

SUPPORTING INFORMATION:

**Product Formation in the Prato Reaction on $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$:
Preference for [5,6]-Bonds, and not Pyracylenic Bonds.**

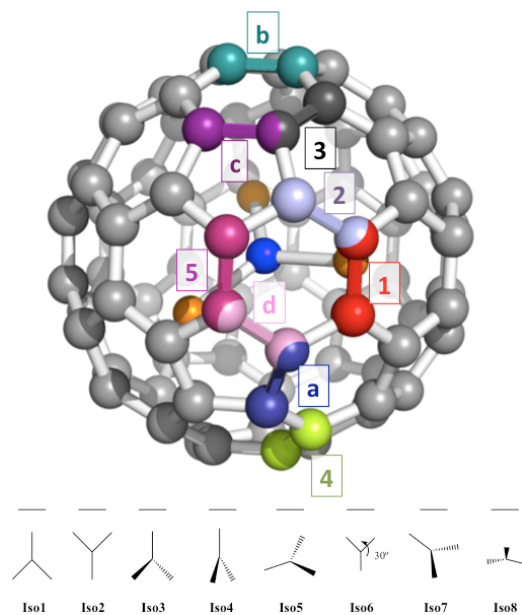
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Figure S1. Representation of all non-equivalent bonds present in $\text{Sc}_3\text{N}@D_{5h}\text{-C}_{80}$ and the different orientations considered for the Sc_3N cluster.



Sc₃N@D_{5h}-C₈₀
84

Sc	1.991282	0.053371	0.065926
Sc	-0.949192	-1.751162	0.066487
Sc	-1.041726	1.697727	0.061184
N	0.000022	0.000080	0.102867
C	0.000382	-3.237318	2.515492
C	-0.634805	-3.831303	1.380305
C	-2.023126	-3.510788	1.123848
C	-1.656193	3.883462	-0.257295
C	1.399636	-2.910601	2.509926
C	3.227563	-2.177863	1.086915
C	2.188919	-3.125715	1.356414
C	1.592529	-3.758481	0.235642
C	-0.299698	-3.944262	-1.111665
C	-1.650366	-3.548106	-1.385372
C	-2.535082	-3.376992	-0.246001
C	-1.826084	-2.682319	-2.511500
C	0.802661	-3.515926	-1.932072
C	1.648485	-1.727097	-3.356633
C	0.606976	-2.644575	-3.039664
C	-0.727225	-2.263602	-3.339509
C	3.643504	-1.848622	-0.245829
C	2.960961	-2.434016	-1.370613
C	1.965165	-3.415849	-1.103227
C	2.804577	-1.625346	-2.522446
C	-3.226426	0.247989	2.501640
C	-3.804531	-0.330174	1.347772
C	-3.421889	-2.231423	-0.250008
C	-3.502331	-1.704076	1.081552
C	-2.325716	-0.491830	3.335511
C	-0.666632	-2.274485	3.352847
C	-1.978109	-1.836293	3.040550
C	-2.624559	-2.461723	1.917685
C	1.027477	0.965550	3.854068
C	-0.002612	0.006712	4.066102
C	-1.348125	0.418713	3.853334
C	0.313227	-1.365151	3.857299
C	3.444790	2.213397	0.233080
C	3.897385	0.340431	-1.387944
C	3.565284	1.709029	-1.118294
C	3.235083	-0.248086	-2.512070
C	2.458944	3.259026	0.224698
C	0.272956	3.887269	1.074953
C	1.613248	3.462540	1.345216
C	1.822084	2.675000	2.501097
C	0.004421	3.233697	-2.532395
C	0.627044	3.776918	-1.382426
C	1.975343	3.406314	-1.114443
C	-0.220708	4.078775	-0.258198
C	2.322665	0.491652	-3.341924
C	1.985670	1.838490	-3.046068
C	2.642906	2.447031	-1.940617
C	0.670231	2.280797	-3.363910
C	1.347797	-0.419836	-3.856154
C	-1.027892	-0.964547	-3.856892
C	0.002861	-0.006741	-4.073832
C	-0.311755	1.365232	-3.860236
C	-0.824103	3.507497	1.909161
C	-0.608476	2.637066	3.034277
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C	-4.051654	0.500558	0.224829
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C	-3.937979	0.004003	-1.112854

ylide
44

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C	-1.014372	0.169051	-4.030310	C	-5.662249	-0.473232	0.878072
C	-2.057211	-1.874161	-3.645944	C	-5.779330	-0.828970	-0.514000
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C	1.265345	-0.687461	-2.626100	C	-4.281849	-0.898569	-2.998391
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C	-3.085083	-0.864796	-3.770505	C	-5.486013	1.478707	-0.366526
C	0.976846	-2.978729	-1.040088	C	-4.834713	1.565880	2.032077
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C	1.067319	0.709164	-2.902550	C	-4.056858	3.297949	0.400309
C	2.030453	-0.835697	-1.437317	C	-4.107889	2.762233	1.721959
C	1.939366	-1.988135	-0.617417	C	-2.826376	4.029256	0.248739
C	0.132031	-3.684833	-0.107193	C	-2.899883	3.121636	2.396154
Sc	-0.060703	-1.121534	0.276127	C	-2.098810	3.944956	1.509894
C	-1.113224	-3.989261	-0.763493	N	-1.732028	-0.016811	0.087936
C	1.741533	1.436073	-1.902804	C	4.101859	0.609221	-1.380336
C	2.587446	0.529308	-1.046544	H	4.359085	1.655237	-1.651952
C	-0.700714	2.422490	-3.059203	H	4.377635	-0.064170	-2.203695
C	1.180326	2.601301	-1.428605	C	4.061634	1.121312	0.831292
C	-0.017386	3.116509	-2.022577	H	4.294418	2.186550	0.612749
C	-2.111002	2.616788	-3.139846	H	4.318029	0.892466	1.875018
C	-2.965694	1.580779	-3.617101	N	4.690019	0.205911	-0.111186
C	2.061249	-1.762443	0.818973	C	6.161604	0.078712	-0.058639
C	2.567449	0.840892	0.537469	C	6.552681	-0.474137	1.315536
C	2.125114	-0.402017	1.277214	C	7.842518	-0.276419	1.812257
C	1.174719	-2.474831	1.750363	C	5.665897	-1.288842	2.025340
C	0.180884	-3.417393	1.299024	C	8.228847	-0.851539	3.021816
C	1.447982	-0.310722	2.519807	H	8.546860	0.340591	1.253335
C	0.791231	-1.545675	2.788132	C	6.049172	-1.859451	3.237453
C	1.166572	2.912145	-0.015433	H	4.669983	-1.474642	1.624404
Sc	-1.739176	1.925636	0.463838	C	7.330795	-1.639158	3.742779
C	-0.729628	3.847823	-1.011318	H	9.237607	-0.683488	3.400554
C	0.005324	3.740729	0.235116	H	5.342231	-2.483419	3.785157
C	1.672481	2.028067	0.949763	H	7.631454	-2.086012	4.691112
C	0.978900	0.899758	3.051413	C	6.761044	1.447977	-0.367894
C	-2.829664	3.329380	-2.119894	C	6.954635	1.851903	-1.694213
C	-4.185156	1.592422	-2.875166	C	6.913543	2.396544	0.650221
C	-4.116448	2.702092	-1.959543	C	7.326290	3.161853	-1.993603
C	-2.152683	3.952542	-1.030195	H	6.817292	1.131335	-2.501139
C	-1.042818	-3.505039	2.022904	C	7.284823	3.707093	0.353749
C	-0.466547	-1.570623	3.480992	H	6.744357	2.103744	1.687001
C	-1.340935	-2.628441	3.134395	C	7.497746	4.093149	-0.969645
C	-2.279192	-3.825307	1.368080	H	7.479512	3.454640	-3.033043
C	-2.327905	-4.012175	-0.028905	H	7.405642	4.429186	1.162201
C	-2.752044	-2.442386	3.165296	H	7.790905	5.117571	-1.202678
C	-3.341826	-3.131526	2.058714	C	6.588312	-1.022182	-1.034824
C	1.064565	2.056868	2.222079	C	7.889417	-1.051612	-1.540471
C	-0.266565	0.895405	3.737371	C	5.719594	-2.077606	-1.327113
C	-0.120068	2.848985	2.473182	C	8.304396	-2.099308	-2.361198
C	-1.016052	-0.306041	3.951985	H	8.580114	-0.243361	-1.298311
C	-0.935126	2.123318	3.419285	C	6.131132	-3.122454	-2.151874
C	-2.429411	-0.173851	4.022776	H	4.715728	-2.077411	-0.903223
C	-3.287867	-1.234891	3.606971	C	7.423937	-3.134624	-2.676544
C	-0.657194	3.750599	1.506326	H	9.321749	-2.105828	-2.753911
C	-3.507744	-3.558020	-0.708077	H	5.438408	-3.933272	-2.379518
C	-4.466343	-2.593122	1.379169	H	7.746823	-3.952460	-3.321759
C	-4.613465	-2.934475	-0.025344				
C	-3.452309	-3.043188	-2.042334				
C	-5.296599	-2.086541	-0.982983				
Sc	-3.404615	-0.923370	-0.510121	b25_down.xyz			
C	-4.533690	-2.099892	-2.219099	125			
C	-4.446967	-0.685656	2.978864	C	0.689202	-4.114039	-0.348762
C	-3.099139	1.065408	3.722763	C	-0.477944	-3.429330	-0.864989
				C	1.012705	-4.026226	1.080652
				C	1.939200	-3.968824	-1.079951

