

Cartesian coordinates all of the calculated structures

trans-butadiene

C	-2.586712	0.188456	0.000000
H	-2.097550	-0.783323	0.000000
H	-3.672523	0.186803	0.000000
C	-1.881388	1.328904	0.000000
H	-2.407329	2.284215	0.000000
C	-0.425034	1.394578	0.000000
H	0.100884	0.439254	0.000000
C	0.280318	2.535006	0.000000
H	-0.208802	3.506805	0.000000
H	1.366130	2.536615	0.000000

cis-butadiene

C	-2.693898	0.224298	0.113820
H	-2.314202	-0.737446	0.449915
H	-3.765830	0.297506	-0.045684
C	-1.884995	1.274093	-0.080933
H	-2.329738	2.228448	-0.365011
C	-0.423472	1.276546	0.080943
H	0.018063	2.232386	0.365034
C	0.388951	0.229476	-0.113825
H	0.012485	-0.733529	-0.449941
H	1.460631	0.306282	0.045681

styrene

C	-3.650711	1.198853	0.000220
C	-2.245143	1.222289	0.000589
C	-1.606947	2.476660	-0.000094
C	-2.347302	3.655299	-0.001158
C	-3.745330	3.613420	-0.001544
C	-4.394649	2.378417	-0.000831
H	-4.162925	0.239145	0.000775
H	-0.522108	2.530843	0.000228
H	-1.832600	4.612703	-0.001689
H	-4.320156	4.535564	-0.002371
H	-5.480501	2.331760	-0.001105
C	-1.512896	-0.055258	0.001714
H	-2.150928	-0.939388	0.002418
C	-0.186244	-0.238522	0.001969
H	0.524047	0.583954	0.001319
H	0.238031	-1.237878	0.002855

1Nd

Nd	-0.055608	-1.152804	0.042312
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C	-1.724946	-2.348387	1.804407
N	2.419947	-1.722235	0.395976
C	0.507200	-2.098913	2.483469
C	1.959628	-2.382592	2.749684
H	2.317718	-1.751184	3.573881
H	2.087214	-3.412770	3.110837
C	-0.444819	-3.019133	1.930361
C	-2.791387	-2.973760	1.110231
H	-3.759115	-2.483839	1.034718
C	2.907976	-2.184308	1.574014
C	-2.595321	-4.226226	0.549247
H	-3.409028	-4.718157	0.025704
C	0.192772	0.299343	3.476401
H	1.213091	0.417335	3.831751
C	-2.505420	0.024597	2.601736
H	-3.542472	-0.082302	2.293968
C	-1.583684	-1.030795	2.395487
C	-0.215455	-0.903464	2.842358
C	-0.284286	-4.308120	1.350725
H	0.658974	-4.840265	1.445737
C	3.276439	-1.533779	-0.637134
H	2.844558	-1.155949	-1.562060
C	-1.346572	-4.891260	0.680228
H	-1.229128	-5.882334	0.251666
C	4.271895	-2.470610	1.716806
H	4.637220	-2.841989	2.669341
C	5.141899	-2.274895	0.651003
H	6.200328	-2.492307	0.758530
C	-0.733773	1.304694	3.676276
H	-0.431340	2.215877	4.184031
C	4.634818	-1.792820	-0.559445
H	5.274265	-1.622646	-1.418492
C	-2.077595	1.172891	3.240556
H	-2.778022	1.981551	3.424986
C	-0.037826	1.269373	-0.267151
H	-0.746129	1.838368	0.347530
H	0.968821	1.661183	-0.049843
Si	-0.431318	1.375815	-2.096593
C	-0.472782	-0.455177	-2.812357
H	0.459495	-1.047277	-2.726840
H	-1.326114	-1.082220	-2.492294
H	-0.615034	-0.362296	-3.896047
C	0.887448	2.256385	-3.125182
H	0.941519	3.314716	-2.844700

H	1.886134	1.829091	-2.968391
H	0.668291	2.206217	-4.198419
C	-2.160669	2.056084	-2.432916
H	-2.429040	1.986987	-3.493617
H	-2.930419	1.523929	-1.859418
H	-2.215086	3.112292	-2.144424

2Nd_{BD}

Nd	0.484048	-0.886361	-0.192920
C	-1.656029	-1.976744	1.321650
N	2.881750	-1.436659	0.629600
C	0.551490	-2.282862	2.056649
C	1.889511	-2.901372	2.359063
H	2.059746	-2.963196	3.442847
H	1.898102	-3.943708	2.009834
C	-0.545399	-2.905772	1.366632
C	-2.849544	-2.323503	0.645323
H	-3.696666	-1.642231	0.649407
C	3.083994	-2.196669	1.734587
C	-2.943309	-3.556123	0.018085
H	-3.866102	-3.844000	-0.476357
C	0.670877	-0.053515	3.410739
H	1.676552	-0.203450	3.794732
C	-1.984179	0.356271	2.469701
H	-3.005243	0.510719	2.131655
C	-1.279233	-0.810989	2.103567
C	0.060879	-1.032643	2.587432
C	-0.664302	-4.146275	0.685053
H	0.143975	-4.873254	0.716697
C	3.943551	-0.825333	0.056697
H	3.733218	-0.215275	-0.818473
C	-1.853133	-4.460458	0.042654
H	-1.959384	-5.430556	-0.435418
C	4.366775	-2.348778	2.273716
H	4.499736	-2.956846	3.162977
C	5.453076	-1.720380	1.673949
H	6.450402	-1.832340	2.088744
C	-0.048900	1.076688	3.759770
H	0.403361	1.817381	4.413004
C	5.239779	-0.937657	0.536759
H	6.053361	-0.421113	0.039465
C	-1.369597	1.284500	3.293131
H	-1.907603	2.177009	3.597343
C	0.500140	1.559945	-0.133816

C	-1.217736	-1.491409	-2.788234
H	-1.037275	-0.460743	-3.089111
H	-2.251257	-1.767195	-2.605044
C	-0.239821	-2.420674	-2.717071
C	1.203106	-2.194145	-2.929677
H	0.349210	1.835061	0.923071
H	-0.521149	-3.440232	-2.463575
C	1.805506	-1.012756	-3.182500
H	1.259931	-0.079316	-3.313885
H	1.552338	1.828365	-0.362098
Si	-0.613661	2.677197	-1.167928
C	-2.419539	2.083295	-1.069361
H	-2.551133	1.061764	-1.454264
H	-2.782095	2.093419	-0.034415
H	-3.083334	2.732246	-1.653445
C	-0.077202	2.636778	-2.996856
H	0.986614	2.881389	-3.111749
H	-0.250879	1.665535	-3.481801
H	-0.640313	3.375503	-3.579927
C	-0.548199	4.478433	-0.582581
H	-1.204579	5.120927	-1.182787
H	-0.865184	4.565875	0.463657
H	0.468111	4.884469	-0.652500
H	1.825637	-3.085080	-2.864605
H	2.878824	-0.964175	-3.339333

TS23Nd_{BD}

Nd	0.390084	-1.064397	-0.148985
C	-1.332586	-2.785780	1.285200
N	2.871581	-1.472794	0.567461
C	0.663850	-2.082174	2.307158
C	2.070567	-2.084631	2.840768
H	2.180197	-1.285718	3.587381
H	2.271460	-3.013208	3.393330
C	0.021445	-3.170415	1.620954
C	-2.172794	-3.681644	0.580192
H	-3.204903	-3.413240	0.368936
C	3.182243	-1.905081	1.815002
C	-1.676348	-4.914246	0.194767
H	-2.317771	-5.616956	-0.328167
C	-0.287239	0.201802	3.156491
H	0.613027	0.524833	3.673254
C	-2.694493	-0.620702	1.873785
H	-3.623088	-0.938141	1.406300

C	-1.556215	-1.463607	1.842337
C	-0.334274	-1.066443	2.513607
C	0.508583	-4.430752	1.182747
H	1.521833	-4.742695	1.422464
C	3.876143	-1.279197	-0.319788
H	3.584764	-0.938659	-1.310516
C	-0.338563	-5.281338	0.493074
H	0.021708	-6.258954	0.185593
C	4.512235	-2.158718	2.175119
H	4.730768	-2.512234	3.178058
C	5.535113	-1.953890	1.256865
H	6.567886	-2.146462	1.531659
C	-1.420520	0.996088	3.173630
H	-1.395146	1.948089	3.696227
C	5.212162	-1.499307	-0.024466
H	5.973720	-1.325925	-0.776799
C	-2.622244	0.590447	2.537949
H	-3.495017	1.234029	2.587140
C	0.161238	1.409215	-0.740971
C	-1.101973	0.138466	-2.384957
H	-0.341029	0.526188	-3.052478
H	-1.940892	0.797805	-2.206230
C	-1.290676	-1.237743	-2.244708
C	-0.319897	-2.243897	-2.618019
H	0.037650	1.407694	0.364314
H	-2.253163	-1.591902	-1.882608
C	1.013084	-2.043181	-2.850837
H	1.426955	-1.043530	-3.002977
H	1.247819	1.322155	-0.959274
Si	-0.381374	3.156330	-1.268355
C	-2.216723	3.393994	-0.868906
H	-2.876179	2.775887	-1.489656
H	-2.429888	3.156283	0.180452
H	-2.508479	4.438260	-1.033558
C	-0.051278	3.421106	-3.115246
H	0.989478	3.193357	-3.378657
H	-0.701730	2.820927	-3.761561
H	-0.224153	4.472217	-3.376262
C	0.636685	4.411022	-0.279193
H	0.356529	5.437190	-0.548197
H	0.479630	4.301111	0.800627
H	1.711117	4.304277	-0.472026
H	-0.673009	-3.274148	-2.581401
H	1.664710	-2.871482	-3.107183

3Nd_{BD}

Nd	0.056056	-1.006203	0.351078
C	-1.382235	-3.170449	1.607024
N	2.635687	-1.044267	0.790747
C	0.851343	-2.785793	2.227070
C	2.339935	-2.932168	2.380863
H	2.618895	-2.972937	3.443153
H	2.651859	-3.901393	1.969113
C	-0.029934	-3.671026	1.513684
C	-2.450750	-3.865562	0.985924
H	-3.471302	-3.504807	1.083661
C	3.195300	-1.863782	1.713448
C	-2.178980	-5.023416	0.287245
H	-2.987798	-5.578115	-0.178367
C	0.383962	-0.580798	3.519742
H	1.404373	-0.414704	3.855128
C	-2.315671	-0.983904	2.694622
H	-3.349608	-1.132361	2.393525
C	-1.345642	-1.979582	2.428040
C	0.033272	-1.788133	2.851630
C	0.212884	-4.860782	0.773488
H	1.217716	-5.266959	0.695816
C	3.425922	-0.143264	0.163164
H	2.943336	0.484508	-0.583133
C	-0.848146	-5.516056	0.184468
H	-0.669733	-6.437636	-0.362131
C	4.556012	-1.762534	2.032182
H	4.975044	-2.425875	2.782556
C	5.357032	-0.829754	1.384135
H	6.413605	-0.751519	1.622170
C	-0.589007	0.382598	3.746853
H	-0.322100	1.299609	4.264352
C	4.780497	0.000821	0.419795
H	5.363403	0.740615	-0.117829
C	-1.934887	0.188337	3.334314
H	-2.673285	0.955877	3.543687
C	-0.447068	1.457019	-1.325388
C	-1.108565	0.484063	-2.347888
H	-0.422099	0.380110	-3.199143
H	-2.001414	0.984596	-2.738794
C	-1.547486	-0.906886	-1.880557
C	-0.756610	-2.048275	-1.992611
H	-1.023078	1.509896	-0.381298

H	-2.621964	-1.057865	-1.796800
C	0.657819	-2.070977	-1.968368
H	1.205612	-1.217466	-2.383464
H	0.597502	1.166658	-1.086899
Si	-0.289806	3.293044	-1.920709
C	-2.023693	3.967121	-2.238491
H	-2.538546	3.429060	-3.042707
H	-2.653212	3.914117	-1.342022
H	-1.971533	5.021018	-2.537301
C	0.763071	3.326832	-3.487760
H	1.763141	2.908196	-3.319520
H	0.298733	2.765245	-4.306365
H	0.897554	4.357713	-3.836699
C	0.554221	4.244225	-0.520758
H	0.676742	5.300676	-0.787931
H	-0.032599	4.212233	0.405722
H	1.554756	3.851137	-0.299401
H	-1.261328	-3.002680	-1.830156
H	1.169819	-3.022408	-2.077044

2Nd_{st}

Nd	0.434068	-1.018737	-0.207696
C	-1.743751	-1.979864	1.364262
N	2.814379	-1.525866	0.699373
C	0.456208	-2.309912	2.110869
C	1.780596	-2.945169	2.437247
H	1.930980	-3.020102	3.523234
H	1.786818	-3.982971	2.074411
C	-0.660104	-2.936535	1.457513
C	-2.953830	-2.332044	0.720717
H	-3.780981	-1.627335	0.690761
C	2.987517	-2.240191	1.839619
C	-3.088099	-3.595466	0.168607
H	-4.022893	-3.885539	-0.301435
C	0.644704	-0.014996	3.342838
H	1.646932	-0.172985	3.732352
C	-2.000888	0.419573	2.387110
H	-3.018674	0.584624	2.044202
C	-1.329935	-0.784478	2.079390
C	0.004829	-1.019136	2.573295
C	-0.821566	-4.212314	0.853484
H	-0.034968	-4.959932	0.925756
C	3.884392	-0.913085	0.145994
H	3.698050	-0.347417	-0.762801

C	-2.023247	-4.528369	0.238337
H	-2.162333	-5.521581	-0.180269
C	4.248851	-2.342802	2.436175
H	4.357827	-2.913821	3.352770
C	5.345113	-1.710107	1.858027
H	6.326025	-1.780980	2.318652
C	-0.042011	1.151259	3.634160
H	0.433065	1.911939	4.247032
C	5.161930	-0.976906	0.684170
H	5.983687	-0.458691	0.202171
C	-1.358395	1.371330	3.160429
H	-1.870557	2.292860	3.419403
C	0.525064	1.428800	-0.274020
C	-1.316073	-1.670582	-2.714788
H	-1.118618	-0.661644	-3.072340
H	-2.349733	-1.905267	-2.482557
C	-0.368224	-2.629266	-2.637319
C	1.075805	-2.479904	-2.905475
H	0.415501	1.740969	0.777932
H	-0.677530	-3.622087	-2.314370
C	1.922909	-3.587238	-2.688819
C	3.290694	-3.503640	-2.946793
C	3.843068	-2.309060	-3.416336
C	3.020851	-1.196294	-3.626004
C	1.650792	-1.275356	-3.373434
H	1.493510	-4.524139	-2.342896
H	3.922045	-4.373667	-2.793765
H	4.905554	-2.248275	-3.632202
H	3.440631	-0.272400	-4.013242
H	1.025507	-0.415539	-3.598341
H	1.575152	1.662930	-0.543416
Si	-0.584797	2.548559	-1.308630
C	-2.401833	1.994840	-1.184479
H	-2.556085	0.969912	-1.550613
H	-2.757132	2.030604	-0.147638
H	-3.055889	2.647381	-1.775613
C	-0.072329	2.472162	-3.142470
H	0.991491	2.707754	-3.273949
H	-0.255362	1.490728	-3.602162
H	-0.639172	3.201604	-3.733516
C	-0.481728	4.357274	-0.749865
H	-1.134514	5.002917	-1.350691
H	-0.784346	4.464574	0.298852
H	0.540331	4.745382	-0.837273

