Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Binding of Saturated Hydrocarbons to the Electrophilic Anion $[B_{12}Br_{11}]^-$: A Systematic Mechanistic Study

Xin Ma, Markus Rohdenburg, Harald Knorke, Sebastian Kawa, Judy Kuan-Yu Liu, Edoardo Apra, Knut R. Asmis, Vladimir A. Azov, Julia Laskin, Carsten Jenne, Hilkka I. Kenttämaa, Jonas Warneke*

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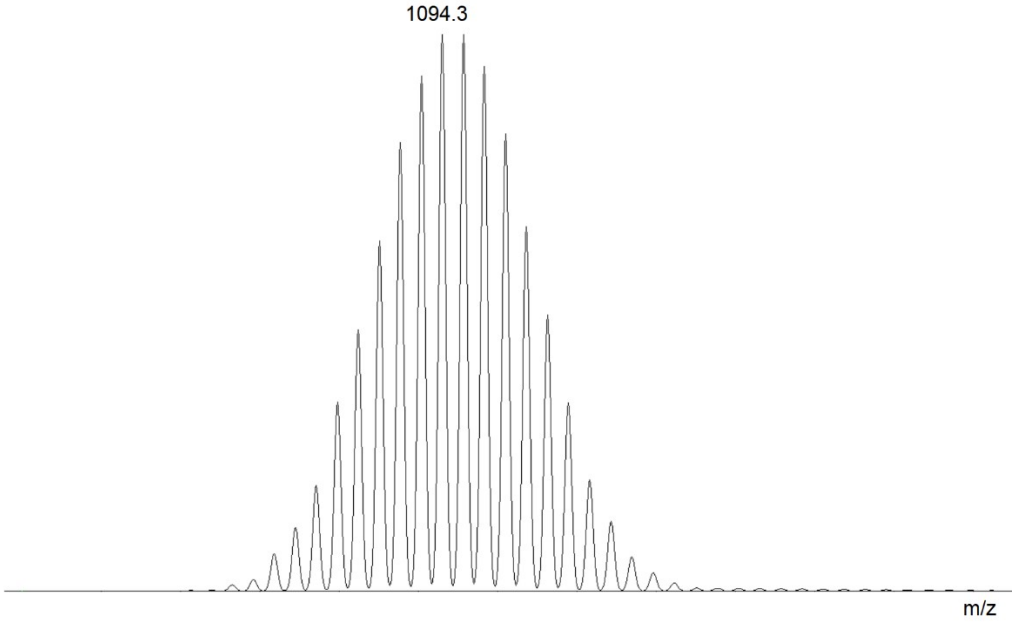


Figure S1. Simulated isotopic pattern of $[B_{12}Br_{11}(C_6H_{14})]^-$.

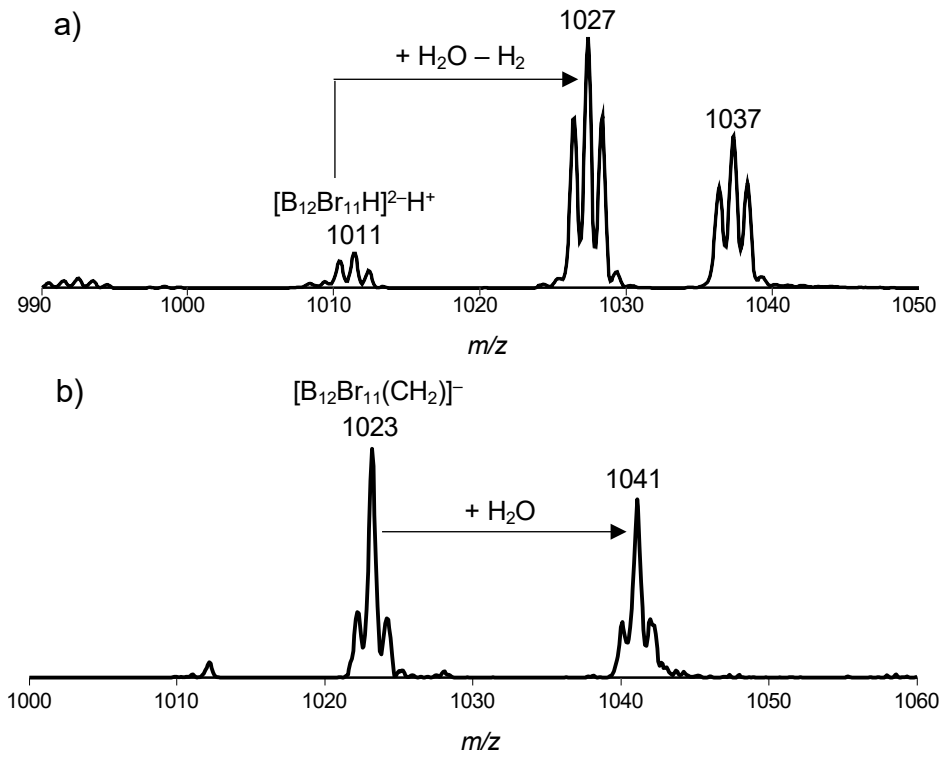


Figure S2. a) Reactions of the ion of *m/z* 1011 with water after 30 ms and b) reactions of the ion of *m/z* 1023 with water after 30 ms. The ions of *m/z* 1011 and 1023 were generated and isolated from the CID of the adduct formed upon reactions of $[B_{12}Br_{11}]^-$ with *n*-hexane. The ion of *m/z* 1027 was formed upon addition of water to *m/z* 1011 followed by elimination of H_2. The isolation window was slightly broader than *m/z* 1 and explaining the appearance of the signal as a triplet.