Sc	1.222480	-1.932334	0.075426	C	2.382802	3.728062	1.479599
C	-0.388764	-2.820007	-2.153780	C	4.206071	-3.070305	-0.395419
C	-1.353510	-2.790044	0.073158	C	5.519129	-1.147075	0.432429
C	0.198958	-3.248656	2.000110	C	5.686901	1.197473	0.566810
C	2.440792	-3.895665	1.181705	C	4.819956	-2.369775	0.719377
C	2.040725	-3.300167	-2.352740	C	5.571926	-0.030327	1.343417
C	3.008912	-3.825270	-0.127653	C	4.930148	2.354490	1.001635
C	-1.130172	-1.637692	-2.467465	C	4.842728	-0.118441	2.581762
C	0.840746	-2.780845	-2.912388	C	4.227255	1.074927	3.057066
C	-1.036441	-2.734998	1.494958	C	4.246889	2.276564	2.259706
C	-2.128773	-1.647048	-0.251464	C	2.999859	1.038667	3.783723
C	-1.946883	-1.019146	-1.483134	C	3.013882	2.971955	2.504829
C	-0.377834	-0.882178	-3.417315	C	2.254541	2.207651	3.441120
C	0.842865	-1.582860	-3.682626	N	1.643736	0.000073	0.018746
C	-1.659614	-1.580471	2.021819	C	-4.107815	-1.306940	1.348249
C	-2.594189	-0.943498	1.016573	H	-4.129894	-1.660744	2.394629
C	0.839338	-2.513333	3.092662	H	-4.473048	-2.118193	0.703598
C	-1.047027	-0.889712	3.037693	C	-4.060434	1.019646	1.497587
C	0.184553	-1.360788	3.600171	H	-4.006720	1.185674	2.591550
C	2.267474	-2.543014	3.214090	H	-4.426315	1.941513	1.025936
C	3.066711	-3.225219	2.251592	N	-4.909207	-0.112229	1.215651
C	-1.993507	0.410871	-1.493336	C	-5.933560	-0.011014	0.153705
C	-2.602962	0.678507	1.022380	C	-6.874910	1.158823	0.489503
C	-2.247952	1.219356	-0.351906	C	-7.040430	1.590056	1.808080
C	-1.261944	1.167033	-2.452692	C	-7.689328	1.706586	-0.506802
C	-0.397540	0.537342	-3.402255	C	-7.970444	2.581702	2.118291
C	-1.726733	2.533199	-0.625025	H	-6.443073	1.140833	2.599131
Sc	0.196025	1.400947	-0.220702	C	-8.620252	2.695431	-0.198304
C	-1.038710	2.482501	-1.908744	H	-7.591139	1.360537	-1.535497
C	-1.034446	0.556246	3.054551	C	-8.759872	3.143136	1.115875
C	0.924248	-0.215059	4.047632	H	-8.080530	2.911296	3.152040
C	0.176606	0.959341	3.712659	H	-9.241915	3.114950	-0.989935
C	-1.601924	1.301194	2.012139	H	-9.486792	3.919153	1.358003
C	-1.077198	3.228572	0.448765	C	-6.870218	-1.226541	0.247473
C	3.005193	-1.396283	3.651407	C	-7.639118	-1.615683	-0.853633
C	4.261668	-2.482459	2.021537	C	-7.084548	-1.860116	1.475322
C	4.243092	-1.357459	2.923330	C	-8.567862	-2.648489	-0.741582
C	2.342092	-0.202430	4.037585	H	-7.509870	-1.111156	-1.810505
C	0.765914	1.244081	-3.769839	C	-8.010845	-2.895172	1.588339
C	0.250815	3.102430	-2.142952	H	-6.528231	-1.532616	2.351483
C	1.083138	2.506970	-3.139836	C	-8.751770	-3.299240	0.478158
C	1.992043	0.546768	-4.015550	H	-9.152609	-2.942226	-1.613913
C	2.054973	-0.868295	-3.921646	H	-8.158421	-3.382372	2.552829
C	2.503475	2.582880	-3.053077	H	-9.476331	-4.109560	0.565464
C	3.073112	1.370059	-3.542933	C	-5.282312	0.138246	-1.222739
C	-1.015052	2.569310	1.732697	C	-4.968225	1.406245	-1.732472
C	0.201893	3.856655	0.235002	C	-4.936506	-0.987383	-1.978283
C	0.209484	2.976368	2.384081	C	-4.371144	1.545697	-2.982996
C	0.888815	3.813252	-1.032438	H	-5.217526	2.297762	-1.155833
C	0.961254	3.768333	1.468138	C	-4.340788	-0.851400	-3.232957
C	2.318769	3.899315	-0.997595	H	-5.158883	-1.984670	-1.596487
C	3.108418	3.271460	-2.001698	C	-4.063743	0.415698	-3.742879
C	0.833593	2.163290	3.361578	H	-4.131149	2.541599	-3.357753
C	3.262411	-1.442762	-3.445589	H	-4.077408	-1.742472	-3.804273
C	4.231920	0.803291	-2.939758	H	-3.588657	0.522435	-4.719228
C	4.345521	-0.618374	-2.989590				
C	3.259161	-2.646631	-2.665023				
C	5.025750	-1.336988	-1.963287				
Sc	3.532231	0.582727	0.153017	b25_up.xyz			
C	4.341629	-2.561477	-1.712943	125			
C	4.301678	2.758082	-1.407724	C	0.697225	3.986202	1.023840
C	3.053196	3.842292	0.236202	C	-0.423242	3.204395	1.498926
C	4.886402	1.532419	-1.840274	C	0.939588	4.111518	-0.418227
C	4.283499	3.138348	-0.004827	C	1.989836	3.776809	1.659418
C	5.652614	0.802343	-0.851135	Sc	1.278583	1.906840	0.262112
C	5.608032	-0.632679	-0.895669	C	-0.258476	2.425492	2.682742
				C	-1.338251	2.681030	0.527539
				C	0.087187	3.454671	-1.393981

