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Supporting Information: Ruthenium Based Catalysts for Olefin Hydrosilylation: Dichloro(*p*-cymene)ruthenium and Related Complexes

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1. σ-Bond metathesis mechanism for B1H.

2. Energy and thermochemical data for all optimized structures.

3. Cartesian coordinates for all optimized structures in XYZ format.

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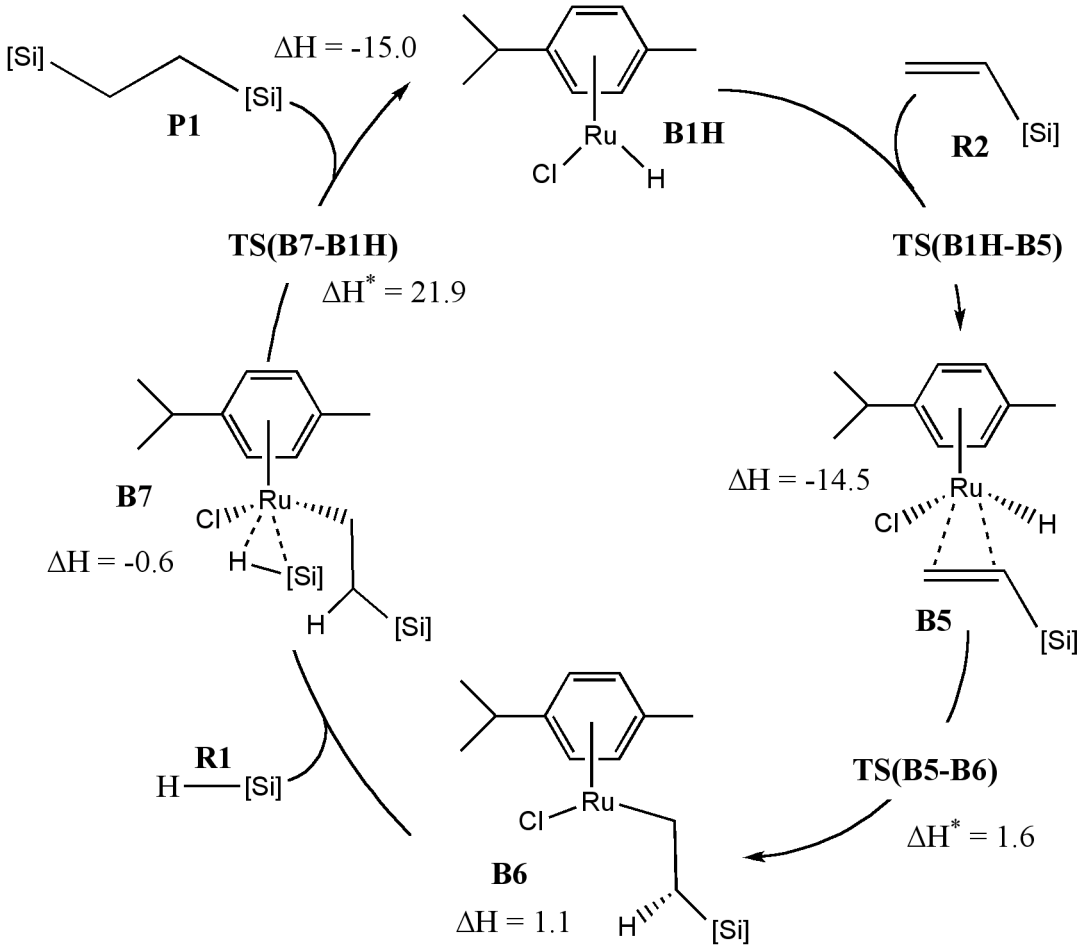
1. σ-Bond metathesis mechanism for B1H.

Scheme S1. σ-Bond metathesis Mechanism.

All enthalpies (ΔH) are given relative to the preceding minimum in kcal/mol.



As in the case of the CH and mCH mechanisms, the σ-bond metathesis (SBM) pathway benefits from the initial exchange of one of the chloride ligands for a hydride ligand in the induction phase (Figure 3, main text). Thus, the starting point for the SBM catalytic cycle is **B1H**. Within the catalytic cycle, the first step involves the η^2-coordination of **R2** in an unhindered process, which lowers the enthalpy by 14.5 kcal/mol (**B5**, Scheme S1). **R2** is in a position to abstract the hydride ligand from Ru in order to form the σ-bonded complex (**B6**). This abstraction reaction has a low barrier (ΔH^* = 1.6 kcal/mol), but is slightly endothermic (ΔH(**B6**) = 1.1 kcal/mol). The addition of **R1** at this point in the mechanism

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results in a weak (ΔH = -0.6 kcal/mol), agostic-like, interaction between **R1** and **B6** to form the intermediate complex **B7**. The final step, closing cycle, is a concerted reaction where the silyl group of **R1** is abstracted by the β-carbon atom (relative to the silicon) of **R2** and the H atom of **R1** forms a bond with Ru. Despite its exothermicity (ΔH(**B1H**) = -15.0 kcal/mol), this concerted process requires an activation enthalpy of 21.9 kcal/mol.

In contrast, the hydride CH mechanism, described in the main text, has an activation enthalpy of only 15.7 kcal/mol, which corresponds to the formation of the CH intermediate (**B3H**). The product-forming step in the CH mechanism is not rate-determining, with a barrier of 13.6 kcal/mol for this step. The rate-limiting transition state in the catalytic cycle lies 7.9 kcal/mol above **B1H** in the SBM mechanism, compared with 1.4 kcal/mol in the hydride CH mechanism. Given its larger activation enthalpy, the SBM mechanism is disfavored relative to the hydride CH mechanism, and therefore does not offer a competitive pathway for the production of **P1**.

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2. Energy and thermochemical data for all optimized structures.

Table S1: Energy and thermochemical data for B3LYP optimized structures.[a]

Structure	E	ZPE	H	S	G	μ
B1	-1404.91555	136.38	-1404.68193	128.27	-1404.74288	8.87
TS(B1-B2)	-1965.28211	220.03	-1964.90492	174.04	-1964.98761	7.79
B2	-1965.28250	219.82	-1964.90477	179.64	-1964.99013	7.67
TS(B2-B3)	-2602.99864	136.38	-2602.44307	234.10	-2602.55430	6.32
B3	-2603.03668	136.38	-2602.47469	240.79	-2602.58910	7.73
TS(B3-B1)	-2603.02490	136.38	-2602.46438	237.97	-2602.57745	7.18
B4	-2603.03049	324.44	-2602.47244	249.86	-2602.59116	9.08
TS(B2-B1H)	-1965.26990	219.95	-1964.89333	171.36	-1964.97475	6.09
B1H	-945.26566	140.12	-945.02753	119.33	-945.08422	6.79
B2H	-1505.64964	223.27	-1505.26793	170.28	-1505.34884	6.36
TS(B2H-B3H)	-2143.40019	328.10	-2142.83780	241.75	-2142.95266	2.67
B3H	-2143.43295	331.34	-2142.86588	235.66	-2142.97785	6.59
TS(B3H-B1H)	-2143.40966	331.23	-2142.84396	230.22	-2142.95335	5.78
B4H	-2.43.39959	328.43	-2142.83754	235.14	-2142.94926	5.82
B1-Ben	-1247.63787	66.01	-1247.52260	97.99	-1247.56916	8.46
B2-Ben	-1808.00363	149.33	-1807.74414	154.60	-1807.81760	7.64
TS(B2-Ben-B3-Ben)	-2445.72336	253.03	-2445.28619	207.70	-2445.38488	6.42
B3-Ben	-2445.75807	256.90	-2445.31437	214.55	-2445.41631	7.70
TS(B3-Ben-B1-Ben)	-2445.75417	256.87	-2445.31164	208.11	-2445.41051	6.63
B1-COT	-1326.24039	102.29	-1326.06532	105.02	-1326.11521	8.35
B2-COT	-1886.60695	185.49	-1886.28762	163.33	-1886.36523	6.38
TS(B2-COT-B3-COT)	-2524.32248	288.81	-2523.82590	224.19	-2523.93242	9.27
B3-COT	-2524.34839	291.66	-2523.84645	229.70	-2523.95558	9.59
TS(B3-COT-B1-COT)	-2524.34727	291.62	-2523.84619	225.20	-2523.95319	9.47
B1-Me	-564.24161	179.13	-563.93870	128.47	-563.99974	3.68
B2-Me	-1124.63573	263.95	-1124.18734	175.58	-1124.27077	3.41
TS(B2-Me-B3-Me)	-1762.30110	367.41	-1761.67452	241.22	-1761.78913	3.20
B3-Me	-1762.39725	371.70	-1761.76400	241.93	-1761.87895	3.87

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TS(B3-Me-B1-Me)	-1762.36982	370.82	-1761.73877	237.09	-1761.85141	3.67
B1-I	-507.37522	135.75	-507.14196	136.61	-507.20686	9.37
B2-I	-1067.74348	219.22	-1067.36619	184.31	-1067.45376	8.55
TS(B2-I-B3-I)	1705.44789	322.42	-1704.89332	242.96	-1705.00876	9.21
B3-I	-1705.48973	326.81	-1704.92793	249.94	-1705.04669	9.05
TS(B3-I-B1-I)	-1705.47822	326.56	-1704.91771	243.58	-1705.03345	8.67
TS(B2-BEN-B1H-Ben)	-1807.99317	149.44	-1807.73497	145.11	-1807.80392	5.89
B1H-Ben	-787.98984	69.62	-787.87005	90.50	-787.91305	6.46
B2H-Ben	-1348.37614	152.72	-1348.11277	143.55	-1348.18097	6.11
TS(B2H-Ben-B3H-Ben)	-1986.14458	257.99	-1985.70038	211.47	-1985.80085	4.97
B3H-Ben	-1986.16034	260.62	-1985.71183	211.68	-1985.81240	6.09
TS(B3H-Ben-B1H-Ben)	-1986.13973	260.61	-1985.69250	202.53	-1985.78872	4.68
TS(B2-COT-B1H-COT)	-1886.60550	185.12	-1886.28742	160.76	-1886.36380	6.91
B1H-COT	-866.59208	105.96	-866.41255	97.20	-866.45873	6.14
B2H-COT	-1426.98153	189.52	-1426.65750	152.75	-1426.73008	4.61
B3H-COT	-2064.76628	296.86	-2064.25846	213.44	-2064.35988	2.84
TS(B2-Me-B1H-Me)	-1124.60621	263.42	-1124.15947	173.80	-1124.24205	3.19
B1H-Me	-524.92614	161.10	-524.65391	119.90	-524.71087	3.71
B2H-Me	-1085.34004	245.46	-1084.92347	166.56	-1085.00261	4.66
TS(B2H-Me-B3H-Me)	-1723.01028	348.65	-1722.41471	240.35	-1722.52891	3.91
B3H-Me	-1723.11083	353.01	-1722.50896	234.27	-1722.62027	3.75
TS(B3H-Me-B1H-Me)	-1723.08117	352.63	-1722.48088	230.25	-1722.59028	4.79
TS(B2-I-B1H-I)	-1067.71648	218.68	-1067.34080	182.78	-1067.42764	6.79
B1H-I	-496.49674	139.76	-496.25887	123.14	-496.31737	7.36
B2H-I	-1056.88142	223.15	-1056.49970	173.57	-1056.58216	7.18
TS(B2H-I-B3H-I)	-1694.61999	326.54	-1694.06054	234.30	-1694.17186	4.23
B3H-I	-1694.67249	330.47	-1694.10606	245.50	-1694.22271	4.58
TS(B3H-I-B1H-I)	-1694.64111	331.24	-1694.07525	233.00	-1694.18596	6.48
R1	-560.36581	82.43	-560.22373	97.68	-560.27014	2.82
R2	-637.77374	103.74	-637.59485	114.45	-637.64923	2.15
P1	-1198.19087	189.47	-1197.86486	168.81	-1197.94506	2.03
Cl—Si	-1020.02712	78.38	-1019.89020	105.51	-1019.94033	1.76
Me—Si	-599.70078	100.09	-599.52848	108.27	-599.57992	2.04
I—Si	-571.22517	78.01	-571.08860	108.24	-571.14003	2.52
B5	-1583.06561	246.06	-1582.64551	184.06	-1582.73296	5.33

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TS(B5-B6)	-1583.06141	245.32	-1582.64303	179.21	-1582.72818	4.74
B6	-1583.06592	247.00	-1582.64381	189.93	-1582.73405	4.813
B7	-2143.43540	331.08	-2142.86849	241.61	-2142.98329	5.14
TS(B7-B1H)	-2143.39947	331.18	-2142.83368	229.81	-2142.94287	5.51

[a]Energy (E), enthalpy (H) and Gibbs free enthalpy (G) in Hartree. Zero-point energies (ZPE) in kcal/mol. Entropy (S) in e.u. Dipole moment (μ) in debye.

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3. Cartesian coordinates for all optimized structures in XYZ format.

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B1

Ru	-0.547640	-0.279421	0.062707
Cl	-2.428192	-1.153013	-0.995371
Cl	-0.063167	-2.365137	0.981214
C	-1.149550	1.867603	0.196707
C	-0.510971	1.652468	-1.046609
H	-1.053209	1.845655	-1.965351
C	0.747995	0.983984	-1.108965
H	1.140440	0.708843	-2.081146
C	1.492818	0.648075	0.073974
C	0.868096	0.900618	1.318678
H	1.333610	0.542377	2.230173
C	-0.456701	1.425103	1.375922
H	-0.963016	1.476662	2.334450
C	-2.538268	2.438154	0.283229
H	-3.075015	2.032746	1.144449
H	-3.113970	2.206485	-0.615129
H	-2.490621	3.528146	0.394946
C	2.867130	0.001979	0.015849
H	2.999004	-0.530284	0.965131
C	3.030963	-1.024848	-1.114845
H	4.008736	-1.508165	-1.028134
H	2.992309	-0.556730	-2.104805
H	2.261833	-1.799125	-1.060410
C	3.941138	1.107571	-0.068861
H	3.864620	1.812834	0.764851
H	3.847432	1.675914	-1.001179
H	4.941218	0.663487	-0.046755

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TS(B1-B2)

C	-0.095680	0.793579	-1.821697
C	-0.394458	2.065265	-1.221947
C	-1.549946	2.129680	-0.413608
C	-2.429260	1.004382	-0.255957
C	-2.161523	-0.225473	-0.893111
C	-0.953823	-0.321271	-1.665584
C	0.528769	3.241052	-1.396828
C	-3.045508	-1.450667	-0.743877
C	-3.900616	-1.614869	-2.019271
C	-3.915634	-1.446769	0.518928
Ru	-0.345456	0.429526	0.347310
Cl	-0.225994	-1.754848	1.400937
Cl	-0.547417	1.379731	2.559709
H	-1.746883	3.027010	0.161805
H	-3.260361	1.090856	0.431423
H	-0.663294	-1.277215	-2.085364
H	0.834135	0.670896	-2.366523
H	1.571583	2.915509	-1.376558
H	0.379537	3.976012	-0.602530
H	0.335806	3.732631	-2.358235
H	-2.365067	-2.307414	-0.672020
H	-4.439966	-2.403410	0.602976
H	-4.679979	-0.661821	0.486751
H	-3.305612	-1.314015	1.415949
H	-3.283466	-1.667876	-2.922102
H	-4.596948	-0.776954	-2.135791
H	-4.489376	-2.535439	-1.958809
H	1.242336	0.691737	0.853621
Si	2.346899	-0.249924	0.214119
O	3.087376	1.033580	-0.547353
C	3.229186	-0.831217	1.752097
O	2.257185	-1.406535	-0.965338
C	4.341583	0.918260	-1.214756
H	4.573932	1.886734	-1.666276
H	5.146439	0.664751	-0.512955
H	4.306250	0.157063	-2.002314
H	4.205060	-1.265320	1.507999
H	3.383236	0.015550	2.427654
H	2.627469	-1.576148	2.277479
C	2.139899	-2.819382	-0.805416
H	2.463364	-3.283531	-1.742020
H	2.775304	-3.188303	0.007723
H	1.105523	-3.093701	-0.586031

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B2

C	-0.048660	0.886443	-1.751224
C	-0.215571	2.138580	-1.074804
C	-1.319953	2.240141	-0.202316
C	-2.317823	1.206569	-0.110500
C	-2.188315	0.008528	-0.822436
C	-0.985748	-0.163993	-1.594501
C	0.782306	3.252011	-1.242574
C	-3.181490	-1.135824	-0.744220
C	-3.993683	-1.202591	-2.056052
C	-4.098790	-1.086052	0.482924
Ru	-0.193166	0.404058	0.429176
Cl	-0.296218	-1.840204	1.325679
Cl	-0.395056	1.171161	2.704637
H	-1.421798	3.117359	0.426324
H	-3.133388	1.340883	0.588416
H	-0.792623	-1.116532	-2.074247
H	0.837314	0.722951	-2.353955
H	1.796493	2.848352	-1.281640
H	0.718051	3.962657	-0.415389
H	0.584717	3.794729	-2.174944
H	-2.577024	-2.048229	-0.668005
H	-4.713831	-1.990181	0.516265
H	-4.783497	-0.230668	0.447746
H	-3.518410	-1.037798	1.408031
H	-3.346186	-1.286852	-2.934841
H	-4.614883	-0.308576	-2.179323
H	-4.655958	-2.073654	-2.041562
H	1.302646	0.737058	0.919732
Si	2.140433	-0.513767	0.060530
O	2.971950	0.722656	-0.714063
C	3.097938	-1.154098	1.537607
O	2.019489	-1.659057	-1.144943
C	4.221872	0.507232	-1.361422
H	4.518707	1.442112	-1.846305
H	5.004175	0.232256	-0.641887
H	4.149673	-0.279716	-2.120850
H	4.076785	-1.538645	1.229396
H	3.255677	-0.340858	2.252685
H	2.550114	-1.946583	2.050683
C	1.857500	-3.064959	-0.992562
H	2.178321	-3.539327	-1.925704
H	2.468199	-3.458667	-0.171807
H	0.812590	-3.314893	-0.790812

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TS(B2-B3)

C	2.074297	1.767143	1.289203
C	1.493352	0.718305	2.043624
C	0.077758	0.591117	1.944186
C	-0.683841	1.530934	1.197454
C	-0.100593	2.739214	0.669371
C	1.288122	2.814993	0.692865
Ru	0.840775	0.590683	-0.168537
Si	1.882506	-1.545261	-0.332453
O	3.472459	-1.613692	0.214659
C	4.668599	-1.497324	-0.538450
H	-0.413277	-0.249929	2.420856
H	1.808324	3.619527	0.187725
Cl	2.645089	0.891118	-1.767678
O	1.179183	-2.564711	0.870486
C	1.763725	-3.811245	1.219234
C	1.754963	-2.466784	-1.980206
Cl	-0.572887	0.670256	-2.145763
H	-1.751226	1.374186	1.080369
C	-1.004800	3.763748	0.010745
H	3.154973	1.825152	1.219583
C	2.321592	-0.196902	2.903537
C	-1.064473	-3.022796	0.219681
H	1.159709	-4.270360	2.010543
H	1.796896	-4.503705	0.366055
H	2.784948	-3.668374	1.585856
H	2.287269	-1.909463	-2.754184
H	2.179358	-3.475871	-1.919427
H	0.714072	-2.544106	-2.307705
H	5.486411	-1.915252	0.060123
H	4.615165	-2.053945	-1.482926
H	4.888532	-0.451796	-0.772811
H	-0.630504	-3.777515	-0.428695
H	-1.191726	-3.316346	1.256560
C	-1.515319	-1.790128	-0.261742
Si	-3.196529	-1.244447	0.469570
H	-0.634247	-0.905641	-0.009658
H	-1.483231	-1.704377	-1.351039
O	-4.356515	-2.209532	-0.224154
C	-3.307565	-1.483459	2.319829
O	-3.546310	0.353597	0.208097
H	-4.356777	-1.386692	2.616599
H	-2.965407	-2.472089	2.639075
H	-2.739931	-0.726384	2.868857
C	-4.042325	0.916839	-1.009264
H	-4.390148	1.930048	-0.788132
H	-3.249098	0.963482	-1.761604