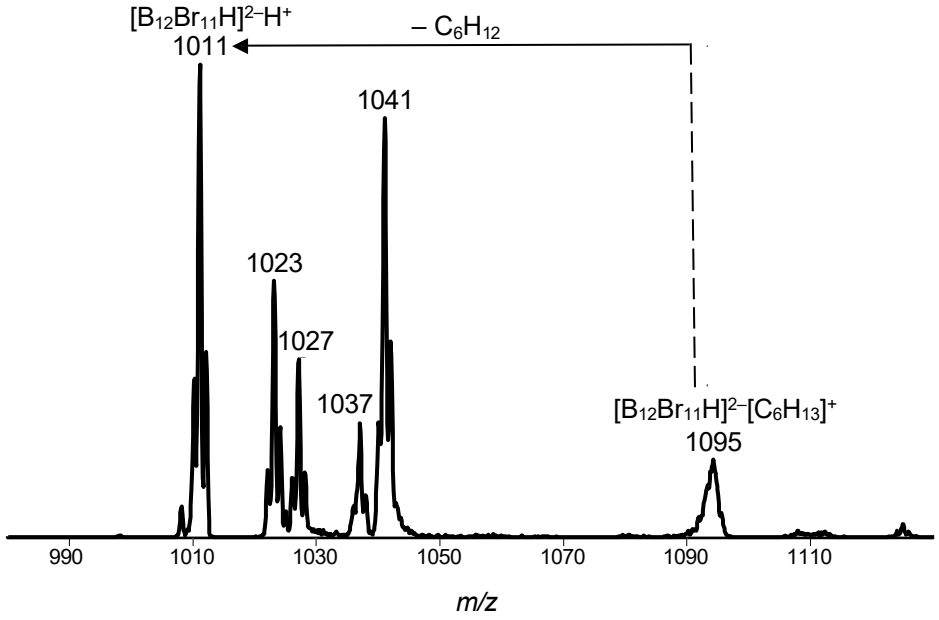


Figure S3. Mass spectrum of 2,3-dimethylbutane reacting with $[B_{12}Br_{11}]^-$ after 30 ms. No CID energy was applied. The ion of *m/z* 1011 ($[B_{12}Br_{11}H]^{2-}H^+$) was the predominant product as the result of instant dissociation of the adduct ion of *m/z* 1095 ($[B_{12}Br_{11}H]^{2-}[C_6H_{13}]^+$) by loss of C_6H_{12}.

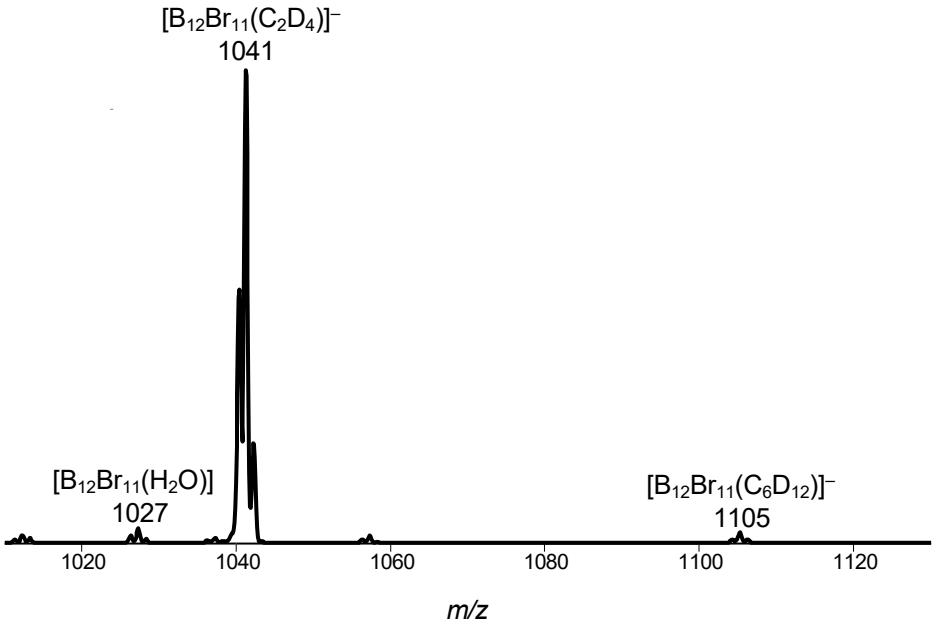


Figure S4. CID mass spectrum of the adduct formed upon reactions of cyclohexane-d_{12} with $[B_{12}Br_{11}]^-$. The ion of *m/z* 1037 was negligible in the spectrum, indicating no $[B_{12}Br_{11}(N_2)]^-$ was formed in the reaction. The ion of *m/z* 1037 observed in Figure 4a is proved to be $[B_{12}Br_{11}(C_2H_4)]^-$. It also suggests a ring opening has occurred during fragmentation of the cyclohexane adduct.

$[B_{12}Br_{11}(C_6H_{12})]^-$

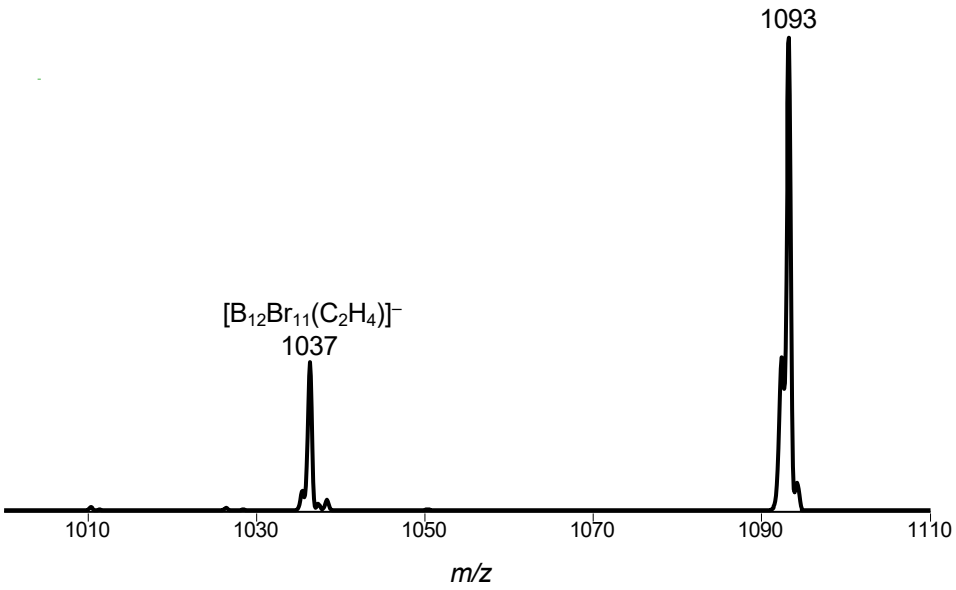


Figure S5. CID mass spectrum of the adduct formed upon reactions of 1-hexene with $[B_{12}Br_{11}]^-$. The fragmentation pattern is identical to that of the adduct formed with cyclohexane (Figure 3a).

