991
C -2.373882 0.802125 3.979227
C -1.635573 -0.289821 3.497397
C -1.181137 -0.568273 -1.990544
C -2.504028 -0.048967 -2.010245
C -2.831680 1.063168 -2.798100

C	-1.860803	1.675649	-3.611341
C	-0.550413	1.175500	-3.618120
C	-0.214820	0.072437	-2.813483
H	0.305170	4.795294	2.230645
H	-0.339133	6.880038	1.043631
H	-1.108196	6.784759	-1.331618
H	-1.199980	4.581918	-2.523151
H	-0.509808	2.511630	-1.363334
H	4.360732	-0.735733	-0.408329
H	6.663173	0.151196	-0.600043
H	7.088882	2.607424	-0.403920
H	5.180134	4.175633	-0.016864
H	2.869496	3.304014	0.171835
H	2.672119	-3.348257	-2.022321
H	4.785764	-4.659060	-2.050406
H	6.162829	-4.861914	0.025747
H	5.402603	-3.760312	2.136662
H	3.292965	-2.445933	2.168744
H	-1.360455	-1.088461	4.191812
H	-2.639081	0.845763	5.038450
H	-3.392737	2.661536	3.493266
H	-2.730325	2.561163	1.071971
H	-1.521376	0.598085	0.204517
H	-3.680169	-1.437528	1.814794
H	-5.791213	-0.263456	1.313721
H	-7.034558	-0.742552	-0.808373
H	-6.139229	-2.455524	-2.400062
H	-4.021322	-3.635709	-1.902917
H	-3.274887	-0.506754	-1.393462
H	0.804038	-0.320396	-2.857799
H	0.213481	1.639858	-4.246324
H	-2.126691	2.531399	-4.236242
H	-3.853573	1.449638	-2.779000

B8

Si	-0.123988	-1.622688	0.128116
Si	-1.474570	-0.147343	-1.125902
Si	-1.444975	0.011803	1.172744
Si	-0.277917	1.604167	-0.121966
Si	2.001446	1.164207	-0.322244
Si	2.109842	-0.972797	0.254283
C	-2.536877	-0.302580	-2.632523
C	-2.468792	0.069951	2.712523
C	-0.992303	3.303040	-0.283154
C	3.331299	2.397259	0.043240
C	3.536474	-2.077961	-0.152941
C	-0.672027	-3.380356	0.309107
C	4.831754	-1.723503	0.242799
C	5.911368	-2.559843	-0.065371

C	5.695703	-3.750641	-0.769280
C	4.400423	-4.105098	-1.165020
C	3.320809	-3.268759	-0.856851
H	4.999511	-0.797232	0.790340
H	6.918911	-2.284125	0.242458
H	6.535489	-4.401194	-1.008992
H	4.232666	-5.031369	-1.712561
H	2.313266	-3.544477	-1.164680
C	3.533012	3.484463	-0.815421
C	4.539386	4.417582	-0.538839
C	5.344048	4.263498	0.596405
C	5.142335	3.176294	1.455066
C	4.135960	2.243175	1.178484
H	2.907101	3.604318	-1.698479
H	4.696291	5.263271	-1.206754
H	6.126864	4.989332	0.811547
H	5.768246	3.056438	2.338124
H	3.979055	1.397485	1.846400
C	-2.031807	-3.702067	0.222508
C	-2.446539	-5.032194	0.359475
C	-1.501490	-6.040610	0.583040
C	-0.141710	-5.718898	0.669639
C	0.273022	-4.388771	0.532673
H	-2.766920	-2.917664	0.048606
H	-3.504254	-5.282440	0.292113
H	-1.824092	-7.075259	0.689580
H	0.593403	-6.503301	0.843541
H	1.330737	-4.138526	0.600035
C	-3.222654	0.814781	-3.123656
C	-4.026562	0.697304	-4.263802
C	-4.144692	-0.537536	-4.912814
C	-3.458915	-1.654898	-4.421680
C	-2.655006	-1.537420	-3.281535
H	-3.130765	1.775310	-2.618817
H	-4.559998	1.566451	-4.645833
H	-4.770017	-0.628917	-5.799684
H	-3.550803	-2.615426	-4.926519
H	-2.121570	-2.406567	-2.899503
C	-3.152051	1.242939	3.054950
C	-3.926831	1.286942	4.220188
C	-4.018353	0.157957	5.042998
C	-3.335094	-1.015031	4.700571
C	-2.560314	-1.059034	3.535333
H	-3.080859	2.121128	2.414921
H	-4.458308	2.199359	4.486547
H	-4.621021	0.192186	5.949387
H	-3.406286	-1.893220	5.340600
H	-2.028837	-1.971451	3.268974
C	-2.372482	3.497424	-0.151551

C	-2.913098	4.783058	-0.273532
C	-2.073535	5.874309	-0.527115
C	-0.693355	5.679925	-0.658719
C	-0.152740	4.394291	-0.536738
H	-3.025543	2.648586	0.045701
H	-3.986681	4.934260	-0.171163
H	-2.494057	6.874348	-0.621999
H	-0.040295	6.528762	-0.855971
H	0.920843	4.243089	-0.639107

B7-TS

C	2.056217	4.022750	0.591161
C	1.046965	3.368028	-0.152823
C	0.648066	3.933442	-1.385497
C	1.239640	5.114711	-1.858267
C	2.240290	5.753135	-1.106993
C	2.646338	5.205368	0.120219
Si	0.287048	1.759377	0.514689
Si	1.715205	0.243671	1.743083
C	3.473108	0.612271	0.766792
C	3.730219	1.365840	-0.419735
C	5.040702	1.581437	-0.886061
C	6.132528	1.053564	-0.186246
C	5.913870	0.296466	0.982603
C	4.613456	0.074562	1.440942
Si	-0.528186	0.272113	-1.132521
Si	-2.022714	1.710075	0.459125
C	-2.976206	0.965114	1.907369
C	-4.213079	0.294849	1.725071
C	-4.836137	-0.352387	2.800310
C	-4.241789	-0.342707	4.074151
C	-3.020737	0.322294	4.273294
C	-2.396475	0.976095	3.201082
Si	-2.517856	1.348508	-1.752615
C	-4.124479	0.308123	-1.833988
C	-4.112226	-1.105284	-1.930911
C	-5.308006	-1.837831	-1.906204
C	-6.543123	-1.177036	-1.795982
C	-6.576861	0.225049	-1.722321
C	-5.380542	0.958517	-1.750158
C	-0.836756	-1.563447	-0.654107
C	-1.454223	-1.965150	0.556619
C	-1.683406	-3.319323	0.835826
C	-1.328068	-4.307424	-0.099579
C	-0.726280	-3.933509	-1.310817
C	-0.474014	-2.578106	-1.578241
Si	2.072576	-0.935019	-0.234163
C	3.151960	-2.499793	-0.253434
C	2.569604	-3.726018	0.153831

C	3.300512	-4.921355	0.086258
C	4.621102	-4.914290	-0.392666
C	5.208106	-3.706946	-0.809129
C	4.477881	-2.511815	-0.749769
H	4.943118	-1.579300	-1.076773
H	6.235250	-3.698386	-1.182453
H	5.189861	-5.845653	-0.443931
H	2.840953	-5.857741	0.412445
H	1.543115	-3.746549	0.529113
H	2.901850	1.802942	-0.974699
H	5.197209	2.163051	-1.797110
H	7.149940	1.223847	-0.545511
H	6.761576	-0.123075	1.529096
H	4.461172	-0.531547	2.338136
H	2.396033	3.595763	1.538103
H	3.426645	5.694011	0.708539
H	2.702046	6.671447	-1.477136
H	0.920224	5.534989	-2.814989
H	-0.130039	3.447438	-1.980252
H	0.015468	-2.303905	-2.516805
H	-0.440072	-4.693283	-2.041415
H	-1.517740	-5.361229	0.116702
H	-2.146359	-3.602167	1.784099
H	-1.755850	-1.215965	1.287396
H	-3.163348	-1.639551	-1.998313
H	-5.273203	-2.928550	-1.964534
H	-7.472786	-1.750372	-1.773365
H	-7.533465	0.747467	-1.643432
H	-5.422442	2.049800	-1.687030
H	-4.675688	0.261071	0.738626
H	-1.441463	1.483175	3.362579
H	-2.553574	0.329562	5.260677
H	-4.728323	-0.852883	4.908671
H	-5.784051	-0.871722	2.641590

B8-TS

C	-3.765371	-2.516074	-1.156692
C	-2.798533	-2.052247	-2.081159
C	-3.217219	-1.800955	-3.410770
C	-4.555929	-1.974610	-3.793591
C	-5.504648	-2.412593	-2.854009
C	-5.105062	-2.687877	-1.535733
Si	-0.992150	-1.679591	-1.542884
Si	-1.034245	0.572395	-0.801401
C	-2.685791	1.403047	-0.382464
C	-2.766733	2.321556	0.693557
C	-3.993715	2.884304	1.071995
C	-5.169302	2.535719	0.385881
C	-5.108025	1.630496	-0.685465