TS23Nd_{st}

Nd	0.682297	-1.162920	-0.149815
C	-1.484467	-2.296336	1.307906
N	3.070761	-1.601166	0.819203
C	0.672689	-2.337444	2.241945
C	2.021995	-2.808677	2.714570
H	2.124067	-2.662584	3.798725
H	2.098798	-3.895396	2.568362
C	-0.309619	-3.113812	1.534037
C	-2.602492	-2.825813	0.619403
H	-3.500858	-2.226693	0.494057
C	3.228854	-2.174456	2.038894
C	-2.549927	-4.120596	0.135519
H	-3.408030	-4.543420	-0.377690
C	0.550882	0.066931	3.251315
H	1.535250	0.051769	3.712291
C	-2.063167	0.128448	2.121774
H	-3.068944	0.151614	1.710382
C	-1.251683	-1.018598	1.955313
C	0.063468	-1.072857	2.555756
C	-0.276800	-4.427109	0.988449
H	0.589624	-5.065796	1.140779
C	4.158686	-1.093009	0.195353
H	3.989472	-0.666290	-0.789884
C	-1.386365	-4.911815	0.316740
H	-1.374875	-5.928909	-0.065165
C	4.486575	-2.218677	2.652607
H	4.582789	-2.675575	3.632578
C	5.596227	-1.683644	2.007022
H	6.573991	-1.713817	2.478590
C	-0.266733	1.175733	3.389375
H	0.090933	2.035743	3.948373
C	5.432227	-1.109717	0.744416
H	6.267504	-0.683739	0.199443
C	-1.571715	1.208041	2.834773
H	-2.192290	2.086241	2.984071
C	-0.096126	1.141203	-0.966036
C	-0.864690	-0.378336	-2.474221
H	-0.386405	0.273823	-3.194004
H	-1.908605	-0.149802	-2.293308
C	-0.464500	-1.723959	-2.376002
C	0.863029	-2.201845	-2.769985
H	-0.299298	1.150164	0.126795

H	-1.199304	-2.469398	-2.073570
C	1.194854	-3.576801	-2.656011
C	2.476840	-4.037517	-2.947062
C	3.485398	-3.147314	-3.336831
C	3.193019	-1.786669	-3.425588
C	1.909873	-1.310524	-3.128141
H	0.417622	-4.282626	-2.374106
H	2.688509	-5.101049	-2.880999
H	4.478838	-3.513886	-3.575477
H	3.958485	-1.085073	-3.747122
H	1.699064	-0.252789	-3.265920
H	0.989006	1.319876	-1.118235
Si	-0.989168	2.712391	-1.582629
C	-2.856313	2.523573	-1.336056
H	-3.293745	1.746217	-1.973404
H	-3.101445	2.281849	-0.294755
H	-3.366797	3.463022	-1.580526
C	-0.588329	3.028534	-3.407380
H	0.493079	3.036866	-3.593793
H	-1.042080	2.294883	-4.083500
H	-0.970726	4.013010	-3.703584
C	-0.361611	4.171475	-0.551835
H	-0.852067	5.104232	-0.857033
H	-0.562668	4.027658	0.516525
H	0.719213	4.316645	-0.670146

3Nd_{st}

Nd	0.768662	-1.139766	0.055349
C	-1.491269	-1.841096	1.652480
N	3.028571	-2.248643	0.721093
C	0.665114	-2.505449	2.313248
C	1.875111	-3.349991	2.609765
H	2.087661	-3.361901	3.687438
H	1.659146	-4.395962	2.350782
C	-0.559860	-2.946217	1.692585
C	-2.773529	-2.008707	1.080041
H	-3.487885	-1.189471	1.086269
C	3.144792	-2.950569	1.876701
C	-3.120101	-3.236152	0.544198
H	-4.108336	-3.382303	0.119393
C	1.314023	-0.218647	3.387405
H	2.301439	-0.522076	3.725750
C	-1.287713	0.607031	2.575809
H	-2.288014	0.922975	2.290599

C	-0.855660	-0.715746	2.313994
C	0.449931	-1.155571	2.758269
C	-0.935832	-4.182172	1.101672
H	-0.259527	-5.032912	1.122968
C	4.152517	-1.946042	0.030977
H	4.010636	-1.415004	-0.905582
C	-2.200044	-4.313637	0.553124
H	-2.500808	-5.268636	0.131678
C	4.399245	-3.332102	2.363901
H	4.461488	-3.886068	3.295376
C	5.550265	-3.003923	1.654055
H	6.527693	-3.295402	2.026878
C	0.865789	1.073201	3.614143
H	1.514081	1.781754	4.121627
C	5.425978	-2.297984	0.456419
H	6.292358	-2.024715	-0.136012
C	-0.432940	1.485420	3.220104
H	-0.759484	2.497617	3.437688
C	-0.872879	0.962674	-1.398447
C	-1.238475	-0.249691	-2.310556
H	-1.024951	0.037346	-3.350778
H	-2.324570	-0.375446	-2.248943
C	-0.594964	-1.607305	-1.991337
H	-1.176978	0.786835	-0.349864
H	-1.298724	-2.437028	-1.922062
H	0.210483	1.195224	-1.411073
Si	-1.715765	2.632846	-1.883927
C	-3.590311	2.412863	-1.798156
H	-3.949311	1.652286	-2.501101
H	-3.922535	2.124669	-0.793254
H	-4.097072	3.352197	-2.050259
C	-1.166151	3.101340	-3.629501
H	-0.076424	3.206106	-3.700376
H	-1.481442	2.361795	-4.374517
H	-1.603515	4.063486	-3.922385
C	-1.138315	3.929164	-0.633790
H	-1.603697	4.901174	-0.836682
H	-1.402182	3.649535	0.393564
H	-0.051802	4.077488	-0.671659
C	0.687345	-1.956048	-2.569545
C	1.149886	-3.308140	-2.577781
C	1.648479	-0.964694	-2.936520
C	2.427479	-3.641347	-3.009571
H	0.453749	-4.095779	-2.297616

C	2.932652	-1.318067	-3.386007
H	1.338539	0.073966	-3.028797
C	3.333327	-2.649784	-3.423546
H	2.720290	-4.687403	-3.044528
H	3.606861	-0.535856	-3.726914
H	4.320798	-2.922093	-3.782682

4Nd_{BD-BD}

Nd	0.746267	-0.703033	-0.903285
C	-1.940493	-1.347404	-1.770694
N	1.416370	-2.487956	0.946129
C	-1.298723	-1.717615	0.459335
C	-0.926361	-2.425764	1.732978
H	-1.004507	-1.721867	2.573341
H	-1.641523	-3.228415	1.963874
C	-1.462507	-2.337671	-0.830768
C	-2.215527	-1.712203	-3.107984
H	-2.631922	-0.983550	-3.799147
C	0.471521	-3.016642	1.762617
C	-1.987934	-3.016117	-3.518403
H	-2.222164	-3.312507	-4.536453
C	-2.031727	0.644892	1.310414
H	-1.814007	0.467481	2.360537
C	-2.686291	1.137528	-1.416515
H	-2.964302	1.322162	-2.451018
C	-2.142940	-0.113402	-1.034989
C	-1.812161	-0.375414	0.346138
C	-1.193277	-3.653724	-1.295251
H	-0.834563	-4.416838	-0.609221
C	2.671045	-2.987221	1.007126
H	3.397999	-2.533235	0.340536
C	-1.468359	-3.977343	-2.615277
H	-1.306012	-4.994627	-2.960403
C	0.779864	-4.064380	2.639318
H	-0.001132	-4.472218	3.273309
C	2.074204	-4.569488	2.692667
H	2.320831	-5.381420	3.370372
C	-2.573369	1.850464	0.909195
H	-2.770684	2.620422	1.649762
C	3.047685	-4.016887	1.857611
H	4.070765	-4.377157	1.858851
C	-2.897405	2.102917	-0.451310
H	-3.333731	3.058434	-0.725939
C	1.278949	-0.123289	-3.991545

H	2.141689	0.530759	-3.951432
H	0.396963	0.273474	-4.484161
C	1.323761	-1.425275	-3.602038
C	2.450936	-2.071236	-2.919808
H	0.465216	-2.060095	-3.812191
C	3.528344	-1.442745	-2.388831
H	3.703320	-0.377174	-2.514890
C	3.444260	0.658023	2.092263
C	2.914478	0.949301	0.675391
H	3.145821	0.059732	0.026300
H	3.507900	1.743283	0.195883
C	1.409870	1.955601	-1.773214
H	3.130399	1.482100	2.748992
H	2.954859	-0.240825	2.494005
Si	5.341660	0.493387	2.292862
C	6.013015	-0.877845	1.161523
H	5.590580	-1.857911	1.416367
H	5.806841	-0.680053	0.101670
H	7.101664	-0.960708	1.264230
C	5.693618	0.051676	4.096804
H	5.314100	0.820735	4.780181
H	5.230050	-0.901004	4.381044
H	6.771304	-0.041352	4.276852
C	6.160521	2.137444	1.840656
H	7.245987	2.084571	1.987754
H	5.989762	2.416792	0.793722
H	5.786221	2.956685	2.466292
H	0.892651	2.472340	-2.574398
C	0.886019	1.985848	-0.480838
C	1.451472	1.339300	0.632857
H	2.376185	-3.152470	-2.809038
H	4.323872	-2.004397	-1.909346
H	-0.128296	2.367229	-0.360608
H	2.476726	1.799899	-1.927592
H	0.936279	1.424226	1.586124

TS45Nd_{BD-BD}

Nd	0.771494	-0.835263	-0.915452
C	-1.966292	-1.407249	-1.718481
N	1.455792	-2.660378	0.873818
C	-1.257347	-1.837165	0.480883
C	-0.863653	-2.578796	1.728706
H	-0.921576	-1.896487	2.588524
H	-1.580322	-3.381748	1.953625

C	-1.473800	-2.424508	-0.817453
C	-2.289051	-1.735971	-3.054837
H	-2.715167	-0.985346	-3.715942
C	0.529626	-3.181421	1.717017
C	-2.084054	-3.029040	-3.504828
H	-2.345540	-3.296438	-4.524125
C	-1.861617	0.538507	1.392821
H	-1.605719	0.338900	2.430584
C	-2.626469	1.089531	-1.292852
H	-2.947717	1.297312	-2.310468
C	-2.115788	-0.185296	-0.952173
C	-1.736132	-0.480289	0.410563
C	-1.235087	-3.732079	-1.321912
H	-0.863904	-4.516283	-0.667006
C	2.706576	-3.176303	0.894670
H	3.412829	-2.735923	0.198890
C	-1.547485	-4.017296	-2.641690
H	-1.401421	-5.025782	-3.018293
C	0.851157	-4.234938	2.581402
H	0.083402	-4.636927	3.235043
C	2.140667	-4.754709	2.595913
H	2.397219	-5.572368	3.262995
C	-2.367040	1.773537	1.029880
H	-2.494017	2.542284	1.786984
C	3.094932	-4.211153	1.733534
H	4.112708	-4.584631	1.701371
C	-2.747868	2.054067	-0.308811
H	-3.159494	3.028876	-0.552378
C	1.357900	0.332936	-3.649321
H	2.343228	0.671439	-3.956951
H	0.546240	0.847591	-4.154288
C	1.181178	-1.073839	-3.486801
C	2.226367	-1.944615	-3.031194
H	0.264299	-1.524030	-3.857071
C	3.355380	-1.543794	-2.360863
H	3.672760	-0.503941	-2.349530
C	3.380629	0.882619	2.047858
C	2.953286	1.016024	0.573791
H	3.162492	0.050650	0.049153
H	3.610486	1.721450	0.043224
C	1.611028	1.784969	-2.102605
H	3.080846	1.796932	2.579722
H	2.819543	0.064736	2.523430
Si	5.252270	0.629958	2.375434

C	5.858901	-0.925582	1.473344
H	5.347207	-1.825568	1.836082
H	5.709241	-0.862189	0.387608
H	6.932657	-1.073479	1.639846
C	5.483414	0.423645	4.239504
H	5.132085	1.305217	4.788901
H	4.935671	-0.445838	4.623086
H	6.541121	0.282142	4.491668
C	6.200841	2.141826	1.748802
H	7.271978	2.042169	1.961762
H	6.100033	2.280704	0.665268
H	5.856531	3.062606	2.234885
H	1.245390	2.508805	-2.824223
C	0.981445	1.895834	-0.805824
C	1.520915	1.467955	0.389066
H	2.031946	-3.014844	-3.112034
H	4.094216	-2.270160	-2.038460
H	-0.039658	2.277377	-0.778987
H	2.699188	1.741860	-2.077991
H	0.928330	1.611834	1.289782

5Nd_{BD-BD}

Nd	0.674545	-1.453768	-1.027853
C	-2.131486	-1.167226	-1.585577
N	1.344101	-3.409044	0.576842
C	-1.384959	-2.710686	0.024322
C	-1.051182	-4.002675	0.721746
H	-1.714068	-4.161774	1.583232
H	-1.258626	-4.843985	0.045290
C	-1.813549	-2.557856	-1.343469
C	-2.558599	-0.745888	-2.865038
H	-2.843405	0.289654	-3.033216
C	0.386686	-4.143680	1.194713
C	-2.641659	-1.670916	-3.893078
H	-2.985648	-1.360652	-4.874767
C	-1.292394	-0.994569	1.985650
H	-0.972896	-1.703157	2.745748
C	-2.196402	0.881293	0.046523
H	-2.563260	1.599497	-0.682682
C	-1.977595	-0.462356	-0.324060
C	-1.553079	-1.429811	0.661442
C	-1.860941	-3.469459	-2.431730
H	-1.626530	-4.520800	-2.283145
C	2.634303	-3.582549	0.947286

H	3.366675	-2.995657	0.401309
C	-2.284838	-3.022366	-3.674957
H	-2.357858	-3.728784	-4.496946
C	0.716119	-5.045753	2.213364
H	-0.072972	-5.616506	2.692883
C	2.043309	-5.206661	2.596376
H	2.307345	-5.905690	3.384412
C	-1.515472	0.334525	2.319696
H	-1.353867	0.661658	3.343012
C	3.028820	-4.459407	1.947278
H	4.078053	-4.555811	2.204379
C	-1.971926	1.268845	1.360129
H	-2.159587	2.295136	1.660862
C	1.704396	0.578242	-3.691559
H	2.431087	0.691186	-4.510006
H	0.831249	1.171856	-3.991384
C	1.265844	-0.889415	-3.649460
C	2.046553	-1.999278	-3.294512
H	0.483063	-1.102175	-4.375505
C	3.010151	-2.110593	-2.276876
H	3.620901	-1.252284	-1.994829
C	3.502497	2.051511	1.547412
C	2.994793	0.863298	0.690674
H	2.872726	-0.010438	1.350490
H	3.746970	0.597398	-0.059776
C	2.330645	1.271452	-2.451754
H	3.621833	2.931047	0.900158
H	2.731156	2.321325	2.282939
Si	5.146517	1.748681	2.487945
C	4.924448	0.266816	3.649919
H	4.117813	0.439095	4.373009
H	4.694450	-0.658859	3.106647
H	5.841444	0.084150	4.222964
C	5.537806	3.307666	3.479786
H	5.659057	4.180365	2.827002
H	4.744359	3.539655	4.200332
H	6.470027	3.189591	4.045135
C	6.526225	1.393737	1.240410
H	7.486877	1.259107	1.751978
H	6.340865	0.482003	0.658662
H	6.649135	2.221637	0.531588
H	2.583147	2.296191	-2.762823
C	1.401138	1.386741	-1.268511
C	1.671145	1.196027	0.045691

H	1.668024	-2.953686	-3.675002
H	3.495712	-3.072282	-2.134646
H	0.391190	1.727909	-1.514466
H	3.280341	0.807376	-2.173222
H	0.856884	1.395654	0.746609