C	0.046507	3.749392	1.254024	C	4.809819	-1.818097	-1.977544
C	-1.074629	1.285690	-2.688156	C	4.838606	-2.506369	-0.702725
C	-2.582044	0.972024	-0.846850	C	3.665061	-2.316271	-2.699562
C	-2.547783	1.030173	0.728483	C	3.738342	-3.425656	-0.669931
C	-0.873451	1.965572	2.443232	C	3.026965	-3.315453	-1.903723
C	0.160349	2.950360	2.454388	N	1.620735	0.045441	0.008687
C	-1.452876	-0.100714	-2.643537	C	-4.043542	1.368151	1.136473
C	-2.165498	-0.364509	-1.457605	H	-4.060613	2.431543	1.444596
C	1.001813	0.690419	-3.903324	H	-4.373131	0.758079	1.989263
C	-0.633220	-1.055249	-3.237080	C	-4.067358	1.388234	-1.198428
C	0.581632	-0.667903	-3.875210	H	-4.046859	2.466671	-1.441553
C	2.406197	0.931729	-3.928908	H	-4.443441	0.845774	-2.075707
C	2.968935	2.108710	-3.345253	N	-4.876879	1.165915	-0.025667
C	-2.100094	-0.276066	1.319611	C	-5.925578	0.124888	-0.034016
C	-2.095346	-1.548389	0.679879	C	-6.865870	0.384471	-1.224731
C	-1.400243	-0.382477	2.549203	C	-7.049299	1.682351	-1.710335
Sc	0.236484	-1.309106	0.551288	C	-7.662726	-0.644761	-1.735182
C	-0.761780	0.733222	3.166022	C	-7.976395	1.938502	-2.718993
C	-1.407011	-2.484643	1.550666	H	-6.466897	2.499317	-1.288397
C	-1.971593	-1.583957	-0.772310	C	-8.592255	-0.389746	-2.741516
C	-0.903389	-1.730002	2.678101	H	-7.554068	-1.657586	-1.348513
C	-0.453249	-2.319335	-2.600047	C	-8.747594	0.902053	-3.244004
C	1.513689	-1.744633	-3.695355	H	-8.099756	2.956270	-3.090898
C	0.879246	-2.764252	-2.905441	H	-9.199461	-1.207085	-3.131940
C	-1.084269	-2.594124	-1.353695	H	-9.472389	1.101370	-4.034037
C	-0.536229	-3.458635	0.966420	C	-6.855724	0.339906	1.171060
C	3.336417	-0.138170	-3.727836	C	-7.691934	-0.695419	1.601825
C	4.202760	1.782854	-2.724649	C	-6.999765	1.604339	1.748388
C	4.457870	0.373030	-2.978533	C	-8.617757	-0.483953	2.620533
C	2.899792	-1.479467	-3.570271	H	-7.617717	-1.678693	1.138308
C	0.409541	0.497590	3.891424	C	-7.924713	1.817401	2.769891
C	0.388676	-1.940334	3.291932	H	-6.394010	2.433242	1.388281
C	0.974079	-0.833584	3.964560	C	-8.732548	0.772589	3.215883
C	1.490786	1.449951	3.866496	H	-9.256019	-1.305954	2.946246
C	1.398326	2.651810	3.123764	H	-8.017265	2.809596	3.212974
C	2.393190	-0.677559	4.008265	H	-9.455708	0.938508	4.015062
C	2.722801	0.710696	3.898740	C	-5.308067	-1.275776	-0.067646
C	-0.392179	-3.507492	-0.469409	C	-4.968707	-1.873791	-1.287685
C	0.773770	-3.666270	1.536382	C	-5.028833	-1.972733	1.115088
C	0.962077	-3.917191	-0.766619	C	-4.407868	-3.149798	-1.328250
C	1.261402	-2.952206	2.694970	H	-5.169403	-1.348296	-2.222197
C	1.674346	-4.024502	0.468989	C	-4.476981	-3.252555	1.076576
C	2.666143	-2.793323	2.809048	H	-5.270646	-1.522792	2.078834
C	3.226062	-1.642446	3.454387	C	-4.169431	-3.848812	-0.145684
C	1.616321	-3.520782	-1.966722	H	-4.147976	-3.592765	-2.290827
C	2.573310	3.154858	2.514354	H	-4.269693	-3.776400	2.010361
C	3.870924	1.137379	3.181979	H	-3.731470	-4.847409	-0.175963
C	3.799692	2.425780	2.563325				
C	2.506706	3.859462	1.248420	b35_up.xyz			
C	4.512014	2.719753	1.360993	125			
C	3.724752	3.554975	0.524878	C	0.989424	2.814503	1.319498
C	4.414840	-1.251646	2.770912	C	1.904916	1.852374	0.778314
C	3.559245	-3.167153	1.743889	C	0.247544	2.536050	2.524011
C	4.737894	0.117206	2.596571	C	0.169215	3.668431	0.480900
C	4.634223	-2.213998	1.715684	Sc	-0.277749	1.374617	-0.344373
Sc	3.490001	-0.363851	-0.506269	C	2.012953	1.814845	-0.678236
C	5.462250	0.452320	1.406764	C	2.052218	0.643712	1.486194
C	5.313780	1.727504	0.787264	C	0.338753	1.278021	3.183276
C	3.067068	-3.740797	0.550354	C	-0.983508	3.252948	2.457129
C	3.720908	3.395402	-0.889360	C	0.221111	3.600929	-0.952307
C	5.397429	1.571860	-0.628731	C	-1.082871	3.889696	1.190469
C	5.758396	-0.507705	0.367484	C	2.061119	0.532014	-1.287187
C	4.582561	2.376370	-1.492469	C	1.196163	2.684670	-1.530227
C	5.748220	0.189949	-0.912713	C	1.303702	0.376483	2.655792
C	5.277293	-1.854226	0.498182	C	2.562668	-0.675865	0.912127
C	5.232149	-0.444586	-2.102836	C	2.544882	-0.753019	-0.672431