C	-3.878400	1.074253	-1.071506
Si	-0.680933	-1.317083	0.703309
C	-1.506860	-1.084210	2.381417
C	-0.798383	-1.277661	3.590652
C	-1.430914	-1.085155	4.827731
C	-2.780781	-0.699734	4.876796
C	-3.497510	-0.507528	3.683675
C	-2.869640	-0.700455	2.445491
Si	1.542955	-1.530402	0.155325
C	2.426333	-3.192204	0.243558
C	1.906807	-4.343881	-0.396399
C	2.569964	-5.575628	-0.306888
C	3.767833	-5.683746	0.419423
C	4.297688	-4.553057	1.060948
C	3.633518	-3.320186	0.974969
Si	2.580841	0.465445	0.234679
C	4.313879	0.829346	-0.426839
C	5.305245	-0.182842	-0.441806
C	6.596800	0.080459	-0.920562
C	6.931016	1.363953	-1.381987
C	5.962548	2.381637	-1.369380
C	4.668649	2.117484	-0.899309
Si	0.845900	1.767393	-0.426691
C	0.820631	3.630933	-0.216089
C	1.875002	4.314282	0.442428
C	1.849838	5.707636	0.589737
C	0.766896	6.449062	0.087520
C	-0.290888	5.789866	-0.561607
C	-0.265042	4.397221	-0.713660
H	0.983098	-4.268133	-0.975113
H	2.154867	-6.451459	-0.810997
H	4.285016	-6.643591	0.484241
H	5.225598	-4.630190	1.632511
H	4.048858	-2.453075	1.495228
H	5.061807	-1.189580	-0.094098
H	7.342423	-0.718114	-0.934100
H	7.938046	1.569377	-1.751789
H	6.212855	3.380856	-1.733790
H	3.925080	2.918156	-0.910879
H	2.715425	3.748370	0.852693
H	2.670538	6.214648	1.102355
H	0.745321	7.534692	0.205623
H	-1.137853	6.361476	-0.947886
H	-1.098878	3.897115	-1.211315
H	-1.863199	2.587158	1.246701
H	-4.033413	3.585889	1.908632
H	-6.127209	2.967356	0.685762
H	-6.017051	1.353985	-1.224825
H	-3.851113	0.369554	-1.902984

H	0.253567	-1.574171	3.562706
H	-0.869989	-1.234834	5.753355
H	-3.271811	-0.549533	5.840996
H	-4.545450	-0.200448	3.715244
H	-3.434485	-0.532743	1.526452
H	-2.493304	-1.442562	-4.148673
H	-4.860647	-1.764286	-4.821810
H	-6.548376	-2.542570	-3.149372
H	-5.838561	-3.030154	-0.801520
H	-3.467717	-2.721051	-0.125276

B9

C	0.641275	-1.749454	3.200038
C	1.405201	-1.387987	2.064405
C	2.737192	-0.945225	2.262960
C	3.277734	-0.859951	3.553355
C	2.503896	-1.217456	4.670119
C	1.183763	-1.662234	4.490511
Si	0.671183	-1.498521	0.324476
Si	1.289183	-1.635722	-1.909330
C	3.210122	-1.800131	-1.997687
C	3.868313	-1.429322	-3.197439
C	5.266312	-1.477315	-3.308644
C	6.042714	-1.912013	-2.221369
C	5.410642	-2.313016	-1.032831
C	4.012488	-2.264057	-0.927016
Si	1.100489	0.550172	-0.927175
C	2.633748	1.439508	-0.241190
C	2.549482	2.171413	0.970102
C	3.684391	2.768358	1.535837
C	4.933867	2.642319	0.905657
C	5.037595	1.923645	-0.295519
C	3.899345	1.332927	-0.866327
Si	-0.796788	1.720882	-0.543913
Si	-2.530970	0.436016	0.121792
C	-4.334912	0.877240	-0.197837
C	-4.691084	2.016512	-0.961026
C	-6.037058	2.341518	-1.182504
C	-7.055380	1.534501	-0.648685
C	-6.721207	0.403507	0.114541
C	-5.375712	0.082392	0.344032
C	-0.808025	3.577431	-0.282407
C	0.320558	4.363359	-0.630261
C	0.317319	5.750286	-0.432009
C	-0.813775	6.383250	0.110972
C	-1.942761	5.621762	0.458345
C	-1.940141	4.233946	0.265551
Si	-1.628613	-1.590267	0.083892
C	-2.565565	-3.202415	-0.064216

C	-3.910308	-3.231404	-0.515941
C	-4.602106	-4.443905	-0.628346
C	-3.963850	-5.653282	-0.301775
C	-2.629960	-5.644885	0.138593
C	-1.938685	-4.431812	0.260576
H	1.209328	3.881986	-1.043550
H	1.198580	6.337846	-0.699088
H	-0.815259	7.464771	0.263986
H	-2.823260	6.109407	0.883144
H	-2.824452	3.654797	0.543795
H	-3.910067	2.648649	-1.390672
H	-6.291019	3.221352	-1.778169
H	-8.103364	1.786378	-0.825042
H	-7.508729	-0.225319	0.536387
H	-5.130480	-0.795304	0.947750
H	-4.412248	-2.299392	-0.786208
H	-5.636954	-4.448053	-0.978335
H	-4.503768	-6.598426	-0.392282
H	-2.130086	-6.582990	0.390057
H	-0.901535	-4.436566	0.606745
H	4.004852	0.769519	-1.793446
H	6.005165	1.816602	-0.791405
H	5.820882	3.099721	1.350509
H	3.595038	3.321157	2.473960
H	1.589355	2.259590	1.483156
H	3.278937	-1.077430	-4.050021
H	5.750021	-1.174986	-4.241018
H	7.131637	-1.946063	-2.303110
H	6.007805	-2.658066	-0.184939
H	3.538460	-2.571854	0.007886
H	3.347688	-0.648049	1.409568
H	-0.388101	-2.097186	3.072704
H	0.576685	-1.941194	5.355142
H	2.927211	-1.150154	5.674996
H	4.302339	-0.504618	3.685713

B9-TS

C	-3.156946	-2.248087	1.011937
C	-2.251933	-2.618256	-0.011868
C	-2.434080	-3.872188	-0.644824
C	-3.482664	-4.724762	-0.266592
C	-4.366389	-4.342152	0.755733
C	-4.198519	-3.103547	1.396879
Si	-0.899740	-1.410783	-0.558457
Si	-1.890658	0.450372	-1.519606
C	-3.791582	0.450417	-1.610167
C	-4.550759	-0.741737	-1.714892
C	-5.946129	-0.697457	-1.845992
C	-6.615476	0.536512	-1.894160

C	-5.879001	1.730589	-1.822726
C	-4.483686	1.686149	-1.690393
Si	-0.877582	1.535176	0.168071
C	-1.709725	2.714541	1.382617
C	-3.114055	2.916524	1.378320
C	-3.724574	3.748379	2.326124
C	-2.948374	4.391227	3.305624
C	-1.558490	4.191220	3.339224
C	-0.947800	3.358853	2.391183
Si	1.207205	-2.181799	-0.872763
C	1.722047	-3.549832	0.360050
C	2.979852	-3.511040	1.011286
C	3.378024	-4.540394	1.876490
C	2.527359	-5.631502	2.118358
C	1.278566	-5.689396	1.479361
C	0.886631	-4.667350	0.602015
Si	2.368244	-0.225716	-0.555724
C	4.245131	-0.370034	-0.598446
C	4.858798	-1.359308	-1.409234
C	6.253075	-1.498368	-1.451385
C	7.069141	-0.653158	-0.681388
C	6.481783	0.328662	0.134582
C	5.087765	0.466158	0.178282
Si	1.441054	1.624339	0.260486
C	2.114437	3.334309	-0.235076
C	1.357426	4.516171	-0.038808
C	1.871740	5.774312	-0.386553
C	3.157320	5.885692	-0.938223
C	3.922646	4.725304	-1.142790
C	3.409423	3.468000	-0.796400
H	-0.087557	-4.735512	0.114616
H	0.607955	-6.533228	1.660491
H	2.836131	-6.430298	2.796691
H	4.352456	-4.485344	2.368295
H	3.654332	-2.668779	0.843786
H	4.644924	1.222645	0.830506
H	7.110273	0.982080	0.744246
H	8.155464	-0.762592	-0.712119
H	6.702725	-2.266691	-2.084569
H	4.236331	-2.026160	-2.012466
H	4.019861	2.581174	-0.976780
H	4.921607	4.797316	-1.579992
H	3.557720	6.864905	-1.210175
H	1.262666	6.667848	-0.228445
H	0.353081	4.459548	0.385320
H	0.132963	3.200436	2.438353
H	-0.951628	4.679606	4.104816
H	-3.425894	5.038428	4.044701
H	-4.807259	3.892331	2.303818

H	-3.733274	2.411846	0.635677
H	-4.053125	-1.710948	-1.677589
H	-6.510963	-1.630529	-1.908254
H	-7.702464	0.568176	-1.997165
H	-6.389652	2.695063	-1.876082
H	-3.923659	2.624858	-1.648499
H	-3.052426	-1.276371	1.501725
H	-4.884474	-2.800481	2.191073
H	-5.183217	-5.005014	1.049600
H	-3.610159	-5.685394	-0.771037
H	-1.757969	-4.177872	-1.447541

B10

Si	-2.208010	0.001625	0.226719
Si	-1.102598	-1.913005	-0.226719
Si	1.102598	-1.913005	0.226719
Si	2.208010	0.001625	-0.226719
Si	1.105412	1.911380	0.226719
Si	-1.105412	1.911380	-0.226719
C	-2.024740	3.550398	-0.000922
C	2.024740	3.550398	0.000922
C	4.087105	-0.021723	-0.000922
C	2.062365	-3.528675	0.000922
C	-2.062365	-3.528675	-0.000922
C	-4.087105	-0.021723	0.000922
C	4.860211	-1.023373	-0.640201
C	6.256167	-1.049530	-0.508467
C	6.910778	-0.068394	0.253865
C	6.161284	0.938396	0.884868
C	4.764824	0.961367	0.759797
H	4.366335	-1.795320	-1.234187
H	6.831901	-1.834725	-1.004126
H	7.998321	-0.087105	0.354815
H	6.663626	1.704809	1.479779
H	4.197870	1.750822	1.257042
C	3.214980	3.645775	-0.759797
C	3.893317	4.866630	-0.884868
C	3.396158	6.019106	-0.253865
C	2.219164	5.942765	0.508467
C	1.543838	4.720753	0.640201
H	3.615191	2.760051	-1.257042
H	4.808221	4.918465	-1.479779
H	3.923725	6.970302	-0.354815
H	1.827032	6.833962	1.004126
H	0.628375	4.679017	1.234187
C	-1.543838	4.720753	-0.640201
C	-2.219164	5.942765	-0.508467
C	-3.396158	6.019106	0.253865
C	-3.893317	4.866630	0.884868