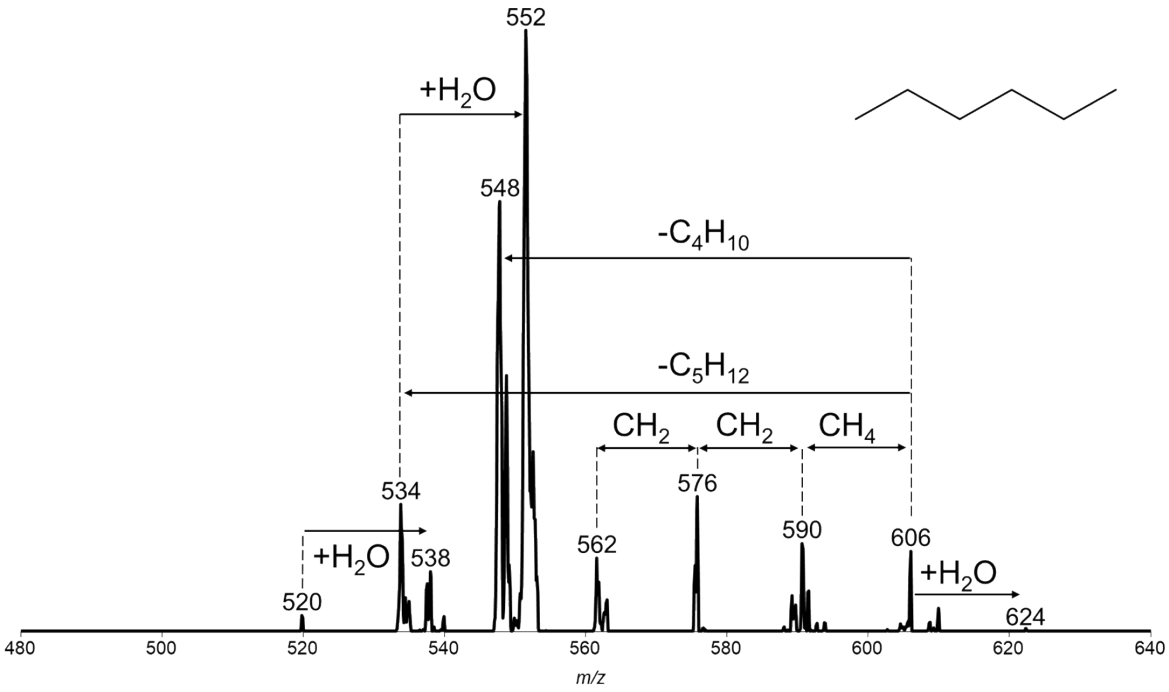
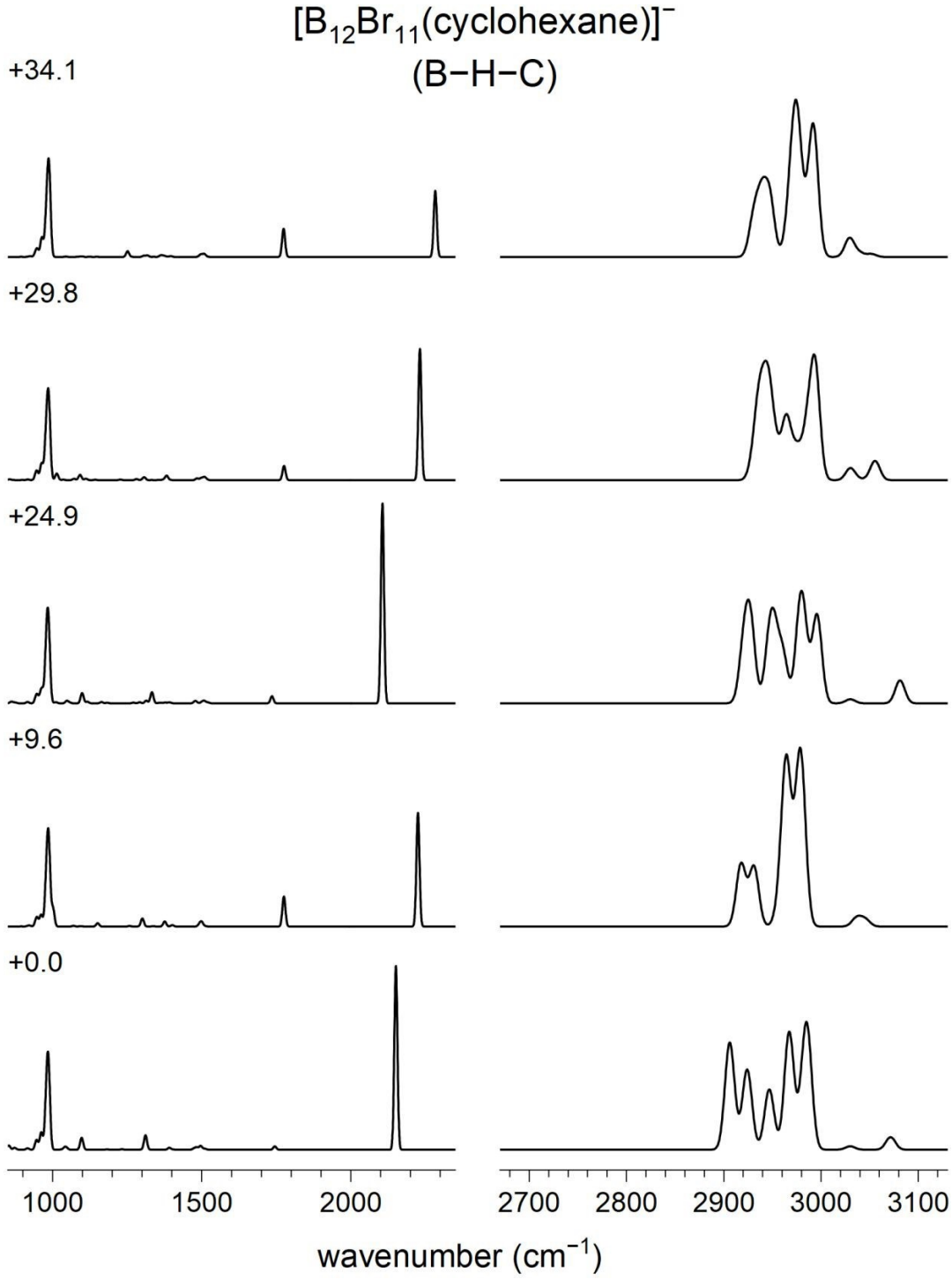