C	1.354345	0.574808	-2.513338	C	-4.242668	-2.367984	2.145676
C	0.783140	1.875108	-2.657369	N	-1.657505	-0.021093	0.017272
C	1.117940	-1.047702	2.752500	N	4.666571	-0.220672	0.069523
C	1.672544	-1.682985	1.625453	C	4.070289	-0.844879	1.242947
C	-0.842037	0.736911	3.845251	H	4.348456	-0.338975	2.177358
C	-0.002133	-1.554432	3.399503	H	4.312461	-1.926554	1.318223
C	-0.973713	-0.674817	3.958447	C	4.045079	-0.954842	-1.022339
C	-2.046895	1.495936	3.801202	H	4.286494	-2.039952	-1.000383
C	-2.120847	2.734190	3.090326	H	4.299687	-0.539427	-2.007339
C	1.658029	-1.860492	-1.161047	C	6.136789	-0.076926	0.044303
C	1.185839	-2.980363	-0.405604	C	6.557183	0.833782	1.201613
C	0.951884	-1.801774	-2.388965	C	5.680448	1.807553	1.687970
Sc	-0.842963	-1.821529	-0.349283	H	4.671804	1.872684	1.280577
C	0.783934	-0.588498	-3.124432	C	6.088825	2.690210	2.685961
C	0.167188	-3.646264	-1.207371	H	5.389437	3.437202	3.062735
C	1.047194	-2.812566	1.047496	C	7.386224	2.622449	3.194066
C	-0.021220	-2.861981	-2.410900	H	7.706890	3.313300	3.974613
C	-0.650359	-2.711240	2.872152	C	8.274036	1.671507	2.689781
C	-2.245744	-1.328547	3.843293	H	9.294612	1.618272	3.070382
C	-2.048995	-2.584962	3.170841	C	7.862230	0.785368	1.695780
C	-0.170041	-3.336082	1.683609	H	8.558373	0.041874	1.306449
C	-1.015184	-4.135076	-0.566241	C	6.741999	-1.476717	0.107307
C	-3.315539	0.846012	3.667780	C	6.933487	-2.107470	1.342285
C	-3.386771	2.841486	2.458722	H	6.791942	-1.540329	2.262963
C	-4.159174	1.668337	2.833458	C	7.309779	-3.448257	1.406939
C	-3.424481	-0.568596	3.647322	H	7.461701	-3.919378	2.378837
C	-0.388093	-0.431227	-3.866804	C	7.488244	-4.183633	0.235188
C	-1.297627	-2.623592	-3.050712	H	7.785515	-5.231928	0.284369
C	-1.417459	-1.448527	-3.840297	C	7.277246	-3.571084	-0.999939
C	-1.022714	0.859797	-3.969861	H	7.403645	-4.138621	-1.922728
C	-0.476069	2.004354	-3.339780	C	6.900466	-2.230265	-1.061725
C	-2.668847	-0.768566	-3.949678	H	6.732860	-1.759996	-2.031273
C	-2.442571	0.645628	-3.978275	C	6.525666	0.713056	-1.209736
C	-1.164105	-3.990568	0.862067	C	7.813339	0.607009	-1.738792
C	-2.305424	-3.883706	-1.159919	H	8.519717	-0.099147	-1.301384
C	-2.571272	-3.824734	1.146997	C	8.195019	1.387397	-2.829124
C	-2.488609	-3.161755	-2.397205	H	9.202043	1.289049	-3.235929
C	-3.272215	-3.770965	-0.098199	C	7.294618	2.289983	-3.395746
C	-3.726715	-2.493774	-2.575971	H	7.591566	2.897632	-4.251299
C	-3.805578	-1.283292	-3.340050	C	6.015253	2.417446	-2.853890
C	-3.020136	-3.092702	2.279595	H	5.306801	3.129120	-3.278999
C	-1.368484	2.974098	-2.820785	C	5.636849	1.640709	-1.760864
C	-3.339198	1.545626	-3.346967	H	4.642879	1.752847	-1.328992
C	-2.779466	2.764062	-2.845307				
C	-1.033986	3.722175	-1.622214	b58_down.xyz			
C	-3.324064	3.423629	-1.700813	125			
C	-2.275123	3.974021	-0.917562	C	0.523309	-2.900616	-2.557746
C	-4.752446	-0.403836	-2.736376	C	-0.030369	-3.465391	-1.351572
C	-4.690844	-2.393246	-1.513579	C	1.932714	-3.131899	-2.565049
C	-4.528926	0.996266	-2.700667	C	-0.051695	-1.763832	-3.183192
C	-5.319819	-1.103102	-1.608487	Sc	1.444331	-2.027813	0.034397
Sc	-3.546202	0.272791	0.546106	C	-1.151627	-2.805132	-0.707965
C	-5.067819	1.698670	-1.577202	C	1.035224	-4.153327	-0.658376
C	-4.446608	2.877523	-1.070621	C	2.835707	-2.221227	-3.191225
C	-4.450836	-2.989047	-0.256598	C	2.268969	-3.845626	-1.354011
C	-2.329348	3.965395	0.505052	C	-1.215504	-1.222812	-2.606494
C	-4.573107	2.902728	0.349347	C	0.845800	-0.880059	-3.859300
C	-5.687994	1.021640	-0.462919	C	-1.764875	-1.762430	-1.402928
C	-3.514176	3.414082	1.165068	C	-2.634874	-0.699943	-0.773758
C	-5.405445	1.780242	0.745690	C	-1.151961	-2.782948	0.787543
C	-5.774430	-0.409118	-0.452357	C	-1.434965	0.200886	-2.615982
C	-5.190213	1.124988	2.010318	C	-2.634393	-0.676622	0.788961
C	-5.341653	-0.312585	2.032951	C	-2.110433	0.565452	-1.420656
C	-5.629954	-1.059355	0.821452	C	-1.764145	-1.718762	1.449909
C	-4.455149	-1.130095	2.826494	C	-0.031941	-3.424650	1.452348
C	-4.948580	-2.320056	0.904909	C	1.034441	-4.133229	0.781367