C	-3.214980	3.645775	0.759797
H	-0.628375	4.679017	-1.234187
H	-1.827032	6.833962	-1.004126
H	-3.923725	6.970302	0.354815
H	-4.808221	4.918465	1.479779
H	-3.615191	2.760051	1.257042
C	-4.860211	-1.023373	0.640201
C	-6.256167	-1.049530	0.508467
C	-6.910778	-0.068394	-0.253865
C	-6.161284	0.938396	-0.884868
C	-4.764824	0.961367	-0.759797
H	-4.366335	-1.795320	1.234187
H	-6.831901	-1.834725	1.004126
H	-7.998321	-0.087105	-0.354815
H	-6.663626	1.704809	-1.479779
H	-4.197870	1.750822	-1.257042
C	-3.316373	-3.697380	-0.640201
C	-4.037003	-4.893235	-0.508467
C	-3.514620	-5.950712	0.253865
C	-2.267967	-5.805026	0.884868
C	-1.549844	-4.607142	0.759797
H	-3.737960	-2.883697	-1.234187
H	-5.004869	-4.999237	-1.004126
H	-4.074596	-6.883197	0.354815
H	-1.855405	-6.623274	1.479779
H	-0.582679	-4.510873	1.257042
C	1.549844	-4.607142	-0.759797
C	2.267967	-5.805026	-0.884868
C	3.514620	-5.950712	-0.253865
C	4.037003	-4.893235	0.508467
C	3.316373	-3.697380	0.640201
H	0.582679	-4.510873	-1.257042
H	1.855405	-6.623274	-1.479779
H	4.074596	-6.883197	-0.354815
H	5.004869	-4.999237	1.004126
H	3.737960	-2.883697	1.234187

B11

Si	-1.176663	0.289844	0.893112
Si	-0.588715	2.334110	-0.095977
Si	1.447148	1.570278	-0.453606
Si	1.157550	-0.290418	0.932940
Si	0.607445	-2.332089	-0.082822
Si	-1.418611	-1.571820	-0.502382
C	-2.962316	-2.282181	-1.291084
C	-2.221814	0.374203	2.471079
C	2.131709	-0.373000	2.554809
C	3.002897	2.264380	-1.232671
C	-1.677220	3.411651	-1.190773

C 1.739279 -3.397209 -1.145129
C -2.339549 1.578772 3.203757
C -3.091996 1.633614 4.386281
C -3.747022 0.484074 4.857628
C -3.644278 -0.720131 4.142285
C -2.890666 -0.772621 2.960230
H -1.832667 2.479914 2.846541
H -3.169847 2.573474 4.938147
H -4.336565 0.527290 5.776375
H -4.152483 -1.617463 4.503579
H -2.816756 -1.716459 2.412243
C 2.559551 0.812916 3.197861
C 3.249515 0.763351 4.417644
C 3.531914 -0.475811 5.016563
C 3.119663 -1.663148 4.390863
C 2.427349 -1.611099 3.171315
H 2.344133 1.783325 2.740847
H 3.568304 1.690397 4.900299
H 4.072538 -0.515446 5.965090
H 3.338036 -2.629753 4.851248
H 2.107062 -2.542417 2.695264
C 2.952612 3.295879 -2.205163
C 4.126843 3.791447 -2.785965
C 5.375552 3.264481 -2.411800
C 5.445204 2.239755 -1.453625
C 4.271292 1.744603 -0.868846
H 1.986400 3.706172 -2.511326
H 4.070836 4.586521 -3.533134
H 6.290248 3.651994 -2.865858
H 6.414237 1.830281 -1.159042
H 4.336734 0.955228 -0.114812
C -1.150999 4.532388 -1.880749
C -1.967673 5.320364 -2.702538
C -3.331811 5.012513 -2.844492
C -3.873674 3.913011 -2.159124
C -3.056217 3.122936 -1.337894
H -0.092971 4.787879 -1.772206
H -1.542000 6.176218 -3.231946
H -3.968366 5.627825 -3.484119
H -4.933320 3.669136 -2.265979
H -3.490105 2.266066 -0.814832
C 3.121241 -3.100429 -1.239879
C 3.972963 -3.882267 -2.033722
C 3.462883 -4.981557 -2.743347
C 2.096088 -5.297309 -2.653340
C 1.245133 -4.517442 -1.859095
H 3.530724 -2.243386 -0.697587
H 5.034420 -3.632046 -2.100345
H 4.125987 -5.590485 -3.361753

H 1.695107 -6.153008 -3.201913
H 0.185132 -4.778511 -1.791244
C -4.237446 -1.780512 -0.924717
C -5.404611 -2.285883 -1.514418
C -5.321441 -3.302391 -2.480213
C -4.065983 -3.811543 -2.856544
C -2.898501 -3.306114 -2.270662
H -4.313498 -0.998480 -0.164027
H -6.378884 -1.890449 -1.217932
H -6.230775 -3.697345 -2.938599
H -3.999493 -4.600404 -3.609420
H -1.927143 -3.702876 -2.578433

B12

Si -1.384828 -0.214298 1.188253
Si 0.987748 -0.334977 1.505660
Si 1.245158 -1.077927 -0.746856
Si -1.120409 -0.994509 -1.034135
Si -1.103081 1.362038 -0.559917
Si 1.259483 1.241611 -0.268663
C 2.043160 -0.648895 3.042923
C 2.600657 -2.093390 -1.590855
C -2.258113 -2.108869 -2.053236
C -2.175196 2.824541 -1.102104
C 2.609598 2.520844 -0.607819
C -2.862268 -0.515598 2.338120
C -1.808187 3.626288 -2.214415
C -2.604684 4.719161 -2.609785
C -3.787061 5.024465 -1.902988
C -4.166018 4.237700 -0.799105
C -3.365329 3.149741 -0.398539
H -0.895657 3.397120 -2.773117
H -2.306658 5.327605 -3.467457
H -4.406206 5.870337 -2.211224
H -5.078831 4.473868 -0.246520
H -3.661900 2.551392 0.467924
C 3.969466 2.217481 -0.389994
C 4.968309 3.160459 -0.663608
C 4.626686 4.424905 -1.158433
C 3.286421 4.744520 -1.373732
C 2.283405 3.802789 -1.100032
H 4.252091 1.237625 0.004801
H 6.016406 2.907641 -0.487465
H 5.406432 5.158571 -1.372521
H 3.014534 5.731171 -1.755809
H 1.236618 4.069518 -1.269891
C 3.390199 -1.061862 2.914266
C 4.191728 -1.264584 4.049296
C 3.658719 -1.068283 5.331893

C 2.322981 -0.667884 5.477380
C 1.521570 -0.457502 4.342298
H 3.814293 -1.231345 1.920058
H 5.230317 -1.583046 3.931693
H 4.281378 -1.230704 6.214458
H 1.902194 -0.518386 6.474612
H 0.480623 -0.147256 4.470089
C -3.678271 -1.676694 2.181355
C -4.795124 -1.896382 3.016405
C -5.113302 -0.969458 4.023171
C -4.309861 0.186748 4.198111
C -3.196618 0.409494 3.358776
H -3.435356 -2.406204 1.403461
H -5.409937 -2.789607 2.880126
H -5.977836 -1.139422 4.669668
H -4.554664 0.910207 4.980434
H -2.588261 1.308249 3.497769
C -1.731676 -2.944263 -3.064894
C -2.564296 -3.775965 -3.813346
C -3.929165 -3.789240 -3.573221
C -4.469394 -2.966090 -2.574357
C -3.639783 -2.137427 -1.821687
H -0.657198 -2.941929 -3.267621
H -2.138831 -4.415312 -4.589720
H -4.580770 -4.440155 -4.159552
H -5.544512 -2.974951 -2.381209
H -4.074275 -1.507661 -1.041853
C 2.462565 -3.476849 -1.792652
C 3.479976 -4.214931 -2.398522
C 4.654738 -3.585992 -2.802813
C 4.809667 -2.220553 -2.610013
C 3.791264 -1.475683 -2.016375
H 1.548533 -3.984023 -1.472867
H 3.355022 -5.289047 -2.551647
H 5.451125 -4.165389 -3.273292
H 5.727125 -1.724577 -2.933235
H 3.916623 -0.397888 -1.889700

B13

C -1.446532 -1.195312 3.028567
C -2.146401 -0.592142 1.952822
C -3.557769 -0.704947 1.916822
C -4.241133 -1.412948 2.915735
C -3.534461 -2.019359 3.967212
C -2.135271 -1.905865 4.022594
Si -1.176221 0.299574 0.603368
Si 1.103856 -0.182696 0.385191
C 2.012822 -1.338137 1.562055
C 3.017843 -0.777467 2.386334