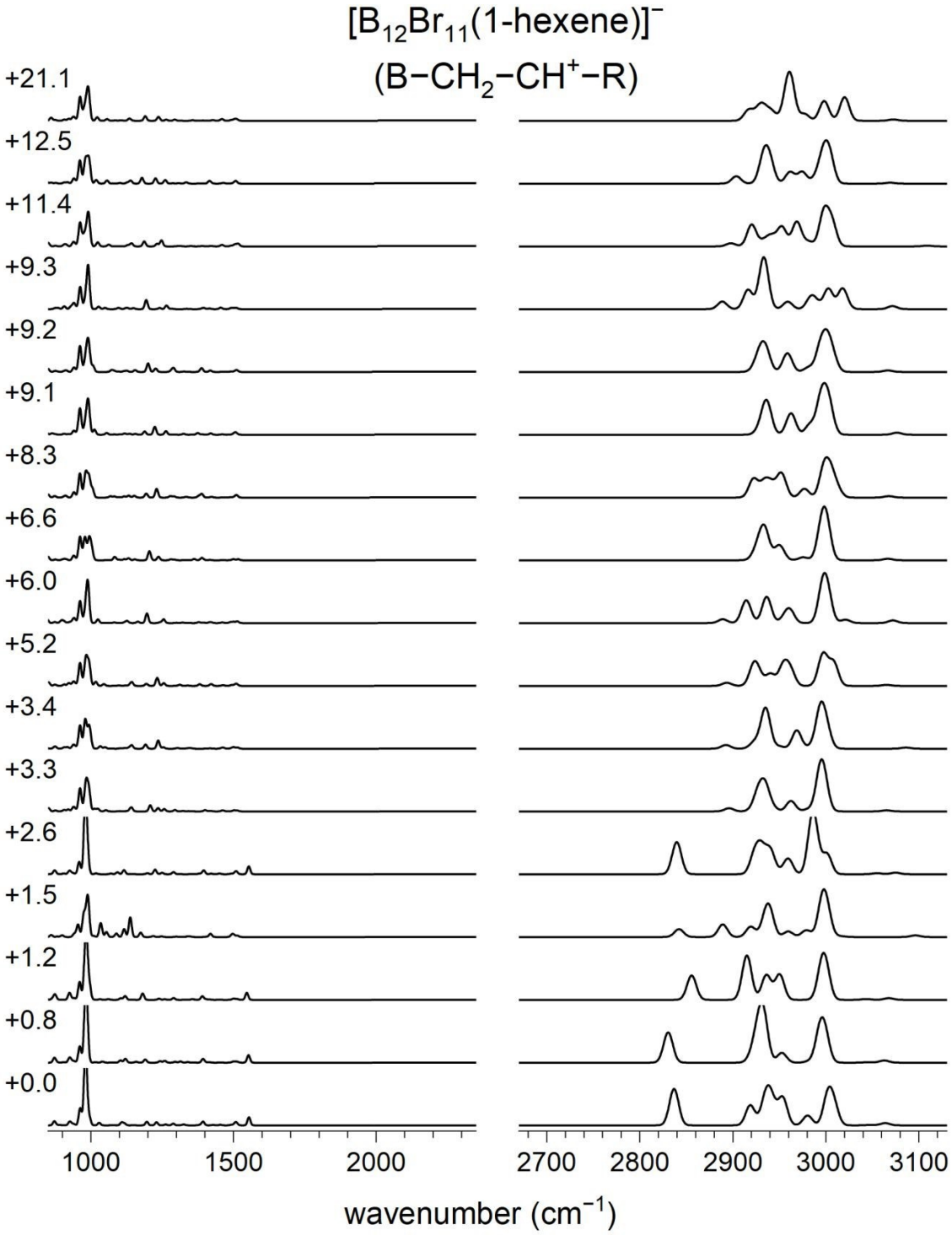