C	-0.353570	2.364099	-2.667863	H	-4.396632	-0.425628	-2.090155
C	-1.020889	2.715304	-1.457703	H	-4.388906	-1.960491	-1.139684
C	0.942830	3.020120	-2.694946	C	-4.138023	-0.846467	1.142981
C	-0.518361	1.085898	-3.243322	H	-4.384831	-1.929449	1.187585
Sc	2.150111	0.755274	-1.785756	H	-4.395854	-0.370519	2.098812
C	-0.171766	3.625515	-0.756237	C	-6.221140	-0.049224	0.000323
C	-1.856232	1.770648	-0.770170	C	-6.634512	0.792861	-1.211038
C	2.074936	2.477878	-3.372970	C	-5.752437	1.729563	-1.756440
C	1.047744	3.783972	-1.468065	H	-4.742105	1.812829	-1.355646
C	0.615454	0.526785	-3.928712	C	-6.158507	2.552539	-2.805454
C	-2.112312	0.607956	1.398996	H	-5.455431	3.271702	-3.226976
C	-1.217478	-1.144039	2.638033	C	-7.456975	2.461717	-3.307072
C	-1.437621	0.279152	2.605145	H	-7.775222	3.106228	-4.127323
C	-1.856925	1.792964	0.713029	C	-8.349443	1.547796	-2.745409
C	-0.172459	3.646656	0.645475	H	-9.370941	1.477193	-3.120754
C	0.520827	-2.822716	2.640891	C	-7.940739	0.721835	-1.699871
C	2.267810	-3.804774	1.468758	H	-8.640528	0.007668	-1.264628
C	1.930275	-3.053623	2.656560	C	-6.819502	-1.453396	0.006609
C	-0.054659	-1.667861	3.232257	C	-7.003767	-2.148428	-1.194268
C	1.888300	1.205439	-4.054456	H	-6.860587	-1.629220	-2.142543
C	3.342929	2.674541	-2.720934	C	-7.374535	-3.492342	-1.190321
C	2.291803	3.913472	-0.789675	H	-7.521593	-4.013831	-2.136950
C	2.914454	0.169284	-3.991764	C	-7.553518	-4.166694	0.017458
C	3.441917	3.411103	-1.468705	H	-7.846111	-5.217455	0.021601
C	4.356902	1.638158	-2.677960	C	-7.348986	-3.489802	1.219828
C	4.155968	0.356120	-3.279084	H	-7.475560	-4.009396	2.170436
C	2.254898	-1.103578	-3.877747	C	-6.978805	-2.145793	1.212864
C	4.545670	2.884302	-0.743393	H	-6.817486	-1.623892	2.156694
C	5.079927	1.763007	-1.434848	C	-6.633226	0.805873	1.202767
C	-1.022185	2.757675	1.372961	C	-7.926477	0.716686	1.721509
C	1.046310	3.826475	1.353514	H	-8.619990	-0.021204	1.317085
C	-0.355978	2.442846	2.593752	C	-8.330192	1.555273	2.759432
C	2.291031	3.935306	0.672706	H	-9.341418	1.470335	3.158855
C	0.940369	3.099486	2.602647	C	-7.445788	2.498473	3.283540
C	3.440488	3.453495	1.367823	H	-7.759898	3.151780	4.098404
C	4.544781	2.905083	0.659503	C	-6.160438	2.606722	2.751769
C	-0.521494	1.182304	3.206894	H	-5.463840	3.348290	3.144313
Sc	2.150857	0.813562	1.759250	C	-5.760004	1.772453	1.709952
C	4.746603	-0.768180	-2.636832	H	-4.760288	1.867858	1.285599
C	5.586170	0.623429	-0.737641				
C	5.480001	-0.626027	-1.403373				
C	4.110898	-2.058923	-2.626005	b58_up.xyz			
C	5.314860	-1.835509	-0.668547	125			
C	4.438347	-2.708509	-1.377856	C	0.523309	-2.900616	-2.557746
C	5.078387	1.805055	1.384825	C	-0.030369	-3.465391	-1.351572
C	3.340744	2.755437	2.641954	C	1.932714	-3.131899	-2.565049
C	5.585503	0.645199	0.722443	C	-0.051695	-1.763832	-3.183192
C	4.354478	1.717789	2.630657	Sc	1.444331	-2.027813	0.034397
C	5.478868	-0.583847	1.425101	C	-1.151627	-2.805132	-0.707965
C	5.314194	-1.814671	0.726476	C	1.035224	-4.153327	-0.658376
C	2.071787	2.578062	3.297986	C	2.835707	-2.221227	-3.191225
C	3.510414	-3.535751	-0.681924	C	2.268969	-3.845626	-1.354011
C	4.436797	-2.665995	1.460582	C	-1.215504	-1.222812	-2.606494
C	4.744206	-0.689031	2.661555	C	0.845800	-0.880059	-3.859300
C	3.509768	-3.514023	0.788739	C	-1.764875	-1.762430	-1.402928
C	4.108373	-1.979414	2.688660	C	-2.634874	-0.699943	-0.773758
C	4.152586	0.453944	3.268971	C	-1.151961	-2.782948	0.787543
C	2.832554	-2.124689	3.256948	C	-1.434965	0.200886	-2.615982
C	2.250961	-0.987498	3.909530	C	-2.634393	-0.676622	0.788961
C	2.910221	0.288343	3.984938	C	-2.110433	0.565452	-1.420656
C	0.841900	-0.764661	3.883214	C	-1.764145	-1.718762	1.449909
C	1.884241	1.325832	4.015598	C	-0.031941	-3.424650	1.452348
C	0.611528	0.643723	3.909683	C	1.034441	-4.133229	0.781367
N	1.947261	-0.080192	0.001032	C	-0.353570	2.364099	-2.667863
N	-4.750519	-0.183270	0.001492	C	-1.020889	2.715304	-1.457703
C	-4.139426	-0.877381	-1.122512	C	0.942830	3.020120	-2.694946
				C	-0.518361	1.085898	-3.243322

Sc	2.150111	0.755274	-1.785756	H	-4.395854	-0.370519	2.098812
C	-0.171766	3.625515	-0.756237	C	-6.221140	-0.049224	0.000323
C	-1.856232	1.770648	-0.770170	C	-6.634512	0.792861	-1.211038
C	2.074936	2.477878	-3.372970	C	-5.752437	1.729563	-1.756440
C	1.047744	3.783972	-1.468065	H	-4.742105	1.812829	-1.355646
C	0.615454	0.526785	-3.928712	C	-6.158507	2.552539	-2.805454
C	-2.112312	0.607956	1.398996	H	-5.455431	3.271702	-3.226976
C	-1.217478	-1.144039	2.638033	C	-7.456975	2.461717	-3.307072
C	-1.437621	0.279152	2.605145	H	-7.775222	3.106228	-4.127323
C	-1.856925	1.792964	0.713029	C	-8.349443	1.547796	-2.745409
C	-0.172459	3.646656	0.645475	H	-9.370941	1.477193	-3.120754
C	0.520827	-2.822716	2.640891	C	-7.940739	0.721835	-1.699871
C	2.267810	-3.804774	1.468758	H	-8.640528	0.007668	-1.264628
C	1.930275	-3.053623	2.656560	C	-6.819502	-1.453396	0.006609
C	-0.054659	-1.667861	3.232257	C	-7.003767	-2.148428	-1.194268
C	1.888300	1.205439	-4.054456	H	-6.860587	-1.629220	-2.142543
C	3.342929	2.674541	-2.720934	C	-7.374535	-3.492342	-1.190321
C	2.291803	3.913472	-0.789675	H	-7.521593	-4.013831	-2.136950
C	2.914454	0.169284	-3.991764	C	-7.553518	-4.166694	0.017458
C	3.441917	3.411103	-1.468705	H	-7.846111	-5.217455	0.021601
C	4.356902	1.638158	-2.677960	C	-7.348986	-3.489802	1.219828
C	4.155968	0.356120	-3.279084	H	-7.475560	-4.009396	2.170436
C	2.254898	-1.103578	-3.877747	C	-6.978805	-2.145793	1.212864
C	4.545670	2.884302	-0.743393	H	-6.817486	-1.623892	2.156694
C	5.079927	1.763007	-1.434848	C	-6.633226	0.805873	1.202767
C	-1.022185	2.757675	1.372961	C	-7.926477	0.716686	1.721509
C	1.046310	3.826475	1.353514	H	-8.619990	-0.021204	1.317085
C	-0.355978	2.442846	2.593752	C	-8.330192	1.555273	2.759432
C	2.291031	3.935306	0.672706	H	-9.341418	1.470335	3.158855
C	0.940369	3.099486	2.602647	C	-7.445788	2.498473	3.283540
C	3.440488	3.453495	1.367823	H	-7.759898	3.151780	4.098404
C	4.544781	2.905083	0.659503	C	-6.160438	2.606722	2.751769
C	-0.521494	1.182304	3.206894	H	-5.463840	3.348290	3.144313
Sc	2.150857	0.813562	1.759250	C	-5.760004	1.772453	1.709952
C	4.746603	-0.768180	-2.636832	H	-4.760288	1.867858	1.285599
C	5.586170	0.623429	-0.737641				
C	5.480001	-0.626027	-1.403373	bb2_down.xyz			
C	4.110898	-2.058923	-2.626005	125			
C	5.314860	-1.835509	-0.668547	C	-1.030980	-2.852914	1.165746
C	4.438347	-2.708509	-1.377856	C	-1.650165	-1.691489	1.698608
C	5.078387	1.805055	1.384825	C	0.151688	-3.438582	1.760815
C	3.340744	2.755437	2.641954	C	-1.019091	-3.144724	-0.244381
C	5.585503	0.645199	0.722443	Sc	1.128385	-1.907120	0.197979
C	4.354478	1.717789	2.630657	C	-1.084286	-1.132564	2.832552
C	5.478868	-0.583847	1.425101	C	-2.640008	-0.922212	0.852987
C	5.314194	-1.814671	0.726476	C	0.815637	-2.765078	2.852754
C	2.071787	2.578062	3.297986	C	0.865698	-4.131917	0.716729
C	3.510414	-3.535751	-0.681924	C	-1.591698	-2.186680	-1.156750
C	4.436797	-2.665995	1.460582	C	0.178039	-3.901040	-0.543927
C	4.744206	-0.689031	2.661555	C	0.124421	-1.668536	3.424506
C	3.509768	-3.514023	0.788739	C	-1.070466	0.305121	3.028514
C	4.108373	-1.979414	2.688660	C	-2.645820	0.671603	1.084536
C	4.152586	0.453944	3.268971	C	-2.284744	-1.077312	-0.614776
C	2.832554	-2.124689	3.256948	C	0.832745	-0.579783	4.011842
C	2.250961	-0.987498	3.909530	C	-1.643083	1.166717	2.093486
C	2.910221	0.288343	3.984938	C	0.138426	0.633278	3.732868
C	0.841900	-0.764661	3.883214	C	2.281655	-2.771469	2.899861
C	1.884241	1.325832	4.015598	C	2.225423	-0.591009	4.067960
C	0.611528	0.643723	3.909683	C	2.955749	-1.700599	3.543763
N	1.947261	-0.080192	0.001032	C	2.978844	-3.425608	1.836722
N	-4.750519	-0.183270	0.001492	C	2.282719	-4.049612	0.744939
C	-4.139426	-0.877381	-1.122512	C	-1.024348	2.428636	1.892644
H	-4.396632	-0.425628	-2.090155	C	0.208183	2.740598	2.581048
H	-4.388906	-1.960491	-1.139684	C	-1.077605	3.187564	0.654171
C	-4.138023	-0.846467	1.142981	Sc	0.361755	1.544205	-0.062558
H	-4.384831	-1.929449	1.187585	C	0.942215	3.641456	1.766693