C	3.781748	-1.589461	3.238368
C	3.552133	-2.973257	3.280410
C	2.555171	-3.542265	2.470529
C	1.792041	-2.733627	1.618909
Si	-1.428444	2.158553	-0.787344
Si	0.549662	3.126060	-1.684371
Si	1.974026	1.258365	-1.207571
Si	1.687551	-0.916512	-2.110543
Si	-0.437712	-1.362875	-1.292505
C	-0.972487	-3.152644	-1.004927
C	-1.007064	-4.031359	-2.114370
C	-1.478639	-5.345560	-1.977740
C	-1.924768	-5.805346	-0.727868
C	-1.898780	-4.945008	0.381308
C	-1.430313	-3.629747	0.244904
C	-2.958331	3.182407	-0.343364
C	-3.726797	2.917413	0.814721
C	-4.897397	3.641188	1.082641
C	-5.317971	4.652175	0.202847
C	-4.557634	4.940951	-0.942004
C	-3.388451	4.213022	-1.212473
Si	-2.110204	0.142311	-1.779555
C	-3.889331	-0.444979	-1.472259
C	-4.925986	0.517479	-1.378083
C	-6.240491	0.130352	-1.076384
C	-6.551436	-1.224455	-0.876296
C	-5.540724	-2.192622	-0.998084
C	-4.226130	-1.809574	-1.297824
C	1.249367	4.031187	-0.087369
C	2.198007	5.059230	-0.305740
C	2.837122	5.713458	0.760159
C	2.535156	5.360565	2.084372
C	1.588436	4.351372	2.331168
C	0.961114	3.697250	1.259376
C	3.801735	1.678080	-0.931350
C	4.203966	2.391099	0.224320
C	5.549614	2.732577	0.424125
C	6.519460	2.373819	-0.525838
C	6.136416	1.678629	-1.684109
C	4.789893	1.338096	-1.885342
C	2.898839	-2.267878	-1.508431
C	2.590111	-3.629977	-1.739877
C	3.433607	-4.651864	-1.278955
C	4.616280	-4.332614	-0.593727
C	4.950006	-2.986267	-0.375330
C	4.101615	-1.965901	-0.825052
H	-4.704715	1.576782	-1.513291
H	-7.018604	0.892594	-0.992077
H	-7.574033	-1.524013	-0.635409

H	-5.772470	-3.250427	-0.852409
H	-3.457048	-2.577278	-1.378202
H	-0.671802	-3.683136	-3.095107
H	-1.500464	-6.007461	-2.846322
H	-2.293953	-6.827713	-0.620991
H	-2.249000	-5.291858	1.356024
H	-1.436097	-2.973224	1.113515
H	1.674281	-3.899098	-2.269460
H	3.165844	-5.696349	-1.456995
H	5.273860	-5.127034	-0.233132
H	5.864494	-2.727762	0.163243
H	4.366339	-0.928982	-0.620624
H	3.460506	2.698584	0.961198
H	5.836376	3.286667	1.321018
H	7.567484	2.639092	-0.367836
H	6.884140	1.400832	-2.430739
H	4.506908	0.793101	-2.789555
H	2.454798	5.343006	-1.331079
H	3.573820	6.494638	0.555625
H	3.028997	5.867794	2.916812
H	1.343762	4.068845	3.358869
H	0.246647	2.898079	1.476739
H	-2.808974	4.442363	-2.110779
H	-4.875839	5.730477	-1.626821
H	-6.230469	5.215571	0.410816
H	-5.480230	3.416445	1.979005
H	-3.417873	2.130597	1.506757
H	3.219511	0.296157	2.347862
H	4.558719	-1.141755	3.862342
H	4.151473	-3.607722	3.937372
H	2.381806	-4.620432	2.489705
H	1.045044	-3.195746	0.974444
H	-4.123879	-0.256559	1.101075
H	-5.328814	-1.498398	2.862094
H	-4.070327	-2.575042	4.740061
H	-1.577434	-2.370943	4.838795
H	-0.357181	-1.128194	3.079060

B14

C	-2.309101	-1.933230	4.565225
C	-1.194470	-2.280353	3.763588
C	-0.462657	-3.447392	4.091397
C	-0.831982	-4.240186	5.188106
C	-1.939705	-3.882179	5.973715
C	-2.678202	-2.728716	5.659059
Si	-0.677959	-1.203734	2.301615
Si	1.042861	-1.392929	0.753525
C	2.794922	-1.773158	1.358095
C	3.065348	-2.082504	2.712482

C	4.383091	-2.262908	3.160162
C	5.456980	-2.144772	2.261879
C	5.205791	-1.845412	0.913159
C	3.888381	-1.665004	0.467215
Si	-1.798638	0.179961	0.766854
C	-3.244643	1.265079	1.314179
C	-4.475329	1.200520	0.617540
C	-5.537432	2.056708	0.949953
C	-5.391480	2.988888	1.989619
C	-4.179011	3.059524	2.697674
C	-3.116551	2.208779	2.361203
Si	0.335753	0.723728	1.441383
C	1.355858	2.286554	1.661854
C	2.687961	2.198356	2.135376
C	3.488142	3.345639	2.222701
C	2.975372	4.595332	1.834003
C	1.657611	4.693826	1.358209
C	0.848308	3.550277	1.275471
Si	-1.589826	-0.329850	-1.510663
C	-3.064640	-1.125528	-2.397018
C	-3.386371	-0.811665	-3.737787
C	-4.455281	-1.445255	-4.390847
C	-5.223642	-2.406506	-3.714135
C	-4.920363	-2.730367	-2.381327
C	-3.852273	-2.094969	-1.730497
Si	0.493816	-1.500097	-1.528929
C	0.648084	-3.165625	-2.411134
C	1.692314	-4.062174	-2.079779
C	1.804407	-5.304210	-2.722523
C	0.868758	-5.675394	-3.702266
C	-0.178360	-4.801110	-4.036580
C	-0.288315	-3.556613	-3.397761
Si	1.420144	0.521548	-2.238236
C	3.195008	1.115394	-2.057217
C	4.280085	0.346104	-2.547465
C	5.605181	0.744006	-2.319961
C	5.870597	1.920067	-1.598207
C	4.807751	2.697083	-1.109760
C	3.481492	2.302635	-1.337150
Si	-0.526833	1.539592	-2.430686
C	-0.897295	3.308699	-1.891491
C	0.025254	4.363063	-2.098442
C	-0.219197	5.643148	-1.582302
C	-1.388431	5.897686	-0.844156
C	-2.320747	4.866661	-0.640223
C	-2.084296	3.589841	-1.171172
H	4.084073	-0.573032	-3.106792
H	6.429357	0.139013	-2.705610
H	6.902902	2.227354	-1.415321

H	5.005399	3.603680	-0.534821
H	2.669840	2.905272	-0.924757
H	0.950637	4.175568	-2.649514
H	0.508714	6.441293	-1.747023
H	-1.571424	6.893060	-0.432917
H	-3.229801	5.047327	-0.062423
H	-2.817195	2.801414	-0.990450
H	-2.790738	-0.066412	-4.272602
H	-4.688929	-1.188075	-5.426844
H	-6.055266	-2.900242	-4.222087
H	-5.514648	-3.477639	-1.849969
H	-3.624138	-2.359069	-0.693472
H	2.421104	-3.788498	-1.310950
H	2.617047	-5.984153	-2.455291
H	0.952880	-6.644500	-4.199698
H	-0.912852	-5.089758	-4.792352
H	-1.113691	-2.890137	-3.659755
H	3.104206	1.228433	2.418231
H	4.515765	3.262597	2.584071
H	3.602389	5.487914	1.898495
H	1.254194	5.657040	1.040745
H	-0.166777	3.641980	0.884459
H	-4.601206	0.483323	-0.198527
H	-6.477201	1.995426	0.396059
H	-6.215983	3.657802	2.246653
H	-4.058221	3.786065	3.504929
H	-2.171871	2.288936	2.905906
H	2.241152	-2.174768	3.425167
H	4.571353	-2.498326	4.210526
H	6.482253	-2.284547	2.612141
H	6.033242	-1.738083	0.207854
H	3.714195	-1.408820	-0.579706
H	0.396456	-3.738077	3.480936
H	-0.258066	-5.138720	5.426856
H	-2.228054	-4.500262	6.826926
H	-3.542087	-2.449478	6.266851
H	-2.890997	-1.037817	4.330025

C1

C	-4.005462	0.133981	-1.372232
C	-4.093136	0.871979	-0.168429
C	-5.063381	0.491186	0.784813
C	-5.917020	-0.592890	0.543378
C	-5.819164	-1.317821	-0.657159
C	-4.858857	-0.953464	-1.611867
C	-3.216419	2.054011	0.059116
C	-1.800466	1.976785	-0.124660
C	-1.035115	3.177254	-0.001783
C	-1.662659	4.372249	0.397866

C	-3.042932	4.419202	0.637900
C	-3.815840	3.267507	0.450132
Si	-1.020846	0.239933	-0.274701
Si	1.020291	-0.240210	0.275509
C	1.800402	-1.976755	0.124568
C	3.216329	-2.053714	-0.059525
C	3.815758	-3.266986	-0.451263
C	3.042944	-4.418674	-0.639432
C	1.662718	-4.371994	-0.399074
C	1.035167	-3.177250	0.001288
C	4.093028	-0.871754	0.168384
C	5.063412	-0.490813	-0.784672
C	5.917176	0.593080	-0.542883
C	5.819289	1.317736	0.657819
C	4.858818	0.953275	1.612320
C	4.005328	-0.134022	1.372345
C	-0.427792	-3.204095	0.282134
C	-1.353014	-3.497621	-0.738670
C	-2.730233	-3.479164	-0.473809
C	-3.195995	-3.192820	0.818790
C	-2.279072	-2.935207	1.849974
C	-0.905007	-2.931385	1.580783
C	0.427908	3.203896	-0.282281
C	1.352835	3.498248	0.738555
C	2.730128	3.479758	0.474074
C	3.196258	3.192530	-0.818192
C	2.279631	2.934032	-1.849422
C	0.905497	2.930280	-1.580602
H	-4.899606	3.301911	0.582066
H	-3.516470	5.355735	0.939957
H	-1.055011	5.274281	0.499078
H	4.899502	-3.301238	-0.583422
H	3.516533	-5.355000	-0.942050
H	1.055127	-5.274030	-0.500592
H	-0.984952	-3.703917	-1.746089
H	-3.442076	-3.674327	-1.278134
H	-4.268312	-3.157695	1.015758
H	-2.635923	-2.717281	2.858955
H	-0.187649	-2.707832	2.372720
H	5.129749	-1.046954	-1.721908
H	6.658607	0.876445	-1.293454
H	6.488970	2.159856	0.846027
H	4.780820	1.503457	2.552100
H	3.297372	-0.451786	2.141000
H	0.984477	3.705239	1.745724
H	3.441722	3.675690	1.278434
H	4.268625	3.157389	-1.014863
H	2.636773	2.715389	-2.858145
H	0.188375	2.706097	-2.372573