4Nd_{BD-st}

Nd	0.628436	-0.591646	-0.633699
C	-2.050236	-1.263448	-1.515903
N	1.392407	-2.456649	1.078682
C	-1.362308	-1.781707	0.670949
C	-0.943072	-2.568893	1.882494
H	-1.050645	-1.939078	2.776574
H	-1.614816	-3.422945	2.050702
C	-1.530350	-2.307530	-0.659242
C	-2.340286	-1.536179	-2.872020
H	-2.786634	-0.769808	-3.500933
C	0.483503	-3.088489	1.861520
C	-2.092669	-2.801206	-3.380089
H	-2.339628	-3.028184	-4.412850
C	-2.159269	0.483020	1.709500
H	-1.921248	0.232689	2.739988
C	-2.859682	1.165082	-0.964943
H	-3.154741	1.420609	-1.979460
C	-2.273040	-0.094363	-0.687157
C	-1.916373	-0.451209	0.666418
C	-1.244069	-3.580494	-1.222720
H	-0.856977	-4.383062	-0.599985
C	2.670193	-2.894924	1.089586
H	3.367534	-2.366944	0.445173
C	-1.538551	-3.814033	-2.557059
H	-1.367263	-4.801761	-2.976441
C	0.853595	-4.177198	2.660283
H	0.101833	-4.667554	3.270845
C	2.172873	-4.617290	2.667980
H	2.468257	-5.459209	3.287184
C	-2.746249	1.696033	1.408656
H	-2.960913	2.398687	2.208919
C	3.106651	-3.961249	1.863788
H	4.146143	-4.268772	1.830110
C	-3.091782	2.043955	0.074392
H	-3.560730	3.003502	-0.120869
C	0.985956	0.253656	-3.655800
H	1.777237	0.992284	-3.608563

H	0.024097	0.604310	-4.016688
C	1.184292	-1.064105	-3.410211
H	0.357863	-1.749966	-3.596341
C	3.398396	0.613002	2.510126
C	2.818030	0.937096	1.120212
H	3.078199	0.097262	0.426038
H	3.350187	1.793095	0.678310
C	1.183007	2.118529	-1.169853
H	3.074672	1.405429	3.200555
H	2.945969	-0.312726	2.894588
Si	5.302491	0.503312	2.668237
C	5.969097	-0.989042	1.699839
H	5.581706	-1.933069	2.102588
H	5.709985	-0.943892	0.634336
H	7.063049	-1.032928	1.765200
C	5.715001	0.294720	4.501443
H	5.363746	1.149850	5.091232
H	5.254533	-0.607877	4.921414
H	6.797646	0.213829	4.655888
C	6.084202	2.089646	1.992885
H	7.170789	2.081311	2.141499
H	5.904769	2.217904	0.918330
H	5.692617	2.978931	2.501371
H	0.627453	2.709854	-1.890167
C	0.714405	2.006987	0.140619
C	1.328730	1.247414	1.150383
H	-0.302412	2.348733	0.335074
H	2.247226	2.005671	-1.378973
H	0.849183	1.223409	2.125617
C	2.435156	-1.694363	-2.944660
C	2.495815	-3.102702	-2.850992
C	3.589406	-0.952123	-2.603537
C	3.670996	-3.744849	-2.465811
H	1.618650	-3.687757	-3.114341
C	4.763275	-1.600847	-2.216926
H	3.589270	0.130241	-2.696073
C	4.809484	-2.996651	-2.150559
H	3.702948	-4.829603	-2.425368
H	5.648955	-1.015390	-1.988541
H	5.730266	-3.497026	-1.865863

TS45Nd_{BD-st}

Nd	0.695058	-0.748236	-0.605093
C	-2.039167	-1.335816	-1.453664

N	1.462149	-2.654254	1.019810
C	-1.290065	-1.942507	0.690800
C	-0.860736	-2.782147	1.863577
H	-0.979574	-2.201005	2.788824
H	-1.524261	-3.650117	1.987150
C	-1.521172	-2.419300	-0.650102
C	-2.381970	-1.552808	-2.807411
H	-2.818511	-0.751042	-3.397743
C	0.570731	-3.289652	1.820532
C	-2.187422	-2.805313	-3.363437
H	-2.466447	-2.989214	-4.396464
C	-1.921398	0.334149	1.813800
H	-1.644011	0.051177	2.826335
C	-2.740708	1.100030	-0.802554
H	-3.083441	1.387920	-1.793274
C	-2.193812	-0.186975	-0.583174
C	-1.790746	-0.593157	0.744622
C	-1.299720	-3.683165	-1.260457
H	-0.914701	-4.516175	-0.677744
C	2.741341	-3.093242	0.996866
H	3.418142	-2.575542	0.323422
C	-1.642307	-3.861935	-2.590610
H	-1.512312	-4.838798	-3.048245
C	0.961098	-4.376582	2.611334
H	0.223211	-4.870953	3.235533
C	2.281575	-4.812800	2.590668
H	2.592082	-5.654530	3.202693
C	-2.460937	1.583236	1.567592
H	-2.593150	2.279655	2.390884
C	3.195618	-4.157047	1.763845
H	4.233364	-4.466197	1.703004
C	-2.870262	1.970511	0.264090
H	-3.309389	2.952082	0.113335
C	1.152726	0.628532	-3.215763
H	2.051607	1.073572	-3.636529
H	0.245399	1.063383	-3.627112
C	1.122384	-0.801035	-3.104596
H	0.238924	-1.318084	-3.473417
C	3.297935	0.939626	2.436997
C	2.853837	1.115049	0.972408
H	3.103644	0.186866	0.405151
H	3.469341	1.878394	0.473233
C	1.421239	1.938559	-1.659651
H	2.974316	1.825491	3.002268

H	2.761874	0.090221	2.885966
Si	5.175161	0.728661	2.754695
C	5.805682	-0.831003	1.876775
H	5.311292	-1.732966	2.258158
H	5.645472	-0.790866	0.791625
H	6.882966	-0.956478	2.039202
C	5.421181	0.557308	4.620501
H	5.061820	1.443718	5.156785
H	4.886962	-0.312266	5.022441
H	6.482178	0.433496	4.868132
C	6.095431	2.246429	2.099322
H	7.167347	2.173556	2.319404
H	5.997049	2.359471	1.012569
H	5.730359	3.170616	2.563374
H	1.033563	2.724484	-2.302605
C	0.817035	1.962414	-0.335392
C	1.395448	1.505747	0.827036
H	-0.217516	2.300954	-0.270575
H	2.511514	1.943912	-1.642389
H	0.816049	1.585031	1.743793
C	2.311248	-1.606411	-2.850784
C	2.261684	-3.022936	-2.964786
C	3.527697	-1.036589	-2.389253
C	3.375215	-3.807356	-2.694447
H	1.341218	-3.487299	-3.308662
C	4.647234	-1.838204	-2.124452
H	3.634419	0.043137	-2.336991
C	4.579448	-3.221214	-2.273672
H	3.314702	-4.884172	-2.826099
H	5.578663	-1.367690	-1.820990
H	5.451937	-3.838498	-2.082324

5Nd_{BD-St}

Nd	0.738126	-1.280971	-0.645659
C	-2.090087	-1.142996	-1.254920
N	1.520754	-3.353826	0.724190
C	-1.260983	-2.781060	0.215797
C	-0.837455	-4.104785	0.796243
H	-1.490357	-4.390420	1.632510
H	-0.981474	-4.890729	0.041528
C	-1.720064	-2.535015	-1.129332
C	-2.570919	-0.637407	-2.485247
H	-2.882634	0.400761	-2.566087
C	0.605710	-4.193662	1.269649

C	-2.669545	-1.485481	-3.572751
H	-3.051641	-1.113752	-4.518337
C	-1.199540	-1.223233	2.308733
H	-0.836238	-1.974499	3.005529
C	-2.218292	0.761493	0.540062
H	-2.627594	1.517902	-0.124919
C	-1.940033	-0.536691	0.055221
C	-1.469838	-1.566741	0.956795
C	-1.814971	-3.373148	-2.273134
H	-1.558671	-4.427641	-2.207332
C	2.818584	-3.486615	1.079802
H	3.522075	-2.818834	0.588679
C	-2.291372	-2.847743	-3.461354
H	-2.392500	-3.495777	-4.327401
C	0.987556	-5.156000	2.211548
H	0.233537	-5.809562	2.639029
C	2.322978	-5.273250	2.584697
H	2.626140	-6.018462	3.314144
C	-1.475320	0.062497	2.750694
H	-1.310313	0.313768	3.794713
C	3.264786	-4.422932	2.002190
H	4.318188	-4.482300	2.253381
C	-1.994524	1.050075	1.876863
H	-2.226194	2.037427	2.264503
C	1.662382	0.907443	-3.347514
H	2.412777	0.982454	-4.150083
H	0.763733	1.402116	-3.736241
C	1.292800	-0.550372	-3.055946
H	0.434803	-0.891964	-3.643241
C	3.225079	2.152028	1.958678
C	2.783875	1.057812	0.954798
H	2.694354	0.107586	1.512800
H	3.562763	0.908441	0.198790
C	2.169144	1.741122	-2.144146
H	3.320401	3.103858	1.418665
H	2.424986	2.305313	2.697154
Si	4.855028	1.808249	2.907408
C	4.668125	0.186976	3.874600
H	3.827994	0.233338	4.578516
H	4.504759	-0.676031	3.215847
H	5.571440	-0.022359	4.460218
C	5.148009	3.247171	4.094967
H	5.232933	4.200569	3.560028
H	4.331044	3.344765	4.819889

H	6.075559	3.106258	4.662658
C	6.285193	1.661625	1.674526
H	7.233756	1.493205	2.198477
H	6.149834	0.826294	0.975963
H	6.399980	2.576632	1.080850
H	2.279258	2.788432	-2.462889
C	1.209515	1.707188	-0.984089
C	1.456929	1.400555	0.312235
H	0.185930	1.998690	-1.231906
H	3.165861	1.418903	-1.829653
H	0.622535	1.497730	1.011846
C	2.302219	-1.580627	-2.903296
C	1.898817	-2.954124	-2.857692
C	3.665486	-1.328532	-2.559601
C	2.806076	-3.986106	-2.589247
H	0.883528	-3.207593	-3.161718
C	4.555734	-2.366711	-2.286053
H	4.048003	-0.314396	-2.606928
C	4.139749	-3.704950	-2.295991
H	2.462263	-5.016595	-2.628288
H	5.597511	-2.127839	-2.085789
H	4.846597	-4.505131	-2.100939

4Nd_{St-BD}

Nd	0.544657	-0.246471	0.735066
C	-1.992019	-1.015445	1.912841
N	1.360336	-1.829081	-1.182017
C	-1.222590	-2.095791	-0.024652
C	-0.716214	-3.155924	-0.962030
H	-1.461358	-3.369098	-1.741714
H	-0.600184	-4.103188	-0.417187
C	-1.372516	-2.218533	1.400047
C	-2.254769	-0.884145	3.298155
H	-2.751075	0.005013	3.679044
C	0.606017	-2.853624	-1.646757
C	-1.923572	-1.920757	4.152524
H	-2.148025	-1.842610	5.211993
C	-2.145913	-0.306817	-1.687091
H	-1.826285	-0.814597	-2.593612
C	-3.060047	1.022276	0.657724
H	-3.436227	1.522850	1.546315
C	-2.340365	-0.187795	0.771685
C	-1.899277	-0.883613	-0.414495
C	-1.030627	-3.256436	2.308914

H	-0.594203	-4.184241	1.946595
C	2.551226	-1.578769	-1.774466
H	3.115575	-0.736371	-1.386259
C	-1.322795	-3.106148	3.653193
H	-1.102150	-3.917199	4.341909
C	1.039970	-3.638971	-2.721854
H	0.408478	-4.447463	-3.077327
C	2.267981	-3.380097	-3.319440
H	2.613470	-3.985920	-4.151965
C	-2.859974	0.877812	-1.764507
H	-3.086762	1.302052	-2.738627
C	3.044791	-2.325585	-2.834149
H	4.005914	-2.078325	-3.271592
C	-3.319624	1.540452	-0.600165
H	-3.892821	2.457168	-0.699621
C	1.665881	0.108856	3.686558
H	2.388141	0.865065	3.388485
H	0.927633	0.413079	4.421435
C	1.734048	-1.179304	3.274477
C	2.679883	-1.730788	2.291731
H	1.008116	-1.882254	3.675809
C	3.714848	-1.071574	1.726366
H	3.995037	-0.063299	2.013746
C	0.591978	4.187965	1.614877
C	0.082811	2.736214	1.409893
H	0.560814	2.105235	2.199737
H	-0.989398	2.696911	1.634799
C	0.270733	2.148581	0.018913
H	0.137422	4.813073	0.833380
H	1.673804	4.236163	1.431380
Si	0.215694	4.992857	3.308737
C	1.040157	3.988406	4.693765
H	2.122680	3.895505	4.538668
H	0.621229	2.977334	4.776616
H	0.894640	4.474843	5.665785
C	0.914261	6.749462	3.295790
H	0.467022	7.355192	2.498577
H	2.000120	6.749959	3.141654
H	0.716431	7.259746	4.246072
C	-1.658222	5.030868	3.588713
H	-1.901400	5.503489	4.547922
H	-2.095460	4.024434	3.603090
H	-2.168790	5.603038	2.804539
H	-0.560093	2.338889	-0.659732

C	1.571675	2.086001	-0.614122
C	1.693347	2.011776	-2.035192
C	2.777861	1.945582	0.133584
C	2.924848	1.881563	-2.652321
H	0.792908	2.111161	-2.636355
C	4.024472	1.814974	-0.507609
H	2.761784	2.106720	1.209080
C	4.108150	1.782021	-1.892684
H	2.980055	1.873831	-3.737740
H	4.929665	1.772106	0.093121
H	5.072321	1.707137	-2.386224
H	2.513087	-2.770414	2.014155
H	4.358785	-1.561952	1.003548

TS45Nd_{St-BD}

Nd	0.658039	-0.803239	0.556776
C	-2.071726	-1.306221	1.327372
N	1.544620	-2.312840	-1.427484
C	-1.165442	-2.425275	-0.529171
C	-0.622247	-3.505139	-1.424749
H	-1.318117	-3.712756	-2.249802
H	-0.560167	-4.447748	-0.862915
C	-1.495519	-2.551701	0.865729
C	-2.489959	-1.171398	2.673402
H	-2.961268	-0.251237	3.009565
C	0.750572	-3.236531	-2.019874
C	-2.333937	-2.236094	3.542303
H	-2.674212	-2.151606	4.569829
C	-1.706426	-0.534465	-2.245498
H	-1.333303	-1.062202	-3.119545
C	-2.755670	0.854055	0.007797
H	-3.184049	1.380318	0.857088
C	-2.192620	-0.432451	0.175402
C	-1.672764	-1.150432	-0.966445
C	-1.323500	-3.615357	1.793691
H	-0.909992	-4.567622	1.470588
C	2.784177	-2.109993	-1.927061
H	3.387680	-1.361369	-1.421023
C	-1.753125	-3.452963	3.098579
H	-1.658732	-4.279000	3.797935
C	1.192175	-3.958425	-3.135867
H	0.529719	-4.686614	-3.593544
C	2.467996	-3.740217	-3.643509
H	2.819331	-4.296969	-4.507216