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H	-4.890894	0.336398	-1.389592
C	-4.360867	-2.821041	-1.503940
H	-5.242846	-3.464533	-1.568475
H	-4.412765	-2.079575	-2.310840
H	-3.468554	-3.441031	-1.658638
H	1.826181	-1.159946	3.036530
H	3.296779	-0.381281	2.449074
H	2.468458	0.262452	3.888795
C	-1.825627	4.514190	1.081151
C	-0.267941	4.740210	-0.913201
H	-1.701170	3.184866	-0.610189
H	-2.537849	5.194931	0.603835
H	-2.392182	3.825768	1.716171
H	-1.171904	5.109729	1.728397
H	-0.990498	5.393042	-1.412410
H	0.421749	5.386262	-0.356940
H	0.295302	4.207494	-1.684447

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B3

C	-2.938419	0.288371	0.843826
C	-1.946677	0.519059	1.834320
C	-1.152809	-0.553787	2.321693
C	-1.357670	-1.817412	1.718734
C	-2.472340	-2.070620	0.851129
C	-3.302873	-1.035829	0.421843
Ru	-0.955482	-0.380106	-0.015207
Si	-0.470620	2.031766	-0.339401
O	-1.975875	2.795105	-0.250744
C	-2.080593	4.201709	-0.100182
C	-0.118385	-0.341277	3.390702
C	-4.459327	-1.212282	-0.543278
C	-4.418217	-2.532254	-1.322758
C	-5.800457	-1.033843	0.200026
Cl	-1.632484	0.304907	-2.232339
O	0.279788	2.629351	1.066589
C	1.459083	3.405655	1.149988
C	0.472606	2.685007	-1.845778
Cl	-0.038061	-2.283954	-1.219054
H	-0.692798	-2.638803	1.963473
H	-2.595951	-3.072651	0.460264
H	-3.452261	1.146319	0.428381
H	-1.772934	1.526569	2.193188
H	0.230656	0.693502	3.396478
H	0.740776	-1.001704	3.250813
H	-0.555530	-0.560959	4.372040
H	-4.359721	-0.395627	-1.269877
H	-5.218319	-2.542698	-2.068804
H	-4.574668	-3.398350	-0.668683
H	-3.465207	-2.653333	-1.845273
H	-5.852922	-0.073321	0.722787
H	-5.949438	-1.829219	0.938995
H	-6.631617	-1.074837	-0.510883
C	1.215216	-0.186958	0.434041
H	1.648940	3.630167	2.205510
H	2.334721	2.874884	0.754288
H	1.366211	4.359936	0.613734
H	-0.211426	3.319813	-2.418287
H	1.348115	3.282612	-1.573455
H	0.784953	1.875426	-2.505157
H	-3.142575	4.460619	-0.038029
H	-1.580542	4.551295	0.812593
H	-1.652742	4.738685	-0.958679
H	1.311106	0.566241	1.215390
H	1.341562	-1.179174	0.865597
C	2.251964	0.008730	-0.663020
Si	4.009651	-0.354146	-0.101932

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H	2.054123	-0.663411	-1.504263
H	2.250048	1.026377	-1.065360
O	4.914558	-0.511549	-1.492334
C	4.765419	0.986583	0.991262
O	3.945900	-1.780228	0.761165
H	5.742932	0.696836	1.392436
H	4.900405	1.925816	0.443197
H	4.112708	1.188460	1.847256
C	5.064666	-2.574507	1.107501
H	4.723417	-3.391603	1.750996
H	5.536322	-3.013984	0.218967
H	5.826078	-2.003526	1.659472
C	6.311071	-0.344526	-1.644648
H	6.526282	-0.180694	-2.705373
H	6.693573	0.517909	-1.081865
H	6.861260	-1.238133	-1.320239

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TS(B3-B1)

C	-3.096178	0.570252	0.361816
C	-2.290807	1.099077	1.397936
C	-1.645964	0.243276	2.353258
C	-1.835458	-1.143691	2.204398
C	-2.684785	-1.671392	1.175160
C	-3.340638	-0.838805	0.244358
Ru	-1.107158	-0.401463	0.207836
Si	-0.030706	1.947964	-0.503809
O	-1.537906	2.525634	-1.013518
C	-1.735477	3.892342	-1.338417
C	-0.768270	0.819248	3.429530
C	-4.212884	-1.357262	-0.885092
C	-3.953640	-2.824881	-1.247319
C	-5.697752	-1.111510	-0.543109
Cl	-1.042785	-0.308080	-2.208097
O	0.161987	2.926781	0.881962
C	1.317860	3.660470	1.238156
C	1.172705	2.550044	-1.828935
Cl	-0.042346	-2.617110	-0.019422
H	-1.285942	-1.836225	2.831516
H	-2.720816	-2.745250	1.051034
H	-3.470272	1.244492	-0.397314
H	-2.108288	2.164996	1.435711
H	-0.233408	1.693081	3.051496
H	-0.045646	0.082434	3.789218
H	-1.381537	1.136195	4.281777
H	-3.954869	-0.749466	-1.760599
H	-4.531899	-3.088109	-2.138115
H	-4.267437	-3.504673	-0.446214
H	-2.896209	-2.999378	-1.462674
H	-5.899269	-0.056684	-0.329395
H	-6.003112	-1.697559	0.331202
H	-6.330127	-1.410278	-1.384913
C	1.193293	0.308220	0.207520
H	1.087118	4.256285	2.127696
H	2.170484	3.008590	1.484901
H	1.634580	4.344157	0.439848
H	0.944710	3.601051	-2.037990
H	2.224217	2.488585	-1.538683
H	1.033848	1.992218	-2.757806
H	-2.814347	4.081398	-1.366050
H	-1.288234	4.563354	-0.593138
H	-1.326014	4.136608	-2.327426
H	1.637827	1.183598	0.692591
H	1.090089	-0.376927	1.050829
C	2.123585	-0.311374	-0.838331
Si	3.895612	-0.483393	-0.246592

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H	1.774179	-1.316917	-1.082115
H	2.132525	0.241000	-1.780313
O	4.604952	-1.644621	-1.204496
C	4.896871	1.114670	-0.351810
O	3.807741	-0.963201	1.349698
H	5.903716	1.003503	0.065788
H	5.006282	1.451224	-1.388907
H	4.405130	1.917725	0.208459
C	4.872541	-1.532192	2.088811
H	4.532445	-1.695064	3.116428
H	5.177983	-2.500482	1.671967
H	5.753318	-0.873597	2.124077
C	5.977567	-1.804242	-1.507715
H	6.065403	-2.513848	-2.336134
H	6.448233	-0.860604	-1.814868
H	6.539225	-2.207062	-0.653713

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B4

C	-2.514484	-0.003856	2.412252
C	-1.560333	-0.882418	2.967803
C	-1.106099	-1.992223	2.272125
C	-1.609076	-2.202960	0.956588
C	-2.563635	-1.321054	0.406532
C	-3.047087	-0.204849	1.147054
C	-0.158085	-2.989816	2.883283
C	-4.148913	0.691434	0.599986
C	-3.708030	1.466608	-0.655890
C	-5.445744	-0.099875	0.337625
Ru	-0.558626	-0.933901	-1.022924
Si	2.790392	-0.840526	0.146665
O	3.963999	0.352573	0.188088
C	5.356944	0.182172	-0.028250
Cl	-0.152474	0.077226	-3.110735
O	2.469794	-1.359596	1.700014
C	3.477786	-1.732502	2.629863
C	3.336004	-2.246679	-0.964472
Cl	-1.159481	-2.837028	-2.235033
H	-1.425473	-3.149564	0.460780
H	-3.075398	-1.618883	-0.504702
H	-2.861402	0.838486	3.005518
H	-1.202645	-0.701701	3.978408
H	0.002492	-2.784879	3.945494
H	0.811736	-2.952216	2.378071
H	-0.547091	-4.010021	2.789147
H	-4.367212	1.429955	1.382271
H	-4.518297	2.115048	-1.006493
H	-3.451711	0.790681	-1.479392
H	-2.839320	2.096758	-0.444232
H	-5.778626	-0.630473	1.235333
H	-5.311794	-0.838819	-0.459952
H	-6.247167	0.577573	0.024575
H	0.396798	-1.962627	-0.409792
H	2.988231	-2.101859	3.535615
H	4.121129	-2.533111	2.239538
H	4.106562	-0.874868	2.898539
H	4.253662	-2.728303	-0.609631
H	2.557366	-3.012003	-1.029818
H	3.518316	-1.883358	-1.981673
H	5.812867	1.172303	-0.120281
H	5.837109	-0.338321	0.811121
H	5.563635	-0.378610	-0.948028
C	1.271432	0.034044	-0.499729
C	0.325389	0.816335	0.338755
H	1.554480	0.543920	-1.421846

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Si	0.550391	2.714087	0.386152
H	-0.731701	0.789335	-0.116606
H	0.237078	0.435225	1.359110
O	-0.860330	3.232441	1.088360
C	2.062030	3.115172	1.418252
O	0.608370	3.414467	-1.103847
H	2.253695	4.193113	1.441382
H	1.917653	2.773567	2.448854
H	2.951145	2.610831	1.026036
C	1.632805	3.385452	-2.091715
H	1.436707	2.579020	-2.805116
H	1.621382	4.341780	-2.623404
H	2.628812	3.245380	-1.652362
C	-1.205364	4.605651	1.241638
H	-2.201767	4.656389	1.689370
H	-0.501908	5.125406	1.905556
H	-1.225424	5.120347	0.274784

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TS(B2-B1H)

C	-0.598695	1.454382	-1.476735
C	-0.814183	2.321832	-0.354549
C	-1.827342	1.956341	0.571683
C	-2.657323	0.800031	0.362643
C	-2.446755	-0.058996	-0.724767
C	-1.356788	0.270327	-1.614575
C	0.041517	3.544091	-0.155627
C	-3.245090	-1.328600	-0.969248
C	-4.294352	-1.078551	-2.073611
C	-3.892656	-1.909088	0.294756
Ru	-0.435158	0.278350	0.402290
Cl	0.682709	-1.905582	0.114160
Cl	-0.492256	-0.174886	2.763799
H	-1.955961	2.537837	1.477062
H	-3.374818	0.539199	1.130578
H	-1.103261	-0.426879	-2.407164
H	0.227306	1.650522	-2.149999
H	1.079328	3.323879	-0.415877
H	0.005909	3.883238	0.882218
H	-0.315828	4.360577	-0.794846
H	-2.531115	-2.071140	-1.349467
H	-4.335585	-2.883850	0.069222
H	-4.699086	-1.267651	0.667762
H	-3.159101	-2.042454	1.095001
H	-3.834351	-0.706706	-2.994945
H	-5.035109	-0.340863	-1.745863
H	-4.823894	-2.006515	-2.311763
H	1.095706	0.698089	0.790950
Si	2.382370	-0.273291	0.036290
O	2.573096	1.199904	-0.760191
C	3.161864	-0.412531	1.736511
O	3.252916	-1.184888	-1.068537
C	3.662772	1.491997	-1.634531
H	3.534575	2.521264	-1.985312
H	4.627530	1.419809	-1.117586
H	3.682030	0.814506	-2.492351
H	3.782856	-1.310092	1.815789
H	3.798302	0.463147	1.904879
H	2.392835	-0.441562	2.511907
C	3.577546	-2.559350	-0.995296
H	4.411953	-2.746411	-1.679022
H	3.884845	-2.863733	0.014137
H	2.729280	-3.183744	-1.297900

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B1H

Cl	-0.857078	0.507913	-0.222830
H	-0.413126	2.768394	-0.001631
C	-2.241006	0.892576	-0.909050
C	-1.539646	-1.530192	0.284142
C	-0.779567	-0.947771	1.351482
C	0.633273	-0.672441	1.238608
C	1.239766	-0.678293	-0.010553
C	0.384119	-0.985027	-1.142694
C	-0.920780	-1.545315	-0.990025
C	-2.948417	-2.013569	0.497893
C	2.684498	-0.285376	-0.261876
C	3.264802	0.659917	0.798176
H	3.549336	-1.554469	-0.421776
H	-1.261115	-0.813724	2.315256
H	1.167870	-0.323656	2.114250
H	0.793573	-0.889702	-2.144099
H	-1.481243	-1.853168	-1.865345
H	-3.537601	-1.933625	-0.418415
H	-3.448591	-1.431649	1.276339
H	-2.945248	-3.064393	0.812600
H	2.696277	0.246146	-1.222917
H	4.266285	0.983559	0.498502
H	3.364294	0.166347	1.771680
H	2.638991	1.548487	0.920785
H	3.160657	-2.215794	-1.203256
H	3.581038	-2.123098	0.514130
Cl	4.576081	-1.283952	-0.688484

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B2H

C	1.042594	1.561081	1.320140
C	1.539990	2.293685	0.199416
C	2.323215	1.570838	-0.755784
C	2.485741	0.186705	-0.652743
C	1.986859	-0.550056	0.478053
C	1.323686	0.174268	1.481670
Ru	0.135629	0.711823	-0.539573
Cl	-0.531665	-0.948735	-2.154889
C	1.375224	3.789353	0.105358
C	2.252164	-2.038496	0.661973
C	3.509908	-2.237330	1.535587
C	2.366979	-2.821171	-0.654352
H	-1.234719	1.513131	-0.530394
H	2.717846	2.091451	-1.622694
H	2.985735	-0.344307	-1.453075
H	0.941000	-0.348657	2.352600
H	0.485419	2.086065	2.087531
H	0.470705	4.117660	0.622895
H	1.307800	4.113899	-0.935848
H	2.230888	4.299834	0.564390
H	1.392698	-2.437150	1.215427
H	2.411786	-3.893552	-0.439779
H	3.284386	-2.566800	-1.198141
H	1.512330	-2.629120	-1.308163
H	3.415662	-1.737670	2.505119
H	4.399830	-1.837838	1.035968
H	3.679109	-3.303476	1.718666
H	-0.295886	1.584416	-1.766359
Si	-1.933971	0.054382	0.541242
C	-2.259296	1.021512	2.135468
O	-3.255207	0.220236	-0.464897
O	-1.844382	-1.509771	1.131410
H	-3.220639	0.716936	2.563786
H	-1.496908	0.828455	2.897115
H	-2.298732	2.099874	1.950161
C	-4.564299	-0.206615	-0.126678
C	-1.911816	-2.723485	0.393909
H	-5.206622	-0.054486	-0.999305
H	-4.595287	-1.269872	0.143717
H	-4.979169	0.372256	0.710485
H	-2.228333	-3.515490	1.081985
H	-2.625425	-2.661681	-0.434248
H	-0.936227	-2.982399	-0.029089

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TS(B2H-B3H)

C	1.347367	1.706197	0.650434
C	0.522215	1.610199	1.802564
C	-0.556261	2.540077	1.996697
C	-0.786357	3.479374	1.015464
C	0.029826	3.565812	-0.145209
C	1.099824	2.714948	-0.336737
Ru	0.074239	-0.318968	0.679648
Si	2.806763	-1.799513	0.376748
O	2.569523	-2.066731	-1.230259
C	1.920508	-3.183704	-1.838559
C	-1.392928	2.459525	3.246766
C	2.088349	2.854325	-1.488609
C	1.496473	3.499855	-2.749662
C	3.347029	3.621370	-1.028292
Cl	-0.632247	-2.592463	0.714031
O	4.066903	-0.732131	0.502392
C	5.318527	-0.881333	-0.162205
C	3.011452	-3.369449	1.365259
H	1.780547	-0.954972	1.115759
H	-1.602293	4.188154	1.136430
H	-0.185852	4.345202	-0.869696
H	2.324717	1.233540	0.642481
H	0.892165	1.081781	2.686102
H	-1.982582	1.535120	3.265080
H	-2.086493	3.301662	3.318591
H	-0.765467	2.458856	4.146434
H	2.407989	1.837647	-1.755469
H	2.222757	3.464177	-3.568010
H	1.246993	4.553957	-2.585303
H	0.588491	2.985222	-3.079314
H	3.811782	3.146110	-0.159046
H	3.090953	4.649890	-0.750482
H	4.092055	3.661115	-1.830817
C	-0.348100	-0.119573	-1.360115
H	5.898013	0.031060	0.001914
H	5.886030	-1.729080	0.243018
H	5.181795	-1.027686	-1.239071
H	3.790510	-4.013867	0.943716
H	3.285495	-3.132068	2.398035
H	2.068170	-3.923166	1.382082
H	2.024842	-3.074356	-2.921301
H	2.389143	-4.127772	-1.534956
H	0.860488	-3.213314	-1.571779
H	0.316015	0.562406	-1.886168
H	-0.436891	-1.098097	-1.828113
C	-1.489014	0.413786	-0.653839
Si	-3.265372	-0.187957	-0.869453

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H	-1.427567	0.097701	0.945570
H	-1.498532	1.504084	-0.587277
O	-3.913709	-0.197939	0.666139
C	-4.122607	1.068277	-1.973781
O	-3.474101	-1.630469	-1.651084
H	-5.180473	0.821873	-2.110367
H	-4.057861	2.079286	-1.558047
H	-3.660667	1.081940	-2.966554
C	-3.502291	-2.952625	-1.125477
H	-4.358343	-3.477379	-1.565039
H	-2.581961	-3.481089	-1.388082
H	-3.591550	-2.961003	-0.035263
C	-5.290821	-0.385935	0.950780
H	-5.441788	-0.240113	2.024547
H	-5.922075	0.334537	0.413297
H	-5.624427	-1.398951	0.691517

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B3H

C	-1.570406	1.288978	1.387549
C	-2.820203	0.840813	0.872920
C	-3.354113	1.368483	-0.343747
C	-2.518425	2.224310	-1.074178
C	-1.296242	2.737132	-0.518931
C	-0.850706	2.355309	0.750197
Ru	-1.233488	0.282526	-0.583812
Si	-1.548189	-1.978094	0.210823
O	-0.946815	-2.153047	1.776643
C	0.118945	-2.996874	2.181612
C	-4.701368	0.922871	-0.846174
C	0.353025	2.970396	1.448854
C	1.123860	3.989889	0.599595
C	-0.090601	3.620057	2.778599
Cl	-0.493076	0.113393	-2.881404
O	-3.216400	-2.166631	0.430335
C	-3.763357	-3.272408	1.133682
C	-0.923813	-3.406954	-0.852420
H	-2.025682	-0.923833	-1.220107
H	-2.810564	2.541640	-2.069166
H	-0.726258	3.443148	-1.110058
H	-1.213693	0.875004	2.324157
H	-3.383514	0.091220	1.415327
H	-4.856818	-0.137087	-0.630546
H	-4.794240	1.080730	-1.923294
H	-5.496873	1.491947	-0.349596
H	1.033843	2.144026	1.696079
H	2.002315	4.339898	1.149870
H	0.507120	4.867540	0.374944
H	1.472055	3.566857	-0.346557
H	-0.598322	2.908822	3.436024
H	-0.774862	4.455311	2.593097
H	0.779941	4.010243	3.315253
C	0.758523	-0.422519	-0.056378
H	-4.839877	-3.108571	1.249029
H	-3.620628	-4.213341	0.584437
H	-3.314923	-3.377987	2.129102
H	-1.234247	-4.372402	-0.435940
H	-1.342888	-3.320105	-1.859403
H	0.164730	-3.421962	-0.952966
H	0.186654	-2.957583	3.274201
H	-0.049848	-4.041846	1.889282
H	1.079552	-2.673471	1.762237
H	0.794956	-0.370708	1.037394
H	0.913660	-1.466421	-0.331400
C	1.913236	0.372836	-0.680589
Si	3.593182	-0.198415	-0.071293