H	-5.129699	1.047563	1.721910
H	-6.658331	-0.876182	1.294094
H	-6.488751	-2.160077	-0.845090
H	-4.780910	-1.503858	-2.551526
H	-3.297574	0.451642	-2.140992

C2

C	5.151103	0.444130	-0.179485
C	4.500745	0.547578	1.065545
C	4.379649	-0.603439	1.872815
C	4.888404	-1.834164	1.437257
C	5.522928	-1.929904	0.188646
C	5.650762	-0.790142	-0.619209
C	3.954022	1.853651	1.531230
C	2.568523	2.038471	1.817837
C	2.144036	3.280505	2.380400
C	3.076971	4.324023	2.555272
C	4.417313	4.158960	2.190921
C	4.853534	2.924276	1.694422
Si	1.291559	0.721074	1.286388
Si	1.399038	-1.163899	0.264338
C	1.781424	-3.031349	0.281450
C	2.415791	-3.688614	-0.817053
C	2.746738	-5.057915	-0.697946
C	2.504198	-5.767408	0.481813
C	1.921096	-5.116171	1.576279
C	1.547571	-3.762842	1.483691
C	2.830151	-2.985111	-2.066029
C	4.112993	-3.243057	-2.604588
C	4.557344	-2.598546	-3.765138
C	3.724497	-1.677736	-4.422762
C	2.445743	-1.417662	-3.910867
C	2.004782	-2.064077	-2.745873
C	0.965622	-3.098252	2.687236
C	1.738477	-2.955302	3.857594
C	1.225519	-2.270329	4.969252
C	-0.075091	-1.738881	4.930237
C	-0.862548	-1.901378	3.779828
C	-0.341148	-2.573286	2.665707
C	0.737807	3.520260	2.807294
C	0.027012	2.556588	3.558370
C	-1.294862	2.790775	3.963066
C	-1.922895	4.007156	3.655491
C	-1.217959	4.987870	2.938412
C	0.094504	4.743446	2.512799
Si	-0.465194	0.149733	-0.222016
C	-0.593155	0.296103	-2.144463
C	-1.483176	-0.575120	-2.845904
C	-1.653932	-0.443937	-4.241982

C	-0.920525	0.495762	-4.974196
C	0.014157	1.297707	-4.311679
C	0.185337	1.211919	-2.913329
C	-2.221991	-1.718234	-2.215232
C	-1.547811	-2.759365	-1.536976
C	-2.231708	-3.902548	-1.098412
C	-3.612237	-4.025428	-1.318064
C	-4.298111	-2.992590	-1.974514
C	-3.610466	-1.856048	-2.420983
C	1.209067	2.118124	-2.318348
C	0.882197	3.018618	-1.286588
C	1.830573	3.931115	-0.807883
C	3.132762	3.940906	-1.329158
C	3.476191	3.035285	-2.345422
C	2.518923	2.138555	-2.842623
Si	-2.425128	0.572333	1.087334
C	-3.886462	0.633391	-0.193627
C	-3.992596	1.581781	-1.254868
C	-5.101953	1.562678	-2.125977
C	-6.159861	0.664737	-1.931276
C	-6.114831	-0.219516	-0.850079
C	-4.990938	-0.254321	-0.000076
C	-3.039023	2.713656	-1.419567
C	-2.534349	3.056607	-2.693442
C	-1.797007	4.231005	-2.878698
C	-1.554365	5.094166	-1.796565
C	-2.020880	4.751559	-0.519964
C	-2.750979	3.566874	-0.329742
C	-4.961936	-1.259727	1.087985
C	-3.799602	-2.029149	1.326883
C	-3.766789	-2.973014	2.368724
C	-4.886433	-3.154597	3.189852
C	-6.050546	-2.398719	2.958050
C	-6.088291	-1.465620	1.915238
H	-6.929812	-0.926634	-0.679340
H	-7.018259	0.670924	-2.606715
H	-5.150349	2.298205	-2.932066
H	-3.161593	3.340723	0.657915
H	-1.821067	5.398887	0.333742
H	-0.981151	6.011420	-1.945197
H	-1.397491	4.466224	-3.867208
H	-2.707220	2.378963	-3.530410
H	-2.870429	-3.572947	2.525965
H	-4.859273	-3.886270	4.000247
H	-6.926068	-2.532786	3.597502
H	-6.983560	-0.863029	1.747950
H	-2.977862	-1.992623	0.606822
H	-2.345962	-1.117931	-4.751433
H	-1.059541	0.583890	-6.054219

H	0.611738	2.022764	-4.868677
H	-0.127074	3.024634	-0.884081
H	1.551043	4.627844	-0.018233
H	3.873965	4.639212	-0.936547
H	4.489437	3.027106	-2.754962
H	2.789267	1.426671	-3.624442
H	-0.476321	-2.701881	-1.367579
H	-1.677096	-4.692806	-0.587274
H	-4.150316	-4.908655	-0.967777
H	-5.377040	-3.059738	-2.127159
H	-4.153844	-1.047309	-2.910155
H	3.199726	-5.563407	-1.552898
H	2.768992	-6.824953	0.548284
H	1.735977	-5.653267	2.509083
H	4.774207	-3.936816	-2.083228
H	5.557174	-2.809991	-4.151674
H	4.067976	-1.174879	-5.329725
H	1.771880	-0.723092	-4.413055
H	0.990785	-1.865121	-2.409507
H	2.752737	-3.360374	3.877496
H	1.840884	-2.149362	5.863715
H	-0.473324	-1.203532	5.795360
H	-1.872392	-1.491995	3.732592
H	-0.939360	-2.678755	1.760581
H	2.741967	5.261890	3.003182
H	5.127514	4.977408	2.328594
H	5.906236	2.767456	1.449461
H	3.871364	-0.530139	2.836153
H	4.772403	-2.721858	2.062195
H	5.903710	-2.892117	-0.157917
H	6.115379	-0.868252	-1.603706
H	5.218308	1.327483	-0.816669
H	0.630217	5.498739	1.934380
H	-1.695429	5.941376	2.700935
H	-2.950588	4.191591	3.975143
H	-1.829119	2.021671	4.522497
H	0.520731	1.627624	3.851387

C2-TS

C	3.033941	1.425293	2.895000
C	2.472660	0.353083	3.625116
C	3.333495	-0.664907	4.090898
C	4.707875	-0.626025	3.817379
C	5.251740	0.444479	3.089148
C	4.408730	1.471422	2.634332
C	1.020671	0.359204	3.953005
C	0.029798	0.748309	2.997929
C	-1.295159	1.006527	3.470376
C	-1.643090	0.680563	4.797995

C	-0.689691	0.168421	5.686932
C	0.642960	0.053205	5.278380
Si	0.403227	0.529226	1.118509
Si	-0.845338	1.442419	-0.623369
C	-1.502129	3.026349	-1.422965
C	-2.697315	3.031928	-2.204609
C	-3.189066	4.250237	-2.712097
C	-2.534800	5.459958	-2.444335
C	-1.352289	5.461527	-1.695256
C	-0.813044	4.256849	-1.201600
C	-3.446692	1.782480	-2.528036
C	-3.653560	1.425886	-3.877228
C	-4.306165	0.228491	-4.208597
C	-4.769191	-0.622830	-3.192722
C	-4.598724	-0.260016	-1.847588
C	-3.945435	0.935492	-1.516301
C	0.474975	4.313058	-0.454702
C	1.583503	3.538764	-0.860110
C	2.793778	3.594112	-0.152417
C	2.912470	4.431592	0.967884
C	1.817622	5.211276	1.379966
C	0.610260	5.157789	0.669341
C	-2.315238	1.732836	2.661175
C	-3.658279	1.305491	2.599967
C	-4.623405	2.066563	1.925647
C	-4.267025	3.277408	1.309969
C	-2.936539	3.718290	1.372458
C	-1.968434	2.953076	2.038517
Si	-0.944514	-0.682403	-0.415656
C	-1.601476	-2.281638	-1.202251
C	-1.042520	-2.709612	-2.443486
C	-1.379315	-3.972573	-2.969117
C	-2.307947	-4.793189	-2.319495
C	-2.920674	-4.345886	-1.143839
C	-2.577112	-3.104965	-0.565821
C	-0.150475	-1.835344	-3.257759
C	1.128837	-2.271297	-3.652168
C	1.943686	-1.451575	-4.445087
C	1.492689	-0.186482	-4.851713
C	0.210719	0.248193	-4.475757
C	-0.609187	-0.573853	-3.691878
C	-3.271569	-2.739134	0.701727
C	-4.672804	-2.902100	0.800126
C	-5.347654	-2.652928	2.003178
C	-4.628155	-2.255301	3.142414
C	-3.237658	-2.085747	3.057314
C	-2.568761	-2.307699	1.845275
Si	1.980447	0.042216	-0.539531
C	2.747512	-1.785194	-0.602126

C	3.894173	-1.776663	-1.466956
C	4.336830	-2.943140	-2.119964
C	3.683840	-4.161379	-1.908407
C	2.637063	-4.220217	-0.982377
C	2.178763	-3.065440	-0.304724
C	4.692977	-0.535072	-1.675346
C	5.128803	0.216914	-0.560261
C	5.904649	1.371800	-0.732551
C	6.257244	1.799535	-2.022973
C	5.839696	1.053679	-3.138174
C	5.073347	-0.106954	-2.964913
C	1.217513	-3.307078	0.808028
C	0.238939	-4.325563	0.730645
C	-0.472237	-4.729861	1.866791
C	-0.239722	-4.109554	3.105057
C	0.681623	-3.053636	3.184019
C	1.402786	-2.658598	2.047933
H	-0.815513	6.394267	-1.509880
H	-2.939056	6.397810	-2.831587
H	-4.108514	4.239938	-3.301033
H	5.217357	-2.889481	-2.765167
H	4.022705	-5.068632	-2.413907
H	2.198128	-5.188997	-0.735635
H	1.414271	-0.234140	5.996249
H	-0.971991	-0.074703	6.713737
H	-2.661529	0.878718	5.139121
H	2.912636	-1.509220	4.639781
H	5.352440	-1.435221	4.167007
H	6.322131	0.475364	2.874573
H	4.817467	2.309494	2.067821
H	2.393479	2.242887	2.561527
H	0.036034	-4.797538	-0.231556
H	-1.227820	-5.513109	1.778408
H	-0.801294	-4.419100	3.988766
H	0.841405	-2.533544	4.129823
H	2.159316	-1.879200	2.121666
H	-3.938703	0.360007	3.060238
H	-5.652562	1.704464	1.871553
H	-5.014987	3.866664	0.775810
H	-2.645347	4.648371	0.883305
H	-0.938444	3.308018	2.096099
H	4.870405	-0.125220	0.442538
H	6.238013	1.933336	0.143337
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H	3.629853	2.974758	-0.479709
H	3.852409	4.476858	1.522562