C	-2.272145	0.722658	-2.377021
H	-2.331118	1.183031	-3.359227
C	3.287599	-2.793724	-3.024084
H	4.290514	-2.587893	-3.382130
C	-2.794484	1.417796	-1.256883
H	-3.244020	2.395750	-1.399087
C	1.240451	0.212934	3.245573
H	2.183043	0.747166	3.180538
H	0.484569	0.670297	3.870187
C	1.225886	-1.183441	3.122494
C	2.295770	-1.953456	2.533363
H	0.403660	-1.733265	3.573183
C	3.259987	-1.475054	1.687134
H	3.432047	-0.404583	1.547059
C	0.365685	4.398257	2.241067
C	0.675009	2.963894	2.730918
H	1.669014	2.943109	3.196665
H	-0.033721	2.699659	3.524543
C	0.576308	1.930201	1.618591
H	-0.630393	4.415371	1.774580
H	1.071443	4.676348	1.445550
Si	0.415328	5.756092	3.592623
C	2.160635	5.848755	4.326039
H	2.910184	6.065893	3.554968
H	2.452149	4.914859	4.822429
H	2.225713	6.646172	5.076134
C	-0.035924	7.403306	2.779686
H	-1.043847	7.377136	2.348179
H	0.662907	7.661298	1.974784
H	-0.012943	8.221991	3.509011
C	-0.834292	5.336595	4.953760
H	-0.857331	6.124472	5.716287
H	-0.587930	4.398655	5.466432
H	-1.851203	5.241456	4.553392
H	-0.463760	1.777622	1.308143
C	1.501392	1.971049	0.502951
C	1.077318	1.583089	-0.807592
C	2.883756	2.297531	0.660054
C	1.990466	1.512594	-1.879511
H	0.009826	1.525381	-1.023861
C	3.765399	2.217194	-0.403942
H	3.244193	2.636146	1.626457
C	3.332677	1.806198	-1.682721
H	1.622729	1.254707	-2.869028

H	4.807282	2.487289	-0.253455
H	4.034729	1.765960	-2.509686
H	2.245301	-3.031645	2.684786
H	4.016909	-2.135698	1.277918

5Nd_{St-BD}

Nd	0.299254	-0.780822	0.303208
C	-2.095832	-2.420956	0.576317
N	1.986662	-2.134363	-1.212121
C	-0.852496	-2.456930	-1.418708
C	0.045442	-2.936353	-2.526279
H	-0.115343	-2.316003	-3.419406
H	-0.223989	-3.955870	-2.837815
C	-1.101906	-3.148458	-0.178564
C	-2.554787	-2.921149	1.816545
H	-3.335868	-2.399329	2.363213
C	1.534826	-2.922313	-2.216908
C	-2.022633	-4.099858	2.307799
H	-2.382202	-4.505299	3.248683
C	-2.116933	-0.449531	-2.520922
H	-1.625997	-0.513107	-3.489254
C	-3.502557	-0.297982	-0.039307
H	-4.057683	-0.255125	0.894447
C	-2.518483	-1.295668	-0.236183
C	-1.804631	-1.378677	-1.492631
C	-0.545916	-4.333347	0.374321
H	0.205762	-4.895673	-0.173407
C	3.314201	-2.113887	-0.954999
H	3.627547	-1.494602	-0.120003
C	-1.016092	-4.796687	1.590090
H	-0.619536	-5.721364	1.999516
C	2.418409	-3.699580	-2.977278
H	2.023819	-4.329927	-3.768162
C	3.782580	-3.660191	-2.713832
H	4.474026	-4.259502	-3.298732
C	-3.102418	0.498610	-2.304123
H	-3.372972	1.179721	-3.106829
C	4.245036	-2.846192	-1.676943
H	5.298071	-2.790785	-1.423049
C	-3.786923	0.587397	-1.064943
H	-4.562033	1.336681	-0.935523
C	0.756733	0.981025	3.547385
H	1.836529	0.802916	3.468178
H	0.574258	1.183773	4.612774

C	-0.008841	-0.282233	3.179027
C	0.595306	-1.502655	2.896108
H	-1.034067	-0.324320	3.545546
C	1.838470	-1.725410	2.250932
H	2.635051	-0.984649	2.358934
C	0.670405	4.850507	2.717602
C	1.093570	3.515122	3.350981
H	2.181924	3.383837	3.268048
H	0.876043	3.528767	4.426650
C	0.390932	2.263353	2.763438
H	-0.420298	4.968127	2.807315
H	0.881935	4.841397	1.637554
Si	1.496078	6.414130	3.454312
C	3.374854	6.287926	3.234048
H	3.652130	6.180426	2.177925
H	3.797413	5.435017	3.779422
H	3.872312	7.189837	3.610533
C	0.833311	7.916382	2.513963
H	-0.255395	8.005831	2.612713
H	1.065763	7.859362	1.443454
H	1.273384	8.845709	2.895105
C	1.069219	6.555204	5.293445
H	1.506529	7.463918	5.724435
H	1.450839	5.706148	5.873419
H	-0.014680	6.607350	5.453653
H	-0.692898	2.418274	2.854522
C	0.698838	2.082453	1.285622
C	-0.305504	2.194102	0.304225
C	2.007903	1.776400	0.848299
C	-0.022980	1.999100	-1.058016
H	-1.320530	2.437564	0.605774
C	2.295224	1.580726	-0.508468
H	2.811581	1.704331	1.574606
C	1.278174	1.682171	-1.470354
H	-0.822236	2.083727	-1.785743
H	3.313048	1.359001	-0.816853
H	1.501739	1.537338	-2.522910
H	-0.060593	-2.373654	2.958685
H	2.192221	-2.749948	2.169697

4Nd_{st-st}

Nd	0.324568	-0.178839	0.627717
C	-2.112829	-1.154426	1.791625
N	1.276115	-1.889450	-1.085000

C	-1.470956	-1.912016	-0.336297
C	-0.995827	-2.809281	-1.444968
H	-1.479213	-2.515338	-2.387149
H	-1.326085	-3.842907	-1.270603
C	-1.519765	-2.252186	1.059139
C	-2.278205	-1.244405	3.194803
H	-2.757254	-0.436730	3.742915
C	0.505582	-2.828503	-1.685844
C	-1.876519	-2.394377	3.853264
H	-2.027574	-2.485284	4.924644
C	-2.546143	0.081617	-1.639887
H	-2.305114	-0.283318	-2.635213
C	-3.258754	1.045687	0.941493
H	-3.559472	1.406978	1.921742
C	-2.535444	-0.163435	0.817689
C	-2.185453	-0.669419	-0.490408
C	-1.098640	-3.408678	1.768967
H	-0.676072	-4.256264	1.234855
C	2.606265	-1.884262	-1.333703
H	3.184401	-1.104315	-0.847789
C	-1.297978	-3.474735	3.137452
H	-1.020135	-4.376490	3.676434
C	1.069818	-3.786012	-2.536585
H	0.426805	-4.527778	-3.000449
C	2.438246	-3.776283	-2.783212
H	2.883158	-4.514755	-3.443756
C	-3.265048	1.253345	-1.484267
H	-3.576023	1.810035	-2.363829
C	3.226834	-2.801536	-2.169186
H	4.297736	-2.749329	-2.331882
C	-3.620440	1.737994	-0.200418
H	-4.196930	2.654253	-0.117457
C	1.388532	0.010418	3.489025
H	2.114111	0.816686	3.419995
H	0.444866	0.250341	3.971563
C	1.677309	-1.273111	3.162741
C	2.937850	-1.801677	2.618271
H	0.905483	-2.020835	3.344325
C	2.995620	-3.164710	2.266032
C	4.172726	-3.728254	1.777113
C	5.315527	-2.938437	1.632080
C	5.276453	-1.584003	1.982519
C	4.101843	-1.019385	2.472130
H	2.109250	-3.781291	2.390911

H	4.201744	-4.783221	1.521210
H	6.238143	-3.377184	1.263328
H	6.170662	-0.974099	1.892439
H	4.099389	0.023845	2.773856
C	0.519294	4.300519	1.463990
C	-0.047054	2.864515	1.314847
H	0.419779	2.238218	2.110186
H	-1.116252	2.873031	1.556369
C	0.102426	2.225511	-0.060891
H	0.030720	4.934523	0.710698
H	1.586337	4.308780	1.201822
Si	0.313818	5.125235	3.176355
C	1.240806	4.103284	4.482832
H	2.305121	4.001337	4.234723
H	0.821398	3.095007	4.595340
H	1.183679	4.584039	5.466855
C	1.047874	6.865970	3.095106
H	0.537428	7.482150	2.345210
H	2.113369	6.845610	2.836002
H	0.954156	7.378961	4.059928
C	-1.522206	5.215850	3.637051
H	-1.658357	5.724546	4.599104
H	-1.977651	4.221957	3.729568
H	-2.096420	5.775438	2.888590
H	-0.704363	2.462916	-0.753476
C	1.404528	2.061185	-0.673463
C	1.540988	1.879945	-2.083306
C	2.585450	1.858693	0.103897
C	2.765621	1.595442	-2.666752
H	0.663093	2.019979	-2.709631
C	3.823083	1.577701	-0.502519
H	2.569251	2.080295	1.168718
C	3.923917	1.443094	-1.881732
H	2.832605	1.506656	-3.747915
H	4.710159	1.491129	0.119684
H	4.883192	1.246757	-2.350688

TS45Nd_{st-st}

Nd	0.684866	-0.830340	0.548296
C	-2.064230	-1.222529	1.320251
N	1.514920	-2.345299	-1.438536
C	-1.189827	-2.410631	-0.508353
C	-0.661268	-3.520625	-1.375638
H	-1.373211	-3.767633	-2.175811

H	-0.574435	-4.439032	-0.778096
C	-1.540489	-2.499922	0.885163
C	-2.479004	-1.041781	2.661576
H	-2.905837	-0.093714	2.979026
C	0.694265	-3.259413	-2.012505
C	-2.378140	-2.096672	3.550168
H	-2.715702	-1.976423	4.575003
C	-1.633532	-0.527225	-2.261152
H	-1.275354	-1.084388	-3.122969
C	-2.646543	0.940725	-0.041159
H	-3.061175	1.497412	0.795388
C	-2.136174	-0.364702	0.153345
C	-1.638470	-1.124368	-0.972080
C	-1.435217	-3.556663	1.829887
H	-1.070916	-4.534229	1.524400
C	2.738017	-2.146117	-1.977774
H	3.364100	-1.407849	-1.485704
C	-1.862298	-3.350072	3.129123
H	-1.817605	-4.168565	3.842274
C	1.093408	-3.973765	-3.147861
H	0.410900	-4.692572	-3.590570
C	2.353404	-3.758791	-3.696876
H	2.670507	-4.308839	-4.577991
C	-2.146445	0.748973	-2.418226
H	-2.177828	1.194873	-3.408384
C	3.199058	-2.823589	-3.098097
H	4.189772	-2.619258	-3.489402
C	-2.652095	1.483548	-1.314876
H	-3.061374	2.475770	-1.478241
C	1.286317	0.194274	3.216128
H	2.236868	0.716193	3.280996
H	0.518054	0.581906	3.874024
C	1.283649	-1.205837	3.021035
C	2.409247	-1.961007	2.477561
H	0.463367	-1.779287	3.447880
C	2.413068	-3.380496	2.517759
C	3.448209	-4.114370	1.950556
C	4.510978	-3.471150	1.298185
C	4.516113	-2.081085	1.217952
C	3.473201	-1.329924	1.778165
H	1.607404	-3.890573	3.038849
H	3.437498	-5.198192	2.026404
H	5.322244	-4.051194	0.869530
H	5.340342	-1.565218	0.732120

H	3.541427	-0.243265	1.753371
C	0.370170	4.287050	2.282543
C	0.751110	2.886398	2.809729
H	1.750834	2.922325	3.262828
H	0.066105	2.611358	3.620482
C	0.692656	1.804831	1.730283
H	-0.625656	4.240971	1.816595
H	1.060763	4.581336	1.479531
Si	0.344104	5.685614	3.591861
C	2.075455	5.888727	4.334918
H	2.821897	6.111865	3.562581
H	2.404517	4.988301	4.868088
H	2.095492	6.715478	5.055225
C	-0.180075	7.282229	2.722727
H	-1.182397	7.193936	2.286261
H	0.511743	7.546609	1.913804
H	-0.201505	8.124820	3.424347
C	-0.895272	5.249907	4.957521
H	-0.959853	6.057921	5.696197
H	-0.609579	4.339664	5.498903
H	-1.903809	5.096155	4.554158
H	-0.348903	1.656082	1.416503
C	1.596603	1.923545	0.584283
C	1.149531	1.612639	-0.735566
C	2.972244	2.265395	0.730898
C	2.038799	1.616042	-1.829251
H	0.078877	1.549888	-0.934154
C	3.832553	2.268054	-0.355650
H	3.349147	2.549416	1.708927
C	3.379899	1.923904	-1.645087
H	1.652211	1.407797	-2.823239
H	4.871982	2.550762	-0.210864
H	4.063677	1.944020	-2.488016

5Nd_{st-st}

Nd	0.611525	-0.804972	0.121867
C	-2.219256	-1.465804	0.564880
N	1.892606	-2.404795	-1.491436
C	-0.900059	-2.748100	-0.898452
C	-0.100496	-3.872954	-1.498212
H	-0.653905	-4.369426	-2.308129
H	0.056162	-4.650344	-0.737067
C	-1.495385	-2.707881	0.415349
C	-2.887860	-1.165907	1.775298

H	-3.454714	-0.243374	1.873875
C	1.269298	-3.482405	-2.030604
C	-2.852280	-2.079685	2.812282
H	-3.376790	-1.870259	3.739414
C	-1.266934	-1.203227	-2.973332
H	-0.683191	-1.800439	-3.669101
C	-2.874442	0.345415	-1.207906
H	-3.517422	0.922534	-0.547578
C	-2.195544	-0.795699	-0.721869
C	-1.415643	-1.615200	-1.621273
C	-1.492218	-3.627773	1.496858
H	-1.002503	-4.592951	1.395947
C	3.141615	-2.105046	-1.910150
H	3.614309	-1.250510	-1.433478
C	-2.165727	-3.311428	2.662795
H	-2.184348	-4.028560	3.478656
C	1.889302	-4.248232	-3.024437
H	1.361233	-5.098027	-3.445513
C	3.169802	-3.921030	-3.459638
H	3.656322	-4.511053	-4.230695
C	-1.941771	-0.078361	-3.417458
H	-1.870873	0.208829	-4.462948
C	3.816749	-2.825601	-2.885884
H	4.817675	-2.534007	-3.185060
C	-2.755021	0.688612	-2.544065
H	-3.301334	1.541824	-2.935630
C	1.350668	0.635590	3.397041
H	2.432864	0.802623	3.471074
H	1.009473	0.562910	4.438885
C	1.062530	-0.682807	2.661302
C	2.151951	-1.595462	2.324479
H	0.202905	-1.215119	3.082744
C	1.869955	-2.971570	2.066009
C	2.849361	-3.863983	1.624392
C	4.152814	-3.431024	1.377180
C	4.457536	-2.082841	1.589059
C	3.486460	-1.182663	2.029658
H	0.882803	-3.348778	2.316901
H	2.591376	-4.912545	1.497107
H	4.918275	-4.127622	1.050127
H	5.472662	-1.726626	1.430317
H	3.790855	-0.162354	2.235980
C	0.435706	4.479716	3.110832
C	1.161645	3.190028	3.527752