Figure S6. Fragment ions observed upon CID of the $[B_{12}Cl_{11}(C_6H_{14})]^-$ adduct (*m/z* 606) formed in the reactions of *n*-hexane with $[B_{12}Cl_{11}]^-$.


[B12Br11(cyclohexane)]−
(B−H−C)
+34.1
+29.8
+24.9
+9.6
+0.0
1000
1500
2000
2700
2800
2900
3000
3100
wavenumber (cm−1)


[B12Br11(1-hexene)]−
(B−CH2−CH+−R)
+21.1
+12.5
+11.4
+9.3
+9.2
+9.1
+8.3
+6.6
+6.0
+5.2
+3.4
+3.3
+2.6
+1.5
+1.2
+0.8
+0.0
1000
1500
2000
2700
2800
2900
3000
3100
wavenumber (cm−1)

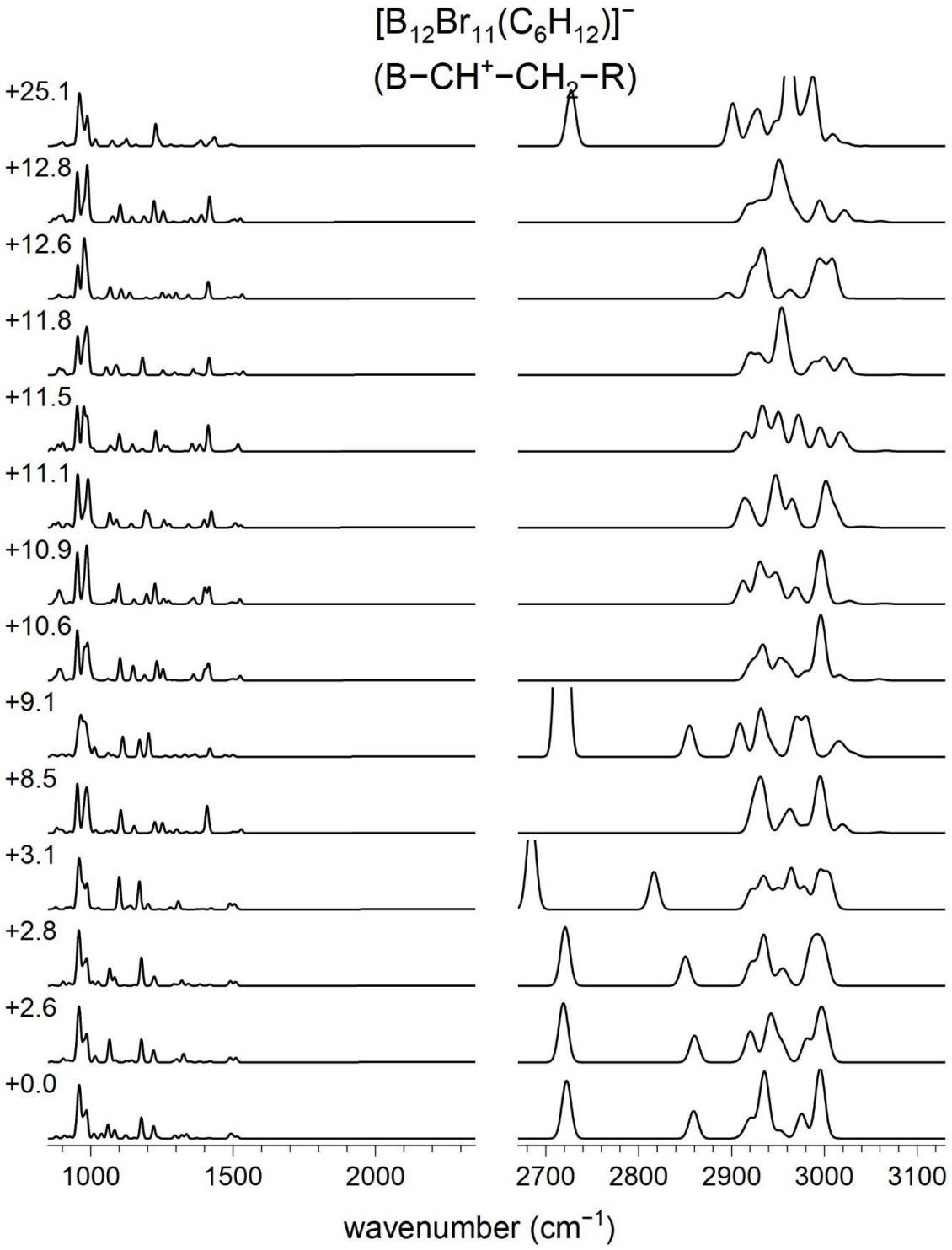


Figure S7. Calculated IR spectra of the found isomers for structure II (top) structure I (middle) and structure III (bottom) in Figure 4.

Table S1. Relative electronic energies for selected isomers as a function of the basis set. In parentheses: zero-corrected relative electronic energies. All values in kJ mol^{-1}.

Isomer	B3LYP+GD3BJ		
	def2SVPP	def2TZVPP	def2QZVPP
B12Br11_Cyclohexane_1	-10.8 (-0.8)	3.4 (12.9)	4.3 (13.7)
B12Br11_Cyclohexane_2	1.9 (12.6)	12.2 (22.5)	12.8 (23.0)
B12Br11_1B-CH2-CH-R_1	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
B12Br11_1B-CH2-CH-R_5	2.1 (2.9)	1.9 (2.6)	1.8 (2.5)
B12Br11_1B-CH-CH2-R_1	35.0 (30.7)	33.7 (29.4)	33.9 (29.6)
B12Br11_1B-CH-CH2-R_14	47.7 (47.7)	55.0 (54.5)	55.6 (54.9)

Table S2. Relative electronic energies for selected isomers as a function of the DFT functional. In parentheses: zero-corrected relative electronic energies. All values in kJ mol^{-1}.

Isomer	def2TZVPP		
	B3LYP+GD3BJ	PBE1PBE+GD3BJ	M062X+GD3
B12Br11_Cyclohexane_1	3.4 (12.9)	-12.3 (-4.4)	-1.7 (3.9)
B12Br11_Cyclohexane_2	12.2 (22.5)	-5.9 (2.5)	6.2 (12.4)
B12Br11_1B-CH2-CH-R_1	0.0 (0.0)	0.0 (0.0)	0.0 (0.0)
B12Br11_1B-CH2-CH-R_5	1.9 (2.6)	2.3 (0.8)	5.3 (2.6)
B12Br11_1B-CH-CH2-R_1	33.7 (29.4)	40.3 (33.3)	51.0 (42.8)
B12Br11_1B-CH-CH2-R_5	36.9 (38.0)	45.4 (44.5)	50.7 (48.2)