C	0.846698	1.830491	3.469436	C	-7.696754	1.761260	-0.439295
C	-1.665222	2.516069	-0.500616	C	-8.018288	2.459632	2.234698
C	0.219716	3.867738	0.546213	H	-6.518301	0.966232	2.641900
C	2.963029	0.610267	3.845004	C	-8.621037	2.740312	-0.080745
C	4.199365	-1.189362	3.030734	H	-7.582092	1.486033	-1.487460
C	4.207227	0.238307	3.218643	C	-8.780401	3.099513	1.257735
C	2.302814	1.826900	3.528415	H	-8.145091	2.719625	3.286255
C	2.347968	3.645416	1.824975	H	-9.221167	3.222169	-0.853288
C	4.230249	-2.926981	1.329758	H	-9.501413	3.867955	1.538569
C	3.041849	-3.829510	-0.451726	C	-5.326799	0.174920	-1.224138
C	4.265964	-3.172809	-0.080295	C	-4.995828	-0.925569	-2.026147
C	4.819252	-1.766160	1.900403	C	-4.968526	1.455134	-1.667010
C	-2.240004	1.235595	-0.270525	C	-4.380861	-0.748708	-3.263730
C	-0.950716	2.675807	-1.746665	H	-5.246761	-1.932890	-1.691630
C	0.972075	3.918642	-0.682350	C	-4.350458	1.636454	-2.902599
C	-2.141393	0.173612	-1.221203	H	-5.204217	2.325162	-1.052883
C	0.309461	3.397541	-1.842198	C	-4.069101	0.535183	-3.711737
C	-0.875263	1.606663	-2.715000	H	-4.129492	-1.618341	-3.872147
C	-1.465876	0.343603	-2.470703	H	-4.079174	2.641234	-3.229311
C	1.066438	2.818140	-2.912747	H	-3.581496	0.675100	-4.677744
C	0.358831	1.703469	-3.440944	C	-6.907221	-1.240574	0.197779
C	3.014834	2.747888	2.706179	C	-7.080836	-1.954296	1.386685
C	3.097245	3.781854	0.626021	C	-7.707810	-1.559913	-0.903371
C	4.259231	2.376938	2.079389	C	-8.003737	-2.996587	1.459918
C	2.442179	3.875956	-0.638545	H	-6.494862	-1.684877	2.263337
C	4.314699	3.017631	0.786403	C	-8.631687	-2.600007	-0.831376
C	3.150131	3.354547	-1.758140	H	-7.604839	-0.993499	-1.828614
C	2.465193	2.813855	-2.879847	C	-8.778417	-3.328637	0.349189
C	4.884343	1.115854	2.320743	H	-8.120917	-3.547091	2.394084
C	-0.900541	-0.791298	-3.080647	H	-9.241939	-2.838805	-1.703007
C	1.040642	0.536566	-3.908730	H	-9.499805	-4.144521	0.405643
C	0.344246	-0.693695	-3.806009				
C	-0.945112	-2.048240	-2.410642	bb2_up.xyz			
C	1.043584	-1.916853	-3.596181	125			
C	0.289658	-2.742544	-2.702525	C	-1.080035	2.985957	0.027914
C	3.182078	1.683744	-3.379831	C	-1.731431	2.049588	-0.822326
C	4.369592	2.591528	-1.590946	C	0.052822	3.773447	-0.410372
C	2.503000	0.526487	-3.867072	C	-0.965770	2.784801	1.450321
C	4.377870	1.561617	-2.601973	Sc	1.146600	1.838050	0.463692
C	3.171299	-0.717522	-3.719666	C	-1.232877	1.902075	-2.105252
C	2.436668	-1.932292	-3.559996	C	-2.631217	1.005056	-0.209845
C	4.994159	2.418821	-0.321615	C	0.648808	3.510271	-1.700299
C	0.930351	-3.592238	-1.754130	C	0.836370	4.097425	0.757628
C	3.120174	-2.779440	-2.641479	C	-1.458772	1.561242	2.030268
C	4.375473	-0.840408	-2.937912	C	0.244300	3.433217	1.906594
C	2.398862	-3.578986	-1.710314	C	-0.068899	2.639848	-2.556863
C	4.343317	-2.109194	-2.268322	C	-1.218383	0.610226	-2.771021
C	4.969016	0.299338	-2.342386	C	-2.636139	-0.433407	-0.962446
Sc	3.550140	0.556490	0.279704	C	-2.181814	0.671880	1.203211
C	4.884621	-2.261068	-0.975901	C	0.605321	1.832747	-3.517896
C	5.539076	-1.123198	-0.394680	C	-1.723784	-0.533395	-2.153127
C	5.626923	0.136617	-1.067292	C	-0.057569	0.573988	-3.617419
C	5.534433	-0.880691	1.016107	C	2.109671	3.578339	-1.835875
C	5.728021	1.187533	-0.074301	C	1.989050	1.905975	-3.654371
C	5.660233	0.540791	1.238894	C	2.745107	2.800120	-2.836718
C	-4.111087	0.977827	1.535369	C	2.874771	3.873747	-0.662810
C	-4.105891	-1.349061	1.218300	C	2.248580	4.074199	0.616169
N	1.650741	0.007894	0.154690	C	-1.072425	-1.769484	-2.416504
N	-4.939276	-0.163189	1.192900	C	0.117319	-1.791572	-3.236258
H	-4.484412	1.906654	1.083629	C	-1.027493	-2.895277	-1.495222
H	-4.093180	1.112799	2.634138	Sc	0.466777	-1.523263	-0.420161
H	-4.475616	-2.125145	0.534427	C	0.918175	-2.887736	-2.815419
H	-4.083165	-1.770031	2.241688	C	0.683734	-0.617354	-3.808621
C	-5.973833	-0.020546	0.145859	C	-1.523612	-2.649633	-0.146333
C	-6.910230	1.135603	0.532557	C	0.282216	-3.532840	-1.701009
C	-7.095988	1.478537	1.874704	C	2.754976	0.725169	-3.894697