H	2.246624	3.306144	3.391207
H	1.013419	3.010533	4.600556
C	0.705183	1.907250	2.787082
H	-0.649362	4.347784	3.241770
H	0.586507	4.668411	2.037055
Si	0.956512	6.059635	4.059632
C	2.808597	6.366290	3.796918
H	3.054827	6.478433	2.733660
H	3.421113	5.549179	4.197562
H	3.126290	7.285944	4.302966
C	-0.044174	7.511414	3.372399
H	-1.121976	7.356556	3.504446
H	0.141054	7.660717	2.301586
H	0.216632	8.446238	3.882996
C	0.597244	5.838724	5.905981
H	0.879262	6.737426	6.467767
H	1.155148	4.998770	6.337589
H	-0.469024	5.659869	6.091296
H	-0.384249	1.825314	2.905445
C	0.983414	1.965970	1.292611
C	-0.057221	2.086665	0.349639
C	2.297505	1.845049	0.789439
C	0.191083	2.022566	-1.032422
H	-1.077067	2.221218	0.700225
C	2.551679	1.756351	-0.582575
H	3.130094	1.805273	1.482545
C	1.493707	1.820175	-1.505081
H	-0.635993	2.101473	-1.729846
H	3.574490	1.651827	-0.934473
H	1.685915	1.756072	-2.571739

1Sc

Sc	0.203956	-0.815977	0.368993
C	-1.745274	-2.011987	1.405828
N	2.388285	-1.345096	0.547176
C	0.415294	-2.159777	2.301427
C	1.818497	-2.626996	2.573707
H	2.139688	-2.323415	3.579208
H	1.862264	-3.724504	2.581631
C	-0.568614	-2.847245	1.512270
C	-2.854722	-2.436364	0.630620
H	-3.756045	-1.830737	0.586869
C	2.839501	-2.113180	1.572486
C	-2.785086	-3.642382	-0.041786

H	-3.633874	-3.987227	-0.624021
C	0.298095	0.098347	3.612433
H	1.289559	0.035176	4.052836
C	-2.326770	0.290596	2.518413
H	-3.334654	0.362470	2.118504
C	-1.514971	-0.829481	2.216146
C	-0.196139	-0.951157	2.792030
C	-0.519231	-4.064785	0.778760
H	0.352803	-4.710733	0.840260
C	3.278090	-0.854841	-0.350471
H	2.871017	-0.231545	-1.142013
C	-1.618130	-4.448088	0.030888
H	-1.596049	-5.393613	-0.503078
C	4.201345	-2.407319	1.696860
H	4.537529	-3.022991	2.525337
C	5.106908	-1.907775	0.767147
H	6.165691	-2.131191	0.857790
C	-0.521124	1.176562	3.890693
H	-0.159895	1.965692	4.543620
C	4.637405	-1.110394	-0.281399
H	5.308479	-0.694481	-1.024680
C	-1.830479	1.272840	3.353429
H	-2.447896	2.128392	3.608753
C	0.116090	1.297792	-0.117989
H	-0.623474	1.879991	0.443508
H	1.087066	1.806564	-0.033119
Si	-0.383328	0.977617	-1.892806
C	-0.363474	-0.999093	-2.052112
H	0.617349	-1.505710	-1.964335
H	-1.114101	-1.576473	-1.476292
H	-0.655022	-1.197205	-3.090246
C	0.858966	1.563518	-3.188576
H	0.883418	2.659170	-3.214516
H	1.879884	1.222772	-2.974194
H	0.594900	1.211861	-4.192870
C	-2.151712	1.477554	-2.311514
H	-2.454448	1.113221	-3.300149
H	-2.869614	1.093517	-1.576627
H	-2.242695	2.570023	-2.316196

2Sc_{BD}

Sc	0.100988	-0.868586	0.075076
C	-1.296637	-2.872755	1.195278
N	2.399680	-0.966439	0.242855

C	0.599207	-1.863777	2.133274
C	2.019192	-1.650053	2.574676
H	2.066088	-0.818965	3.291433
H	2.408590	-2.522834	3.117257
C	0.119386	-3.018819	1.418815
C	-2.024644	-3.905398	0.559747
H	-3.104256	-3.832356	0.454443
C	2.956504	-1.329113	1.425694
C	-1.353951	-5.033972	0.120900
H	-1.906503	-5.846486	-0.341296
C	-0.711327	0.091848	3.279284
H	0.140494	0.523385	3.797847
C	-2.981972	-1.021665	1.970460
H	-3.859667	-1.459884	1.502440
C	-1.712846	-1.635159	1.830201
C	-0.558270	-1.074357	2.486383
C	0.787445	-4.166466	0.917638
H	1.855448	-4.294879	1.072828
C	3.217431	-0.619039	-0.777560
H	2.732639	-0.312550	-1.697604
C	0.049315	-5.156391	0.291942
H	0.547248	-6.058095	-0.052914
C	4.345311	-1.371195	1.586957
H	4.758854	-1.673715	2.543965
C	5.177074	-1.022651	0.528656
H	6.256429	-1.051214	0.644144
C	-1.964629	0.657254	3.411176
H	-2.090889	1.535231	4.037849
C	4.600485	-0.631958	-0.682633
H	5.206249	-0.343893	-1.534815
C	-3.097303	0.111020	2.753107
H	-4.067222	0.580039	2.887001
C	0.039027	1.293657	0.134456
C	-2.050515	-0.179848	-1.944304
H	-1.310951	0.473893	-2.393805
H	-2.983416	0.287517	-1.645362
C	-1.867525	-1.509305	-1.799875
C	-0.639790	-2.253984	-2.125716
H	-0.921568	1.513791	0.631700
H	-2.674833	-2.107047	-1.388549
C	0.515890	-1.727033	-2.589619
H	0.610837	-0.680861	-2.876543
H	0.795130	1.384020	0.940540
Si	0.366379	2.734252	-1.058505

C	-1.272879	3.591574	-1.475484
H	-1.991781	2.922285	-1.964565
H	-1.752865	3.983026	-0.570457
H	-1.108571	4.438480	-2.152694
C	1.176069	2.213362	-2.705869
H	2.143307	1.715689	-2.559067
H	0.543023	1.556138	-3.317382
H	1.373108	3.103313	-3.316647
C	1.539585	3.976315	-0.238413
H	1.746821	4.829227	-0.896252
H	1.111567	4.370864	0.690925
H	2.503279	3.514540	0.013244
H	-0.674889	-3.321004	-1.916301
H	1.373038	-2.364587	-2.783096

TS23Sc_{BD}

Sc	0.072699	-1.050928	-0.013480
C	-1.298615	-2.891079	1.242031
N	2.416147	-1.049494	0.141593
C	0.637887	-1.895906	2.108734
C	2.071147	-1.683333	2.501313
H	2.142757	-0.849742	3.213190
H	2.470576	-2.554674	3.038865
C	0.118340	-3.064249	1.448051
C	-2.061132	-3.922438	0.641557
H	-3.138553	-3.821107	0.539316
C	2.985797	-1.377223	1.329530
C	-1.424370	-5.077322	0.228332
H	-2.001399	-5.886640	-0.208786
C	-0.594771	0.149116	3.177630
H	0.278911	0.581402	3.658272
C	-2.924721	-0.973702	1.981994
H	-3.823971	-1.412862	1.557775
C	-1.673201	-1.623855	1.838721
C	-0.488759	-1.060328	2.439436
C	0.750480	-4.245736	0.973016
H	1.817735	-4.394358	1.114209
C	3.231037	-0.727397	-0.891226
H	2.744780	-0.465019	-1.823247
C	-0.020986	-5.231811	0.387538
H	0.448826	-6.154678	0.059788
C	4.376482	-1.405849	1.483809
H	4.795836	-1.683967	2.445755
C	5.201526	-1.075957	0.415338

H	6.281597	-1.093647	0.526108
C	-1.830936	0.748671	3.313151
H	-1.922552	1.656535	3.902452
C	4.614350	-0.721911	-0.801828
H	5.212154	-0.454459	-1.666309
C	-2.994154	0.196998	2.711021
H	-3.949952	0.693026	2.849335
C	-0.171624	1.193232	-0.158935
C	-1.548658	0.098926	-1.749058
H	-0.899392	0.492764	-2.521568
H	-2.332429	0.768420	-1.417000
C	-1.724826	-1.274327	-1.607509
C	-0.772340	-2.251563	-2.083395
H	-0.956651	1.378123	0.585863
H	-2.616975	-1.639539	-1.110425
C	0.503627	-1.965858	-2.474357
H	0.813935	-0.947993	-2.710258
H	0.760610	0.990069	0.425453
Si	0.197609	2.801672	-1.112583
C	-1.405526	3.557798	-1.775026
H	-1.857840	2.971420	-2.582890
H	-2.155126	3.675863	-0.982964
H	-1.204611	4.557177	-2.179631
C	1.387421	2.441033	-2.547161
H	2.338931	2.030559	-2.186059
H	0.972838	1.742129	-3.285282
H	1.623694	3.365827	-3.087394
C	1.026102	4.017783	0.077770
H	1.266291	4.958812	-0.432521
H	0.372456	4.260178	0.924075
H	1.962993	3.617457	0.484823
H	-1.048125	-3.296140	-1.955815
H	1.199245	-2.754313	-2.740275

3Sc_{BD}

Sc	0.282419	-1.413084	-0.044073
C	-1.376266	-2.866688	1.284867
N	2.556273	-1.136854	0.353358
C	0.684531	-2.148254	2.144113
C	2.123720	-2.119487	2.574422
H	2.231355	-1.582499	3.526598
H	2.474751	-3.139199	2.783074
C	-0.017061	-3.263796	1.562535
C	-2.285080	-3.787564	0.709603

H	-3.320632	-3.504022	0.542303
C	3.064452	-1.495872	1.559027
C	-1.844943	-5.057467	0.392145
H	-2.535920	-5.779840	-0.031401
C	-0.159245	0.208193	2.888467
H	0.775330	0.535398	3.336519
C	-2.646695	-0.626380	1.773884
H	-3.602932	-0.943621	1.366923
C	-1.536898	-1.504534	1.755927
C	-0.277667	-1.095727	2.336061
C	0.414679	-4.565946	1.185685
H	1.435224	-4.886601	1.377437
C	3.398868	-0.612893	-0.569570
H	2.961704	-0.360317	-1.529852
C	-0.496408	-5.439449	0.623866
H	-0.181252	-6.446182	0.365441
C	4.421053	-1.317809	1.855130
H	4.793407	-1.615695	2.830488
C	5.272918	-0.769827	0.904204
H	6.326940	-0.628962	1.124101
C	-1.269910	1.035034	2.905993
H	-1.196932	2.016474	3.366106
C	4.749963	-0.409552	-0.341170
H	5.374763	0.013776	-1.119993
C	-2.509204	0.624026	2.351045
H	-3.360952	1.295792	2.395039
C	-0.196019	0.959158	-0.995150
C	-1.030504	0.201846	-2.075604
H	-0.485407	0.261667	-3.027141
H	-1.962702	0.757681	-2.216816
C	-1.413698	-1.249067	-1.785454
C	-0.608335	-2.341844	-2.078999
H	-0.622558	0.844819	0.018999
H	-2.465480	-1.435028	-1.585781
C	0.802043	-2.275107	-2.155689
H	1.254217	-1.375387	-2.584927
H	0.869263	0.661393	-0.978722
Si	-0.106903	2.880928	-1.254431
C	-1.858435	3.570255	-1.133051
H	-2.511985	3.192786	-1.927854
H	-2.322983	3.326052	-0.170355
H	-1.841618	4.663214	-1.221520
C	0.653514	3.205541	-2.951794
H	1.659342	2.775533	-3.036484

H	0.043525	2.795502	-3.764910
H	0.746670	4.283853	-3.128604
C	0.992469	3.562537	0.122078
H	1.063756	4.654915	0.057760
H	0.595476	3.317956	1.114592
H	2.014342	3.167351	0.061937
H	-1.056825	-3.328041	-1.953928
H	1.371503	-3.184101	-2.327589

2Sc_{st}

Sc	0.196149	-0.852836	0.349872
C	-1.923070	-1.723940	1.460605
N	2.341119	-1.481718	0.750783
C	0.197017	-2.104133	2.379857
C	1.523736	-2.725638	2.713172
H	1.787815	-2.550755	3.764868
H	1.466658	-3.818151	2.611689
C	-0.868214	-2.701494	1.626820
C	-3.086359	-2.048319	0.719142
H	-3.893954	-1.327619	0.625186
C	2.662183	-2.224258	1.841449
C	-3.194642	-3.302785	0.146892
H	-4.090503	-3.570743	-0.404630
C	0.353163	0.188307	3.617377
H	1.322935	0.010384	4.074505
C	-2.213763	0.675169	2.479075
H	-3.202324	0.859195	2.068462
C	-1.543185	-0.542495	2.212094
C	-0.255774	-0.805992	2.806206
C	-1.001775	-3.971722	1.001091
H	-0.233670	-4.731109	1.126856
C	3.334933	-1.023780	-0.047344
H	3.029844	-0.432089	-0.904597
C	-2.153898	-4.258462	0.290457
H	-2.277006	-5.242399	-0.153379
C	3.996531	-2.514887	2.142212
H	4.225356	-3.104694	3.024380
C	5.011433	-2.041594	1.317275
H	6.050663	-2.258398	1.546206
C	-0.329124	1.364632	3.860679
H	0.115630	2.116929	4.505664
C	4.675235	-1.279154	0.195397
H	5.432488	-0.885861	-0.473540
C	-1.609040	1.609404	3.297542

H	-2.120426	2.539376	3.525861
C	0.404575	1.271882	-0.020482
C	-0.448583	-1.738540	-1.975040
H	-0.444092	-0.770065	-2.471003
H	-1.386148	-2.053376	-1.515871
C	0.540512	-2.654102	-2.159554
C	1.778725	-2.515718	-2.922415
H	0.316856	1.715286	0.985830
H	0.399890	-3.628134	-1.689931
C	2.695743	-3.585055	-2.905701
C	3.887483	-3.514395	-3.624098
C	4.179840	-2.372301	-4.372852
C	3.275449	-1.302880	-4.404749
C	2.084559	-1.371963	-3.690138
H	2.461910	-4.479173	-2.332593
H	4.580645	-4.349950	-3.608481
H	5.103517	-2.317079	-4.941525
H	3.496032	-0.422472	-5.000916
H	1.383883	-0.544389	-3.743930
H	1.461261	1.425094	-0.312864
Si	-0.645190	2.345331	-1.178213
C	-2.462526	1.786308	-1.199118
H	-2.582729	0.753742	-1.554260
H	-2.909243	1.850621	-0.200109
H	-3.058168	2.425463	-1.862422
C	0.027701	2.234068	-2.954657
H	1.099866	2.463990	-2.994467
H	-0.122383	1.245490	-3.408482
H	-0.483096	2.955948	-3.603383
C	-0.588826	4.158665	-0.631722
H	-1.180374	4.797909	-1.298874
H	-0.988580	4.279789	0.382547
H	0.438507	4.542527	-0.628187

TS23Sc_{st}

Sc	0.464228	-1.156362	-0.013385
C	-1.607054	-2.207862	1.161835
N	2.680824	-1.285312	0.591601
C	0.556063	-2.317949	2.056976
C	1.943504	-2.775939	2.409373
H	2.121707	-2.725756	3.492334
H	2.064369	-3.835601	2.145465
C	-0.454581	-3.059940	1.353433
C	-2.751659	-2.694582	0.484499