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H	1.897501	0.274886	-1.769891
H	1.838006	1.447025	-0.474062
O	4.727184	0.387084	-1.145828
C	4.019109	0.398305	1.669939
O	3.542030	-1.869295	-0.070642
H	4.954789	-0.030250	2.045566
H	4.121279	1.488859	1.704362
H	3.228975	0.112417	2.372630
C	4.647802	-2.726416	0.140854
H	4.277609	-3.751325	0.245911
H	5.344391	-2.701298	-0.707544
H	5.204691	-2.472609	1.054994
C	6.115124	0.553816	-0.929224
H	6.511573	1.206238	-1.713815
H	6.333474	1.017741	0.042572
H	6.651671	-0.403504	-0.981004

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TS(B3H-B1H)

C	-2.132635	0.914551	1.431915
C	-3.114367	0.005046	0.969931
C	-3.694691	0.176332	-0.325204
C	-3.258949	1.293672	-1.086560
C	-2.394667	2.301592	-0.527507
C	-1.836254	2.151166	0.741434
Ru	-1.481228	0.108106	-0.537719
Si	-0.399412	-2.149954	0.250596
O	0.443629	-2.678117	1.622067
C	1.816277	-2.894984	1.855861
C	-4.698355	-0.810120	-0.860057
C	-0.891608	3.152696	1.384270
C	-0.276116	4.153441	0.397746
C	-1.607219	3.887405	2.538300
Cl	-0.546635	0.368428	-2.755376
O	-1.915408	-2.679585	0.824807
C	-2.059133	-3.894712	1.549256
C	0.111478	-3.216346	-1.223684
H	-1.640735	-1.364325	-1.076745
H	-3.595750	1.403279	-2.110920
H	-2.114584	3.138891	-1.155852
H	-1.637442	0.709831	2.376761
H	-3.325326	-0.892051	1.535883
H	-4.462544	-1.819113	-0.515222
H	-4.706882	-0.807383	-1.952451
H	-5.705138	-0.550703	-0.510412
H	-0.070777	2.569068	1.826224
H	0.470507	4.769279	0.908369
H	-1.032126	4.833538	-0.010709
H	0.213925	3.648540	-0.440429
H	-2.013616	3.187705	3.275163
H	-2.436852	4.492129	2.155566
H	-0.910891	4.555428	3.055395
C	0.755741	-0.342072	0.190188
H	-3.125573	-4.034078	1.761129
H	-1.713167	-4.761111	0.968012
H	-1.504041	-3.873973	2.491961
H	-0.692223	-3.937835	-1.408245
H	0.241322	-2.619867	-2.129538
H	1.030280	-3.784320	-1.044609
H	1.919022	-3.444370	2.799270
H	2.281868	-3.500774	1.064234
H	2.380368	-1.957593	1.944500
H	0.544760	0.708156	-0.045906
H	0.959095	-0.353281	1.261926
C	1.984438	-0.723675	-0.664836
Si	3.513345	0.295085	-0.292233

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H	2.275044	-1.771890	-0.553223
H	1.739127	-0.585463	-1.723033
O	4.770964	-0.483272	-1.059743
C	3.401891	2.084126	-0.868943
O	3.690499	0.250528	1.371332
H	4.299567	2.667053	-0.635870
H	3.242481	2.132180	-1.951227
H	2.554613	2.585087	-0.389094
C	4.751437	0.836217	2.103271
H	4.478314	0.847526	3.163382
H	5.679398	0.258879	1.996056
H	4.950433	1.872151	1.793560
C	6.022053	0.055934	-1.444542
H	6.469015	-0.607666	-2.191262
H	5.925492	1.054853	-1.889807
H	6.711413	0.122411	-0.591632

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B4H

C	2.828701	-0.569073	-2.094397
C	1.894418	-1.510380	-2.567282
C	1.356176	-2.481310	-1.732468
C	1.757598	-2.482865	-0.370135
C	2.676131	-1.519293	0.105554
C	3.250968	-0.553888	-0.771723
C	0.412688	-3.537426	-2.244812
C	4.283185	0.458980	-0.293952
C	3.624422	1.630347	0.463406
C	5.406415	-0.177838	0.544242
Ru	0.765622	-0.817713	1.290132
Si	-2.562517	-1.110638	0.212052
O	-3.829954	-0.022539	0.046580
C	-5.190485	-0.235938	0.384650
Cl	0.378262	0.482153	3.216645
O	-2.303098	-1.859732	-1.262314
C	-3.350814	-2.350178	-2.085791
C	-3.005072	-2.365114	1.537738
H	0.997644	-1.898472	2.392117
H	1.512538	-3.339709	0.246751
H	3.118445	-1.670969	1.093846
H	3.242606	0.156666	-2.790259
H	1.615857	-1.495873	-3.617897
H	0.389410	-3.552690	-3.338104
H	-0.601196	-3.340505	-1.881776
H	0.707430	-4.534045	-1.897124
H	4.746091	0.875770	-1.198126
H	4.378581	2.367715	0.759736
H	3.128246	1.286758	1.379574
H	2.880213	2.138424	-0.157788
H	5.873130	-1.017418	0.019279
H	5.037436	-0.543357	1.508768
H	6.183054	0.563484	0.758197
H	-0.171738	-2.032535	1.348729
H	-2.904402	-2.801669	-2.977058
H	-3.947181	-3.120685	-1.577056
H	-4.019575	-1.540997	-2.403602
H	-3.971334	-2.842968	1.341521
H	-2.251064	-3.154558	1.601753
H	-3.060943	-1.884268	2.520353
H	-5.732369	0.702531	0.232439
H	-5.657221	-1.003276	-0.248153
H	-5.310646	-0.534294	1.433717
C	-1.077870	-0.057702	0.619378
C	-0.300012	0.665046	-0.456983
H	-1.387829	0.610070	1.428236
Si	-0.799426	2.453523	-0.863386

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H	0.762805	0.842249	-0.137904
H	-0.238083	0.086085	-1.383059
O	0.493139	2.988477	-1.762979
C	-2.404457	2.514806	-1.831120
O	-0.851188	3.431158	0.470072
H	-2.709710	3.545716	-2.039285
H	-2.286277	1.995384	-2.788338
H	-3.209097	2.014828	-1.282933
C	-1.804245	3.463456	1.524625
H	-1.465377	2.837260	2.356819
H	-1.894874	4.496868	1.874735
H	-2.795861	3.120815	1.201248
C	0.625461	4.326079	-2.225597
H	1.563632	4.402729	-2.783305
H	-0.196746	4.606228	-2.898211
H	0.653335	5.035907	-1.390830

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Ru	0.121151	-0.000944	-0.001254
Cl	1.756203	1.632334	0.205026
Cl	1.755981	-1.633379	-0.214494
C	-1.582053	1.268510	-0.655222
C	-1.594006	1.215415	0.753718
H	-1.502366	2.127214	1.331756
C	-1.516157	-0.052807	1.406663
H	-1.391357	-0.095281	2.483089
C	-1.582852	-1.269417	0.654162
C	-1.595143	-1.216280	-0.754672
H	-1.504505	-2.127972	-1.333042
C	-1.516676	0.051907	-1.407833
H	-1.392277	0.094505	-2.484280
H	-1.487078	2.221524	-1.162253
H	-1.488792	-2.222483	1.161269

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B2-Ben

C	-0.564213	0.612964	-2.012694
C	-0.634001	1.900030	-1.392416
C	-1.719145	2.207918	-0.546345
C	-2.786533	1.260094	-0.368808
C	-2.719235	0.002164	-0.975025
C	-1.575033	-0.344278	-1.770034
H	0.189687	2.594749	-1.505321
H	-3.469670	-0.748488	-0.757019
Ru	-0.767668	0.333536	0.214419
Cl	-0.805855	-1.896273	1.147764
Cl	-1.031679	1.146016	2.466845
H	-1.734659	3.140227	0.004333
H	-3.585077	1.484467	0.328457
H	-1.473612	-1.348058	-2.163601
H	0.304071	0.341721	-2.600240
H	0.742062	0.584351	0.790449
Si	1.711533	-0.490757	-0.023668
O	2.472133	0.791385	-0.774169
C	2.633803	-1.116466	1.477292
O	1.615238	-1.634755	-1.223602
C	3.728011	0.660930	-1.433776
H	3.974289	1.626118	-1.885549
H	4.526654	0.399612	-0.727381
H	3.690388	-0.101226	-2.220653
H	3.595796	-1.554968	1.189072
H	2.823214	-0.288272	2.166864
H	2.044864	-1.868012	2.007091
C	1.530091	-3.050005	-1.069562
H	1.785806	-3.501766	-2.032859
H	2.234271	-3.417071	-0.313741
H	0.520037	-3.344343	-0.774853

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TS(B2-Ben-B3-Ben)

C	2.333639	-1.725033	-1.440696
C	1.565566	-0.729552	-2.091406
C	0.150277	-0.851322	-2.077957
C	-0.447963	-1.970611	-1.442110
C	0.349378	-3.082916	-1.012043
C	1.728359	-2.951398	-0.989321
Ru	0.900673	-0.879958	0.052451
Si	1.718211	1.347581	0.206832
O	3.282498	1.531569	-0.378397
C	4.498198	1.546161	0.352795
H	-0.463265	-0.062770	-2.497548
H	2.354120	-3.724340	-0.557060
Cl	2.679333	-0.981421	1.693019
O	0.898908	2.251265	-1.008280
C	1.344002	3.539207	-1.410120
C	1.529788	2.289748	1.834576
Cl	-0.537122	-1.204621	1.984362
H	-1.526869	-2.009133	-1.346293
H	-0.131729	-3.964022	-0.603374
H	3.403100	-1.587463	-1.337872
H	2.045249	0.141893	-2.519295
C	-1.394491	2.489529	-0.290306
H	0.688826	3.898418	-2.211997
H	1.306965	4.263592	-0.584046
H	2.372369	3.494612	-1.782524
H	2.131774	1.811435	2.610144
H	1.847664	3.334668	1.737930
H	0.492551	2.272816	2.182038
H	5.274556	1.973423	-0.291950
H	4.424784	2.163556	1.257429
H	4.791386	0.535971	0.653072
H	-1.027000	3.302151	0.329103
H	-1.575556	2.741733	-1.330075
C	-1.684667	1.225152	0.226460
Si	-3.319805	0.468387	-0.430359
H	-0.721792	0.442347	-0.055357
H	-1.603332	1.163185	1.313987
O	-4.530316	1.054529	0.540066
C	-3.678931	1.007874	-2.184189
O	-3.356384	-1.187169	-0.465699
H	-4.657013	0.613922	-2.476832
H	-3.713688	2.096451	-2.284469
H	-2.943321	0.618634	-2.895862
C	-3.762799	-2.059430	0.593909
H	-3.949433	-3.044862	0.157033
H	-2.973977	-2.137258	1.347804
H	-4.691086	-1.704149	1.054987

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C	-4.479539	1.334420	1.932928
H	-5.495845	1.559699	2.267981
H	-4.100926	0.484345	2.512800
H	-3.845922	2.205916	2.139701

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B3-Ben

C	3.412488	-0.659569	-0.746803
C	2.512335	-0.290266	-1.782353
C	1.506355	-1.204084	-2.177196
C	1.408671	-2.452404	-1.524549
C	2.441653	-2.884513	-0.625644
C	3.445981	-2.001063	-0.253029
Ru	1.287901	-0.826898	0.081007
Si	1.313955	1.663245	0.202258
O	2.949852	2.068544	0.134064
C	3.372821	3.398679	-0.123605
H	0.760743	-0.910819	-2.907225
H	4.180578	-2.281353	0.492853
Cl	1.997830	-0.070567	2.258995
O	0.773183	2.269156	-1.289455
C	-0.245149	3.221153	-1.528530
C	0.458444	2.630184	1.584654
Cl	-0.045345	-2.368912	1.386252
H	0.578210	-3.114244	-1.740332
H	2.372364	-3.866198	-0.171657
H	4.101784	0.082933	-0.366445
H	2.556889	0.699532	-2.218751
C	-0.769558	-0.238952	-0.521574
H	-0.334787	3.362719	-2.611143
H	-1.221155	2.892565	-1.148660
H	-0.012996	4.196066	-1.078630
H	1.232487	3.149370	2.159020
H	-0.244588	3.376255	1.201701
H	-0.063569	1.968011	2.275024
H	4.467144	3.408881	-0.151024
H	2.993650	3.766901	-1.085858
H	3.049262	4.090789	0.666357
H	-0.664479	0.443110	-1.365864
H	-1.090108	-1.215825	-0.882074
C	-1.780055	0.270755	0.495720
Si	-3.559555	0.193828	-0.107986
H	-1.745214	-0.335186	1.406845
H	-1.589709	1.305230	0.797362
O	-4.510598	0.390713	1.245941
C	-4.002623	1.508790	-1.387167
O	-3.759960	-1.314665	-0.788930
H	-5.012197	1.373230	-1.790781
H	-3.950816	2.518825	-0.965132
H	-3.307951	1.462856	-2.232640
C	-5.007160	-1.926164	-1.061973
H	-4.822053	-2.873948	-1.577039
H	-5.559500	-2.140619	-0.138002
H	-5.641769	-1.305109	-1.711545

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C	-5.841031	0.869015	1.308510
H	-6.066881	1.123219	2.348832
H	-5.989583	1.769185	0.696791
H	-6.561682	0.107584	0.980383

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TS(B3-Ben-B1-Ben)

C	-3.552363	-0.640942	0.095900
C	-3.008270	-0.102327	1.283395
C	-2.108802	-0.881345	2.073624
C	-1.834274	-2.218023	1.720183
C	-2.460702	-2.778804	0.560931
C	-3.304349	-2.004503	-0.256309
Ru	-1.344703	-0.907701	-0.048677
Si	-0.896726	1.715179	0.032731
O	-2.461269	2.199221	-0.384718
C	-2.913427	2.769198	-1.602650
H	-1.599938	-0.414359	2.908884
H	-3.686021	-2.409216	-1.185630
Cl	-1.264691	-0.058158	-2.314645
O	-0.931599	2.100749	1.683307
C	-1.491404	3.309901	2.176403
C	0.208505	2.941712	-0.882955
Cl	0.202557	-2.635713	-0.846798
H	-1.108860	-2.801272	2.273732
H	-2.171826	-3.770968	0.237926
H	-4.124545	-0.002000	-0.564414
H	-3.188689	0.933106	1.530496
C	0.707698	0.231952	0.401398
H	-1.473197	3.270052	3.270415
H	-0.906771	4.183552	1.857673
H	-2.524989	3.448472	1.838879
H	-0.251142	3.931157	-0.774860
H	1.215808	2.994251	-0.464785
H	0.284426	2.725118	-1.950540
H	-3.903523	3.202342	-1.420403
H	-2.251416	3.570258	-1.954675
H	-2.985979	2.011568	-2.388022
H	0.862048	1.031379	1.133851
H	0.780707	-0.661637	1.022090
C	1.788540	0.194015	-0.677811
Si	3.528357	0.230819	0.024918
H	1.702857	-0.730540	-1.252348
H	1.703429	1.008052	-1.401051
O	4.531645	-0.279783	-1.200760
C	4.075598	1.933961	0.627725
O	3.529293	-0.828026	1.314165
H	5.054741	1.910834	1.118986
H	4.139208	2.650660	-0.198735
H	3.359719	2.327931	1.357613
C	4.686936	-1.309384	1.970584
H	4.374827	-1.872319	2.855974
H	5.264001	-1.982247	1.323026
H	5.347040	-0.494373	2.302587

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C	5.907573	-0.006452	-1.380255
H	6.174672	-0.248822	-2.413669
H	6.150230	1.050365	-1.204409
H	6.532494	-0.618563	-0.715618

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B1-COT

Ru	-0.517045	0.031142	0.152490
Cl	-1.983778	-0.768880	-1.453276
Cl	-2.039140	1.744004	0.669750
C	1.023908	1.277857	1.134796
C	0.846934	0.139399	1.954932
H	0.583763	0.387018	2.981123
C	1.079973	1.361780	-0.305803
H	0.686979	2.321151	-0.645899
C	0.509579	-1.215707	1.611517
H	0.009510	-1.750725	2.416148
C	0.541629	-1.888856	0.345931
H	-0.112719	-2.753241	0.269470
H	0.752370	2.194082	1.656066
C	1.132113	-1.354435	-0.797785
H	0.792540	-1.769553	-1.743338
C	2.171973	0.825788	-1.202676
H	1.827695	0.886789	-2.240776
H	3.066249	1.460893	-1.122404
C	2.451312	-0.619953	-0.822430
H	3.124248	-1.102437	-1.539936
H	2.937204	-0.666655	0.157730

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B2-COT

C	0.408738	-2.375342	-0.704569
C	-0.260310	-3.076732	0.363382
H	0.368479	-3.837591	0.821374
C	0.086127	-1.209758	-1.441107
H	0.986978	-0.734467	-1.829367
C	-1.376190	-2.728348	1.166267
H	-1.423868	-3.256738	2.114828
C	-2.262236	-1.604192	1.028667
H	-2.714200	-1.270649	1.957242
H	1.466521	-2.629584	-0.704412
C	-2.366872	-0.819497	-0.118137
H	-2.838563	0.151449	0.018397
C	-1.142223	-0.893530	-2.259074
H	-1.188996	0.190296	-2.413555
H	-1.044642	-1.350359	-3.254959
C	-2.381730	-1.373254	-1.526662
H	-3.297568	-1.049193	-2.033783
H	-2.400515	-2.468117	-1.499607
Ru	-0.201870	-0.877589	0.763883
H	-0.114458	0.823759	0.309846
Si	0.685999	2.124493	0.180485
Cl	2.172846	-0.806575	1.275241
Cl	-0.624208	0.030773	2.979958
O	-0.584091	2.973378	-0.453911
C	1.320704	2.742983	1.810895
O	1.815736	1.994882	-1.008236
C	-0.472430	4.261200	-1.054555
H	1.771464	3.735486	1.696448
H	0.495186	2.800776	2.523928
H	2.059285	2.048212	2.217132
C	3.230553	1.837936	-0.877833
H	-1.443776	4.516211	-1.486148
H	-0.212616	5.025857	-0.311406
H	0.281210	4.265604	-1.850145
H	3.688637	2.202458	-1.801618
H	3.625225	2.417957	-0.036129
H	3.483645	0.786466	-0.725732

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TS(B2-COT-B3-COT)