C	4.029166	2.186518	-2.606997	H	-7.781842	2.217956	4.644901
C	4.037358	0.911095	-3.266177	C	-8.347215	1.733177	2.616734
C	2.132574	-0.548778	-3.957521	H	-9.365591	2.108475	2.723284
C	2.315447	-2.830130	-2.966568	C	-7.936002	1.191998	1.399870
C	4.159952	3.274581	-0.431375	H	-8.630394	1.149167	0.560150
C	3.090898	3.493131	1.619775	C	-6.803949	0.681019	-1.314355
C	4.296215	3.040446	0.974665	C	-6.975652	2.069067	-1.372532
C	4.710000	2.377900	-1.386159	H	-6.836959	2.665931	-0.470417
C	-2.127435	-1.389545	0.103269	C	-7.327724	2.693930	-2.567859
C	-0.721046	-3.183821	0.926727	H	-7.464130	3.775844	-2.590804
C	1.123189	-3.954166	-0.608305	C	-7.501193	1.940070	-3.728588
C	-2.005338	-0.706706	1.355662	H	-7.778313	2.427976	-4.663893
C	0.543555	-3.859353	0.699742	C	-7.310626	0.559018	-3.686487
C	-0.603151	-2.504575	2.194821	H	-7.433390	-0.039530	-4.589962
C	-1.233517	-1.259855	2.432765	C	-6.958432	-0.063438	-2.489800
C	1.363139	-3.647232	1.853539	H	-6.806733	-1.143060	-2.465601
C	0.683020	-2.794627	2.764014	C	-6.640354	-1.429138	0.135570
C	2.912385	-1.672126	-3.546895	C	-7.929472	-1.845733	-0.200929
C	3.149510	-3.326609	-1.929756	H	-8.613847	-1.146463	-0.682168
C	4.184464	-1.486226	-2.913126	C	-8.340802	-3.151319	0.064020
C	2.586010	-3.850378	-0.731540	H	-9.348858	-3.464756	-0.209522
C	4.341391	-2.504982	-1.904064	C	-7.468697	-4.051064	0.677178
C	3.365853	-3.701854	0.453632	H	-7.788902	-5.073413	0.881345
C	2.756288	-3.580842	1.731828	C	-6.187574	-3.631389	1.037288
C	4.745402	-0.195557	-2.734619	H	-5.502073	-4.321891	1.529634
C	-0.625763	-0.366730	3.336362	C	-5.779827	-2.324951	0.777404
C	1.382920	-1.827725	3.548800	H	-4.784868	-1.990426	1.071854
C	0.670674	-0.655831	3.904317				
C	-0.724528	1.040024	3.124501				
C	1.341120	0.588757	4.071760	bb8_down.xyz			
C	0.517784	1.638142	3.553854	125			
C	3.490167	-2.653607	2.526647	C	1.471682	-2.611250	-0.587191
C	4.567059	-2.893287	0.468713	C	2.153607	-1.355553	-0.499376
C	2.838576	-1.754561	3.419961	C	0.599732	-2.864665	-1.712782
C	4.636651	-2.243129	1.757075	C	0.960812	-3.353538	0.557249
C	3.482595	-0.510910	3.649942	Sc	-0.568773	-1.681390	0.343725
C	2.728893	0.662646	3.954208	C	2.008006	-0.470054	-1.568090
C	5.098797	-2.289253	-0.712479	C	2.658847	-0.877306	0.837121
C	1.081818	2.769936	2.897965	C	0.406635	-1.932225	-2.779735
C	3.338008	1.790413	3.333610	C	-0.448731	-3.729080	-1.279990
C	4.627539	-0.095993	2.876708	C	1.002124	-2.639644	1.824759
C	2.542485	2.824219	2.762438	C	-0.295554	-3.993565	0.123523
C	4.536213	1.325769	2.680108	C	1.204545	-0.764087	-2.725130
C	5.229409	-0.954890	1.911928	C	2.006554	0.961199	-1.382485
Sc	3.646687	-0.495061	-0.002561	C	2.621027	0.716538	1.051683
C	4.993957	1.911896	1.481590	C	1.688862	-1.402782	1.878407
C	5.639214	1.046956	0.525140	C	0.754761	0.475600	-3.261251
C	5.849673	-0.362386	0.742071	C	2.104813	1.529920	-0.115873
C	5.473249	1.274640	-0.878096	C	1.191846	1.535138	-2.415251
C	5.801106	-1.023667	-0.563754	C	-0.898802	-1.885679	-3.418044
C	5.540973	0.010658	-1.548309	C	-0.510210	0.552638	-3.877079
N	1.723340	-0.011414	0.023490	Sc	-1.932104	0.698913	-1.771941
N	-4.748630	0.082001	-0.179227	C	-1.329140	-0.620221	-3.949484
C	-4.124566	1.396483	-0.249825	C	-1.918546	-2.773555	-2.992796
H	-4.402977	2.034962	0.599865	C	-1.703821	-3.684897	-1.916032
H	-4.346117	1.923983	-1.203206	C	1.387838	2.716882	0.116869
C	-4.127725	-0.641336	-1.282450	C	0.543521	3.295257	-0.902038
H	-4.360013	-0.191986	-2.273097	C	0.802258	3.008843	1.394630
H	-4.401448	-1.705522	-1.286716	C	-0.532220	3.947830	-0.244540
C	-6.218663	0.030089	-0.064406	C	0.368301	2.670903	-2.169378
C	-6.633877	0.712749	1.242873	C	0.887137	2.043705	2.431865
C	-5.758676	0.746897	2.332111	C	-0.418766	3.732863	1.166162
H	-4.750853	0.345309	2.222952	C	-1.344851	1.720568	-3.772052
C	-6.167000	1.292801	3.547731	C	-2.703526	-0.197251	-3.939313
H	-5.469423	1.322022	4.385440	C	-2.739502	1.253302	-3.846892
C	-7.461547	1.791889	3.693408	C	-0.938756	2.760865	-2.839365
				C	-1.785788	4.014799	-0.849837