H	-3.631673	-2.066378	0.373539
C	3.030430	-1.986538	1.701618
C	-2.749070	-3.989103	0.001911
H	-3.627309	-4.382032	-0.500960
C	0.489977	0.043966	3.169628
H	1.477132	-0.009337	3.620826
C	-2.131767	0.197380	2.060331
H	-3.141512	0.252689	1.662784
C	-1.338694	-0.955809	1.837597
C	-0.021378	-1.053357	2.420858
C	-0.481794	-4.382631	0.831038
H	0.360950	-5.051892	0.982981
C	3.640643	-0.595613	-0.067450
H	3.322503	-0.062950	-0.957203
C	-1.616410	-4.828735	0.180907
H	-1.654314	-5.849717	-0.188302
C	4.349538	-1.991637	2.164219
H	4.595556	-2.556607	3.057861
C	5.327233	-1.273697	1.483141
H	6.353599	-1.269051	1.837802
C	-0.308420	1.153514	3.365644
H	0.062187	1.979670	3.965637
C	4.965644	-0.558363	0.339713
H	5.690853	0.017266	-0.224841
C	-1.617958	1.231924	2.817593
H	-2.223947	2.110913	3.014989
C	0.068611	0.901076	-0.755265
C	-0.810977	-0.613143	-2.175609
H	-0.403296	0.052400	-2.925666
H	-1.854559	-0.435176	-1.939998
C	-0.309928	-1.911864	-2.018710
C	1.033559	-2.329997	-2.457864
H	-0.012829	0.947889	0.355642
H	-0.990393	-2.691157	-1.679556
C	1.476860	-3.646309	-2.186826
C	2.750254	-4.069614	-2.561749
C	3.623278	-3.191925	-3.211229
C	3.205526	-1.887173	-3.487402
C	1.933740	-1.455698	-3.110795
H	0.795207	-4.340106	-1.702906
H	3.057128	-5.091997	-2.359796
H	4.611155	-3.525883	-3.513792
H	3.866946	-1.205630	-4.015529
H	1.623736	-0.447205	-3.370272

H	1.143572	0.958699	-1.014623
Si	-0.744181	2.523108	-1.365397
C	-2.625638	2.409747	-1.215000
H	-3.059368	1.664681	-1.892187
H	-2.931162	2.157273	-0.193264
H	-3.081686	3.375615	-1.464045
C	-0.241073	2.837556	-3.164504
H	0.849022	2.835349	-3.290878
H	-0.664933	2.111332	-3.868084
H	-0.597189	3.826426	-3.478395
C	-0.095245	3.931924	-0.282722
H	-0.525176	4.891535	-0.595589
H	-0.353962	3.782192	0.772083
H	0.995680	4.024993	-0.348539

3Sc_{st}

Sc	0.515249	-1.363157	0.075317
C	-1.553885	-2.415210	1.272397
N	2.741548	-1.436075	0.648210
C	0.617324	-2.420416	2.160967
C	2.013066	-2.830489	2.542740
H	2.178409	-2.732364	3.624243
H	2.158282	-3.897449	2.324555
C	-0.375516	-3.219675	1.489428
C	-2.687255	-2.961354	0.626270
H	-3.587867	-2.366010	0.501566
C	3.089108	-2.048655	1.811450
C	-2.642396	-4.267941	0.181238
H	-3.509787	-4.707038	-0.301718
C	0.511098	0.015860	3.096840
H	1.506643	0.022427	3.532572
C	-2.130107	0.026325	2.027259
H	-3.145056	0.029112	1.638858
C	-1.313669	-1.122134	1.880866
C	0.009077	-1.153245	2.461035
C	-0.352251	-4.551465	0.992841
H	0.518452	-5.183296	1.147368
C	3.695623	-0.765673	-0.039720
H	3.381874	-0.323281	-0.978595
C	-1.475129	-5.055079	0.362847
H	-1.473881	-6.083776	0.013657
C	4.395401	-1.976940	2.301663
H	4.639346	-2.472965	3.235911
C	5.365586	-1.273936	1.593395

H	6.382959	-1.211841	1.968019
C	-0.309012	1.124641	3.215799
H	0.056612	2.004992	3.736520
C	5.008554	-0.653971	0.394949
H	5.729266	-0.098918	-0.195484
C	-1.629714	1.128785	2.695735
H	-2.253066	2.006758	2.835206
C	-0.260199	0.789611	-1.139187
C	-0.918766	-0.291202	-2.069142
H	-0.762687	0.023572	-3.111415
H	-1.999326	-0.253414	-1.898059
C	-0.435504	-1.725785	-1.835001
C	0.875432	-2.121957	-2.374791
H	-0.579874	0.700602	-0.081205
H	-1.205361	-2.494717	-1.900172
C	1.355572	-3.441990	-2.143636
C	2.624932	-3.840155	-2.555919
C	3.477784	-2.937115	-3.200901
C	3.036626	-1.633496	-3.433988
C	1.767169	-1.224344	-3.016840
H	0.690317	-4.162858	-1.673850
H	2.945181	-4.865122	-2.389162
H	4.462088	-3.252582	-3.533271
H	3.676858	-0.930577	-3.961264
H	1.437467	-0.218350	-3.259897
H	0.845815	0.777145	-1.182336
Si	-0.735289	2.617915	-1.572156
C	-2.612271	2.779252	-1.457678
H	-3.125557	2.139889	-2.185161
H	-2.981230	2.517504	-0.458708
H	-2.919900	3.812229	-1.659979
C	-0.121084	2.996859	-3.317460
H	0.966706	2.882939	-3.403194
H	-0.588902	2.357672	-4.074878
H	-0.358217	4.034979	-3.580451
C	0.127035	3.727061	-0.310027
H	-0.125210	4.780271	-0.482616
H	-0.170319	3.482198	0.716553
H	1.219105	3.641711	-0.372892

4Sc_{BD-BD}

Sc	0.322141	-0.585666	-0.505512
C	-1.921707	-0.767542	-1.872838
N	1.110197	-2.373497	0.769709

C	-1.552507	-1.781171	0.209274
C	-1.265128	-2.816189	1.259181
H	-1.613572	-2.457468	2.237082
H	-1.833205	-3.738934	1.074314
C	-1.568111	-2.003659	-1.215002
C	-2.000784	-0.709787	-3.284195
H	-2.298118	0.210604	-3.779314
C	0.203150	-3.172384	1.387730
C	-1.737420	-1.850425	-4.022818
H	-1.819398	-1.825414	-5.105066
C	-2.368039	0.263454	1.621362
H	-2.251910	-0.206830	2.594154
C	-2.745880	1.517678	-0.909573
H	-2.913438	1.993948	-1.871690
C	-2.235683	0.199659	-0.842457
C	-2.054671	-0.447793	0.431265
C	-1.273606	-3.148772	-2.003019
H	-1.023457	-4.094302	-1.528019
C	2.423827	-2.676174	0.896506
H	3.117956	-2.021175	0.383507
C	-1.378649	-3.063969	-3.381227
H	-1.197888	-3.947606	-3.986851
C	0.607307	-4.283172	2.137027
H	-0.146488	-4.902226	2.613633
C	1.959093	-4.579183	2.266543
H	2.282567	-5.435712	2.850502
C	-2.872426	1.544550	1.524651
H	-3.144505	2.082369	2.428248
C	2.891292	-3.756556	1.629091
H	3.957136	-3.945842	1.696719
C	-3.061216	2.174237	0.263300
H	-3.473548	3.178018	0.228277
C	1.732833	-1.088302	-2.813902
H	2.367620	-0.211150	-2.899179
H	0.705090	-0.988582	-3.162291
C	2.245735	-2.312675	-2.545352
C	3.656119	-2.642900	-2.314562
H	1.553811	-3.153128	-2.515053
C	4.699354	-1.911149	-2.737601
H	4.573039	-0.991801	-3.303362
C	3.611379	1.929562	1.368194
C	2.747901	0.681771	1.046996
H	3.001732	-0.121061	1.747949
H	3.030679	0.316640	0.043245

C	0.832805	1.665235	-1.198467
H	3.346623	2.737307	0.671930
H	3.329349	2.295696	2.365684
Si	5.507994	1.686057	1.330356
C	6.002478	0.322111	2.551729
H	5.673870	0.557859	3.571293
H	5.576196	-0.653191	2.283685
H	7.092177	0.201712	2.580868
C	6.323308	3.319959	1.817552
H	6.049754	4.128809	1.129451
H	6.028280	3.630380	2.827049
H	7.416666	3.235022	1.806719
C	6.044079	1.191120	-0.421964
H	7.134209	1.087285	-0.482091
H	5.609557	0.231510	-0.731781
H	5.748189	1.947301	-1.159773
H	0.176245	2.193611	-1.883945
C	0.561922	1.711234	0.178519
C	1.256881	0.974103	1.143334
H	3.845946	-3.591968	-1.816376
H	5.720914	-2.232729	-2.559719
H	-0.410256	2.102549	0.473903
H	1.859158	1.549628	-1.545639
H	0.854985	0.990169	2.155263

TS45Sc_{BD-BD}

Sc	0.605433	-0.792261	-0.866125
C	-1.906823	-1.256490	-1.852205
N	1.496961	-2.442404	0.548322
C	-1.182462	-1.745119	0.323952
C	-0.758666	-2.528295	1.532293
H	-0.858710	-1.904841	2.431328
H	-1.416716	-3.392304	1.705422
C	-1.379936	-2.290505	-0.997938
C	-2.231519	-1.539920	-3.195744
H	-2.680444	-0.777695	-3.827145
C	0.671637	-3.018773	1.460402
C	-2.001755	-2.813147	-3.691415
H	-2.263897	-3.049231	-4.718225
C	-1.970709	0.524593	1.350545
H	-1.746112	0.275307	2.384492
C	-2.661637	1.190306	-1.330323
H	-2.958803	1.438813	-2.345844
C	-2.102002	-0.074875	-1.036700

C	-1.736974	-0.415547	0.313505
C	-1.119083	-3.574578	-1.543959
H	-0.723578	-4.371391	-0.919406
C	2.785074	-2.860629	0.500955
H	3.407754	-2.384761	-0.246244
C	-1.439867	-3.821699	-2.868978
H	-1.278523	-4.812957	-3.282712
C	1.126979	-4.022252	2.322311
H	0.432883	-4.466109	3.029199
C	2.452287	-4.437356	2.267912
H	2.815491	-5.214067	2.934300
C	-2.533551	1.747160	1.038187
H	-2.740290	2.459982	1.831417
C	3.302767	-3.839896	1.335242
H	4.343664	-4.131327	1.245602
C	-2.867810	2.088978	-0.300328
H	-3.316270	3.056214	-0.505548
C	1.033723	0.246577	-3.280841
H	1.895361	0.766699	-3.688244
H	0.083098	0.631113	-3.639828
C	1.121491	-1.153022	-3.078611
C	2.387965	-1.805771	-2.793581
H	0.290438	-1.777302	-3.387973
C	3.560732	-1.191578	-2.493659
H	3.686811	-0.114032	-2.532175
C	3.692484	1.843815	1.367360
C	2.829950	0.625180	0.935291
H	2.920191	-0.164003	1.689140
H	3.241012	0.215475	-0.000460
C	1.359910	1.609657	-1.653635
H	3.601827	2.637427	0.613298
H	3.271685	2.262692	2.292311
Si	5.549299	1.471021	1.664278
C	5.706484	0.117032	2.981253
H	5.243906	0.422558	3.927729
H	5.235555	-0.824220	2.669776
H	6.760516	-0.101638	3.190275
C	6.375138	3.064429	2.253222
H	6.282504	3.865497	1.510160
H	5.929967	3.425736	3.187862
H	7.445017	2.909516	2.437338
C	6.333087	0.883107	0.040675
H	7.402915	0.682350	0.173748
H	5.874535	-0.042789	-0.329507

H	6.241244	1.640610	-0.747552
H	0.915130	2.359890	-2.299899
C	0.806639	1.592201	-0.322110
C	1.374824	1.006824	0.786382
H	2.365449	-2.895416	-2.784057
H	4.460036	-1.768275	-2.299550
H	-0.209647	1.965597	-0.215845
H	2.445908	1.595503	-1.714163
H	0.791764	1.031541	1.704689

5Sc_{BD-BD}

Sc	0.348777	-1.253919	-1.094320
C	-2.078184	-1.609324	-1.949754
N	1.357273	-2.796485	0.354523
C	-1.354374	-2.259340	0.183837
C	-0.882737	-3.107096	1.329039
H	-1.068446	-2.588667	2.279512
H	-1.460945	-4.039094	1.394954
C	-1.628728	-2.723040	-1.152405
C	-2.431665	-1.801324	-3.305819
H	-2.819085	-0.974206	-3.894405
C	0.591157	-3.457997	1.258339
C	-2.302256	-3.059281	-3.863617
H	-2.586920	-3.224507	-4.898207
C	-1.762705	0.066924	1.303058
H	-1.508916	-0.236635	2.315748
C	-2.523393	0.892155	-1.315700
H	-2.837842	1.207527	-2.306827
C	-2.126914	-0.446870	-1.085308
C	-1.747377	-0.876725	0.240648
C	-1.463043	-3.994767	-1.767010
H	-1.114546	-4.846119	-1.188380
C	2.675962	-3.101153	0.290289
H	3.251846	-2.564136	-0.452891
C	-1.808831	-4.147794	-3.097129
H	-1.718203	-5.124249	-3.564022
C	1.136614	-4.430910	2.103690
H	0.488448	-4.945434	2.806406
C	2.491866	-4.729934	2.032013
H	2.925775	-5.484429	2.681434
C	-2.165642	1.365483	1.046552
H	-2.211603	2.081110	1.862582
C	3.281419	-4.047238	1.103122
H	4.342015	-4.249768	1.000458

C	-2.541457	1.782176	-0.257306
H	-2.863702	2.806651	-0.415967
C	1.348408	1.378290	-2.978483
H	2.024475	1.610226	-3.814603
H	0.621989	2.199458	-2.948667
C	0.574868	0.107683	-3.312618
C	1.033862	-1.198545	-3.411368
H	-0.341202	0.305681	-3.865381
C	2.027575	-1.837378	-2.628785
H	2.887839	-1.259749	-2.282961
C	3.719291	1.395844	2.095776
C	3.204432	0.303604	1.120483
H	3.251547	-0.671463	1.620983
H	3.856696	0.252377	0.242139
C	2.166107	1.434747	-1.673113
H	3.662249	2.377116	1.605001
H	3.048301	1.453676	2.965028
Si	5.507414	1.132125	2.738546
C	5.591535	-0.524877	3.655278
H	4.885538	-0.555983	4.494240
H	5.370268	-1.376578	2.999731
H	6.594407	-0.687976	4.067944
C	5.907813	2.552696	3.918020
H	5.850507	3.525006	3.414230
H	5.216146	2.578077	4.768580
H	6.922011	2.452973	4.323055
C	6.707692	1.126808	1.274233
H	7.741979	1.020603	1.622834
H	6.515719	0.299894	0.579107
H	6.651546	2.062065	0.704066
H	2.538421	2.462958	-1.555619
C	1.336222	1.087448	-0.456440
C	1.784459	0.591621	0.722652
H	0.357050	-1.876603	-3.937350
H	2.248912	-2.880824	-2.839576
H	0.289051	1.407535	-0.493483
H	3.059317	0.805545	-1.735288
H	1.049344	0.486156	1.522668

4Sc_{BD-St}

Sc	0.102843	-0.616578	-0.166827
C	-2.192265	-0.532542	-1.460622
N	0.908940	-2.622568	0.687463
C	-1.763688	-1.914537	0.384683