C	2.518915	2.056099	-0.443379
C	1.916336	3.098064	-1.290865
H	2.593496	3.373981	-2.097803
C	2.243194	1.495311	0.803894
H	3.072956	0.905443	1.182779
C	0.700306	3.706972	-1.358947
Ru	1.565116	0.064389	-0.995373
Si	1.434298	-1.669129	0.591707
O	1.126762	-1.133962	2.142152
C	0.885505	-1.986072	3.257141
H	0.557716	4.342565	-2.232846
C	-0.465570	3.602529	-0.499114
H	-1.426225	3.707118	-1.002460
H	3.513668	1.811492	-0.804603
Cl	3.805954	-0.631620	-1.289749
O	-0.077488	-2.625172	0.321964
C	-0.148549	-3.809299	-0.507857
C	2.724928	-3.035267	0.634772
Cl	0.903837	-1.375361	-2.777149
C	-0.467669	3.453476	0.839401
H	-1.432692	3.374182	1.337707
C	1.349561	2.000574	1.918846
H	0.565384	1.281758	2.171812
H	1.988118	2.032598	2.811570
C	0.746151	3.411997	1.715362
H	0.477440	3.802475	2.703675
H	1.522994	4.069780	1.308541
C	-0.436019	0.202928	-0.272856
H	-1.202134	-4.087379	-0.584549
H	0.258033	-3.604110	-1.500067
H	0.403025	-4.612276	-0.016813
H	3.682248	-2.618786	0.955759
H	2.429254	-3.823093	1.337549
H	2.876431	-3.468793	-0.356470
H	0.305498	-2.873606	2.977348
H	1.829542	-2.306077	3.714962
H	0.312711	-1.420847	3.998061
H	-0.493722	0.751773	0.660186
H	-0.012208	0.832327	-1.180315
C	-1.531374	-0.636494	-0.560506
Si	-3.125372	-0.464858	0.381162
H	-1.582502	-0.983872	-1.595708
H	-0.872258	-1.786863	-0.035689
O	-4.047918	0.717131	-0.343622
C	-4.085904	-2.081572	0.449983
O	-2.659479	0.011023	1.910847
H	-4.961976	-2.029143	1.105207

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H	-4.435707	-2.384296	-0.543495
H	-3.438418	-2.877444	0.833190
C	-3.556575	0.471474	2.908113
H	-2.985657	0.668813	3.820186
H	-4.055209	1.401117	2.603892
H	-4.326634	-0.275962	3.145292
C	-5.458713	0.783027	-0.461706
H	-5.703054	1.432409	-1.307760
H	-5.909018	-0.201025	-0.644604
H	-5.916112	1.209513	0.441191

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B3-COT

C	2.422736	1.542844	0.828638
C	2.570279	2.807218	0.088485
H	3.599725	2.963981	-0.226091
C	1.466194	1.030515	1.700085
H	1.789114	0.112884	2.184200
C	1.672860	3.685251	-0.433126
Ru	1.051681	0.371420	-0.587354
Si	1.630257	-1.854635	0.165525
O	3.063698	-1.688115	1.019792
C	3.528728	-2.642495	1.963676
H	2.088280	4.425811	-1.115743
C	0.224691	3.733499	-0.280220
H	-0.333113	4.011495	-1.173345
H	3.331790	0.951109	0.787211
Cl	3.131125	-0.028895	-1.634212
O	0.555414	-2.499999	1.304418
C	0.181289	-3.862920	1.413888
C	1.752916	-3.089589	-1.247236
Cl	0.144770	0.151286	-2.775753
C	-0.452389	3.521105	0.862635
H	-1.539379	3.566848	0.830764
C	0.379955	1.738027	2.484605
H	-0.579470	1.215062	2.396971
H	0.664932	1.624676	3.540977
C	0.175542	3.237381	2.194423
H	-0.462132	3.645825	2.987160
H	1.145006	3.743141	2.265719
C	-0.674271	-0.348000	0.192479
H	-0.580105	-3.946650	2.196369
H	-0.241233	-4.251632	0.478178
H	1.029198	-4.501509	1.696291
H	2.460038	-2.728215	-1.994357
H	2.088867	-4.066323	-0.878660
H	0.782106	-3.218603	-1.735889
H	4.439796	-2.247143	2.422724
H	2.788838	-2.828067	2.752331
H	3.778498	-3.598801	1.483554
H	-0.691138	-0.491177	1.269979
H	-0.729933	0.784819	-0.048675
C	-1.773247	-1.118532	-0.474397
Si	-3.487366	-0.556063	0.093954
H	-1.731311	-1.046005	-1.562111
H	-1.691308	-2.174808	-0.189807
O	-4.541900	-1.019047	-1.098628
C	-3.993769	-1.291950	1.750679
O	-3.369027	1.103594	0.225755
H	-4.930718	-0.867312	2.126892

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H	-4.125640	-2.377212	1.682129
H	-3.222535	-1.097381	2.503854
C	-4.472834	1.983902	0.375080
H	-4.088600	2.999682	0.506424
H	-5.114431	1.973066	-0.514576
H	-5.083057	1.734107	1.254479
C	-5.932243	-1.276688	-0.990850
H	-6.239615	-1.864967	-1.860145
H	-6.180317	-1.844963	-0.084911
H	-6.510905	-0.343961	-0.985394

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TS(B3-COT-B1-COT)

C	-2.411335	1.548710	-0.843542
C	-2.570808	2.801389	-0.086707
H	-3.603571	2.949825	0.220911
C	-1.440338	1.049899	-1.706914
H	-1.752454	0.134467	-2.202232
C	-1.681432	3.674335	0.457667
Ru	-1.051193	0.377913	0.578638
Si	-1.631342	-1.846470	-0.173405
O	-3.037271	-1.656152	-1.073225
C	-3.522951	-2.648069	-1.963986
H	-2.106613	4.401669	1.148425
C	-0.232266	3.733097	0.318934
H	0.315034	4.003345	1.220851
H	-3.318423	0.952915	-0.821373
Cl	-3.139537	-0.049661	1.598302
O	-0.542034	-2.508991	-1.290319
C	-0.177687	-3.873685	-1.392658
C	-1.814341	-3.077309	1.246347
Cl	-0.167639	0.141955	2.776265
C	0.457506	3.540094	-0.819877
H	1.543765	3.593160	-0.776114
C	-0.347035	1.770466	-2.469436
H	0.613701	1.251310	-2.373653
H	-0.617260	1.666427	-3.530640
C	-0.154239	3.267866	-2.161453
H	0.490009	3.688217	-2.942524
H	-1.125642	3.769187	-2.238192
C	0.678749	-0.342481	-0.188875
H	0.346097	-4.015376	-2.345102
H	0.498905	-4.176423	-0.581392
H	-1.047156	-4.544253	-1.380507
H	-2.736686	-3.676116	1.106522
H	-0.954946	-3.768052	1.296081
H	-1.893990	-2.537276	2.201005
H	-4.432073	-2.262404	-2.437601
H	-2.792338	-2.888024	-2.745357
H	-3.788791	-3.574410	-1.434524
H	0.700811	-0.485948	-1.266319
H	0.736849	0.789738	0.052565
C	1.772872	-1.114464	0.484535
Si	3.490032	-0.566751	-0.088705
H	1.730684	-1.033823	1.571621
H	1.683938	-2.172462	0.208674
O	4.540416	-1.005600	1.116657
C	4.001439	-1.337232	-1.728101
O	3.375481	1.090554	-0.254458
H	4.940130	-0.921726	-2.110113

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H	4.131676	-2.420972	-1.636318
H	3.232734	-1.157987	-2.487624
C	4.482504	1.964103	-0.418792
H	4.102053	2.978741	-0.568841
H	5.123582	1.967043	0.471333
H	5.092490	1.696407	-1.293068
C	5.929542	-1.272853	1.018130
H	6.231323	-1.845410	1.899815
H	6.177133	-1.860275	0.124354
H	6.513289	-0.343515	0.995897

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B1-Me

Ru	0.784044	0.619592	-0.128091
C	1.349772	-1.649142	-0.196206
C	0.567422	-1.348995	-1.324255
H	0.957010	-1.568769	-2.314100
C	-0.744534	-0.763415	-1.217287
H	-1.291130	-0.563929	-2.132092
C	-1.308945	-0.432771	0.024345
C	-0.436963	-0.546546	1.161772
H	-0.777159	-0.198488	2.132209
C	0.862432	-1.150811	1.056527
H	1.477039	-1.240817	1.946842
C	2.685345	-2.334073	-0.299251
H	3.429546	-1.846161	0.337983
H	3.057872	-2.322211	-1.327432
H	2.612264	-3.380944	0.019688
C	-2.714594	0.111947	0.209106
H	-2.643669	0.902894	0.968309
C	-3.319156	0.737567	-1.054440
H	-4.287796	1.189720	-0.819964
H	-3.493254	-0.012886	-1.834053
H	-2.672435	1.518432	-1.465578
C	-3.635768	-0.990746	0.772590
H	-3.234094	-1.416966	1.697342
H	-3.752563	-1.806798	0.050582
H	-4.630144	-0.586945	0.990707
C	2.685549	1.337485	0.305571
H	3.425111	0.549059	0.494725
H	2.959441	1.840976	-0.642731
H	2.760437	2.087103	1.098563
C	0.144815	2.518513	0.438455
H	-0.909674	2.563273	0.738365
H	0.746727	3.034277	1.192165
H	0.254872	3.086655	-0.506524

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B2-Me

C	-0.026895	-0.123946	0.099335
C	0.001111	-0.077856	1.520229
C	1.270064	0.005773	2.136919
C	2.477843	-0.123513	1.375569
C	2.449530	-0.246464	-0.022171
C	1.170668	-0.163033	-0.661287
C	-1.279611	-0.055925	2.313582
C	3.695400	-0.422600	-0.876531
C	3.750257	-1.862439	-1.431120
C	5.005915	-0.065896	-0.163037
Ru	1.204986	1.747599	0.615968
H	1.335423	0.116784	3.214394
H	3.424902	-0.093685	1.901190
H	1.107323	-0.170811	-1.743878
H	-0.983015	-0.094431	-0.410612
H	-2.023862	0.567513	1.812022
H	-1.113789	0.338184	3.319484
H	-1.685057	-1.070475	2.410271
H	3.582915	0.259513	-1.729870
H	5.840828	-0.129381	-0.867440
H	5.220621	-0.759620	0.657882
H	4.984023	0.950074	0.241623
H	2.842511	-2.118682	-1.985585
H	3.864008	-2.587987	-0.617874
H	4.603233	-1.977079	-2.107864
H	0.151195	2.768784	1.208712
Si	-0.384744	2.986585	-0.640218
O	-1.912183	2.416333	-0.169447
C	-0.423172	4.876638	-0.513832
O	-0.344615	2.584825	-2.285826
C	-3.090957	2.734127	-0.892176
H	-3.925215	2.173753	-0.456329
H	-3.333483	3.804471	-0.827924
H	-3.000662	2.462728	-1.951438
H	-1.240999	5.302611	-1.106556
H	-0.584540	5.163166	0.530792
H	0.507286	5.347126	-0.844746
C	0.062302	3.394076	-3.369917
H	-0.446610	3.046156	-4.276595
H	-0.191100	4.452457	-3.223556
H	1.145439	3.325405	-3.539152
C	2.441844	2.899261	-0.710055
H	2.322219	2.569500	-1.746783
H	2.307030	3.983542	-0.674075
H	3.473380	2.699855	-0.399149
C	2.171895	3.082578	1.985462

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H	1.765449	2.968218	2.996078
H	3.238745	2.830723	2.005026
H	2.078502	4.131834	1.694723

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TS(B2-Me-B3-Me)

C	-3.341040	-0.146682	0.824564
C	-2.485427	-0.423027	1.915145
C	-1.692792	-1.607744	1.930960
C	-1.792132	-2.476295	0.813473
C	-2.746737	-2.253821	-0.225424
C	-3.540131	-1.096666	-0.240589
Ru	-1.285961	-0.353855	-0.035200
Si	-0.164666	1.494350	0.911853
O	-1.330566	2.608110	1.480976
C	-1.261632	4.014615	1.397096
C	-0.828495	-1.924479	3.124885
C	-4.596243	-0.810425	-1.294967
C	-4.369916	-1.538017	-2.626691
C	-6.001546	-1.113454	-0.733012
O	0.651644	1.046547	2.362177
C	1.039781	1.997638	3.336423
C	1.124150	2.526246	-0.046331
H	-1.184204	-3.376493	0.782819
H	-2.808770	-2.970601	-1.036634
H	-3.897104	0.785088	0.817002
H	-2.402773	0.294523	2.724097
H	-0.197528	-1.067359	3.378792
H	-0.191181	-2.795031	2.944697
H	-1.456330	-2.159098	3.992970
H	-4.547826	0.268189	-1.495508
H	-5.107229	-1.205212	-3.364125
H	-4.485683	-2.622851	-2.521057
H	-3.372549	-1.336629	-3.028442
H	-6.190460	-0.566425	0.195882
H	-6.114245	-2.182760	-0.521258
H	-6.773548	-0.828511	-1.456012
C	1.623071	-1.351209	0.788875
H	1.538295	1.473328	4.160276
H	1.745822	2.739298	2.933822
H	0.172613	2.535944	3.741050
H	0.726408	2.900410	-0.994093
H	1.471874	3.390739	0.531733
H	2.005412	1.914673	-0.261567
H	-2.164750	4.435496	1.854984
H	-0.393012	4.429786	1.930431
H	-1.216075	4.366767	0.356445
H	1.741842	-0.483688	1.429595
H	0.975012	-2.139807	1.139196
C	2.466728	-1.575173	-0.336409
Si	3.955377	-0.551149	-0.836232
H	2.336930	-2.536172	-0.832852
H	1.312510	-0.972139	-0.458905

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O	5.269218	-1.570594	-0.901673
C	3.756801	0.341084	-2.474042
O	4.172946	0.488656	0.426272
H	4.675032	0.869623	-2.754332
H	3.512101	-0.351575	-3.286352
H	2.948101	1.076120	-2.417565
C	5.181170	1.487594	0.506674
H	5.005310	2.071965	1.413565
H	6.179004	1.037504	0.565615
H	5.148369	2.167714	-0.354192
C	5.635893	-2.405070	-1.987652
H	4.950334	-3.257214	-2.091119
H	5.657057	-1.859100	-2.939854
H	6.638398	-2.797709	-1.794593
C	-1.712359	1.269545	-1.388975
H	-2.159516	2.138548	-0.894958
H	-0.850911	1.607916	-1.972180
H	-2.442870	0.874939	-2.106057
C	-0.190429	-0.920263	-1.800832
H	0.110052	-1.979190	-1.787093
H	-0.845855	-0.792244	-2.670455
H	0.699530	-0.307487	-2.019415

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B3-Me

C	-2.974360	0.106188	0.884017
C	-1.968804	0.092367	1.890607
C	-1.201325	-1.070545	2.122698
C	-1.420247	-2.179044	1.265001
C	-2.513725	-2.202722	0.351189
C	-3.340506	-1.081539	0.177575
Ru	-1.025413	-0.384154	-0.198347
Si	-0.502433	1.953316	-0.269570
O	-1.980719	2.781493	-0.048759
C	-2.018053	4.167322	0.235678
C	-0.158818	-1.117695	3.206494
C	-4.558828	-1.063006	-0.731901
C	-4.623659	-2.232306	-1.723500
C	-5.845778	-0.998990	0.118842
O	0.395843	2.406649	1.105980
C	1.393977	3.400472	1.197387
C	0.312740	2.779551	-1.781177
H	-0.787044	-3.056437	1.353985
H	-2.678354	-3.099121	-0.235134
H	-3.513372	1.028749	0.705206
H	-1.777916	0.990765	2.467321
H	0.170871	-0.112652	3.479797
H	0.714951	-1.694380	2.891449
H	-0.571499	-1.596830	4.102378
H	-4.498688	-0.132702	-1.311800
H	-5.476445	-2.101323	-2.396432
H	-4.760500	-3.190530	-1.208948
H	-3.720179	-2.298688	-2.336896
H	-5.839632	-0.140679	0.797143
H	-5.959861	-1.905918	0.723294
H	-6.724545	-0.911949	-0.528446
C	1.140973	-0.380108	0.250150
H	1.751460	3.437721	2.232853
H	2.256845	3.184591	0.551568
H	1.019527	4.401227	0.936399
H	-0.463570	3.084354	-2.489564
H	0.879927	3.675861	-1.508645
H	0.990021	2.102184	-2.306006
H	-3.065188	4.489107	0.268306
H	-1.557824	4.395485	1.207008
H	-1.507954	4.763888	-0.535329
H	1.228569	0.181547	1.182244
H	1.278988	-1.441595	0.471879
C	2.261747	0.065249	-0.695986
Si	3.975853	-0.445886	-0.137707
H	2.136316	-0.342255	-1.705386
H	2.285029	1.154711	-0.810214

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O	5.014705	-0.042574	-1.382484
C	4.547797	0.387679	1.455796
O	3.919886	-2.100493	0.093594
H	5.505150	-0.000794	1.819794
H	4.660718	1.468972	1.319343
H	3.807407	0.229432	2.246856
C	5.037895	-2.931076	0.339562
H	4.677442	-3.930642	0.603580
H	5.675099	-3.022756	-0.550304
H	5.656792	-2.564323	1.171804
C	6.412799	0.155983	-1.303836
H	6.738369	0.690792	-2.202075
H	6.701067	0.753959	-0.428378
H	6.956528	-0.798020	-1.261757
C	-1.733994	0.421918	-2.086397
H	-2.363668	1.310004	-1.978530
H	-0.947296	0.629063	-2.812195
H	-2.352845	-0.381809	-2.496376
C	-0.191805	-1.668158	-1.708132
H	0.458032	-2.423682	-1.254089
H	-1.018080	-2.175369	-2.219147
H	0.379789	-1.121039	-2.458459

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TS(B3-Me-B1-Me)

C	-3.109039	0.237524	0.397584
C	-2.345847	0.774052	1.455347
C	-1.550852	-0.068777	2.297224
C	-1.550895	-1.453194	2.047418
C	-2.317240	-1.984737	0.963394
C	-3.139005	-1.172224	0.140811
Ru	-1.006025	-0.458787	-0.011962
Si	-0.190852	2.036201	-0.495467
O	-1.781834	2.446692	-0.965948
C	-2.181734	3.793287	-1.152874
C	-0.740614	0.534897	3.414423
C	-4.077419	-1.715059	-0.926421
C	-3.723790	-3.119041	-1.433635
C	-5.529548	-1.677634	-0.404149
O	-0.098434	2.985874	0.922078
C	0.982372	3.812609	1.294507
C	0.832276	2.889443	-1.852762
H	-0.933797	-2.117139	2.643814
H	-2.247908	-3.046924	0.759522
H	-3.649056	0.912885	-0.254389
H	-2.316137	1.846512	1.601911
H	-0.317061	1.492252	3.100320
H	0.070584	-0.129786	3.724344
H	-1.376835	0.720437	4.288645
H	-4.009897	-1.025520	-1.777713
H	-4.393751	-3.395847	-2.253749
H	-3.844121	-3.875637	-0.649510
H	-2.697484	-3.168254	-1.805397
H	-5.820089	-0.671305	-0.087328
H	-5.652295	-2.348497	0.453979
H	-6.225282	-2.000166	-1.185972
C	1.190839	0.588800	0.062138
H	0.738247	4.296183	2.246996
H	1.918988	3.249806	1.437496
H	1.176805	4.599300	0.552545
H	0.347157	3.827642	-2.139880
H	1.852973	3.132813	-1.542445
H	0.898568	2.270863	-2.752896
H	-3.276709	3.834092	-1.104067
H	-1.780438	4.457081	-0.375975
H	-1.877169	4.179372	-2.136070
H	1.529992	1.268321	0.850932
H	1.004153	-0.325716	0.646686
C	2.316206	0.284140	-0.942834
Si	3.850898	-0.476371	-0.177002
H	1.970244	-0.402055	-1.720958
H	2.642926	1.185027	-1.470361