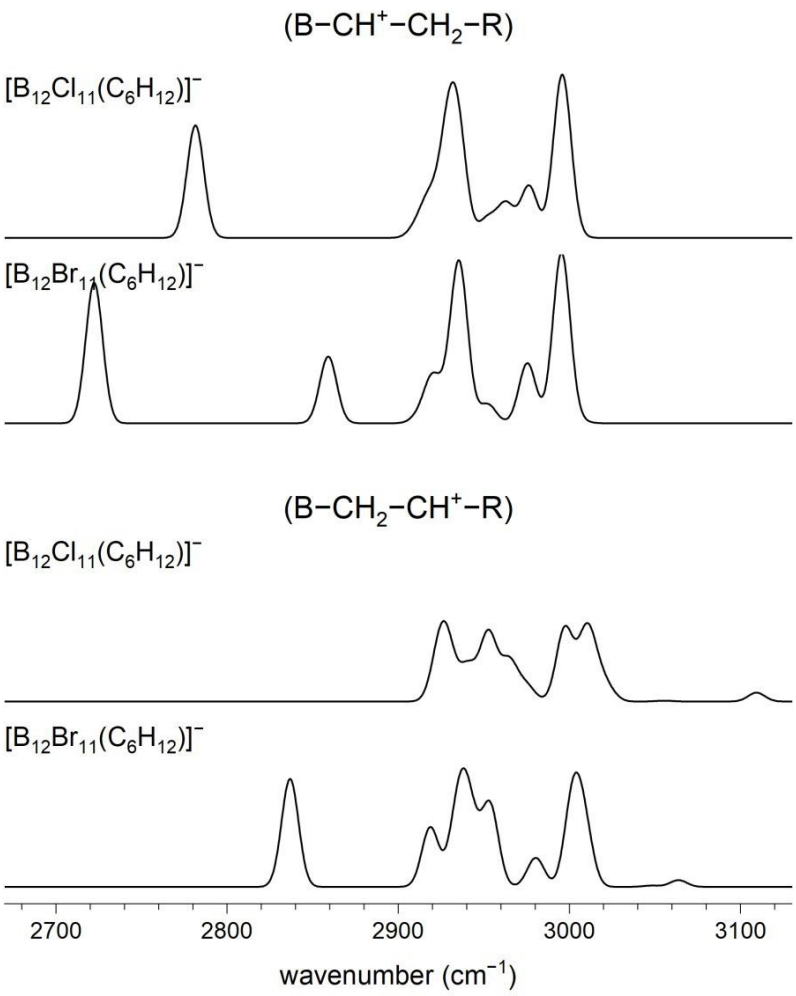


Figure S8. Comparison of the computed harmonic vibrational spectrum of $[B_{12}Cl_{11}(C_6H_{12})]^-$ and $[B_{12}Br_{11}(C_6H_{12})]^-$.

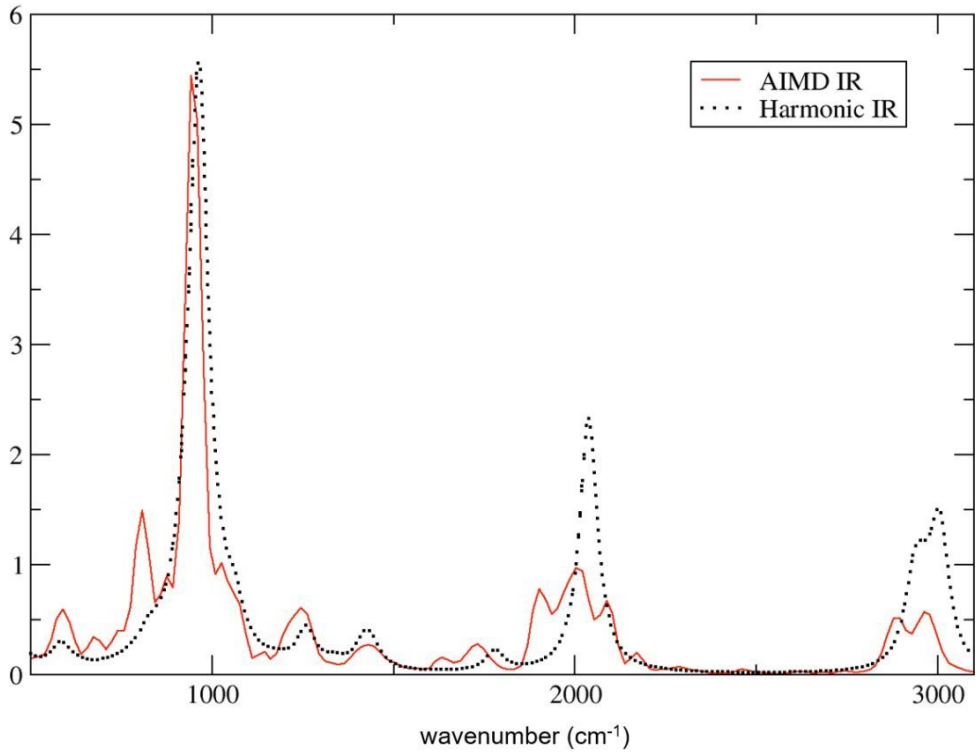


Figure S9. AIMD simulations (PBE/def2-TZVP) of the vibrational spectrum of the binding of cyclohexane to $[B_{12}Br_{11}]^-$ for structure II of Figure 4.