C	-1.445223	-3.126382	1.213471
H	-1.729226	-2.943581	2.258571
H	-2.044528	-3.993204	0.900509
C	-1.830538	-1.870250	-1.054425
C	-2.318433	-0.215115	-2.833573
H	-2.621021	0.782559	-3.139962
C	0.019632	-3.518241	1.187780
C	-2.093557	-1.201336	-3.778358
H	-2.211503	-0.976680	-4.833928
C	-2.521017	-0.166523	2.176202
H	-2.381046	-0.810462	3.040350
C	-2.959355	1.539087	-0.064527
H	-3.150094	2.186607	-0.915995
C	-2.459565	0.229472	-0.259148
C	-2.245368	-0.643965	0.866094
C	-1.575637	-2.851647	-2.049653
H	-1.318944	-3.869207	-1.765426
C	2.220330	-2.955884	0.675076
H	2.898945	-2.221496	0.257752
C	-1.727630	-2.514120	-3.384122
H	-1.578591	-3.271983	-4.148247
C	0.440941	-4.757125	1.681903
H	-0.297964	-5.450383	2.071795
C	1.792150	-5.085390	1.672056
H	2.128979	-6.043126	2.057668
C	-3.017609	1.111300	2.334396
H	-3.260692	1.471607	3.329841
C	2.704643	-4.164191	1.153382
H	3.767539	-4.374743	1.112254
C	-3.235968	1.966420	1.218602
H	-3.640685	2.960330	1.383420
C	1.429769	-0.658798	-2.530264
H	2.087695	0.202112	-2.467869
H	0.388167	-0.454454	-2.780464
C	1.905247	-1.925525	-2.631696
H	1.173634	-2.717421	-2.784712
C	3.400793	1.401432	2.251621
C	2.540614	0.265663	1.638871
H	2.772297	-0.678149	2.145268
H	2.843609	0.131411	0.585481
C	0.659461	1.727675	-0.377593
H	3.178576	2.340687	1.726353
H	3.073310	1.560089	3.289217
Si	5.294655	1.138235	2.263433

C	5.713182	-0.424465	3.252616
H	5.354054	-0.350552	4.286351
H	5.270368	-1.326970	2.812303
H	6.797585	-0.582523	3.294966
C	6.093004	2.651421	3.066864
H	5.860580	3.570213	2.515092
H	5.746203	2.788531	4.098085
H	7.184849	2.553579	3.097911
C	5.921947	0.948365	0.481768
H	7.015663	0.867414	0.461107
H	5.521185	0.048995	-0.002836
H	5.647971	1.814934	-0.133105
H	0.022802	2.404405	-0.940660
C	0.379847	1.489447	0.975972
C	1.049272	0.548036	1.767792
H	-0.586147	1.833045	1.342574
H	1.683555	1.652310	-0.741884
H	0.633074	0.360969	2.756604
C	3.297380	-2.373950	-2.590774
C	3.560285	-3.752250	-2.711313
C	4.387772	-1.488737	-2.466037
C	4.867621	-4.235220	-2.703609
H	2.729514	-4.444715	-2.824931
C	5.692108	-1.972037	-2.453637
H	4.218448	-0.418450	-2.395225
C	5.936015	-3.345906	-2.571868
H	5.052696	-5.300154	-2.807972
H	6.522123	-1.278111	-2.361822
H	6.956581	-3.717318	-2.570236

TS45Sc_{BD-st}

Sc	0.399201	-0.848406	-0.507302
C	-2.036977	-1.097509	-1.618523
N	1.287421	-2.680747	0.591419
C	-1.407742	-2.033243	0.437045
C	-0.985315	-3.034263	1.473976
H	-1.140301	-2.615599	2.477717
H	-1.609982	-3.938412	1.439676
C	-1.576365	-2.299902	-0.969606
C	-2.318527	-1.097744	-3.002967
H	-2.714796	-0.207730	-3.484704
C	0.468129	-3.449091	1.355589
C	-2.119509	-2.257922	-3.730764
H	-2.351559	-2.278086	-4.791183

C	-2.142708	0.023992	1.871725
H	-1.952310	-0.428844	2.841442
C	-2.742506	1.222716	-0.642140
H	-3.004926	1.674070	-1.595453
C	-2.224469	-0.093995	-0.591510
C	-1.913100	-0.707308	0.675490
C	-1.346830	-3.463883	-1.749843
H	-1.001327	-4.382361	-1.282637
C	2.590391	-3.034683	0.483425
H	3.208283	-2.411195	-0.152850
C	-1.631334	-3.433456	-3.104141
H	-1.498234	-4.332498	-3.699277
C	0.950840	-4.578698	2.022959
H	0.266074	-5.174086	2.618810
C	2.293380	-4.926000	1.917240
H	2.678064	-5.800408	2.433840
C	-2.661674	1.301084	1.792082
H	-2.868017	1.853072	2.704681
C	3.132366	-4.136575	1.128299
H	4.183035	-4.372254	1.000560
C	-2.953169	1.907585	0.538876
H	-3.370513	2.909681	0.518262
C	0.992513	0.581752	-2.643829
H	1.840006	1.171454	-2.981236
H	0.037386	1.008863	-2.939531
C	1.081885	-0.837605	-2.690939
H	0.251434	-1.370966	-3.145958
C	3.488341	1.310983	2.372529
C	2.687192	0.223428	1.605745
H	2.755958	-0.723544	2.151897
H	3.157108	0.058527	0.625961
C	1.282305	1.614510	-0.845518
H	3.419154	2.262331	1.827502
H	3.006094	1.488192	3.344367
Si	5.335601	0.906915	2.683388
C	5.466124	-0.691163	3.693543
H	4.937391	-0.605312	4.650663
H	5.052038	-1.556263	3.160339
H	6.513902	-0.922271	3.920661
C	6.092645	2.350844	3.637795
H	6.019761	3.289475	3.075532
H	5.593705	2.502393	4.602426
H	7.155179	2.172621	3.842527
C	6.218503	0.686241	1.019629

H	7.285610	0.484506	1.172138
H	5.809574	-0.152606	0.441956
H	6.144000	1.589061	0.400808
H	0.879187	2.494384	-1.339097
C	0.695648	1.379746	0.457818
C	1.234956	0.624057	1.470735
H	-0.320633	1.742458	0.601506
H	2.370181	1.593241	-0.868576
H	0.627239	0.503874	2.365898
C	2.372216	-1.547777	-2.662463
C	2.419842	-2.922923	-2.989723
C	3.588422	-0.918378	-2.310579
C	3.618821	-3.627541	-2.974548
H	1.499642	-3.426109	-3.274808
C	4.790901	-1.630973	-2.293448
H	3.610235	0.144269	-2.088299
C	4.813442	-2.988094	-2.619482
H	3.627030	-4.678423	-3.250577
H	5.713095	-1.115621	-2.039043
H	5.750132	-3.537474	-2.616627

5Sc_{BD-St}

Sc	0.344747	-1.226114	-0.857235
C	-2.062111	-1.601187	-1.687345
N	1.386129	-2.769812	0.491834
C	-1.351450	-2.258942	0.448031
C	-0.810520	-3.098876	1.570384
H	-0.944340	-2.575681	2.527014
H	-1.377393	-4.034400	1.674830
C	-1.628539	-2.721843	-0.884578
C	-2.408377	-1.793461	-3.047939
H	-2.767419	-0.960126	-3.645683
C	0.662120	-3.445089	1.421708
C	-2.321120	-3.060480	-3.592358
H	-2.605713	-3.224868	-4.627061
C	-1.808487	0.053552	1.581677
H	-1.560289	-0.254754	2.594175
C	-2.565686	0.885049	-1.038908
H	-2.881341	1.200967	-2.029498
C	-2.124521	-0.444555	-0.820550
C	-1.743446	-0.877824	0.505801
C	-1.514966	-4.006421	-1.486757
H	-1.194510	-4.862775	-0.899315
C	2.701288	-3.058026	0.352267

H	3.233152	-2.505676	-0.415290
C	-1.875870	-4.161626	-2.811097
H	-1.830559	-5.146692	-3.266697
C	1.258135	-4.421919	2.225708
H	0.652728	-4.950332	2.955621
C	2.612011	-4.707116	2.081089
H	3.083296	-5.463882	2.701275
C	-2.256365	1.335536	1.335892
H	-2.341612	2.038351	2.159811
C	3.351898	-4.010533	1.122322
H	4.407504	-4.204900	0.966976
C	-2.630199	1.756787	0.028973
H	-2.988444	2.770765	-0.119410
C	1.298503	1.556745	-2.487790
H	1.948321	1.899919	-3.307442
H	0.392201	2.171023	-2.547784
C	0.877961	0.098472	-2.647312
H	-0.014464	-0.026726	-3.268392
C	3.577202	1.275047	2.534458
C	3.115608	0.291535	1.427946
H	3.223526	-0.735687	1.797394
H	3.766671	0.386722	0.552432
C	1.983215	1.848264	-1.134707
H	3.489601	2.304559	2.161262
H	2.890905	1.208130	3.391518
Si	5.359345	0.995006	3.179471
C	5.455364	-0.718311	3.986972
H	4.749073	-0.807720	4.821564
H	5.236488	-1.525837	3.276674
H	6.458782	-0.904146	4.388594
C	5.738262	2.338286	4.453208
H	5.689947	3.339561	4.008704
H	5.029754	2.312249	5.289801
H	6.744391	2.213235	4.871138
C	6.579597	1.093011	1.733259
H	7.610638	0.974048	2.087397
H	6.401783	0.308730	0.986799
H	6.521657	2.060925	1.220510
H	2.036732	2.934579	-0.972675
C	1.197841	1.225941	-0.007843
C	1.675538	0.539094	1.058778
H	0.128033	1.449454	-0.019377
H	3.016858	1.490578	-1.126409
H	0.949455	0.247325	1.820676

C	1.849022	-0.958554	-2.877837
C	1.364335	-2.296994	-3.006660
C	3.264920	-0.805873	-2.806439
C	2.238096	-3.392281	-3.130231
H	0.302987	-2.460448	-3.200982
C	4.115547	-1.895689	-2.938676
H	3.687965	0.190165	-2.732657
C	3.613204	-3.200818	-3.096253
H	1.823961	-4.385188	-3.282342
H	5.190328	-1.731709	-2.939328
H	4.292673	-4.039332	-3.212998

4Sc_{st-BD}

Sc	0.146911	-0.309664	0.557100
C	-2.002544	-1.273081	1.650344
N	1.365528	-1.684202	-0.830999
C	-1.387975	-1.720649	-0.565056
C	-0.791748	-2.407977	-1.761139
H	-1.032347	-1.842412	-2.671833
H	-1.225231	-3.405691	-1.915445
C	-1.413081	-2.253386	0.768300
C	-2.156700	-1.558759	3.028658
H	-2.632311	-0.838390	3.689199
C	0.718174	-2.535009	-1.669831
C	-1.752868	-2.791348	3.511944
H	-1.901927	-3.035986	4.559312
C	-2.512933	0.414007	-1.569615
H	-2.304243	0.184060	-2.611203
C	-3.164338	1.016465	1.138083
H	-3.437944	1.240483	2.165625
C	-2.446261	-0.162069	0.829514
C	-2.121065	-0.481311	-0.539656
C	-0.969763	-3.492650	1.304385
H	-0.542289	-4.250992	0.653716
C	2.714864	-1.738019	-0.767576
H	3.190489	-1.023176	-0.105672
C	-1.168258	-3.755206	2.648551
H	-0.882585	-4.722312	3.053101
C	1.421679	-3.466590	-2.436221
H	0.874515	-4.136963	-3.091732
C	2.810489	-3.525775	-2.352877
H	3.366359	-4.247326	-2.944253
C	-3.221680	1.552806	-1.236432
H	-3.554124	2.223827	-2.023332

C	3.472697	-2.640805	-1.501535
H	4.553221	-2.642513	-1.408052
C	-3.543955	1.859723	0.111543
H	-4.112390	2.758202	0.330650
C	1.422897	-0.295621	2.829320
H	2.196147	0.423931	2.569393
H	0.477934	0.104702	3.196902
C	1.689458	-1.621131	2.934107
C	2.988060	-2.263081	2.713729
H	0.874382	-2.283415	3.219442
C	4.172308	-1.676763	2.949818
H	4.248413	-0.662071	3.332299
C	0.264340	4.299619	1.506775
C	0.212557	2.779859	1.791176
H	1.077887	2.504004	2.409391
H	-0.670648	2.563676	2.407951
C	0.136443	1.921083	0.522167
H	-0.618390	4.577569	0.911899
H	1.130540	4.517836	0.864770
Si	0.346062	5.449964	3.030242
C	1.917845	5.074831	4.025653
H	2.820824	5.208952	3.416870
H	1.925563	4.048636	4.414781
H	2.005181	5.746712	4.888126
C	0.386687	7.241365	2.422086
H	-0.510992	7.490060	1.843124
H	1.256159	7.429659	1.780604
H	0.444054	7.943997	3.262499
C	-1.177268	5.177197	4.126878
H	-1.159924	5.850210	4.992630
H	-1.230223	4.151949	4.514385
H	-2.107113	5.374696	3.579252
H	-0.766913	2.171508	-0.044241
C	1.301913	1.827566	-0.369074
C	1.118474	1.497604	-1.740556
C	2.647827	1.913454	0.085198
C	2.199314	1.300740	-2.601554
H	0.105703	1.470060	-2.137877
C	3.722286	1.722071	-0.781369
H	2.846316	2.212258	1.110628
C	3.508824	1.406861	-2.128951
H	2.015572	1.088329	-3.651559
H	4.736511	1.841873	-0.408433
H	4.350264	1.275003	-2.802397

H	2.961230	-3.308625	2.411954
H	5.105036	-2.214569	2.808805

TS45Sc_{St-BD}

Sc	0.272153	-0.627708	0.651920
C	-2.058561	-1.552154	1.527934
N	1.449601	-1.893265	-0.868042
C	-1.316137	-1.774059	-0.684832
C	-0.721767	-2.365150	-1.931343
H	-0.940365	-1.716865	-2.790960
H	-1.182295	-3.332617	-2.176004
C	-1.442232	-2.448908	0.580244
C	-2.322451	-1.982256	2.848681
H	-2.827601	-1.324873	3.551349
C	0.782173	-2.550637	-1.851395
C	-1.958829	-3.263177	3.224218
H	-2.172279	-3.613245	4.229507
C	-2.263840	0.529242	-1.488897
H	-2.011391	0.406558	-2.539296
C	-3.042775	0.853113	1.231882
H	-3.371056	0.969880	2.261404
C	-2.374193	-0.327626	0.824815
C	-1.974060	-0.502435	-0.551809
C	-1.046948	-3.745133	1.008061
H	-0.581686	-4.437612	0.311564
C	2.795930	-2.016070	-0.803117
H	3.284538	-1.485876	0.006227
C	-1.319266	-4.137299	2.306211
H	-1.053134	-5.139406	2.629842
C	1.461170	-3.354192	-2.771582
H	0.896418	-3.875820	-3.538026
C	2.844917	-3.477649	-2.695607
H	3.381318	-4.100992	-3.404962
C	-2.920152	1.666089	-1.060878
H	-3.168350	2.442145	-1.779331
C	3.528486	-2.791072	-1.690496
H	4.606059	-2.858350	-1.587558
C	-3.302592	1.836474	0.297875
H	-3.831181	2.738020	0.591734
C	0.879223	0.053846	3.028693
H	1.720224	0.684961	3.291126
H	-0.062943	0.352929	3.478108
C	1.083318	-1.303269	2.734875
C	2.404574	-1.941800	2.605580