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O	4.704798	-1.157347	-1.435557
C	4.930845	0.779778	0.726524
O	3.319282	-1.623839	0.913503
H	5.765464	0.316375	1.263660
H	5.351577	1.515379	0.032197
H	4.333628	1.323936	1.466531
C	4.140809	-2.561406	1.584978
H	3.537895	-3.069355	2.344010
H	4.530311	-3.320627	0.894094
H	4.991078	-2.082510	2.092187
C	6.082767	-1.476653	-1.482029
H	6.385225	-1.553776	-2.531229
H	6.706261	-0.709679	-1.002899
H	6.287614	-2.440460	-0.996925
C	-1.156259	-0.236470	-2.137658
H	-1.908767	0.510940	-2.399129
H	-0.205742	0.042942	-2.608853
H	-1.444617	-1.202992	-2.564085
C	0.101286	-2.154522	-0.723507
H	0.753589	-2.533996	0.071603
H	-0.589391	-2.950314	-1.019178
H	0.716288	-1.922528	-1.595056

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Ru	-0.501464	0.287764	0.013956
I	-1.469368	1.715159	2.065343
I	-0.943186	2.263345	-1.741512
C	-1.199268	-1.779050	-0.168155
C	-0.501732	-1.669401	1.075081
H	-1.027822	-1.878237	1.999788
C	0.797372	-1.115940	1.126728
H	1.244064	-0.915779	2.093110
C	1.464058	-0.682791	-0.067803
C	0.813160	-0.914460	-1.321330
H	1.275528	-0.551160	-2.232407
C	-0.497919	-1.436000	-1.372036
H	-1.022699	-1.470796	-2.320471
C	-2.623803	-2.262834	-0.218247
H	-3.157685	-1.829092	-1.066898
H	-3.161287	-2.003730	0.696418
H	-2.640867	-3.354489	-0.327849
C	2.845492	-0.047958	-0.040996
H	2.923680	0.560224	-0.950153
C	3.089834	0.874717	1.162365
H	4.051527	1.382660	1.043929
H	3.134852	0.316880	2.104086
H	2.309500	1.635241	1.250827
C	3.912655	-1.161134	-0.119962
H	3.778211	-1.790502	-1.005354
H	3.872888	-1.807164	0.764117
H	4.912567	-0.719050	-0.167568

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B2-I

C	-0.456767	-0.993806	2.255787
C	-0.244642	0.336231	2.737622
C	0.976278	0.947187	2.375786
C	2.024510	0.223543	1.713676
C	1.852594	-1.114250	1.330980
C	0.550138	-1.685340	1.533062
C	-1.293872	1.060207	3.535895
C	2.940815	-1.952034	0.685423
C	3.472126	-2.970425	1.719328
C	4.084134	-1.135351	0.072419
Ru	0.038760	0.226332	0.449226
I	0.602638	-0.733578	-2.092576
I	0.484668	2.786668	-0.535054
H	1.136957	1.992286	2.614934
H	2.940311	0.747718	1.472251
H	0.333692	-2.676604	1.152008
H	-1.414384	-1.473175	2.420785
H	-2.287833	0.838925	3.142346
H	-1.133688	2.140342	3.502915
H	-1.250255	0.741177	4.584353
H	2.456772	-2.510744	-0.124850
H	4.775661	-1.806615	-0.445307
H	4.661300	-0.603208	0.837351
H	3.709524	-0.411608	-0.656254
H	2.671171	-3.592891	2.130732
H	3.967732	-2.461844	2.553632
H	4.203463	-3.632655	1.246132
H	-1.358741	0.942500	0.121939
Si	-2.292363	-0.519565	-0.202455
O	-3.232548	-0.085303	1.119911
C	-3.080059	0.100789	-1.787239
O	-2.316226	-2.188128	-0.122255
C	-4.562637	-0.562254	1.297572
H	-4.917538	-0.221396	2.274891
H	-5.238207	-0.162071	0.530691
H	-4.604208	-1.657306	1.267714
H	-4.107560	-0.271461	-1.873165
H	-3.110870	1.194718	-1.778822
H	-2.519897	-0.208601	-2.671474
C	-2.244570	-3.121135	-1.193940
H	-2.640688	-4.075444	-0.832073
H	-2.841953	-2.800850	-2.055858
H	-1.209778	-3.257980	-1.522901

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TS(B2-I-B3-I)

C	-2.049891	-0.079445	2.047334
C	-0.939802	0.723267	2.405297
C	0.360734	0.147456	2.455453
C	0.476333	-1.216732	2.071327
C	-0.669831	-2.059200	1.917779
C	-1.953170	-1.516544	1.924321
Ru	-0.598259	-0.147572	0.356725
Si	-0.642416	2.135373	-0.341860
O	-1.965276	2.977206	0.274122
C	-3.059538	3.549287	-0.421652
C	1.544961	0.941898	2.929250
C	-3.223323	-2.331176	1.774519
C	-3.009627	-3.710363	1.139614
C	-3.928863	-2.445239	3.143986
I	-2.843400	-0.137827	-1.331736
O	0.601159	2.951032	0.535853
C	0.642282	4.367634	0.622883
C	-0.382063	2.593058	-2.162343
I	0.493891	-1.794399	-1.640744
H	1.469992	-1.642905	1.996781
H	-0.517604	-3.112575	1.717890
H	-3.022603	0.389743	1.950908
H	-1.082351	1.778006	2.611293
H	1.612156	1.891481	2.392161
H	2.468214	0.374703	2.805330
H	1.430073	1.161548	3.997568
H	-3.874718	-1.755528	1.104745
H	-3.977336	-4.195032	0.978626
H	-2.420708	-4.371526	1.786304
H	-2.507742	-3.628300	0.171447
H	-4.125453	-1.462679	3.585208
H	-3.321126	-3.018197	3.853374
H	-4.888492	-2.959238	3.029554
C	2.690046	2.248572	-0.441061
H	1.475124	4.651659	1.276504
H	0.800420	4.836051	-0.358882
H	-0.290113	4.757176	1.043929
H	-1.263513	2.329842	-2.751151
H	-0.186130	3.663974	-2.293935
H	0.456909	2.031900	-2.584841
H	-3.468987	4.359791	0.192413
H	-2.760585	3.971250	-1.389776
H	-3.846042	2.807588	-0.599481
H	2.433905	2.939668	-1.237815
H	3.135745	2.697545	0.440380
C	2.525237	0.866950	-0.572710

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Si	3.967492	-0.152811	0.146832
H	2.302475	0.549578	-1.593881
H	1.379204	0.533368	-0.057598
O	4.814541	-0.541760	-1.227961
C	5.027288	0.870558	1.316047
O	3.566180	-1.517565	1.007238
H	5.820887	0.244409	1.736411
H	5.500855	1.706954	0.791234
H	4.463367	1.280836	2.158774
C	3.520832	-2.857180	0.510775
H	2.527922	-3.279293	0.686809
H	3.713377	-2.900405	-0.564218
H	4.269242	-3.455124	1.043485
C	6.121129	-1.100522	-1.247320
H	6.425173	-1.212961	-2.291421
H	6.847535	-0.450140	-0.742822
H	6.149714	-2.089004	-0.771441

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C	-2.650333	0.878147	1.311373
C	-1.547324	1.271199	2.118951
C	-0.730297	0.299648	2.757971
C	-1.018032	-1.054733	2.468706
C	-2.214033	-1.439086	1.776982
C	-3.079073	-0.485329	1.230037
Ru	-0.759669	-0.040768	0.434062
Si	-0.218623	2.275767	-0.340268
O	-1.699619	3.089836	-0.332184
C	-1.769515	4.505322	-0.390345
C	0.404702	0.702011	3.656334
C	-4.378160	-0.824460	0.522831
C	-4.462447	-2.276760	0.036389
C	-5.570048	-0.467430	1.437919
I	-1.752194	0.085276	-2.167627
O	0.615377	3.059237	0.921835
C	1.692155	3.970259	0.802087
C	0.676991	2.680438	-1.963842
I	0.087755	-2.646412	-0.406894
H	-0.354378	-1.832403	2.831226
H	-2.406626	-2.495722	1.640396
H	-3.201725	1.651694	0.790665
H	-1.319724	2.323482	2.236706
H	0.793884	1.681943	3.372311
H	1.219126	-0.025453	3.621946
H	0.047791	0.760010	4.691644
H	-4.420479	-0.173284	-0.359157
H	-5.377376	-2.414238	-0.547416
H	-4.502593	-2.985892	0.871708
H	-3.612181	-2.533552	-0.601543
H	-5.545252	0.581529	1.750523
H	-5.574081	-1.089414	2.340219
H	-6.512201	-0.638134	0.907702
C	1.463427	0.163730	0.628742
H	1.931790	4.349764	1.801467
H	2.593129	3.492358	0.396426
H	1.444020	4.830088	0.165204
H	0.017641	3.320592	-2.560136
H	1.620204	3.213467	-1.810252
H	0.872744	1.786259	-2.555424
H	-2.824742	4.795176	-0.414629
H	-1.298078	4.970880	0.485437
H	-1.289745	4.904481	-1.295042
H	1.628029	1.065838	1.215702
H	1.625210	-0.704323	1.266423
C	2.421626	0.092995	-0.552446
Si	4.222357	-0.064950	-0.028194

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H	2.208478	-0.773818	-1.185291
H	2.361215	0.971681	-1.200160
O	5.056914	-0.574345	-1.376917
C	4.980150	1.543643	0.607209
O	4.261601	-1.200260	1.192984
H	6.003945	1.408463	0.973467
H	5.011649	2.308591	-0.176848
H	4.389851	1.939692	1.440333
C	5.432638	-1.823097	1.688318
H	5.163127	-2.418398	2.566305
H	5.874882	-2.495492	0.942005
H	6.195587	-1.092167	1.994769
C	6.434285	-0.404173	-1.653842
H	6.597111	-0.589524	-2.720073
H	6.782015	0.612648	-1.426544
H	7.051730	-1.113964	-1.086713

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TS(B3-I-B1-I)

C	-3.287067	-0.439802	0.510877
C	-2.980548	0.954115	0.616339
C	-2.139732	1.449946	1.643773
C	-1.517309	0.572055	2.590441
C	-1.737242	-0.808044	2.421223
C	-2.621323	-1.302111	1.404975
Ru	-0.998208	-0.056233	0.419878
I	-1.020438	-0.126353	-2.364604
C	-0.628736	1.110980	3.677147
C	-4.274233	-0.919458	-0.538279
C	-5.707646	-0.595379	-0.063218
Si	0.091767	2.334744	-0.218747
C	1.302615	0.670604	0.457308
C	2.287026	0.123561	-0.579546
Si	4.047713	-0.005946	0.068273
O	3.913380	-0.475751	1.663283
C	4.955705	-1.036805	2.441361
O	-1.407674	2.897197	-0.757780
C	-1.609023	4.252774	-1.129847
O	0.248289	3.275512	1.193926
C	1.393298	4.008271	1.589586
C	1.323460	2.989453	-1.493664
C	-4.129178	-2.401039	-0.905559
O	4.805195	-1.156529	-0.861816
C	6.190452	-1.298289	-1.115799
C	5.017240	1.612183	-0.014795
I	0.200776	-2.692807	0.304595
H	-1.209044	-1.521080	3.043362
H	-2.723219	-2.372975	1.293963
H	-3.364416	1.648877	-0.119124
H	-1.935943	2.511381	1.695880
H	-0.078758	1.982899	3.317613
H	0.080035	0.353714	4.021359
H	-1.235940	1.421428	4.536162
H	-4.071351	-0.328652	-1.439004
H	-4.796091	-2.636641	-1.740160
H	-4.408661	-3.057028	-0.072765
H	-3.106881	-2.637688	-1.211574
H	-5.836344	0.470623	0.150769
H	-5.959716	-1.155741	0.844243
H	-6.427992	-0.871726	-0.839406
H	1.144857	4.570005	2.496042
H	2.248653	3.356006	1.824095
H	1.711535	4.721882	0.819104
H	1.088722	4.044302	-1.673175
H	2.368105	2.930939	-1.179862
H	1.215409	2.464787	-2.445843

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H	-2.688300	4.436107	-1.165250
H	-1.166166	4.949992	-0.406139
H	-1.197892	4.461898	-2.125515
H	1.711555	1.534487	0.992177
H	1.199491	-0.045615	1.274471
H	1.994393	-0.885941	-0.875390
H	2.304659	0.706734	-1.502242
H	6.013894	1.519928	0.431099
H	5.149609	1.948582	-1.049171
H	4.495862	2.406780	0.530389
H	4.577412	-1.206166	3.454195
H	5.285956	-2.000407	2.033548
H	5.826618	-0.368346	2.510920
H	6.316430	-1.999246	-1.946339
H	6.660962	-0.346391	-1.396420
H	6.722959	-1.702694	-0.244373

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TS(B2-Ben-B1H-Ben)

C	-0.596313	1.255283	-1.595850
C	-0.704669	2.188438	-0.521408
C	-1.702240	2.020146	0.477037
C	-2.614710	0.917220	0.390271
C	-2.501986	-0.023004	-0.643202
C	-1.443735	0.122383	-1.602744
H	0.019860	2.989491	-0.434394
H	-3.137683	-0.900080	-0.661332
Ru	-0.442365	0.223048	0.391202
Cl	0.700093	-1.939853	0.120485
Cl	-0.568957	-0.250022	2.737980
H	-1.744143	2.690779	1.326040
H	-3.323464	0.754768	1.194288
H	-1.283511	-0.657360	-2.339500
H	0.206184	1.348993	-2.316260
H	1.053269	0.659181	0.857729
Si	2.371242	-0.259363	0.063841
O	2.537132	1.254124	-0.650933
C	3.152070	-0.459809	1.756295
O	3.236412	-1.109984	-1.088512
C	3.633423	1.618744	-1.487937
H	3.485461	2.661637	-1.786438
H	4.591090	1.543696	-0.957866
H	3.684831	0.988114	-2.379874
H	3.708703	-1.399344	1.825124
H	3.848944	0.368461	1.924866
H	2.389724	-0.445294	2.538633
C	3.579544	-2.482897	-1.083985
H	4.417690	-2.622833	-1.774112
H	3.888583	-2.832918	-0.090369
H	2.739867	-3.101204	-1.420053

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B1H-Ben

Ru	0.275603	-0.358965	-0.000026
Cl	2.511230	0.203782	0.000000
H	0.720535	-1.883093	-0.000340
C	-1.745236	-0.839319	-0.706769
C	-1.232312	0.307559	-1.389083
C	-1.010945	1.553275	-0.692455
C	-1.010875	1.553380	0.692330
C	-1.232108	0.307712	1.389145
C	-1.745143	-0.839235	0.707050
H	-2.003513	-1.733620	-1.260698
H	-0.720410	2.438090	1.248042
H	-1.115380	0.271957	-2.466871
H	-0.720645	2.437937	-1.248337
H	-1.114952	0.272136	2.466901
H	-2.003353	-1.733454	1.261146

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B2H-Ben

C	1.072654	1.548986	1.350982
C	1.579910	2.251089	0.218398
C	2.347492	1.548625	-0.760787
C	2.452115	0.158518	-0.683892
C	1.906657	-0.551205	0.437975
C	1.301767	0.149850	1.488113
Ru	0.125418	0.736365	-0.521158
Cl	-0.527970	-0.910023	-2.143164
H	1.447440	3.323742	0.142228
H	1.983174	-1.631252	0.473284
H	-1.236091	1.551942	-0.487960
H	2.756934	2.079749	-1.613016
H	2.919525	-0.397174	-1.488077
H	0.913620	-0.383546	2.348670
H	0.546125	2.090986	2.127223
H	-0.325262	1.631564	-1.723860
Si	-1.949989	0.072574	0.552162
C	-2.283290	1.049345	2.137436
O	-3.258030	0.235805	-0.467769
O	-1.850776	-1.484743	1.150996
H	-3.243119	0.742172	2.567324
H	-1.520427	0.868363	2.901618
H	-2.329732	2.125506	1.941832
C	-4.564256	-0.222376	-0.158467
C	-1.835027	-2.709376	0.428598
H	-5.198495	-0.052888	-1.033604
H	-4.579532	-1.293866	0.077768
H	-4.997586	0.322918	0.691719
H	-2.085059	-3.512426	1.130551
H	-2.561760	-2.711239	-0.390506
H	-0.848146	-2.901032	-0.003791

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TS(B2H-Ben-B3H-Ben)

C	-3.400787	-1.492921	0.670690
C	-2.243484	-1.173735	1.410499
C	-1.270942	-2.168944	1.639367
C	-1.468455	-3.466813	1.139094
C	-2.618556	-3.766433	0.417790
C	-3.584034	-2.778651	0.178679
Ru	-0.377459	-0.452550	-0.257648
Si	-0.757632	1.766472	0.455513
O	-2.134792	2.079436	-0.464893
C	-2.197200	2.247704	-1.876014
Cl	-1.180207	-1.746591	-2.111337
O	-1.354576	1.877244	2.021458
C	-2.175620	2.947304	2.468446
C	0.508629	3.145563	0.226655
C	1.701298	-0.625875	-0.994014
Si	3.356349	-0.245724	-0.154802
O	3.257479	-0.926845	1.349405
C	4.227793	-0.777088	2.379424
C	0.960405	0.412939	-1.687215
O	3.581680	1.388681	0.054827
C	4.215231	2.275742	-0.856462
C	4.739172	-0.983971	-1.188850
H	-0.725868	-4.236345	1.327967
H	-4.150555	-0.726466	0.499745
H	-0.429211	-1.961500	2.290815
H	-2.175721	-0.222597	1.926966
H	-2.768170	-4.770019	0.030568
H	-4.473594	-3.020633	-0.394746
H	-1.647701	3.910166	2.424725
H	-3.090708	3.025963	1.870820
H	-2.446006	2.755320	3.511337
H	1.498909	2.824021	0.561689
H	0.590906	3.477807	-0.812978
H	0.205352	4.011954	0.824582
H	-2.089693	1.288891	-2.395180
H	-3.175310	2.672882	-2.120985
H	-1.423700	2.938135	-2.239244
H	1.267026	1.443505	-1.537790
H	0.596505	0.190402	-2.686302
H	1.712376	-1.581414	-1.525658
H	3.638338	2.383930	-1.783661
H	4.286800	3.257060	-0.379525
H	5.227831	1.940144	-1.113167
H	5.720759	-0.793292	-0.741502
H	4.751201	-0.576326	-2.205383
H	4.613539	-2.068619	-1.268876
H	5.185535	-1.234818	2.098715

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H	3.852715	-1.283073	3.272828
H	4.395003	0.279665	2.615549
H	1.082876	-0.998144	0.210417
H	0.146293	0.299788	1.095246