C	-3.296916	-2.349603	-2.926945	H	6.500049	-1.503692	2.328821
C	-2.891311	-3.774492	-1.134703	C	8.733989	-2.547052	-0.655731
C	-3.890700	-2.962400	-1.774908	C	8.857606	-3.211313	0.564967
C	-3.698478	-1.057208	-3.349210	H	8.146122	-3.335463	2.599703
C	1.692461	0.898703	2.241617	H	9.370539	-2.822757	-1.497170
C	-0.240702	1.929776	3.300781	H	9.587215	-4.013208	0.682815
C	-1.590539	3.534516	1.956160	C	6.926543	1.229473	0.467074
C	1.276796	-0.340386	2.736524	C	7.070609	1.641684	1.794606
C	-1.448852	2.694756	3.118675	C	7.729838	1.818207	-0.514029
C	-0.597593	0.685840	3.891705	C	7.968549	2.653878	2.128966
Sc	-2.449462	0.966954	1.606852	H	6.480576	1.158643	2.571076
C	0.135252	-0.485766	3.592622	C	8.629426	2.828725	-0.181122
C	-2.549156	1.948248	3.694228	C	8.747350	3.256391	1.141420
C	-2.035137	0.657805	4.074721	H	8.063025	2.968165	3.169015
C	-1.986559	3.432150	-2.141276	H	9.449123	4.049380	1.402076
C	-2.976791	3.867301	-0.079625	N	4.947394	-0.067834	1.130891
C	-3.361239	2.968445	-2.196224	C	4.113640	1.093527	1.386094
C	-2.906616	3.605680	1.320845	H	4.153429	1.377929	2.453114
C	-3.961657	3.235604	-0.921181	H	4.447376	1.959385	0.796273
C	-3.991575	2.841222	1.900670	H	4.514459	-2.022610	0.444219
C	-3.840426	2.026190	3.084166	H	4.145741	-1.725390	2.162131
C	-3.748268	1.849745	-2.998726	C	4.138071	-1.270748	1.152173
C	-0.553737	-1.710294	3.562805	H	5.354807	-1.984161	-1.617749
C	-2.755923	-0.574799	3.879269				
C	-1.985061	-1.762667	3.729807				
C	-0.156750	-2.759216	2.665802	bb8_up.xyz			
C	-2.459331	-2.848180	2.939030	125			
C	-1.357506	-3.450112	2.251309	C	1.388244	0.300070	-2.693947
C	-4.568953	0.792811	2.854848	C	2.075507	0.442357	-1.452535
C	-4.941910	2.184035	1.030867	C	0.483985	1.341854	-3.121421
C	-4.074464	-0.508836	3.244609	C	0.921277	-0.965494	-3.241028
C	-5.291600	0.927721	1.614384	Sc	-0.630777	-0.563545	-1.620926
C	-4.532044	-1.627742	2.497714	C	1.932759	1.641228	-0.755811
C	-3.710352	-2.787345	2.331580	C	2.629058	-0.785780	-0.780706
C	-4.930603	2.356527	-0.384809	C	0.266954	2.538191	-2.373571
C	-1.498892	-3.980961	0.929115	C	-0.548480	0.741612	-3.899154
C	-3.900827	-3.316400	1.022710	C	1.015730	-2.106010	-2.339750
C	-5.302054	-1.478463	1.286548	C	-0.347773	-0.681068	-3.935866
C	-2.819429	-3.884103	0.286622	C	1.080439	2.705228	-1.223032
C	-4.909934	-2.515097	0.381359	C	1.946176	1.689028	0.694302
C	-5.652321	-0.195477	0.808160	C	2.600329	-0.746789	0.838307
C	-4.884744	-2.289971	-1.019053	C	1.723849	-1.948496	-1.123638
C	-5.353763	-1.031838	-1.503462	C	0.611688	3.411913	-0.079068
C	-5.725270	0.009655	-0.596956	C	2.054918	0.525313	1.451136
C	-4.763690	-0.426931	-2.650843	C	1.087962	2.769034	1.100202
C	-5.362252	1.263218	-1.179762	C	-1.059209	3.131178	-2.418604
C	-4.764293	1.002491	-2.456726	C	-0.675789	3.984030	-0.090439
N	-1.631248	0.005405	0.057221	Sc	-2.048913	1.884488	0.402997
H	7.711071	-1.009361	-1.762252	C	-1.501917	3.843209	-1.251459
C	5.040369	1.395019	-1.804568	C	-2.068249	2.536470	-3.217946
C	5.080125	-1.003040	-2.006589	C	-1.823170	1.335362	-3.947390
C	4.402916	1.488850	-3.040577	C	1.354291	0.459664	2.663261
H	5.277328	2.306334	-1.254865	C	0.481943	1.529917	3.080440
C	4.442522	-0.911042	-3.241500	C	0.814959	-0.775547	3.161801
C	4.104051	0.336541	-3.765384	C	-0.566491	0.950361	3.841393
H	4.122204	2.469283	-3.428066	C	0.268328	2.675030	2.264105
H	4.195156	-1.821221	-3.789643	C	0.933943	-1.954823	2.380561
H	3.592247	0.408485	-4.725939	C	-0.406783	-0.472694	3.852104
H	7.647409	1.488236	-1.549305	C	-1.502601	4.041874	1.085153
H	9.242714	3.281578	-0.960862	C	-2.873562	3.859595	-0.820643
C	5.399045	0.149402	-1.275478	C	-2.900838	4.000809	0.626235
C	6.021448	0.040967	0.115070	C	-1.061237	3.304082	2.256956
C	6.967442	-1.159854	0.256463	C	-1.838752	1.516939	3.822602
C	7.115056	-1.809683	1.484554	C	-3.442023	2.495499	-2.776743
C	7.799398	-1.525031	-0.806216	C	-2.984267	0.511844	-3.900557
C	8.048274	-2.834205	1.636065	C	-4.000259	1.241473	-3.191452
				C	-3.852152	3.107043	-1.565777

C	2.914190	0.942555	3.836366	C	-7.364417	-1.382698	3.857665
C	1.402992	-4.037432	-0.543597	H	-5.364397	-0.834036	4.464049
C	2.794908	-3.724498	1.298707	H	-7.670726	-1.697675	4.855857
C	2.741080	-3.807520	-1.025276	N	-4.707587	-0.134348	-0.226033
C	3.074282	-2.932415	2.461060	C	-4.096853	-1.456275	-0.171697
C	3.595908	-3.622964	0.109138	H	-4.375105	-2.001401	0.741192
C	4.272450	-2.162853	2.438798	H	-4.341614	-2.074862	-1.062800
C	4.344302	-0.904322	3.110297	H	-4.331035	-0.112318	-2.337646
C	2.966673	-3.104641	-2.235827	H	-4.395653	1.508610	-1.545600
C	1.484443	3.090464	2.694089	C	-4.101997	0.458463	-1.411178
C	3.633326	1.871890	3.037451	H	-6.811024	0.868338	-2.589682
C	2.909914	3.003996	2.552476				
C	0.955821	3.748924	1.534932				
C	3.256287	3.636173	1.323991				
C	2.070332	4.056138	0.660456				
C	5.114779	0.007737	2.333063				
C	5.061104	-2.051742	1.243286				
C	4.770427	1.384746	2.260381				
C	5.593266	-0.709981	1.172424				
C	5.109884	2.058118	1.046183				
C	4.335221	3.153256	0.571014				
C	4.713371	-2.744075	0.064554				
C	1.935603	3.971084	-0.752056				
C	4.254199	3.097920	-0.846848				
C	5.626636	1.350540	-0.107238				
C	3.062148	3.479600	-1.540022				
C	5.082996	1.996930	-1.287488				
C	5.880101	-0.059898	-0.065676				
Sc	3.566030	0.056633	-0.701753				
C	4.764326	1.260124	-2.469517				
C	5.088574	-0.151699	-2.471623				
C	5.643760	-0.806784	-1.287340				
C	4.148353	-1.066869	-3.071260				
C	5.007747	-2.099918	-1.187611				
C	4.126048	-2.268652	-2.300513				
N	1.654377	-0.077710	-0.192853				
H	-8.580403	1.065165	-0.766667				
C	-6.978276	-2.210585	-1.163777				
C	-6.973265	-0.206019	-2.496706				
C	-7.373402	-2.951470	-2.276621				
H	-6.819216	-2.712541	-0.208803				
C	-7.368216	-0.944513	-3.611275				
C	-7.575569	-2.319633	-3.503550				
H	-7.522011	-4.027907	-2.182660				
H	-7.512782	-0.441265	-4.568054				
H	-7.888551	-2.897653	-4.373946				
H	-8.578879	-1.099297	0.689137				
H	-9.281213	-1.807278	2.956582				
C	-6.792456	-0.826241	-1.254954				
C	-6.176208	-0.053622	-0.091251				
C	-6.582785	1.422915	-0.041424				
C	-5.702012	2.378763	0.473074				
C	-7.879592	1.808860	-0.386262				
C	-6.097117	3.709210	0.596049				
H	-4.701152	2.074391	0.778938				
C	-8.278295	3.138556	-0.258186				
C	-7.385790	4.095292	0.225948				
H	-5.395523	4.445105	0.990091				
H	-9.292665	3.426137	-0.536797				
H	-7.696158	5.136279	0.322941				
C	-6.573011	-0.588196	1.288811				
C	-5.683210	-0.497681	2.362935				
C	-7.871914	-1.046930	1.517680				
C	-6.073140	-0.902443	3.638120				
H	-4.679123	-0.107137	2.197393				
C	-8.264965	-1.446675	2.793876				