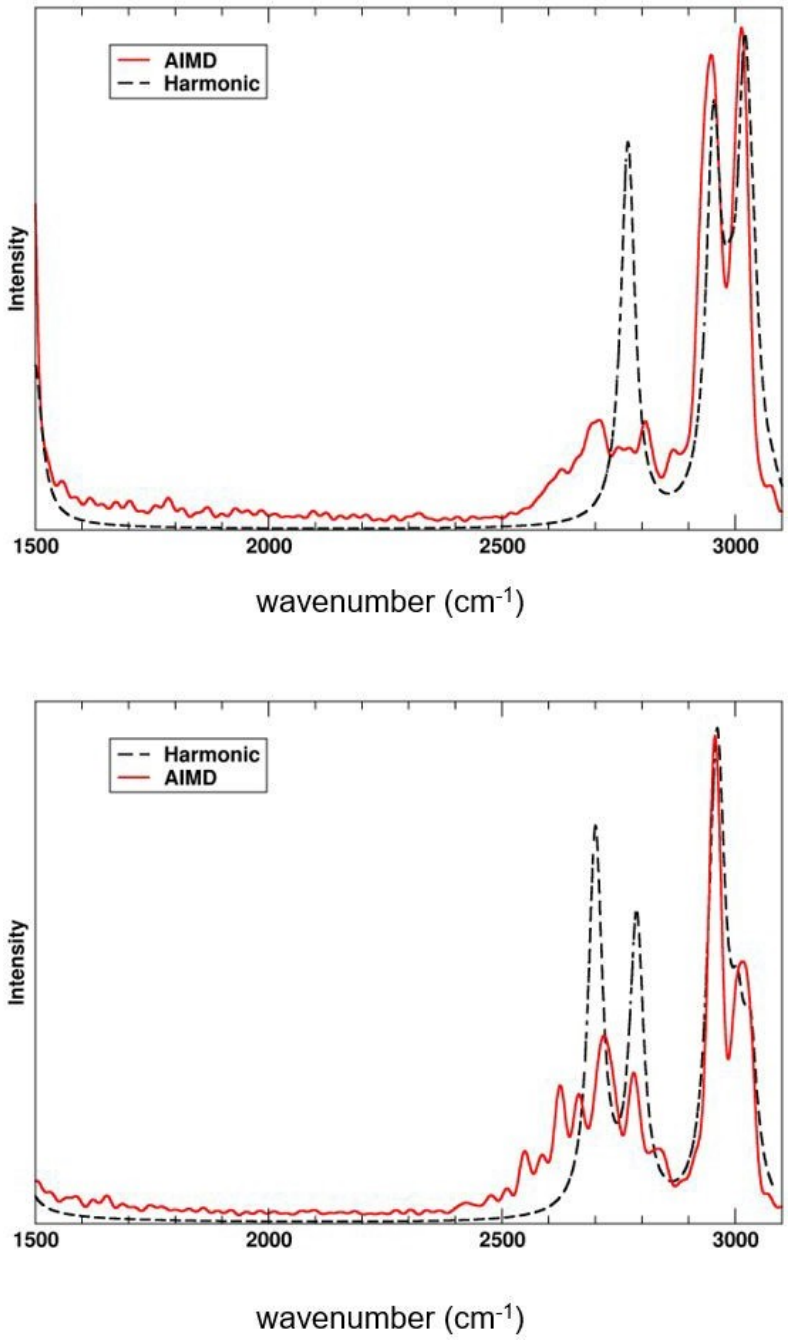


Figure S10. AIMD simulations (compared to harmonic IR spectra (PBE/def2-TZVP) of the IR spectra of minimum structures of geometries I (top) and III (bottom) in Figure 4.

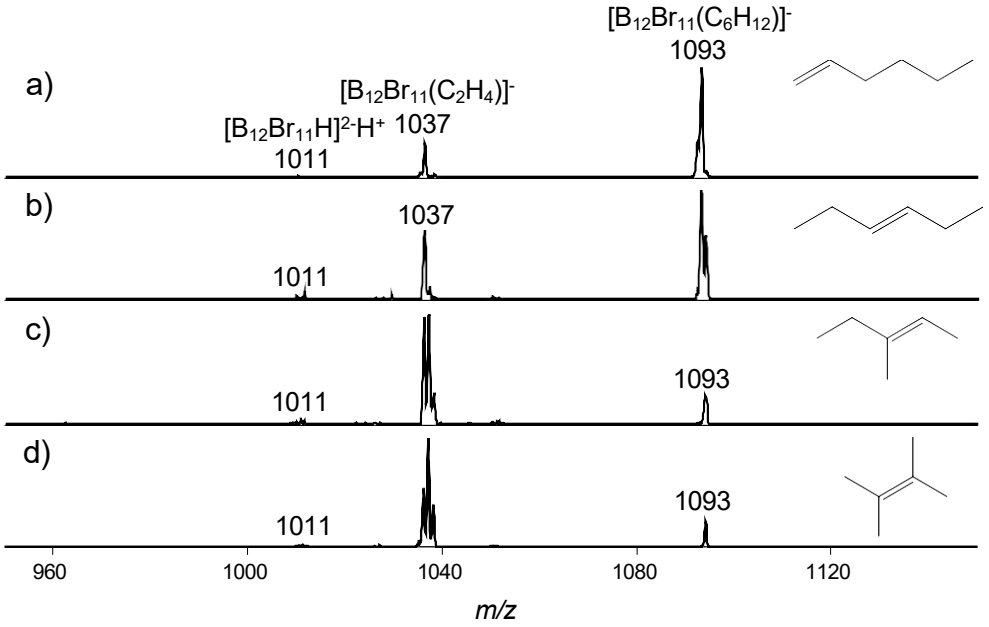


Figure S11. CID mass spectra of the adducts of $[B_{12}Br_{11}]^-$ with a) 1-hexene, b) *trans*-3-hexene, c) 3-methyl-2-petene and d) 2,3-dimethyl-2-butene.

The following geometries were obtained by DFT geometry optimization (B3LYP-GD3BJ/def2TZVPP).