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B3H-Ben

C	-1.878954	-1.033276	-1.949317
C	-3.035611	-1.120191	-1.115137
C	-3.199937	-2.214480	-0.213045
C	-2.126732	-3.082377	-0.005389
C	-0.934330	-2.966870	-0.792930
C	-0.852479	-1.998570	-1.806211
Ru	-1.285761	-0.835606	0.231352
Si	-1.820421	1.530974	0.252748
O	-1.366595	2.219906	-1.221135
C	-0.462360	3.294863	-1.408269
H	-4.100817	-2.297319	0.384090
H	0.042350	-1.925399	-2.414507
Cl	-0.376882	-1.382422	2.399557
O	-3.504646	1.633369	0.217282
C	-4.187709	2.838507	-0.094241
C	-1.163710	2.603746	1.657001
H	-2.085478	0.044679	1.282456
H	-2.176354	-3.834928	0.773365
H	-0.103773	-3.637756	-0.609110
H	-1.790476	-0.230922	-2.671483
H	-3.814159	-0.372429	-1.200168
C	0.640882	0.139862	-0.050922
H	-5.258881	2.620066	-0.152598
H	-4.039407	3.601973	0.682065
H	-3.859102	3.250580	-1.056364
H	-1.603189	3.607360	1.624781
H	-1.426615	2.147720	2.616097
H	-0.076092	2.714382	1.634132
H	-0.570180	3.657359	-2.436249
H	-0.663126	4.132841	-0.728399
H	0.578894	2.979142	-1.261411
H	0.590171	0.674623	-1.004108
H	0.796212	0.867914	0.745720
C	1.829501	-0.830200	-0.042006
Si	3.480010	0.039513	-0.259948
H	1.866241	-1.379029	0.904515
H	1.759371	-1.584291	-0.837210
O	4.665616	-1.087980	0.069864
C	3.741288	0.732132	-1.997095
O	3.494133	1.293529	0.839309
H	4.668908	1.307977	-2.086927
H	3.778188	-0.067610	-2.745441
H	2.917074	1.401941	-2.264579
C	4.621005	2.075808	1.185974
H	4.283826	2.915057	1.802508
H	5.348747	1.495179	1.768031
H	5.131777	2.487555	0.302894

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C	6.019323	-1.043691	-0.339708
H	6.468088	-2.025041	-0.155888
H	6.122945	-0.815683	-1.409480
H	6.591984	-0.297107	0.227311

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TS(B3H-Ben-B1H-Ben)

C	-1.358144	-1.944691	-0.644930
C	-2.605215	-1.400934	-0.248546
C	-2.973226	-1.420726	1.131940
C	-2.063841	-1.937827	2.077850
C	-0.844441	-2.579523	1.658558
C	-0.503664	-2.597362	0.308348
Ru	-1.034438	-0.342551	0.890342
Si	-0.755564	1.763434	-0.611799
O	0.208599	2.364392	-1.880590
C	1.311620	3.230939	-1.767219
H	-3.896134	-0.957103	1.459972
H	0.459951	-2.986915	-0.003396
Cl	-0.284743	0.685515	2.967854
O	-2.066506	1.317483	-1.575739
C	-2.410976	1.982346	-2.788603
C	-1.035130	3.263889	0.504554
H	-1.843633	1.007616	0.823342
H	-2.275781	-1.839259	3.135710
H	-0.164249	-2.971444	2.405519
H	-1.065120	-1.888751	-1.686863
H	-3.232399	-0.905032	-0.977682
C	0.930713	0.517593	0.020320
H	-3.297697	1.485732	-3.197037
H	-2.657653	3.037972	-2.616141
H	-1.598998	1.933358	-3.519291
H	-0.766991	4.205137	0.014197
H	-2.096293	3.311587	0.770724
H	-0.479862	3.169411	1.441889
H	1.468779	3.725016	-2.732727
H	1.164688	4.010267	-1.007168
H	2.237143	2.688731	-1.517788
H	1.350311	1.512798	0.222571
H	1.200076	0.009165	0.948918
C	1.599275	-0.147986	-1.200348
Si	3.241065	-0.962205	-0.812366
H	0.965829	-0.930338	-1.629193
H	1.731119	0.571381	-2.011765
O	3.842278	-1.447646	-2.289068
C	4.473359	0.152729	0.069515
O	2.877256	-2.282308	0.155683
H	5.444737	-0.328621	0.225033
H	4.650683	1.057946	-0.521095
H	4.096532	0.461866	1.050216
C	3.763342	-2.948572	1.041193
H	3.173837	-3.594127	1.699619
H	4.479306	-3.580125	0.498193
H	4.324999	-2.245861	1.669346

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C	5.026255	-2.195747	-2.503205
H	5.247674	-2.192121	-3.574834
H	5.890258	-1.767405	-1.976007
H	4.904704	-3.238711	-2.181819

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TS(B2-COT-B1H-COT)

C	2.112443	0.407282	1.878914
C	3.125748	-0.096869	0.987205
H	3.782457	-0.818982	1.468154
C	0.937546	1.168687	1.663799
H	0.203526	0.971182	2.445490
C	3.200758	-0.144204	-0.430894
H	3.881412	-0.900428	-0.813153
C	2.317183	0.450247	-1.395348
H	2.271662	-0.071515	-2.345966
H	2.107863	-0.177114	2.796529
C	1.381982	1.439538	-1.096787
H	0.581913	1.569040	-1.822469
C	0.767216	2.525866	1.026787
H	-0.282793	2.645206	0.738318
H	0.988208	3.307892	1.768256
C	1.657363	2.625565	-0.198245
H	1.473471	3.551802	-0.754469
H	2.710943	2.634491	0.101484
Ru	1.097253	-0.503080	0.170988
H	-0.685246	-0.340692	0.071494
Si	-2.190568	-0.204131	-0.013289
Cl	0.524296	-2.233434	1.771012
Cl	0.700300	-2.110990	-1.605674
O	-2.312231	1.290696	-0.704638
C	-2.852668	-1.616727	-1.023592
O	-2.804065	-0.099019	1.508806
C	-3.538713	2.003435	-0.863199
H	-3.929742	-1.509514	-1.193013
H	-2.335049	-1.658123	-1.985118
H	-2.665867	-2.566755	-0.514648
C	-3.055371	-1.188625	2.405890
H	-3.311006	2.959404	-1.341370
H	-4.240467	1.454403	-1.503378
H	-4.012962	2.193952	0.105662
H	-3.503269	-0.769770	3.310373
H	-3.758432	-1.905739	1.966175
H	-2.123844	-1.701639	2.659376

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B1H-COT

Ru	0.385427	0.098510	0.156882
Cl	2.363378	-0.758812	-0.720647
C	-0.810998	-1.947836	0.016155
C	-0.905362	-1.577477	1.348897
H	-0.697794	-2.371397	2.064168
C	-0.783852	-1.044929	-1.144789
H	-0.171623	-1.472435	-1.941608
C	-0.828691	-0.243017	1.929125
H	-0.429042	-0.246027	2.942177
C	-1.115249	1.053525	1.405139
H	-0.766624	1.886525	2.011767
H	-0.484279	-2.975973	-0.140502
C	-1.557110	1.257030	0.083577
H	-1.437862	2.267527	-0.298189
C	-2.029427	-0.371800	-1.693024
H	-1.727725	0.282628	-2.518637
H	-2.724412	-1.116708	-2.108560
C	-2.658165	0.444433	-0.573297
H	-3.441437	1.113719	-0.946429
H	-3.125686	-0.221660	0.158988
H	0.944327	1.496652	-0.336325

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B2H-COT

C	2.309728	0.094414	1.630307
C	2.850529	-0.338673	0.340759
H	3.497246	-1.208440	0.433000
C	1.606881	1.189711	2.107802
H	1.210979	1.021679	3.107641
C	2.466242	-0.056291	-0.968882
H	2.863355	-0.736688	-1.719366
C	1.415638	0.843477	-1.400113
H	0.968049	0.630162	-2.366183
H	2.372366	-0.725661	2.343455
C	0.960703	1.929980	-0.632583
H	0.077741	2.428358	-1.022408
C	1.607618	2.635904	1.686947
H	0.631277	3.070771	1.926681
H	2.343671	3.175578	2.303051
C	1.899367	2.787664	0.204248
H	1.796211	3.834895	-0.102577
H	2.938515	2.504137	0.004886
Ru	0.440972	-0.046868	0.319607
H	-0.746032	0.807880	0.910757
Si	-1.942291	-0.141537	-0.302024
Cl	-0.143683	-1.907429	1.783805
O	-2.045843	0.952960	-1.564430
C	-2.621536	-1.828042	-0.798373
O	-2.993961	0.476105	0.849122
C	-3.293797	1.438603	-2.050228
H	-3.711334	-1.791505	-0.906764
H	-2.189532	-2.150037	-1.751829
H	-2.368239	-2.578142	-0.044644
C	-3.437886	-0.200639	2.017299
H	-3.088049	2.170629	-2.837152
H	-3.899187	0.630352	-2.481688
H	-3.870513	1.922161	-1.254247
H	-4.176504	0.435934	2.514256
H	-3.913075	-1.159647	1.773280
H	-2.607993	-0.394466	2.706030
H	-0.316264	-0.850100	-0.841789

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B3H-COT

C	2.206524	-0.674675	-1.256562
C	2.855264	0.599118	-1.672794
H	3.857025	0.520977	-2.093398
C	1.844922	-1.078103	0.006973
H	1.552775	-2.121285	0.098969
C	2.218935	1.779035	-1.646767
H	2.704145	2.671979	-2.039454
C	0.866650	1.928694	-1.054205
H	0.204019	2.654736	-1.521561
H	2.187085	-1.453434	-2.019883
C	0.627680	1.598498	0.289440
H	-0.230769	2.068129	0.757133
C	2.029775	-0.334971	1.311903
H	1.361069	-0.792049	2.047480
H	3.051285	-0.508607	1.681782
C	1.749148	1.178471	1.240960
H	1.500102	1.531353	2.246658
H	2.664713	1.699036	0.941080
Ru	-0.124286	-0.071847	-1.071553
H	-0.369024	-0.658408	0.362942
Si	-2.113313	0.281637	0.277579
Cl	-0.784582	-2.308370	-1.784358
O	-2.546672	1.899869	0.165244
C	-3.566221	-0.850546	-0.122973
O	-1.875123	0.144898	1.950932
C	-3.490926	2.504666	1.042774
H	-4.343169	-0.736930	0.642113
H	-4.007846	-0.617741	-1.094860
H	-3.245754	-1.895377	-0.149909
C	-1.800030	-1.085915	2.644921
H	-3.560777	3.565195	0.782062
H	-4.487493	2.056983	0.930598
H	-3.182169	2.411838	2.089580
H	-1.670272	-0.873876	3.711027
H	-2.711947	-1.684992	2.520128
H	-0.946713	-1.696687	2.312240
C	-1.617413	0.729753	-2.346952
H	-2.476733	0.084494	-2.514684
H	-1.927755	1.755805	-2.160458
C	-0.547181	0.593399	-3.411315
H	-0.081429	1.551813	-3.653464
H	0.309093	-0.072673	-3.082613
Si	-1.101566	-0.244997	-5.031644
O	-1.196814	1.061088	-6.056809
O	-2.625273	-0.886134	-4.928615
C	0.134921	-1.523363	-5.630789
H	-0.143645	-1.931844	-6.608380

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H	1.130640	-1.077155	-5.730640
H	0.204331	-2.354534	-4.921428
C	-2.988306	-2.255278	-4.784944
H	-2.681128	-2.643729	-3.808937
H	-4.076757	-2.322127	-4.873629
H	-2.540257	-2.875579	-5.571844
C	-1.785656	1.010792	-7.349116
H	-1.847603	2.032566	-7.735087
H	-1.177904	0.416645	-8.045484
H	-2.795495	0.586052	-7.312776

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TS(B2-Me-B1H-Me)

C	-0.596954	1.201083	-1.607950
C	-0.617891	2.184316	-0.571091
C	-1.598140	2.050733	0.461651
C	-2.538172	0.969418	0.448947
C	-2.475094	-0.040845	-0.521997
C	-1.436498	0.076736	-1.517647
C	0.326278	3.357717	-0.610372
C	-3.424443	-1.228353	-0.579007
C	-4.489742	-1.006120	-1.673747
C	-4.085404	-1.570930	0.763202
Ru	-0.330088	0.266839	0.495146
H	-1.640256	2.786086	1.257592
H	-3.254560	0.897801	1.259831
H	-1.322387	-0.722627	-2.244901
H	0.169063	1.248026	-2.371654
H	1.310327	3.035006	-0.957210
H	0.436393	3.805597	0.380533
H	-0.052597	4.128839	-1.292518
H	-2.820215	-2.095973	-0.881029
H	-4.661317	-2.496931	0.670524
H	-4.783310	-0.788597	1.082057
H	-3.343805	-1.710495	1.555810
H	-4.031740	-0.804590	-2.647140
H	-5.130228	-0.153496	-1.421736
H	-5.127457	-1.890489	-1.776520
H	1.100241	0.782371	0.964822
Si	2.081234	-0.665080	0.063595
O	2.382031	0.564420	-1.069666
C	3.166624	-0.467291	1.606974
O	2.841532	-1.891798	-0.859058
C	3.548107	0.586268	-1.885704
H	3.519926	1.506862	-2.480072
H	4.468141	0.596711	-1.285480
H	3.590022	-0.276698	-2.556785
H	3.481724	0.577953	1.693978
H	2.633468	-0.723321	2.527115
H	4.070389	-1.083894	1.550087
C	3.204222	-3.175323	-0.416604
H	3.953985	-3.586869	-1.102882
H	3.644427	-3.168022	0.592597
H	2.349572	-3.868609	-0.402992
C	0.522885	-1.913684	0.504265
H	0.438634	-2.530480	-0.389604
H	1.080045	-2.437018	1.289229
H	-0.481151	-1.818510	0.943760
C	-0.364980	0.101452	2.625003

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H	-0.151571	1.057805	3.112173
H	-1.361952	-0.229021	2.945754
H	0.363174	-0.628202	2.997348

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B1H-Me

C	-0.292620	1.278472	-1.529913
C	-0.521567	2.385782	-0.654510
C	-1.668136	2.334724	0.216114
C	-2.601994	1.245426	0.164407
C	-2.310306	0.117671	-0.612761
C	-1.108937	0.138874	-1.416275
C	0.365877	3.602551	-0.681051
C	-3.191630	-1.122168	-0.659169
C	-4.084512	-1.085711	-1.917919
C	-4.034364	-1.344695	0.604025
Ru	-0.395344	0.705782	0.689535
H	-1.856415	3.169188	0.884102
H	-3.466266	1.258265	0.817926
H	-0.849056	-0.753500	-1.978674
H	0.580410	1.264703	-2.172584
H	1.389605	3.337200	-0.956107
H	0.392234	4.087245	0.298089
H	-0.008432	4.330457	-1.412432
H	-2.514714	-1.981988	-0.760852
H	-4.552933	-2.306610	0.543230
H	-4.802280	-0.571813	0.719821
H	-3.413849	-1.347792	1.505221
H	-3.491311	-0.967539	-2.830099
H	-4.790640	-0.249474	-1.866557
H	-4.662037	-2.011898	-2.006985
H	1.116289	1.069794	1.071958
C	-0.514023	0.618792	2.750677
H	0.263262	1.104478	3.343990
H	-1.496721	0.858345	3.175492
H	-0.350160	-0.479377	2.848562

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B2H-Me

C	1.078175	1.414037	1.499737
C	1.539344	2.273565	0.460316
C	2.138902	1.666798	-0.659814
C	2.390747	0.256650	-0.701294
C	2.046973	-0.580274	0.379612
C	1.329924	0.013640	1.459818
Ru	0.095112	0.568567	-0.388374
C	1.351403	3.766102	0.546448
C	2.392290	-2.061144	0.426112
C	3.749895	-2.254050	1.134849
C	2.380653	-2.751639	-0.945013
H	-1.120312	1.561965	-0.622299
H	2.423208	2.277251	-1.510659
H	2.859884	-0.160542	-1.584278
H	0.986175	-0.610346	2.278201
H	0.556393	1.838141	2.350731
H	0.420316	4.017713	1.060403
H	1.329633	4.220940	-0.446924
H	2.177555	4.219728	1.107528
H	1.622788	-2.539602	1.045385
H	2.529722	-3.828667	-0.819796
H	3.187614	-2.388912	-1.591318
H	1.429735	-2.592114	-1.460833
H	3.750679	-1.804397	2.132756
H	4.559823	-1.794301	0.557494
H	3.975896	-3.319939	1.242856
Si	-2.028882	0.128651	0.544509
C	-2.627309	1.396690	1.818353
O	-3.197209	-0.024554	-0.659567
O	-2.089392	-1.273097	1.495898
H	-3.601426	1.109986	2.229404
H	-1.928972	1.466166	2.659244
H	-2.719963	2.391326	1.369358
C	-4.564924	-0.257815	-0.371506
C	-1.923835	-2.581562	0.989101
H	-5.088079	-0.443184	-1.315345
H	-4.707886	-1.130413	0.280487
H	-5.033199	0.610212	0.113325
H	-2.027760	-3.290848	1.817561
H	-2.678441	-2.825126	0.228514
H	-0.932261	-2.724171	0.534411
H	-0.686535	-0.771594	-0.721459
C	-0.301941	0.591459	-2.493818
H	-1.353368	0.410805	-2.719662
H	-0.019920	1.567912	-2.902904
H	0.299749	-0.183424	-2.981716

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TS(B2H-Me-B3H-Me)

C	-2.889405	-0.590638	1.189353
C	-1.918079	-1.328556	1.920573
C	-1.253429	-2.435560	1.329823
C	-1.502876	-2.689183	-0.039498
C	-2.512845	-1.980955	-0.758769
C	-3.250046	-0.944607	-0.148231
Ru	-0.973941	-0.384331	0.017558
Si	-0.485011	1.704606	1.039145
O	-1.973201	2.477044	1.324810
C	-2.091678	3.595938	2.185210
C	-0.300600	-3.284531	2.127553
C	-4.392691	-0.211184	-0.834586
C	-4.229069	-0.077793	-2.354718
C	-5.732815	-0.889217	-0.478725
O	0.176378	1.453523	2.586797
C	1.154475	2.254732	3.221557
C	0.633240	2.943905	0.136222
H	-0.948952	-3.473820	-0.546068
H	-2.685230	-2.232818	-1.798659
H	-3.371824	0.259043	1.658625
H	-1.693389	-1.045760	2.943660
H	0.250434	-2.688147	2.861551
H	0.420846	-3.793559	1.483135
H	-0.852720	-4.052975	2.682503
H	-4.404984	0.800400	-0.410599
H	-5.029539	0.548344	-2.761114
H	-4.292369	-1.048494	-2.859759
H	-3.270612	0.381450	-2.611090
H	-5.880243	-0.946626	0.604349
H	-5.773036	-1.908923	-0.878476
H	-6.570157	-0.326903	-0.905025
C	1.496426	-0.601278	0.780565
H	1.423925	1.782404	4.172834
H	2.068673	2.350561	2.619621
H	0.786496	3.267453	3.440454
H	0.115404	3.288293	-0.765908
H	0.872422	3.826509	0.740228
H	1.574365	2.486692	-0.186821
H	-3.137328	3.922849	2.189395
H	-1.804235	3.347466	3.215946
H	-1.476283	4.443450	1.849203
H	1.823934	0.428167	0.806099
H	1.117915	-0.967035	1.726466
C	2.321271	-1.469580	-0.083362
Si	3.718750	-0.842832	-1.089562
H	2.131009	-2.538301	0.003981
H	1.056996	-0.945100	-0.371510