H	0.264833	-1.984845	2.956010
C	3.618506	-1.375842	2.730284
H	3.758860	-0.320706	2.950010
C	0.291818	4.128895	1.696773
C	0.651920	2.769088	2.331460
H	1.665001	2.818670	2.751161
H	-0.020002	2.575702	3.176527
C	0.561739	1.603675	1.343527
H	-0.734084	4.083544	1.302436
H	0.939690	4.313979	0.827754
Si	0.417508	5.645323	2.860845
C	2.213638	5.860323	3.424738
H	2.891471	6.000101	2.573621
H	2.573203	4.998649	4.000850
H	2.314081	6.742061	4.069123
C	-0.145601	7.167428	1.889615
H	-1.184651	7.070330	1.552173
H	0.477487	7.333711	1.002503
H	-0.085037	8.071929	2.506700
C	-0.699796	5.383707	4.369489
H	-0.670666	6.259327	5.029204
H	-0.389333	4.518663	4.968418
H	-1.746544	5.230638	4.078783
H	-0.465518	1.580787	0.937177
C	1.559404	1.572454	0.246033
C	1.144872	1.435741	-1.100661
C	2.955932	1.640895	0.495402
C	2.079007	1.370591	-2.147980
H	0.085340	1.491522	-1.337586
C	3.871295	1.592027	-0.545066
H	3.311368	1.758691	1.514487
C	3.438686	1.449271	-1.875890
H	1.728405	1.295372	-3.173628
H	4.933093	1.672957	-0.329219
H	4.163935	1.422491	-2.683573
H	2.362434	-3.014268	2.415603
H	4.521991	-1.972956	2.654788

5Sc_{st-BD}

Sc	0.304595	-1.134974	0.530028
C	-2.030116	-2.269088	1.137844
N	1.732046	-2.035177	-1.078877
C	-1.016207	-2.365220	-0.975123
C	-0.295574	-2.890444	-2.183175

H	-0.646145	-2.371235	-3.085510
H	-0.538054	-3.948785	-2.352681
C	-1.233259	-3.083768	0.256839
C	-2.435800	-2.767829	2.396278
H	-3.082059	-2.177459	3.039993
C	1.212499	-2.749014	-2.107400
C	-2.025820	-4.030808	2.781829
H	-2.345836	-4.435069	3.737371
C	-2.082663	-0.146432	-1.853935
H	-1.719096	-0.232108	-2.874917
C	-3.139054	0.074418	0.781772
H	-3.569228	0.150824	1.776753
C	-2.351591	-1.046681	0.428714
C	-1.800990	-1.160256	-0.900784
C	-0.790669	-4.359385	0.699070
H	-0.181370	-4.986501	0.053639
C	3.077584	-1.900553	-1.006926
H	3.455299	-1.333640	-0.164910
C	-1.197197	-4.817666	1.938507
H	-0.893728	-5.806462	2.269873
C	2.036122	-3.338138	-3.074031
H	1.583443	-3.910635	-3.877859
C	3.414877	-3.188556	-2.993143
H	4.063733	-3.643039	-3.735959
C	-2.878661	0.923928	-1.486326
H	-3.125710	1.684032	-2.222140
C	3.949228	-2.449625	-1.934035
H	5.018891	-2.310119	-1.821098
C	-3.394614	1.046026	-0.169848
H	-4.018140	1.898842	0.080271
C	0.904557	0.807174	3.338820
H	1.988337	0.635214	3.344680
H	0.644927	1.119958	4.360077
C	0.166295	-0.496412	3.083028
C	0.778520	-1.716246	2.828997
H	-0.835773	-0.541213	3.506385
C	1.927964	-1.909318	2.029093
H	2.664460	-1.101784	1.967469
C	0.612747	4.582598	2.184488
C	0.983041	3.346719	3.020473
H	2.061194	3.341226	3.232969
H	0.488902	3.400280	3.999263
C	0.578348	1.989113	2.390701
H	-0.466090	4.565449	1.965769

H	1.116177	4.542039	1.207171
Si	1.026624	6.273707	2.981372
C	2.895267	6.387479	3.277486
H	3.460315	6.262073	2.345389
H	3.247893	5.628668	3.986784
H	3.164419	7.366569	3.691761
C	0.480155	7.631856	1.782216
H	-0.598830	7.589859	1.589771
H	0.993150	7.549428	0.816161
H	0.701828	8.626832	2.186640
C	0.101413	6.447001	4.625089
H	0.310038	7.419327	5.087454
H	0.395299	5.675627	5.347315
H	-0.984653	6.377669	4.487255
H	-0.510569	2.010421	2.244453
C	1.218515	1.764237	1.030746
C	0.433048	1.482092	-0.105768
C	2.612301	1.864409	0.853772
C	1.019065	1.358401	-1.381915
H	-0.653314	1.495144	-0.019558
C	3.189961	1.746262	-0.410287
H	3.246658	2.083819	1.707717
C	2.396241	1.498769	-1.537102
H	0.381522	1.191547	-2.244327
H	4.264363	1.866091	-0.521054
H	2.847647	1.431414	-2.522247
H	0.180597	-2.607235	3.022422
H	2.340206	-2.909601	1.928172

4Sc_{st-st}

Sc	0.022808	-0.432856	0.526341
C	-2.143064	-1.352592	1.631172
N	1.175755	-1.820337	-0.906125
C	-1.573797	-1.774164	-0.601347
C	-1.016509	-2.454245	-1.820038
H	-1.250704	-1.861408	-2.714955
H	-1.484322	-3.433923	-1.989462
C	-1.594104	-2.331593	0.722037
C	-2.282584	-1.659522	3.006682
H	-2.727418	-0.938817	3.688042
C	0.489367	-2.632861	-1.751949
C	-1.902691	-2.909966	3.461299
H	-2.039753	-3.169231	4.506783
C	-2.652668	0.409912	-1.547740

H	-2.466395	0.194150	-2.596590
C	-3.244828	0.978796	1.180541
H	-3.495571	1.191200	2.216377
C	-2.566350	-0.214037	0.838699
C	-2.270409	-0.515563	-0.541053
C	-1.178819	-3.593165	1.227735
H	-0.784181	-4.350567	0.555641
C	2.522258	-1.924848	-0.857929
H	3.031853	-1.243201	-0.186725
C	-1.360904	-3.873956	2.570274
H	-1.098964	-4.856965	2.952428
C	1.150758	-3.573699	-2.543617
H	0.572796	-4.211799	-3.204924
C	2.537442	-3.684446	-2.476335
H	3.060369	-4.414910	-3.086595
C	-3.323154	1.561758	-1.182377
H	-3.648055	2.256960	-1.951257
C	3.239527	-2.841329	-1.615256
H	4.319262	-2.886994	-1.526825
C	-3.615430	1.852108	0.176163
H	-4.153822	2.762399	0.421011
C	1.286811	-0.527348	2.779806
H	2.018875	0.256112	2.604814
H	0.313365	-0.207864	3.152713
C	1.630755	-1.840790	2.842632
C	2.951500	-2.429592	2.625545
H	0.843118	-2.550523	3.087979
C	3.054834	-3.831062	2.533438
C	4.290416	-4.443575	2.334602
C	5.444842	-3.663823	2.235442
C	5.360733	-2.269709	2.340157
C	4.127582	-1.656615	2.535165
H	2.156427	-4.436647	2.620857
H	4.354883	-5.525461	2.268419
H	6.411155	-4.138880	2.093046
H	6.261890	-1.665964	2.286913
H	4.080389	-0.577400	2.647509
C	0.299354	4.146292	1.570452
C	0.189471	2.621099	1.807646
H	1.049309	2.293053	2.407216
H	-0.694169	2.421844	2.429260
C	0.066245	1.799730	0.518345
H	-0.590113	4.485116	1.019117
H	1.152072	4.349340	0.905862

Si	0.493218	5.227331	3.134851
C	2.085408	4.737734	4.044398
H	2.966590	4.854626	3.401041
H	2.059487	3.697044	4.391903
H	2.242206	5.368479	4.927775
C	0.593587	7.040770	2.603355
H	-0.310981	7.352769	2.067339
H	1.448663	7.219754	1.940206
H	0.705853	7.702688	3.470618
C	-0.996467	4.974330	4.280801
H	-0.917994	5.610431	5.170755
H	-1.078600	3.937184	4.629407
H	-1.936818	5.232050	3.777928
H	-0.837442	2.089351	-0.027983
C	1.215291	1.687635	-0.391133
C	1.002750	1.389758	-1.765924
C	2.569316	1.722373	0.045330
C	2.064563	1.174743	-2.645514
H	-0.016025	1.399990	-2.148146
C	3.625057	1.513659	-0.840251
H	2.790609	1.995253	1.073325
C	3.383403	1.230678	-2.189899
H	1.859786	0.987101	-3.696358
H	4.647755	1.594447	-0.480097
H	4.210865	1.084587	-2.877601

TS45Sc_{st-st}

Sc	0.263055	-0.655887	0.589399
C	-2.080414	-1.535193	1.507584
N	1.382626	-1.916823	-0.971199
C	-1.379285	-1.766542	-0.717931
C	-0.821632	-2.364835	-1.978336
H	-1.061443	-1.718537	-2.833763
H	-1.294451	-3.330423	-2.206583
C	-1.505510	-2.444108	0.546099
C	-2.334870	-1.963195	2.830890
H	-2.804810	-1.292760	3.545621
C	0.683382	-2.560361	-1.941110
C	-2.013566	-3.259137	3.191975
H	-2.223255	-3.608382	4.198346
C	-2.300975	0.553799	-1.501966
H	-2.069746	0.427848	-2.556946
C	-3.025618	0.887674	1.232070
H	-3.334795	1.008123	2.267091

C	-2.382427	-0.302745	0.812659
C	-2.009958	-0.482664	-0.570813
C	-1.157414	-3.758607	0.957112
H	-0.728772	-4.462013	0.248168
C	2.728147	-2.057994	-0.936989
H	3.247243	-1.544065	-0.135576
C	-1.427885	-4.151184	2.255448
H	-1.201938	-5.167469	2.565758
C	1.330595	-3.361433	-2.885796
H	0.741429	-3.870757	-3.642117
C	2.714718	-3.498371	-2.846122
H	3.226801	-4.119672	-3.575021
C	-2.932176	1.700438	-1.062060
H	-3.181828	2.480296	-1.775880
C	3.429889	-2.830776	-1.850612
H	4.507975	-2.913840	-1.769972
C	-3.287381	1.875678	0.303332
H	-3.797640	2.784561	0.606905
C	0.901393	0.036437	2.945967
H	1.746178	0.644861	3.248100
H	-0.031508	0.312737	3.429166
C	1.096860	-1.326613	2.634384
C	2.422406	-1.969807	2.481162
H	0.289031	-2.005448	2.901875
C	2.488336	-3.372267	2.342651
C	3.709167	-4.030602	2.214166
C	4.905538	-3.307422	2.215451
C	4.861536	-1.918454	2.360526
C	3.639055	-1.258580	2.491225
H	1.565191	-3.945524	2.350642
H	3.727714	-5.113189	2.122354
H	5.858425	-3.819871	2.122268
H	5.784380	-1.345056	2.387106
H	3.638975	-0.181125	2.620780
C	0.324539	4.099699	1.735058
C	0.693550	2.736202	2.354503
H	1.714001	2.779839	2.756746
H	0.037507	2.537672	3.210665
C	0.582730	1.574275	1.361544
H	-0.709236	4.060181	1.361311
H	0.955187	4.288865	0.854369
Si	0.481067	5.608171	2.905824
C	2.287563	5.798892	3.445626
H	2.955446	5.929453	2.585177

H	2.643052	4.932268	4.016847
H	2.409081	6.679115	4.088426
C	-0.076984	7.141908	1.950164
H	-1.120573	7.057531	1.623516
H	0.538112	7.307164	1.057307
H	-0.000346	8.041914	2.572014
C	-0.618557	5.350968	4.427896
H	-0.567680	6.221062	5.093548
H	-0.312340	4.476979	5.015867
H	-1.671230	5.215033	4.150454
H	-0.455380	1.551907	0.986977
C	1.545300	1.568666	0.232540
C	1.089723	1.408385	-1.098660
C	2.946267	1.688370	0.431179
C	1.989501	1.356013	-2.176946
H	0.022698	1.446542	-1.303097
C	3.826387	1.652455	-0.639872
H	3.332780	1.843834	1.433433
C	3.354453	1.475198	-1.953038
H	1.605830	1.260507	-3.188979
H	4.891543	1.771920	-0.461959
H	4.052616	1.458397	-2.784447

5Sc_{st-st}

Sc	0.421611	-1.269530	0.383814
C	-2.087851	-1.489518	1.297965
N	1.433639	-2.444305	-1.314687
C	-1.217414	-2.686570	-0.521150
C	-0.632983	-3.775140	-1.378228
H	-1.304598	-4.046768	-2.204395
H	-0.518647	-4.691316	-0.782507
C	-1.589215	-2.772271	0.869306
C	-2.506070	-1.291318	2.633628
H	-2.906506	-0.330913	2.947101
C	0.726121	-3.415899	-1.948566
C	-2.428608	-2.343975	3.525225
H	-2.760713	-2.212695	4.550396
C	-1.584158	-0.779977	-2.270112
H	-1.211883	-1.331818	-3.129254
C	-2.637433	0.677716	-0.060620
H	-3.060174	1.231378	0.773378
C	-2.134571	-0.630866	0.132224
C	-1.638481	-1.392810	-0.988913
C	-1.524982	-3.833923	1.810185

H	-1.188914	-4.821792	1.506074
C	2.667009	-2.136292	-1.775952
H	3.202682	-1.368795	-1.229521
C	-1.947040	-3.612219	3.107494
H	-1.925944	-4.429614	3.822670
C	1.243697	-4.073031	-3.067078
H	0.648783	-4.838732	-3.555062
C	2.509436	-3.740885	-3.542383
H	2.920396	-4.245608	-4.411694
C	-2.080276	0.503358	-2.426147
H	-2.082935	0.959277	-3.412199
C	3.238338	-2.751457	-2.881693
H	4.229986	-2.460545	-3.210808
C	-2.614368	1.228671	-1.329860
H	-3.016119	2.223560	-1.495667
C	1.350010	0.270940	3.151412
H	2.416082	0.391659	3.387771
H	0.831564	0.303527	4.117744
C	1.084763	-1.100619	2.505423
C	2.203862	-1.961287	2.089241
H	0.347913	-1.674501	3.074686
C	1.990104	-3.359468	1.929039
C	2.986565	-4.207113	1.440367
C	4.233101	-3.697255	1.074203
C	4.468172	-2.324341	1.207818
C	3.475334	-1.470551	1.684705
H	1.049883	-3.783704	2.270894
H	2.794334	-5.274897	1.374222
H	5.015823	-4.357630	0.713462
H	5.442030	-1.915227	0.949977
H	3.699927	-0.415836	1.794402
C	0.440529	4.074879	2.523532
C	1.016258	2.812294	3.186778
H	2.072894	2.968660	3.444150
H	0.505375	2.629303	4.141185
C	0.880232	1.518190	2.348424
H	-0.615007	3.901024	2.261974
H	0.955685	4.267165	1.570700
Si	0.531821	5.675923	3.568532
C	2.345246	6.079650	3.943678
H	2.928115	6.205734	3.022762
H	2.827834	5.295503	4.539840
H	2.427332	7.014252	4.511537
C	-0.243714	7.076550	2.558700

H	-1.292907	6.867073	2.316870
H	0.289343	7.235821	1.613375
H	-0.218423	8.022921	3.112227
C	-0.425587	5.435644	5.185618
H	-0.398874	6.347964	5.793591
H	-0.006218	4.626816	5.796311
H	-1.480317	5.199139	4.998243
H	-0.191746	1.383667	2.138635
C	1.596206	1.593607	1.008514
C	0.925545	1.267675	-0.190467
C	2.948899	1.961592	0.911307
C	1.581374	1.309393	-1.436782
H	-0.162234	1.166110	-0.177711
C	3.599966	2.003802	-0.321885
H	3.495131	2.239980	1.807964
C	2.925170	1.668946	-1.502410
H	1.020188	1.097072	-2.341812
H	4.641324	2.311492	-0.365421
H	3.434703	1.723066	-2.459803