H	1.902515	5.856464	2.257315
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H	-5.229743	-3.226306	-0.081907
H	-6.431663	-2.779026	2.052955
H	-5.148152	-2.078894	4.087035
H	-2.660862	-1.778803	3.931015
H	-1.486951	-2.209475	1.815001
H	-1.613297	-0.247564	-3.422883
H	-0.156102	1.226392	-4.795407
H	2.136107	0.457611	-5.455425
H	2.938078	-1.801609	-4.727376
H	1.499038	-3.235845	-3.303902

C5

C	3.342303	-1.561219	2.287661
C	1.917312	-1.620546	2.148754
C	1.159119	-1.978219	3.306335
C	1.812440	-2.274671	4.522943
C	3.208106	-2.260898	4.621116
C	3.968620	-1.902308	3.502101
Si	1.289689	-1.507246	0.315015
Si	-0.845420	-1.034052	-0.451060
C	-2.220916	-1.931113	-1.427429
C	-2.562166	-3.307180	-1.225463
C	-3.810128	-3.789185	-1.681142
C	-4.702485	-2.958056	-2.364065
C	-4.325512	-1.644829	-2.666933
C	-3.089558	-1.129584	-2.232027
Si	0.932282	0.517265	-0.764742
C	1.817515	1.328610	-2.249594
C	1.960361	2.742507	-2.416601
C	2.647474	3.251707	-3.541761
C	3.162643	2.405639	-4.526563
C	3.000170	1.022950	-4.390825
C	2.352640	0.477013	-3.265327
Si	-0.937205	1.059469	0.383459
C	-1.616614	2.277276	1.697254
C	-3.013432	2.608510	1.690370
C	-3.445315	3.807592	2.297920
C	-2.539108	4.674918	2.916411
C	-1.186805	4.325665	2.986568

C	-0.716517	3.131094	2.405160
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H	-2.893787	5.598015	3.380426
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H	2.736429	4.334393	-3.650763
H	3.674103	2.820203	-5.398165
H	3.387589	0.343223	-5.152627
C	2.264851	-1.020015	-3.239324
C	-1.628842	-4.288652	-0.611135
H	-4.052827	-4.843180	-1.531018
H	-5.662574	-3.348794	-2.708816
H	-4.974426	-1.008880	-3.272063
C	-2.711456	0.228582	-2.718889
C	-0.333586	-2.008572	3.336499
H	1.206404	-2.537493	5.392889
H	3.696692	-2.515330	5.564323
H	5.057764	-1.846365	3.568241
C	4.240290	-1.092229	1.183958
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C	-2.045329	2.738463	-3.830155
C	-1.168642	1.649453	-3.975493
C	-1.500802	0.406583	-3.421676
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H	-1.780990	3.712285	-4.247533
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C	-1.209289	-6.207179	0.853161
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H	0.108666	-3.580104	-1.698704
C	1.734950	3.731345	2.447123
C	3.055497	3.443183	2.815954
C	3.364120	2.218142	3.429666
C	2.350583	1.270385	3.640138
C	1.038347	1.541635	3.230664
H	1.489798	4.683663	1.980681
H	3.841338	4.179465	2.630988
H	4.389811	1.995257	3.731415

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C	-6.176349	1.441756	-0.097307
C	-6.066969	0.045634	0.016612
C	-4.960203	-0.509725	0.676854
C	-3.974666	0.321964	1.223103
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H	-6.833925	-0.603778	-0.410418
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H	-3.154709	-0.118516	1.786630
C	2.191305	4.823283	-1.019714
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C	0.254113	5.924457	-0.044502
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H	-0.180675	6.747708	0.526531
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H	-0.656736	3.069888	-1.681892
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C	3.099599	-3.183495	-2.477190
C	2.253407	-3.843637	-3.380117
C	1.412335	-3.093417	-4.219659
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H	3.761049	-3.752179	-1.820241
H	2.243938	-4.934514	-3.429750
H	0.750190	-3.597017	-4.927188
H	0.804809	-1.106701	-4.834768
C	5.261275	-1.928281	0.686611
C	6.141101	-1.473062	-0.308905
C	6.015625	-0.170143	-0.817050
C	5.007733	0.674901	-0.322062
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H	5.353474	-2.943032	1.080975
H	6.918725	-2.138205	-0.691361
H	6.692527	0.181584	-1.598634
H	4.894822	1.687049	-0.715477
H	3.364409	0.880662	1.072282
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C	-3.159689	-2.061348	3.524014
C	-2.495005	-2.833951	2.558849
C	-1.095219	-2.812758	2.464556
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H	-2.916099	-0.650616	5.154806

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H	-0.594968	-3.445512	1.733253

C7

C	-2.846272	-1.257781	-3.741163
C	-1.975289	-0.152996	-3.597759
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C	-3.873728	1.333371	-4.004570
C	-4.713532	0.225395	-4.202998
C	-4.202377	-1.070134	-4.045578
C	-0.494079	-0.296515	-3.604207
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C	1.712521	0.703179	-3.342011
C	2.148370	-0.039247	-4.465164
C	1.326504	-0.980881	-5.079533
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Si	0.229026	0.664204	-0.860266
Si	2.237642	0.848819	0.455833
Si	2.763781	-1.304015	0.105365
C	4.542167	-1.891830	0.702781
C	5.598197	-2.043067	-0.256851
C	6.835696	-2.617247	0.104162
C	7.072749	-3.075090	1.401959
C	6.048795	-2.976421	2.345268
C	4.792725	-2.411675	2.018176
C	5.503476	-1.668997	-1.705744
C	6.521873	-0.886101	-2.294590
C	6.575651	-0.692270	-3.682356
C	5.610426	-1.280640	-4.516024
C	4.580760	-2.042517	-3.941794
C	4.525300	-2.227888	-2.553650
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C	2.071280	-2.475715	5.390090
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C	-2.196301	-1.175176	5.105928
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C	-3.958457	-0.218856	2.525952
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H	-4.281463	2.342617	-4.087244
H	-5.760769	0.375800	-4.460273
H	-4.857969	-1.937110	-4.153731
H	-2.442703	-2.260525	-3.625625
H	-7.577512	0.567412	-2.799164
H	-7.760699	2.916699	-3.567729
H	-6.355019	4.702014	-2.508692
H	-4.782383	4.076919	-0.647172
H	-4.647978	1.733264	0.101641
H	-3.195403	-3.209049	1.542785
H	-1.792904	-5.241031	1.697535
H	-1.881800	-6.978483	-0.090338
H	-3.383459	-6.646219	-2.067632

H -4.826527 -4.613043 -2.198214

C7-TS

C 6.679914 -0.962325 -2.131399
C 5.639221 -1.692983 -1.513902
C 4.667890 -2.291940 -2.342442
C 4.742186 -2.188124 -3.738407
C 5.792409 -1.475665 -4.339427
C 6.756806 -0.855876 -3.527748
C 5.691097 -1.977322 -0.044476
C 4.599714 -1.786336 0.868642
C 4.809301 -2.249559 2.211707
C 6.056707 -2.788667 2.608666
C 7.115730 -2.919010 1.709209
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Si 2.826044 -1.245933 0.188398
Si 2.266116 0.913964 0.470817
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C 4.212236 3.181795 0.523075
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C 2.098486 3.627917 1.647395
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C 3.010679 -1.104972 3.623932
C 2.123732 -1.125001 4.710265
C 1.974084 -2.281680 5.487677
C 2.721359 -3.426719 5.167526
C 3.602502 -3.405265 4.078780
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C 1.801647 0.624495 -3.299966
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C 1.203044 -0.971938 -5.056816
C -0.144111 -0.796791 -4.731438
C -0.524699 0.020498 -3.649426
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C	-1.950395	0.409616	-3.598584
C	-2.282580	1.774653	-3.475794
C	-3.607303	2.199789	-3.634999
C	-4.622917	1.272820	-3.910443
C	-4.316763	-0.094041	-3.976654
C	-2.988710	-0.524083	-3.820459
Si	-2.016478	1.105445	-0.048976
Si	-0.930143	-1.265518	-0.252991
C	-0.170313	-2.818686	0.563701
C	-0.098209	-2.964570	1.978959
C	0.583388	-4.065034	2.540015
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C	1.108152	-4.899518	0.338487
C	0.419780	-3.825480	-0.258870
C	-0.670720	-1.983922	2.939013
C	-1.445806	-2.424255	4.034047
C	-1.923578	-1.512850	4.986740
C	-1.655568	-0.141166	4.846182
C	-0.897806	0.307947	3.756599
C	-0.388349	-0.608772	2.828484
C	0.315799	-3.849717	-1.743783
C	1.440900	-4.178356	-2.532497
C	1.328362	-4.336481	-3.918810
C	0.081735	-4.184194	-4.547947
C	-1.043652	-3.864313	-3.776808
C	-0.927246	-3.694034	-2.390337
Si	-3.095682	-0.754089	-0.751838
C	-4.892508	-1.479791	-0.590104
C	-6.110471	-0.713517	-0.716272
C	-7.354985	-1.337191	-0.457037
C	-7.464063	-2.690906	-0.152832
C	-6.306933	-3.465301	-0.145178
C	-5.038430	-2.887493	-0.367037
C	-6.260715	0.710988	-1.142621
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C	-6.816775	3.422936	-1.785050
C	-7.557270	2.387387	-2.380636
C	-7.284973	1.050987	-2.060906
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C	-3.164258	-5.999163	-1.426141
C	-2.268699	-6.183986	-0.361067
C	-2.213059	-5.240411	0.672512