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O	5.181079	-0.789125	-0.260005
C	3.986703	-1.831010	-2.668802
O	3.387945	0.762940	-1.396112
H	4.850064	-1.456435	-3.229088
H	4.175617	-2.888515	-2.448443
H	3.107044	-1.778734	-3.317611
C	4.351273	1.687198	-1.880375
H	3.899655	2.684025	-1.875304
H	5.247801	1.700315	-1.249989
H	4.651097	1.452308	-2.911026
C	5.720429	-1.877065	0.462972
H	4.987699	-2.306725	1.160869
H	6.072937	-2.678691	-0.202927
H	6.578006	-1.520344	1.043114
C	-0.069219	-0.250224	-1.946911
H	0.770561	0.449211	-1.985560
H	0.294556	-1.242296	-2.246136
H	-0.810945	0.069611	-2.686228
H	-1.261660	1.035093	-0.612333

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B3H-Me

C	-1.951880	1.168055	1.335289
C	-3.012219	0.311246	0.952754
C	-3.663592	0.462652	-0.300539
C	-3.170567	1.464049	-1.170243
C	-2.180134	2.401788	-0.734940
C	-1.581186	2.293511	0.527631
Ru	-1.340345	0.145967	-0.648791
Si	-0.989287	-2.081288	0.135631
O	-0.234390	-2.140268	1.644508
C	1.053367	-2.615941	1.989507
C	-4.796944	-0.449429	-0.691942
C	-0.548206	3.275060	1.056944
C	0.046255	4.204126	-0.009764
C	-1.147653	4.096729	2.218470
O	-2.543957	-2.673948	0.495256
C	-2.727070	-3.885491	1.210953
C	-0.200348	-3.397368	-0.984074
H	-1.659023	-1.184500	-1.439025
H	-3.596733	1.568018	-2.162739
H	-1.876498	3.186337	-1.418038
H	-1.458210	1.005146	2.287324
H	-3.301524	-0.507111	1.601182
H	-4.578216	-1.472603	-0.377291
H	-4.956338	-0.438758	-1.773350
H	-5.727737	-0.126845	-0.209594
H	0.271989	2.669414	1.466439
H	0.839184	4.815371	0.431819
H	-0.706582	4.891376	-0.412887
H	0.479146	3.643673	-0.843911
H	-1.531958	3.453361	3.015423
H	-1.973493	4.724476	1.865366
H	-0.386100	4.752910	2.652487
C	0.793007	0.287373	-0.186084
H	-3.795691	-4.005288	1.421433
H	-2.397419	-4.757736	0.628753
H	-2.180776	-3.877725	2.162283
H	-0.897907	-3.604833	-1.803862
H	0.747967	-3.092775	-1.431973
H	-0.032815	-4.338561	-0.447595
H	1.014186	-3.014530	3.010592
H	1.391513	-3.423553	1.326066
H	1.797851	-1.811400	1.961673
H	0.957250	1.344814	-0.431054
H	0.857896	0.193367	0.901560
C	1.935104	-0.519405	-0.820475
Si	3.647342	0.057603	-0.328664
H	1.886239	-1.578268	-0.547004

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H	1.889157	-0.493151	-1.915655
O	4.722081	-1.055860	-0.959401
C	4.094082	1.783340	-0.947809
O	3.676038	0.041075	1.344707
H	5.074593	2.122053	-0.596086
H	4.108431	1.813982	-2.042981
H	3.353725	2.513174	-0.604458
C	4.798380	0.336547	2.153599
H	4.463446	0.433255	3.191477
H	5.548895	-0.464441	2.110864
H	5.283251	1.280518	1.865683
C	6.100100	-0.870560	-1.218965
H	6.448641	-1.698594	-1.844626
H	6.300220	0.067826	-1.753987
H	6.693218	-0.871552	-0.293865
C	-0.555993	0.290353	-2.633724
H	-1.372639	0.431614	-3.350971
H	0.108174	1.161347	-2.685407
H	0.011931	-0.588604	-2.944896

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TS(B3H-Me-B1H-Me)

C	-2.125335	1.087696	1.399854
C	-3.070007	0.100533	1.060993
C	-3.647493	0.093357	-0.244403
C	-3.324909	1.173009	-1.123837
C	-2.473463	2.244372	-0.700449
C	-1.856923	2.229070	0.559833
Ru	-1.457446	0.158611	-0.605239
Si	-0.450416	-2.136082	0.095148
O	0.294320	-2.751411	1.503305
C	1.652906	-2.994279	1.779305
C	-4.607062	-0.992743	-0.653650
C	-0.940559	3.328148	1.074785
C	-0.315613	4.194331	-0.027301
C	-1.688053	4.206632	2.100685
O	-2.007554	-2.682665	0.555483
C	-2.197526	-3.934323	1.199713
C	0.120397	-3.219706	-1.354947
H	-1.559591	-1.257159	-1.314490
H	-3.747204	1.189482	-2.122616
H	-2.254558	3.039838	-1.404236
H	-1.604856	1.009164	2.350883
H	-3.244179	-0.736445	1.724691
H	-4.253794	-1.955945	-0.280275
H	-4.692358	-1.049629	-1.741861
H	-5.604546	-0.793665	-0.242788
H	-0.120573	2.827025	1.609655
H	0.408971	4.889088	0.408615
H	-1.070477	4.798534	-0.543220
H	0.202860	3.587364	-0.775779
H	-2.104134	3.607768	2.916602
H	-2.515747	4.741200	1.621231
H	-1.012094	4.949777	2.537112
C	0.763005	-0.430232	0.101077
H	-3.277315	-4.102497	1.294603
H	-1.776719	-4.767149	0.617614
H	-1.741322	-3.953881	2.194526
H	-0.684111	-3.926927	-1.585386
H	0.325710	-2.645368	-2.261652
H	1.014696	-3.805839	-1.116753
H	1.720356	-3.535770	2.730840
H	2.128326	-3.619053	1.007413
H	2.239723	-2.070521	1.875976
H	0.518412	0.624549	-0.119189
H	0.971127	-0.423619	1.171893
C	2.023116	-0.752532	-0.736891
Si	3.529929	0.272755	-0.297156
H	2.325303	-1.800630	-0.645200

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H	1.817075	-0.601872	-1.801584
O	4.809951	-0.459781	-1.074209
C	3.411109	2.081074	-0.816101
O	3.673026	0.177269	1.364771
H	4.276837	2.674515	-0.502636
H	3.327340	2.169478	-1.904758
H	2.522931	2.545483	-0.375014
C	4.701711	0.753593	2.148289
H	4.391650	0.733186	3.197854
H	5.638751	0.188296	2.057982
H	4.899666	1.799341	1.873103
C	6.083238	0.089843	-1.357233
H	6.563901	-0.528039	-2.122192
H	6.017689	1.117193	-1.740275
H	6.727888	0.093058	-0.467863
C	-0.604933	0.451348	-2.539112
H	-1.371510	0.749826	-3.262535
H	0.136690	1.260064	-2.479703
H	-0.105946	-0.434944	-2.940416

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TS(B2-I-B1H-I)

C	-0.701059	1.974429	-1.686584
C	-0.850165	2.717764	-0.469871
C	-1.849714	2.283624	0.442929
C	-2.730985	1.189171	0.134683
C	-2.589874	0.454794	-1.051418
C	-1.512604	0.842496	-1.930998
C	0.041164	3.892800	-0.166734
C	-3.462329	-0.733052	-1.423014
C	-4.519453	-0.297604	-2.460294
C	-4.115676	-1.427671	-0.221112
Ru	-0.520452	0.594670	0.038570
I	0.646650	-1.862640	-0.670655
I	-0.528819	-0.140052	2.715108
H	-1.935339	2.767662	1.408844
H	-3.443051	0.878212	0.888767
H	-1.315322	0.236983	-2.810209
H	0.106214	2.217888	-2.366829
H	1.044696	3.726484	-0.564904
H	0.117708	4.058619	0.910388
H	-0.366365	4.802933	-0.623783
H	-2.800722	-1.461967	-1.909989
H	-4.629673	-2.335084	-0.552387
H	-4.866120	-0.788678	0.257778
H	-3.373610	-1.709262	0.531327
H	-4.058883	0.158846	-3.342483
H	-5.212415	0.432109	-2.027094
H	-5.103348	-1.161523	-2.793709
H	1.048735	0.909155	0.345906
Si	2.581749	0.055895	-0.411843
O	2.520549	1.369104	-1.429101
C	3.183304	0.281846	1.349873
O	3.729526	-0.858837	-1.214262
C	3.380423	1.548265	-2.558572
H	3.109460	2.502339	-3.020192
H	4.433033	1.581671	-2.260749
H	3.254334	0.744201	-3.288960
H	4.227481	-0.036983	1.430514
H	3.109639	1.340072	1.616360
H	2.566918	-0.277342	2.057452
C	4.276755	-2.092220	-0.787607
H	5.114397	-2.337531	-1.446811
H	4.647667	-2.044810	0.244713
H	3.535569	-2.899361	-0.852018

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B1H-I

Ru	-0.205747	0.436268	0.862941
I	0.022676	3.070475	0.626970
H	-0.895880	0.723573	2.269163
C	0.303443	-1.646817	1.384118
C	1.373628	-1.012091	0.672062
C	1.256167	-0.608979	-0.707000
C	0.006035	-0.569188	-1.314736
C	-1.124998	-0.957336	-0.495154
C	-0.972720	-1.612208	0.764476
C	0.517193	-2.245448	2.748182
C	-0.245894	-0.058376	-2.722415
C	0.863205	0.852012	-3.264041
C	-0.505674	-1.249376	-3.670350
H	2.337764	-0.918295	1.162205
H	2.129391	-0.212262	-1.210403
H	-2.125787	-0.831561	-0.897259
H	-1.847743	-1.966791	1.297230
H	-0.399426	-2.217481	3.341711
H	1.294690	-1.706337	3.295645
H	0.833660	-3.291887	2.656699
H	-1.169018	0.534904	-2.673117
H	0.567674	1.258336	-4.236005
H	1.799641	0.302721	-3.414901
H	1.054961	1.690878	-2.588897
H	-1.323795	-1.883627	-3.314019
H	0.388982	-1.874959	-3.762360
H	-0.770180	-0.888512	-4.669390

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B2H-I

C	1.465949	2.209753	0.400499
C	1.867178	2.141534	-0.968225
C	2.451578	0.914933	-1.414440
C	2.522893	-0.199079	-0.570201
C	2.130284	-0.128078	0.809806
C	1.649719	1.107088	1.280621
Ru	0.260011	0.613523	-0.613213
I	-0.844880	-1.830428	-1.251863
C	1.802828	3.351934	-1.864506
C	2.328595	-1.283035	1.784783
C	3.570319	-1.008584	2.662037
C	2.430387	-2.662645	1.120520
H	-1.030648	1.461928	-0.975884
H	2.762066	0.818817	-2.449923
H	2.872489	-1.140247	-0.975415
H	1.341277	1.198120	2.317273
H	1.052218	3.135086	0.784178
H	0.992811	4.020413	-1.563424
H	1.636461	3.063258	-2.905089
H	2.742430	3.915804	-1.815076
H	1.449584	-1.287350	2.441120
H	2.454447	-3.438612	1.891759
H	3.353277	-2.762748	0.537293
H	1.579492	-2.858738	0.463175
H	3.487117	-0.060570	3.202769
H	4.479061	-0.969042	2.050776
H	3.696536	-1.808072	3.399187
H	-0.251554	0.732713	-2.091217
Si	-1.675034	0.994743	0.806995
C	-1.689312	2.743898	1.534270
O	-3.126102	0.740641	0.020968
O	-1.620163	0.079756	2.211945
H	-2.605894	2.890980	2.116115
H	-0.850015	2.917976	2.215107
H	-1.662971	3.506749	0.749177
C	-4.389826	0.848149	0.657252
C	-1.902278	-1.304382	2.362576
H	-5.139916	0.392172	0.004137
H	-4.412534	0.331099	1.625249
H	-4.668361	1.898228	0.822114
H	-2.170436	-1.480897	3.410248
H	-2.730722	-1.627186	1.723145
H	-1.029146	-1.917127	2.112176

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TS(B2H-I-B3H-I)

Ru	-0.657813	0.516621	-0.130248
I	-1.168875	-0.190899	2.492137
C	-1.115410	1.299884	-2.145722
C	0.049827	1.973932	-1.666274
C	-0.009637	2.821185	-0.520012
C	-1.207472	2.782148	0.223530
C	-2.378966	2.117445	-0.259681
C	-2.380737	1.444900	-1.495278
C	1.152906	3.691635	-0.055099
C	2.441858	3.498503	-0.865890
C	0.736669	5.178926	-0.069647
C	-3.635293	0.868455	-2.091969
H	0.975295	1.861444	-2.215266
H	-1.045969	0.685109	-3.035107
H	-1.261152	3.287378	1.181876
H	-3.283399	2.149239	0.338175
H	1.358515	3.419013	0.988936
H	2.316316	3.852418	-1.895792
H	2.756983	2.453059	-0.909628
H	3.251687	4.083055	-0.418272
H	1.555208	5.804794	0.300638
H	-0.139433	5.365131	0.557802
H	0.497176	5.504921	-1.087970
H	-4.100632	1.608791	-2.755132
H	-4.354078	0.597446	-1.316723
H	-3.413570	-0.028053	-2.672503
Si	-1.350567	-1.701408	-0.729705
O	-1.097508	-1.807489	-2.402673
C	-1.581125	-2.903825	-3.164254
C	-0.543197	-3.194749	0.098474
O	-3.023035	-1.907160	-0.641571
C	-3.760236	-2.407742	0.459745
H	-0.984437	-3.810426	-2.989700
H	-2.629527	-3.128261	-2.934115
H	-1.503226	-2.648199	-4.227086
H	0.542327	-3.154304	-0.036235
H	-0.745698	-3.212170	1.172743
H	-0.914921	-4.130378	-0.336279
H	-3.769194	-1.700508	1.297532
H	-4.791699	-2.577840	0.130239
H	-3.356606	-3.362067	0.824301
C	2.274971	-0.365902	2.483834
C	2.405076	0.207603	1.241223
Si	3.371536	-0.720392	-0.077238
O	3.039470	-2.348100	0.002771
C	3.810750	-3.361552	0.627316

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C	5.216814	-0.410733	0.122599
O	2.854919	-0.174381	-1.554014
C	2.840974	-0.916985	-2.769022
H	2.276317	-1.444899	2.611354
H	2.072961	0.214815	3.378125
H	2.496719	1.296589	1.239246
H	3.783220	-3.276221	1.721066
H	3.386105	-4.330515	0.349897
H	4.859412	-3.337187	0.304474
H	5.792432	-0.913913	-0.662545
H	5.587692	-0.756187	1.093219
H	5.429184	0.661289	0.050232
H	3.527932	-0.458608	-3.490293
H	1.826000	-0.905565	-3.178717
H	3.131473	-1.961528	-2.613991
H	1.056942	0.192425	0.621093
H	0.316812	-0.650327	-0.600121

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B3H-I

C	-2.721685	-0.491989	1.382005
C	-2.061260	0.508913	2.131096
C	-0.786335	0.274523	2.727910
C	-0.187209	-0.980098	2.467863
C	-0.869998	-2.009215	1.751572
C	-2.155606	-1.792055	1.225157
Ru	-0.609959	-0.013443	0.434686
Si	-1.237522	2.221210	-0.313081
O	-2.909641	2.317442	-0.460409
C	-3.673290	2.209874	-1.652093
C	-0.123737	1.315364	3.590541
C	-2.957369	-2.865585	0.507300
C	-2.127358	-4.060691	0.025302
C	-4.116505	-3.329968	1.417195
I	-1.142195	-0.739915	-2.205673
O	-0.947317	3.226668	1.010945
C	-1.433045	4.561498	1.065245
C	-0.431654	2.983421	-1.835842
H	0.277741	1.273059	0.191459
H	0.804653	-1.180518	2.857901
H	-0.372228	-2.958792	1.599460
H	-3.677162	-0.263106	0.925211
H	-2.527309	1.480312	2.247550
H	-0.287851	2.310375	3.172070
H	0.952228	1.139121	3.663083
H	-0.541542	1.285634	4.604351
H	-3.390513	-2.383123	-0.377595
H	-2.763874	-4.741146	-0.548301
H	-1.713812	-4.634350	0.863212
H	-1.309607	-3.739489	-0.625155
H	-4.753623	-2.495677	1.726215
H	-3.734033	-3.814979	2.322300
H	-4.742401	-4.053778	0.885874
C	1.444693	-0.459989	-0.114979
H	-1.210935	4.966373	2.058012
H	-0.941344	5.201348	0.319972
H	-2.516310	4.603293	0.900690
H	-0.783183	4.011518	-1.982502
H	0.655647	3.012356	-1.711155
H	-0.647224	2.410782	-2.740443
H	-4.690333	2.553045	-1.433310
H	-3.265916	2.833920	-2.457754
H	-3.713800	1.174688	-2.007841
H	1.458814	-1.555586	-0.116988
H	1.577775	-0.139043	-1.148400
C	2.573024	0.103894	0.757262
Si	4.286622	-0.362156	0.140311

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H	2.540506	1.200697	0.784890
H	2.497125	-0.220726	1.802699
O	5.330703	0.152679	1.337838
C	4.509083	-2.210100	-0.153632
O	4.547251	0.478877	-1.274071
H	5.536589	-2.472206	-0.428470
H	4.264260	-2.766603	0.757689
H	3.850127	-2.569978	-0.950892
C	5.315317	0.083868	-2.395266
H	5.005100	0.685156	-3.255556
H	6.388019	0.253622	-2.228972
H	5.168796	-0.974143	-2.648543
C	6.739866	0.211985	1.206648
H	7.161213	0.555296	2.156750
H	7.176306	-0.771204	0.977706
H	7.042688	0.917808	0.421909

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TS(B3H-I-B1H-I)

C	1.957578	-0.260310	2.081980
C	2.988026	0.447445	1.415133
C	3.632423	-0.123626	0.274744
C	3.194637	-1.412210	-0.128921
C	2.271187	-2.187555	0.658518
C	1.653141	-1.641717	1.782628
Ru	1.427890	-0.084423	-0.072743
Si	0.283092	2.280655	0.139853
O	-0.597291	3.030715	1.377308
C	-1.977048	3.269022	1.540609
C	4.701860	0.626128	-0.473877
C	0.637343	-2.375646	2.641177
C	0.070239	-3.645184	1.993515
C	1.246651	-2.689689	4.024724
I	0.705888	-1.019248	-2.597124
O	1.774040	2.960121	0.614569
C	1.862690	4.321933	1.014948
C	-0.192254	3.041160	-1.524028
H	1.586197	1.208078	-0.966818
H	3.582094	-1.840894	-1.045908
H	2.004025	-3.176471	0.306451
H	1.423525	0.234465	2.887778
H	3.194753	1.472537	1.690803
H	4.507659	1.700634	-0.448337
H	4.748228	0.305514	-1.517128
H	5.681950	0.442020	-0.016984
H	-0.197478	-1.677549	2.800142
H	-0.724210	-4.060081	2.620918
H	0.837481	-4.420093	1.885935
H	-0.349708	-3.444727	1.003073
H	1.618309	-1.787375	4.519912
H	2.083579	-3.390027	3.928933
H	0.495427	-3.146449	4.676886
C	-0.853506	0.487309	0.352241
H	2.922129	4.557884	1.166940
H	1.471926	5.002114	0.244758
H	1.314001	4.507545	1.943634
H	0.595101	3.746541	-1.810940
H	-0.269164	2.290418	-2.313858
H	-1.135357	3.595925	-1.483417
H	-2.107418	3.950611	2.389466
H	-2.421483	3.748862	0.656204
H	-2.540414	2.350957	1.751867
H	-0.622580	-0.585781	0.278461
H	-1.103056	0.645670	1.402401
C	-2.065284	0.699794	-0.584514
Si	-3.589554	-0.275833	-0.086563

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H	-2.379481	1.745526	-0.648579
H	-1.799935	0.403003	-1.604473
O	-4.840114	0.353226	-0.988459
C	-3.444197	-2.130941	-0.363114
O	-3.805113	0.039200	1.543059
H	-4.333896	-2.680530	-0.037032
H	-3.278182	-2.356654	-1.421629
H	-2.591379	-2.531528	0.194603
C	-4.921840	-0.379376	2.307796
H	-4.743681	-0.115028	3.354879
H	-5.843607	0.119720	1.980899
H	-5.076757	-1.466324	2.252786
C	-6.036193	-0.282517	-1.400814
H	-6.432328	0.255297	-2.267824
H	-5.873764	-1.328205	-1.692887
H	-6.796114	-0.258576	-0.607995

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R1

Si	-0.000137	0.548358	-0.593735
H	-0.000143	1.211085	-1.911455
O	1.390266	-0.359636	-0.582953
O	-1.390531	-0.359695	-0.582935
C	1.949475	-1.043924	0.524455
H	1.927676	-0.440846	1.442414
H	1.425195	-1.989169	0.716977
H	2.993901	-1.275147	0.295046
C	-1.948877	-1.044419	0.524654
H	-1.927566	-0.441198	1.442539
H	-2.993119	-1.276686	0.295459
H	-1.423653	-1.989124	0.717246
C	-0.000196	1.777813	0.829821
H	-0.885332	2.420449	0.776419
H	0.000313	1.300245	1.815285
H	0.884362	2.421204	0.775877

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R2

C	-3.019996	-0.003467	-0.106261
C	-1.873507	-0.096867	-0.789161
H	-3.041967	0.110774	0.975701
H	-3.993602	-0.036304	-0.59165
H	-1.930767	-0.209491	-1.87272
Si	-0.188318	-0.033536	-0.008493
O	0.538256	-1.474461	-0.418777
O	0.5945	1.261451	-0.703622
C	-0.243666	0.162793	1.861745
H	0.754871	0.115083	2.309113
H	-0.687437	1.120705	2.15223
H	-0.838806	-0.636659	2.314586
C	1.70819	1.973758	-0.196767
H	2.64727	1.432027	-0.372051
H	1.769051	2.934579	-0.716954
H	1.620304	2.174042	0.879442
C	1.863355	-1.854847	-0.093675
H	1.98659	-2.914876	-0.3349
H	2.598792	-1.283149	-0.674776
H	2.083841	-1.721371	0.974783

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P1

Si	-2.218319	-0.117918	-0.173708
C	-0.448839	-0.604836	0.195417
C	0.591733	0.521419	-0.029429
H	-0.19224	-1.480958	-0.412581
H	-0.420081	-0.947467	1.237959
H	0.55978	0.857822	-1.074766
H	0.329054	1.398224	0.576321
O	-3.130517	-1.454308	0.225244
O	-2.54024	1.188197	0.811693
Si	2.358024	0.021927	0.374326
O	2.692851	-1.225756	-0.684079
O	3.423346	1.288753	0.155316
C	-2.518086	0.350217	-1.974702
H	-2.238287	-0.478685	-2.63353
H	-1.915649	1.219519	-2.258394
H	-3.564428	0.595993	-2.185546
C	2.604428	-0.492248	2.159709
H	2.319491	0.322076	2.833636
H	1.99752	-1.367432	2.412394
H	3.651768	-0.735602	2.364386
C	-3.635108	2.081021	0.72932
H	-4.538692	1.65095	1.181412
H	-3.381963	2.992552	1.279924
H	-3.867419	2.363009	-0.306656
C	-4.519307	-1.632311	0.016749
H	-4.75853	-2.68941	0.16818
H	-5.113037	-1.043964	0.729056
H	-4.82704	-1.357224	-1.001582
C	3.544412	2.027901	-1.050321
H	3.722244	1.37615	-1.915517
H	2.646452	2.628343	-1.248014
H	4.395109	2.708834	-0.95113
C	3.889076	-1.989178	-0.65985
H	3.829789	-2.745657	-1.448106
H	4.773905	-1.366136	-0.84357
H	4.023002	-2.50405	0.300719

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Cl-Si

Si	0.041155	-0.367517	-0.372711
O	-1.406554	0.333264	-0.712489
O	1.343188	0.583746	-0.694216
C	-2.094134	1.36432	-0.015527
H	-2.040687	1.222861	1.069616
H	-1.682315	2.348871	-0.267443
H	-3.142955	1.338322	-0.321722
C	1.779441	1.745898	-0.000715
H	1.111722	2.594252	-0.19301
H	1.833125	1.572056	1.079822
H	2.777063	2.000678	-0.366671
C	0.188411	-1.915344	-1.37829
H	1.12096	-2.438518	-1.151845
H	-0.648219	-2.589094	-1.177504
H	0.183585	-1.667952	-2.44415
Cl	0.069186	-0.808327	1.683041

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Me—Si

Si	-0.034159	0.498781	0.014936
O	1.305145	-0.275853	-0.603879
O	-1.459362	-0.189396	-0.507338
C	1.905799	-1.467014	-0.130956
H	1.962423	-1.499685	0.965528
H	1.361345	-2.356357	-0.475302
H	2.925480	-1.520706	-0.524969
C	-1.908396	-1.500582	-0.218407
H	-1.833241	-1.741657	0.851326
H	-2.960611	-1.577446	-0.508995
H	-1.342089	-2.252337	-0.783948
C	0.031170	0.488512	1.897577
H	-0.795652	1.078271	2.307405
H	-0.043430	-0.516908	2.325082
H	0.966369	0.929955	2.258624
C	-0.018303	2.218040	-0.707206
H	-0.904459	2.782118	-0.400437
H	0.869244	2.771497	-0.384962
H	-0.008899	2.172789	-1.800221

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I—Si

Si	0.554946	-0.381684	0.145522
O	-0.071835	-0.166197	1.653215
O	0.438605	-1.970917	-0.228405
C	2.336244	0.129181	-0.029582
C	-0.307076	1.063282	2.329839
C	-0.740971	-2.769432	-0.140669
H	-0.742295	0.829651	3.304496
H	0.626136	1.618293	2.486846
H	-1.007040	1.694708	1.770772
H	-1.490249	-2.437621	-0.868487
H	-0.458975	-3.800267	-0.367334
H	-1.171321	-2.726148	0.865098
H	2.953005	-0.474575	0.644337
H	2.682445	-0.028885	-1.054313
H	2.474206	1.185024	0.220128
I	-0.848459	0.970073	-1.463058

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B5

Ru	-0.024089	0.394246	0.100945
Cl	-0.060247	1.918663	1.982728
H	-1.503700	0.884181	0.036373
C	-0.973760	-1.708393	0.417255
C	-0.114105	-1.415359	1.495173
C	1.289608	-1.161418	1.300174
C	1.860576	-1.149230	0.023091
C	0.938088	-1.222521	-1.074726
C	-0.440781	-1.545925	-0.895965
C	-2.413960	-2.090657	0.633118
C	3.346385	-0.983503	-0.245217
C	4.108755	-0.274383	0.882125
C	3.976449	-2.356457	-0.565109
H	-0.511704	-1.389121	2.503462
H	1.895102	-0.959803	2.175627
H	1.315352	-1.102025	-2.086702
H	-1.082846	-1.670967	-1.760943
H	-3.049028	-1.694991	-0.162726
H	-2.782159	-1.712989	1.589638
H	-2.513802	-3.182936	0.637742
H	3.434753	-0.365583	-1.149340
H	5.139777	-0.081557	0.570163
H	4.155679	-0.890057	1.787136
H	3.643992	0.680743	1.142546
H	3.466204	-2.851576	-1.397316
H	3.922906	-3.020195	0.304750
H	5.030527	-2.238469	-0.836381
C	-0.157546	1.694258	-1.698596
H	-0.002808	1.046332	-2.564099
C	0.989843	2.016741	-0.945350
H	0.999738	2.879763	-0.287499
H	1.973272	1.683429	-1.274318
Si	-1.676161	2.760560	-1.861297
C	-1.963961	3.977341	-0.467051
H	-1.204164	4.766635	-0.465268
H	-2.943414	4.461480	-0.550444
H	-1.907171	3.468436	0.498943
O	-2.957840	1.698092	-2.033829
O	-1.471511	3.577362	-3.309039
C	-4.230861	2.086747	-2.516378
H	-4.174585	2.474316	-3.542425
H	-4.883241	1.207531	-2.518648
H	-4.699299	2.851891	-1.880381
C	-1.957200	4.862153	-3.645798
H	-1.416774	5.216205	-4.529942
H	-3.028767	4.841710	-3.889652

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H	-1.804716	5.591235	-2.838917

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TS(B5-B6)

Ru	-0.513097	0.711395	-0.021897
Cl	0.160223	0.982172	2.303870
H	0.964653	1.291476	-0.292367
C	-1.570031	2.537467	-1.011424
C	-2.234353	2.204222	0.180938
C	-2.770851	0.887630	0.413881
C	-2.640675	-0.137265	-0.536074
C	-1.834366	0.155027	-1.689414
C	-1.312317	1.460083	-1.923804
C	-1.087656	3.935851	-1.294359
C	-3.256660	-1.517009	-0.372972
C	-3.453031	-1.942687	1.088183
C	-4.584257	-1.586488	-1.157692
H	-2.329204	2.946615	0.965490
H	-3.248838	0.693326	1.365721
H	-1.636904	-0.630002	-2.413605
H	-0.730269	1.646693	-2.820822
H	-0.141740	3.927353	-1.841763
H	-0.942957	4.497489	-0.368498
H	-1.823321	4.474172	-1.904923
H	-2.560850	-2.227993	-0.837892
H	-3.775987	-2.987395	1.131664
H	-4.226799	-1.345281	1.582831
H	-2.526419	-1.842335	1.660039
H	-4.444882	-1.327662	-2.212200
H	-5.320621	-0.893566	-0.735935
H	-5.003951	-2.596529	-1.109495
C	1.459806	-0.229276	-0.536364
H	1.531824	-0.254475	-1.625488
C	0.537522	-1.159832	0.045631
H	0.688678	-1.483283	1.071371
H	0.058084	-1.894692	-0.599076
Si	3.149215	0.185268	0.216215
C	3.486397	-0.644395	1.861277
H	3.378480	-1.730199	1.771223
H	4.506554	-0.436965	2.203628
H	2.785241	-0.294140	2.623542
O	3.436426	1.819836	0.275068
O	4.139775	-0.408362	-0.985539
C	3.333924	2.671104	1.412485
H	4.022787	2.358680	2.208220
H	3.610664	3.682261	1.097804
H	2.316102	2.680143	1.814841
C	5.549173	-0.242711	-0.991229
H	5.937686	-0.644516	-1.932189
H	5.828694	0.815415	-0.919695

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H	6.025281	-0.787803	-0.164279

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B6

Ru	0.091525	-0.324790	0.380273
Cl	-0.033236	1.129316	2.234954
H	-2.364116	1.517296	0.308966
C	-0.578939	-2.361715	-0.011971
C	0.233428	-2.585130	1.164757
C	1.507735	-2.049371	1.242407
C	2.023704	-1.250119	0.152358
C	1.330222	-1.282259	-1.109014
C	0.039297	-1.850890	-1.197836
C	-2.005062	-2.850056	-0.040026
C	3.390683	-0.583808	0.227618
C	3.706946	0.041792	1.594034
C	4.480381	-1.594631	-0.189985
H	-0.214964	-3.054770	2.034561
H	2.053382	-2.095873	2.177571
H	1.758115	-0.769393	-1.964575
H	-0.535131	-1.766467	-2.114342
H	-2.590326	-2.326442	-0.800157
H	-2.491014	-2.703598	0.928322
H	-2.034164	-3.922642	-0.271342
H	3.381107	0.224555	-0.514792
H	4.642540	0.606955	1.533834
H	3.843535	-0.721698	2.368159
H	2.910813	0.716942	1.918371
H	4.292842	-2.004142	-1.187841
H	4.527227	-2.433010	0.514093
H	5.462953	-1.111863	-0.200420
C	-2.056588	1.336415	-0.728252
H	-2.541231	0.401434	-1.042437
C	-0.522524	1.242564	-0.837605
H	-0.056224	2.163465	-0.472109
H	-0.219332	1.083913	-1.877954
Si	-2.802634	2.694887	-1.789145
C	-2.296344	4.428824	-1.260018
H	-1.205062	4.513806	-1.242068
H	-2.676565	5.212430	-1.924226
H	-2.661146	4.644528	-0.250113
O	-4.457332	2.514582	-1.663460
O	-2.266661	2.388005	-3.341230
C	-5.449329	3.463763	-2.006908
H	-5.618052	3.496545	-3.092213
H	-6.389182	3.172275	-1.527003
H	-5.193683	4.476529	-1.666735
C	-2.537110	3.169733	-4.488630
H	-1.826749	2.892643	-5.274602
H	-3.552014	2.988362	-4.868089

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H	-2.426842	4.246652	-4.298103

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B7

Ru	1.039334	0.125807	-0.193113
Cl	0.922941	0.858095	-2.496849
H	-1.973932	0.673247	-2.014594
C	0.819265	0.094906	2.108140
C	0.004848	1.185114	1.698274
C	0.516947	2.228331	0.913020
C	1.915139	2.314102	0.602664
C	2.739943	1.270792	1.047779
C	2.193211	0.133549	1.713260
C	0.277292	-0.982225	3.008918
C	2.517795	3.502178	-0.133882
C	1.531079	4.239215	-1.049629
C	3.158727	4.468418	0.886567
H	-1.059177	1.154453	1.917557
H	-0.156288	2.996927	0.554491
H	3.799658	1.289738	0.812077
H	2.845168	-0.687167	1.991859
H	0.798220	-1.926634	2.851429
H	-0.785669	-1.147890	2.818144
H	0.392997	-0.681436	4.057832
H	3.318924	3.098901	-0.765492
H	2.067614	4.996910	-1.629189
H	0.758272	4.763073	-0.475032
H	1.051674	3.547540	-1.746768
H	3.911063	3.968158	1.504777
H	2.400135	4.890202	1.555509
H	3.645441	5.298980	0.365196
C	-1.960406	0.486234	-0.937222
H	-1.697554	1.450186	-0.489244
C	-0.955903	-0.633128	-0.596886
H	-0.959020	-1.351413	-1.417218
H	-1.229601	-1.171248	0.312215
Si	-3.678762	0.102060	-0.304490
C	-4.378558	-1.545222	-0.888012
H	-3.678228	-2.350066	-0.641859
H	-5.343967	-1.795501	-0.435326
H	-4.513692	-1.544809	-1.975274
O	-4.677364	1.356239	-0.767953
O	-3.495673	0.083724	1.367341
C	-6.084949	1.333825	-0.910766
H	-6.591771	1.399718	0.061962
H	-6.385745	2.199695	-1.509217
H	-6.437280	0.427541	-1.421244
C	-4.550569	-0.140468	2.286045
H	-4.124203	-0.239302	3.289604
H	-5.260608	0.697570	2.298557

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H	-5.105854	-1.062328	2.062959
Si	1.372565	-2.246759	-0.453704
H	2.196190	-0.637346	-0.949839
O	0.341966	-3.043966	0.608394
O	2.878254	-2.752591	0.139317
C	1.176577	-2.964209	-2.189410
H	0.128841	-2.987263	-2.502018
H	1.717158	-2.361706	-2.925475
H	1.561814	-3.989747	-2.227458
C	0.414032	-4.447543	0.818211
H	1.419888	-4.759537	1.122966
H	-0.292805	-4.709857	1.612631
H	0.133560	-5.006691	-0.085110
C	4.099254	-2.565535	-0.546837
H	4.319438	-1.500333	-0.717332
H	4.908097	-2.986084	0.060388
H	4.107488	-3.071064	-1.522502

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TS(B7-B1H)

Ru	-1.148774	-0.094657	0.278191
Cl	-1.281793	0.248358	-2.132736
H	2.141283	1.011679	-1.741390
C	-0.796107	-1.050708	2.305961
C	-0.334980	-2.040114	1.366562
C	-1.144143	-2.481200	0.319775
C	-2.464853	-1.935790	0.140132
C	-2.959366	-1.019305	1.106154
C	-2.125730	-0.570788	2.179704
C	0.091122	-0.604419	3.441276
C	-3.383511	-2.378620	-0.994210
C	-2.664360	-3.084902	-2.150991
C	-4.508611	-3.272352	-0.428791
H	0.697210	-2.373072	1.424304
H	-0.745075	-3.175519	-0.408290
H	-3.959063	-0.614502	0.995371
H	-2.500471	0.161748	2.886052
H	-0.179025	0.396661	3.786224
H	1.142697	-0.593359	3.141540
H	-0.003856	-1.294696	4.288990
H	-3.836309	-1.464507	-1.396033
H	-3.377261	-3.280390	-2.958060
H	-2.254154	-4.053817	-1.841766
H	-1.860254	-2.464851	-2.552803
H	-5.084329	-2.764706	0.351250
H	-4.098713	-4.192929	0.002377
H	-5.201558	-3.556819	-1.227287
C	1.896479	0.275379	-0.969054
H	1.325386	-0.496831	-1.491845
C	1.067276	0.906261	0.163371
H	1.624181	1.720834	0.643994
H	0.999370	0.222345	1.009564
Si	3.502539	-0.478722	-0.367846
C	4.780636	0.794263	0.178081
H	4.365243	1.436915	0.961709
H	5.696037	0.343990	0.576262
H	5.069841	1.438332	-0.659646
O	4.104184	-1.396983	-1.620514
O	3.094289	-1.447571	0.945147
C	5.447384	-1.772963	-1.861989
H	5.750301	-2.617569	-1.228252
H	5.535413	-2.084623	-2.907407
H	6.149049	-0.945510	-1.692136
C	4.029302	-2.227316	1.673618
H	3.535628	-2.615326	2.570438
H	4.386406	-3.081828	1.083821

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H	4.899125	-1.638054	1.995370
Si	-0.205290	2.516166	-0.190270
H	-1.857321	1.301238	0.373512
O	0.129698	3.181106	1.319577
O	-1.702847	3.235339	-0.475758
C	0.851664	3.286887	-1.562848
H	1.919569	3.271256	-1.326118
H	0.707881	2.780948	-2.521696
H	0.548955	4.332103	-1.687110
C	-0.461951	4.375592	1.807590
H	-1.549828	4.283254	1.888805
H	-0.043256	4.574304	2.800148
H	-0.241051	5.234587	1.160695
C	-2.427043	3.367237	-1.682753
H	-2.995588	2.458376	-1.901163
H	-3.120463	4.208622	-1.567305
H	-1.772794	3.572324	-2.539555