C	-3.041606	-4.109365	0.647273
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C	-2.540689	3.787919	0.782487
C	-3.010529	4.833623	1.603150
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C	-4.034131	3.224127	3.073620
C	-3.659750	2.153926	2.229186
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C	-2.544108	4.774343	-1.539321
C	-1.870629	5.363109	-2.621054
C	-0.469834	5.459461	-2.610904
C	0.253202	4.932795	-1.528782
C	-0.418843	4.298042	-0.478356
C	-4.416679	0.879052	2.468884
C	-3.868130	-0.414264	2.539880
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C	-6.067653	-1.382064	2.955565
C	-6.637850	-0.104343	2.854058
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H	8.074382	-3.331036	2.032886
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H	-0.921355	-1.242976	-5.353537
H	1.549739	-5.662617	-0.304878
H	1.759100	-5.842434	2.175991
H	0.670769	-4.126303	3.623541
H	-8.255067	-0.722446	-0.485742
H	-8.438732	-3.137188	0.055766
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H	1.274171	-2.290548	6.325795
H	1.537435	-0.236782	4.936619
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H	5.852864	-1.394148	-5.427241
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H	3.861275	-2.859822	-1.884169
H	5.343195	4.952062	0.002106
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H	6.506736	3.503205	-1.009026
H	8.646793	2.301180	-0.752883

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H	4.729132	1.002748	2.024236
H	-0.443773	4.564450	2.331473
H	-1.518712	4.376537	4.544280
H	-0.423694	3.052248	6.373581
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H	1.338651	5.002626	-1.487962
H	0.150165	3.872003	0.341303
H	-2.801932	-0.558434	2.428436
H	-4.227077	-2.509883	2.892693
H	-6.695677	-2.256097	3.136798
H	-7.717893	0.028334	2.946744
H	-6.275790	1.993991	2.516962
H	-1.668188	-3.489464	4.133638
H	-2.525453	-1.872077	5.824404
H	-2.043534	0.576147	5.572242
H	-0.694348	1.365530	3.623731
H	0.305697	-0.263146	2.061508
H	2.403517	-4.323068	-2.043001
H	2.213638	-4.588866	-4.506635
H	-0.009516	-4.317878	-5.628132
H	-2.025295	-3.773486	-4.247354
H	-1.818966	-3.516778	-1.796124
H	4.515153	0.355276	-2.890282
H	6.180882	2.175877	-3.005136
H	5.429790	4.569755	-3.111598
H	2.985180	5.090686	-3.065036
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H	-4.728558	-4.745587	-2.249643

C10

C	2.657931	2.663973	2.828319
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C	5.418196	2.269954	3.117354
C	4.552317	1.930045	4.168267
C	3.170175	2.127376	4.016804
C	3.004311	3.966896	0.717350
C	1.914667	3.661770	-0.156630
C	1.463405	4.697741	-1.034606
C	2.059534	5.979140	-0.993969
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Si	1.083374	1.938117	-0.246275
Si	-1.127248	1.900329	0.222431
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C	-3.363889	6.120385	0.188993
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C	-3.614627	2.964683	-1.808531
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C	-5.471206	2.093568	-3.140664
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C	-2.727469	2.575492	-2.828936
Si	2.212274	0.031078	0.253860
C	4.125573	-0.043018	0.182284
C	4.917448	0.776695	-0.681480
C	6.327070	0.709279	-0.638230
C	6.985669	-0.182693	0.208855
C	6.229016	-1.003016	1.046452
C	4.817347	-0.927871	1.069282
C	4.394397	1.655802	-1.767882
C	4.864793	2.977586	-1.917044
C	4.590711	3.710814	-3.079607
C	3.877330	3.116602	-4.132088
C	3.387191	1.809086	-3.983879
C	3.612461	1.099031	-2.797304
Si	1.139898	-1.899390	-0.244197
C	2.220694	-3.480034	-0.173818
C	1.941232	-4.585013	0.688929
C	2.745027	-5.744720	0.651300
C	3.852708	-5.831733	-0.192720
C	4.150642	-4.756346	-1.030736
C	3.341321	-3.597016	-1.056442
C	0.911597	-4.601676	1.768008
C	0.042640	-5.702521	1.920300

C	-0.735256	-5.849217	3.076804
C	-0.622887	-4.917013	4.119958
C	0.223254	-3.806383	3.967681
C	0.955859	-3.631433	2.786453
Si	-1.077420	-1.941581	0.254121
Si	-2.204113	-0.042126	-0.239509
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C	-4.925594	0.640232	0.679513
C	-6.333508	0.549664	0.624783
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C	-6.193428	-1.155045	-1.065474
C	-4.783204	-1.055979	-1.077055
C	-4.424738	1.516134	1.778681
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C	-3.958774	2.954291	4.166431
C	-3.446961	1.656158	4.008479
C	-3.647087	0.958180	2.810234
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C	-1.782362	-4.651408	-0.694672
C	-2.547005	-5.837703	-0.665219
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C	-3.234510	-3.712507	1.033492
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C	0.166700	-5.701145	-1.908433
C	0.953342	-5.826348	-3.061635
C	0.805593	-4.909688	-4.114019
C	-0.087111	-3.834417	-3.974655
C	-0.828032	-3.677661	-2.796128
H	-6.922909	1.163164	1.308404
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H	-6.673711	-1.842802	-1.763535
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C	-0.620416	4.501684	2.153405
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H	-3.872968	7.086988	0.201652
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H	4.426039	5.446739	1.384170
H	3.599443	7.241236	-0.143552
H	1.696926	6.745075	-1.681602
C	0.466790	4.547583	-2.142072
H	6.900192	1.337032	-1.322859
H	8.076840	-0.236499	0.218264
H	6.726238	-1.683253	1.740106
C	4.202625	-1.737956	2.168748
H	2.514102	-6.562099	1.336614
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H	4.993145	-4.819864	-1.721515

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C	-3.652376	-2.779845	2.129065
H	-4.857871	-4.985273	1.673285
H	-4.257304	-6.878173	0.160772
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H	5.452134	3.428093	-1.116199
H	4.944842	4.739922	-3.166536
H	3.680691	3.677250	-5.048275
H	2.819109	1.337650	-4.788524
H	3.243052	0.083951	-2.687964
H	-5.684668	2.976946	-1.177450
H	-6.536820	1.877198	-3.239239
H	-4.959662	1.327081	-5.104402
H	-2.508628	1.770973	-4.818082
H	-1.667065	2.770875	-2.705835
H	0.253130	-6.437397	-1.108676
H	1.670746	-6.645463	-3.141168
H	1.400511	-5.015991	-5.023481
H	-0.203882	-3.105781	-4.779700
H	-1.525955	-2.852281	-2.693602
H	-0.017058	-6.447990	1.126553
H	-1.418331	-6.696269	3.166104
H	-1.211013	-5.039129	5.031916
H	0.311854	-3.065909	4.765346
H	1.620313	-2.780210	2.674306
H	-5.494350	3.282808	1.131114
H	-5.035145	4.575194	3.205798
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H	-2.883220	1.181862	4.814589
H	-3.262982	-0.050426	2.693546
H	5.588092	3.161867	1.154454
H	6.490808	2.086682	3.206278
H	4.947561	1.489467	5.085848
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H	1.590835	2.829205	2.717088
C	-0.583915	5.476965	-2.297013
C	-1.328150	5.521707	-3.484274
C	-1.024818	4.653546	-4.544878
C	-0.008573	3.698499	-4.385333
C	0.713921	3.634133	-3.185668
H	-0.815297	6.161589	-1.480025
H	-2.147793	6.237020	-3.578294
H	-1.596654	4.701623	-5.473735
H	0.226246	3.000339	-5.192562
H	1.514137	2.911485	-3.067412
C	-4.441410	-3.231044	-2.318784
C	-4.094641	-3.911761	-3.494220
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C	-3.130516	-1.876781	-4.392614

C	-3.446732	-1.206483	-3.202623
H	-4.943933	-3.759660	-1.507877
H	-4.317021	-4.976997	-3.584263
H	-3.211778	-3.760202	-5.469166
H	-2.620089	-1.337335	-5.194205
H	-3.205787	-0.155363	-3.086693
C	5.048118	-2.205428	-2.295198
C	5.468791	-1.572790	-3.473170
C	4.572223	-1.386399	-4.537119
C	3.233550	-1.781101	-4.387585
C	2.805949	-2.382186	-3.195330
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H	6.500804	-1.226310	-3.558205
H	4.907371	-0.907888	-5.459510
H	2.516109	-1.620306	-5.196060
H	1.775482	-2.702143	-3.084533
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C	-0.829142	3.560974	3.181033
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H	1.920526	6.276181	3.617887
H	1.428919	4.693057	5.490695
H	-0.319809	2.920180	5.180089
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C	-4.996378	-2.365633	2.244111
C	-5.458928	-1.759325	3.420194
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H	-5.675200	-2.521638	1.404941
H	-6.498307	-1.430479	3.482270
H	-4.960945	-1.115772	5.430453
H	-2.552920	-1.788776	5.221733
H	-1.740618	-2.830359	3.114249
C	4.527002	-3.102491	2.324433
C	4.204488	-3.782240	3.507342
C	3.568969	-3.108105	4.561968
C	3.205032	-1.762094	4.400830
C	3.501004	-1.091567	3.205818
H	5.031411	-3.626428	1.511559
H	4.450947	-4.841720	3.603091
H	3.333625	-3.636598	5.487947
H	2.690829	-1.228113	5.203667
H	3.240411	-0.044858	3.088487

D1

C	-1.062639	-3.300885	0.088529
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C	0.061219	-3.134684	0.933264
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C	-1.401533	-2.971973	2.868459
C	-2.520457	-3.105305	2.036798
C	-2.348765	-3.275965	0.655484
C	1.422245	-3.028104	0.323985
C	1.953954	-1.745919	0.005176
C	3.238948	-1.665051	-0.594097
C	3.971301	-2.833706	-0.865947
C	3.440732	-4.092637	-0.548823
C	2.169658	-4.183317	0.040104
C	3.810542	-0.326235	-0.956731
C	3.470540	0.272495	-2.198750
C	4.059401	1.501667	-2.546334
C	4.971345	2.129915	-1.687738
C	5.289854	1.541252	-0.455759
C	4.716118	0.316875	-0.072842
Si	1.084499	-0.096174	0.365884
Si	-1.084538	0.096279	0.366606
C	-1.953986	1.745900	0.005247
C	-3.238924	1.664921	-0.594147
C	-3.971197	2.833548	-0.866332
C	-3.440623	4.092540	-0.549441
C	-2.169608	4.183321	0.039582
C	-1.422287	3.028139	0.323830
C	-3.810518	0.326094	-0.956725
C	-3.470003	-0.272833	-2.198515
C	-4.058924	-1.501923	-2.546277
C	-4.971430	-2.129901	-1.688079
C	-5.290404	-1.541071	-0.456301
C	-4.716606	-0.316779	-0.073205
C	-0.061270	3.134777	0.933124
C	1.062574	3.300878	0.088371
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C	2.520427	3.105410	2.036628
C	1.401508	2.972185	2.868316
C	0.102298	2.976032	2.330200
H	4.956004	-2.747762	-1.332120
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H	1.744804	-5.159610	0.286081
H	-4.955861	2.747546	-1.332580
H	-4.012580	4.998428	-0.761746
H	-1.744724	5.159656	0.285340
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H	3.217955	3.368101	0.003097
H	3.526876	3.076873	2.460688
H	1.529026	2.842771	3.946173
C	-1.100835	2.769928	3.229341
C	-2.490218	0.400446	-3.140843

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C	5.042032	-0.298198	1.273994
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H	-2.429085	-0.143481	-4.095794
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H	-1.480235	0.436270	-2.697254
H	-0.809071	2.803616	4.290291
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H	-1.569277	1.789264	3.033181
H	1.867989	3.468752	-1.914114
H	0.321077	2.582747	-1.813474
H	0.326268	4.348500	-1.674414
H	2.431467	0.142139	-4.096973
H	2.785757	-1.443491	-3.343612
H	1.480855	-0.435859	-2.698945
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D5

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C	4.543259	-2.271689	-3.425746
C	0.844370	-1.585556	-3.679473
C	-0.101812	-1.858340	-2.640809
C	-1.342973	-2.453899	-3.054059

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C	0.491781	-1.755470	-5.038254
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C	-2.433337	-4.493632	-2.107489
C	-3.495096	-5.112146	-1.428646
C	-4.472100	-4.347145	-0.777024
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Si	-0.195474	1.723003	-0.042488
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C	0.769990	4.166405	-4.121993
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C	-0.837916	2.894345	-2.773501
C	2.384409	3.665198	-0.790590
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C	3.502512	5.258545	0.673799
C	4.481468	4.301070	0.972889
C	4.419962	3.037895	0.377879
C	3.397428	2.716396	-0.535254
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C	-3.157702	3.450859	-2.013881
C	-4.536632	3.438963	-2.286698
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C	-4.241315	1.691532	-3.933141
C	-2.853406	1.702198	-3.715052
Si	1.167246	0.043660	0.776350
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C	3.965508	-0.384597	1.711287
C	5.107426	0.054957	2.416742
C	5.042792	1.100799	3.337699
C	3.793613	1.637390	3.652275
C	2.615567	1.190716	3.016446
C	4.187391	-1.636921	0.910280
C	5.248234	-1.736684	-0.032547
C	5.592359	-2.999926	-0.549875
C	4.901688	-4.155029	-0.179242
C	3.859577	-4.057003	0.749318
C	3.509538	-2.822166	1.320958
C	1.383384	1.653192	3.764592
C	0.875042	2.966263	3.631555
C	-0.007819	3.475134	4.602359
C	-0.390144	2.703339	5.702213
C	0.091311	1.393768	5.821354
C	0.981977	0.857761	4.875405

C	-2.700700	-0.978509	1.688415
C	-3.969470	-0.306891	1.718357
C	-5.112712	-0.984188	2.197420
C	-5.050221	-2.305226	2.641111
C	-3.802200	-2.924089	2.721196
C	-2.623518	-2.268221	2.306522
C	-4.190832	1.157213	1.462386
C	-5.246232	1.613109	0.624671
C	-5.587525	2.978821	0.629988
C	-4.900975	3.900944	1.421503
C	-3.864967	3.451540	2.247846
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H	5.942851	1.447374	3.850517
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H	5.186210	-5.125846	-0.591630
H	3.335481	-4.955918	1.083608
C	2.521902	-2.826439	2.465289
C	-2.601620	4.447181	-1.016168
H	-5.178980	4.142277	-1.757170
H	-6.155614	2.583372	-3.443528
H	-4.654391	1.002536	-4.674505
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H	3.538917	6.246374	1.140425
H	5.285843	4.537306	1.673155
H	5.175390	2.289853	0.617824

C	3.445414	1.416381	-1.300437
C	-6.067464	0.715203	-0.283784
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H	-5.182967	4.956359	1.412155
H	-3.344806	4.151990	2.906099
C	-2.534788	1.654076	3.364573
C	-1.265959	-4.489001	0.761336
H	0.380446	-5.883562	2.361767
H	1.023769	-5.409548	4.732482
H	0.147158	-3.355049	5.853593
C	-1.587462	-1.522703	4.900487
C	-1.346530	-5.343074	-2.740412
H	-3.531557	-6.203679	-1.383935
H	-5.274244	-4.837386	-0.220817
H	-5.164177	-2.356262	-0.317149
C	-3.439456	-0.804559	-1.751006
C	1.968042	1.027236	-4.504944
H	4.661096	0.892223	-4.702039
H	6.162628	-1.037794	-4.164736
H	5.186858	-3.121572	-3.200094
C	2.607447	-3.691237	-2.642409
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H	-1.353647	-5.265379	-3.840150
H	-0.347052	-5.014062	-2.412169
H	-3.697980	-0.269409	-0.830257
H	-2.489609	-0.406235	-2.118293
H	-4.207302	-0.541423	-2.495597
H	3.383529	-4.469614	-2.633691
H	2.250912	-3.573194	-1.605691
H	1.755099	-4.041030	-3.246917
H	2.553418	1.948633	-4.625933
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H	3.706724	0.568898	-0.657160
H	2.494558	1.190501	-1.791718
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H	-1.172491	0.337319	-3.940062
H	1.479737	6.852157	0.218812
H	1.350950	6.330943	-1.485631
H	0.353012	5.548209	-0.257848
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H	1.862505	3.301258	1.739319
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H	-5.820627	-0.345020	-0.177764
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H	-1.975847	-3.766685	0.351253

D7

C	5.149076	-3.581040	2.232728
C	4.379527	-3.969718	1.102489
C	3.484534	-5.070724	1.219361
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C	4.997024	-4.273006	3.447614
C	4.803554	-3.481603	-0.259660
C	4.833959	-2.129397	-0.774526
C	5.648122	-1.960012	-1.953030
C	6.209305	-3.057890	-2.643800
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Si	3.334357	-0.737449	-0.601276
Si	2.428238	0.712111	0.973140
C	2.756553	1.702678	2.741666
C	2.292965	1.365025	4.066025
C	2.583311	2.200051	5.172577
C	3.372858	3.338625	5.058412
C	3.915633	3.628000	3.812701
C	3.621429	2.851267	2.666797
C	1.707230	0.071213	4.567025
C	2.544760	-1.072744	4.593267
C	2.140327	-2.211305	5.315170
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C	0.506298	0.073386	5.328359
C	4.462746	3.309462	1.504227

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C	6.567465	3.122145	0.280974
C	5.599410	2.548021	1.125567
C	3.908657	-1.049497	3.946599
C	-0.391218	1.291111	5.398679
C	3.226558	5.565744	1.553165
C	5.858368	1.166184	1.679394
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C	7.307269	-0.081061	-1.939465
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C	7.825794	-0.570369	-0.602763
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C	1.776860	2.063081	-2.563121
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C	-0.821899	4.480262	-3.070184
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C	0.740481	4.008655	-0.320337
Si	-1.849533	0.995945	0.679266
C	-2.439461	1.753240	2.349524
C	-3.130111	0.915714	3.301376
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C	-3.476181	2.836129	4.788595
C	-2.816316	3.649891	3.874433
C	-2.261445	3.141695	2.674814

C	-3.341556	-0.578530	3.272349
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C	-4.790168	-2.457533	3.903118
C	-3.677624	-3.295719	4.030578
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C	-1.114158	-5.067629	-3.085250
C	-1.109871	-6.119409	-2.178947
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C	-1.125552	-2.083254	-6.099459
C	0.220248	-1.736605	-6.259826
C	1.123295	-1.978090	-5.218078
C	0.698288	-2.540978	-4.003045
C	-0.771284	-4.496839	1.168168
C	-1.415588	-5.442023	2.033437
C	-0.876925	-5.714230	3.304307
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C	0.377858	-3.824564	1.661788
C	-3.019123	-3.100142	-4.777280
C	1.721850	-2.909788	-2.956603
C	-2.663006	-6.237543	1.685453
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C	-5.915482	-1.480396	-0.492687
C	-7.203760	-1.719038	0.030263
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