B12Br11-C2H4
E(electronic) = -28693.8546282000
E(zero-point) = 0.1214274328

B	0.596700	-0.472913	1.447646
B	-0.925548	-1.219994	0.908944
B	0.572065	-1.524244	0.000000
B	1.531098	-0.018043	0.000000
B	0.609362	1.216018	0.899151
B	-0.907808	0.471108	1.451194
B	-1.838529	0.024919	0.000000
B	-0.925548	-1.219994	-0.908944
B	0.596700	-0.472913	-1.447646
B	0.609362	1.216018	-0.899151
B	-0.890397	1.542606	0.000000
B	-0.907808	0.471108	-1.451194
Br	1.452962	-1.022077	3.109179
Br	-1.769030	-2.648708	1.948782
Br	1.407817	-3.283303	0.000000
Br	3.476415	-0.041431	0.000000
Br	1.482863	2.618967	1.929542
Br	-1.834261	1.011829	3.089900
Br	-1.769030	-2.648708	-1.948782
Br	1.452962	-1.022077	-3.109179
Br	1.482863	2.618967	-1.929542
Br	-1.645911	3.350812	0.000000
Br	-1.834261	1.011829	-3.089900
C	-3.538698	0.795740	0.000000
H	-3.588320	1.353480	0.924346
H	-3.588320	1.353480	-0.924346
C	-3.576162	-0.569067	0.000000
H	-3.675534	-1.124460	-0.921900
H	-3.675534	-1.124460	0.921900

B12Br11-CH2CH2
E(electronic) = -28693.8550292000
E(zero-point) = 0.1230471669

B	-1.049042	1.227795	0.436976
B	-1.115654	0.596150	-1.240996
B	-1.617286	-0.435885	0.124437
B	-0.518257	-0.107563	1.503856
B	0.650742	1.136591	0.990462
B	0.259267	1.562465	-0.696764
B	0.523884	0.112806	-1.704268

B	-0.645766	-1.119483	-1.206163
B	-0.283988	-1.564490	0.492990
B	1.125842	-0.600735	1.025852
B	1.532847	0.419006	-0.328499
B	1.024281	-1.226419	-0.642138
Br	-2.241825	2.638827	1.057746
Br	-2.362179	1.288996	-2.580076
Br	-3.480874	-0.941708	0.393761
Br	-1.108661	-0.231601	3.357606
Br	1.474515	2.431626	2.198488
Br	0.650918	3.341756	-1.428757
Br	-1.351348	-2.401879	-2.504301
Br	-0.595277	-3.363382	1.176573
Br	2.479424	-1.253086	2.272773
Br	3.351632	0.915086	-1.021204
Br	2.268544	-2.599607	-1.302709
C	1.264644	0.322720	-3.101888
H	1.069023	-0.553094	-3.725664
H	0.849125	1.203769	-3.586753
C	2.761591	0.453928	-2.987504
H	3.212801	1.284341	-3.516973
H	3.306909	-0.472044	-3.109511

C2H4

E(electronic) = -78.6293010422

E(zero-point) = 0.0509622100

C	0.000000	0.000000	0.662323
H	0.000000	0.920920	1.231436
H	0.000000	-0.920920	1.231436
C	0.000000	0.000000	-0.662323
H	0.000000	-0.920920	-1.231436
H	0.000000	0.920920	-1.231436

B12Br11_1B-CH2-CH-R_1

E(electronic) = -28851.1986471000

E(zero-point) = 0.2337595732

B	-1.811310	-0.600488	0.597388
B	1.155577	0.603253	-0.498755
B	-1.546153	-0.152587	-1.108998
B	-1.602665	1.117118	0.143463
B	-0.817528	0.472431	1.597005
B	-0.261978	-1.190372	1.252380
B	-0.716795	-1.577049	-0.423727
B	0.162273	-0.467510	-1.504971
B	0.954546	-1.101115	-0.042681

B	0.886476	0.159282	1.193494
B	0.075986	1.575335	0.524180
B	-0.383699	1.199050	-1.152032
Br	-1.152455	-3.400477	-0.959287
Br	-0.157762	-2.549129	2.658098
Br	-3.512750	-1.300300	1.241431
Br	-1.332635	1.017281	3.405594
Br	-3.059281	2.407316	0.265320
Br	0.600568	3.371088	1.125469
Br	-0.431999	2.579856	-2.528801
Br	2.862420	1.318647	-1.178627
Br	0.744729	-1.005875	-3.287587
Br	2.440008	-2.389796	-0.131296
Br	-2.953945	-0.334670	-2.444164
C	6.447434	-0.647016	-0.486228
H	6.232886	0.099290	-1.252296
H	7.313933	-1.224823	-0.810345
H	5.594930	-1.325650	-0.453457
C	6.709609	0.017133	0.864266
H	7.600443	0.645764	0.791870
H	6.937468	-0.746706	1.614668
C	5.546537	0.880075	1.356763
H	5.855161	1.442933	2.241334
H	5.285250	1.610913	0.589071
C	4.305542	0.057891	1.691760
H	4.478204	-0.647512	2.511197
H	4.030078	-0.600085	0.850876
C	3.087899	0.817529	1.963713
H	3.061910	1.868641	1.691467
C	1.927667	0.279304	2.519619
H	2.005324	-0.711628	2.955600
H	1.341176	0.984705	3.111671

B12Br11_1B-CH2-CH-R_2
E(electronic) = -28851.1981290000
E(zero-point) = 0.2335333641

B	1.858401	0.502896	0.644191
B	-1.143291	-0.499855	-0.549499
B	1.634943	0.009139	-1.055563
B	1.529400	-1.209134	0.244236
B	0.734256	-0.444406	1.632923
B	0.335147	1.241802	1.200957
B	0.895639	1.522893	-0.464242
B	-0.021841	0.444909	-1.545880
B	-0.824609	1.199375	-0.147972
B	-0.916362	-0.011394	1.134097

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B     -0.196622   -1.514365    0.559288
B      0.367810   -1.244788   -1.105636
Br     1.504403    3.281976   -1.044309
Br     0.277948    2.659138    2.550397
Br     3.580994    1.088064    1.344227
Br     1.114349   -0.955205    3.484579
Br     2.867362   -2.606930    0.484045
Br    -0.894256   -3.236499    1.199611
Br     0.362827   -2.679813   -2.426827
Br    -2.876229   -1.100262   -1.272820
Br    -0.476703    0.954829   -3.373476
Br    -2.199070    2.593076   -0.349029
Br     3.112353    0.022279   -2.326500
C     -7.970508   -0.180572    0.103186
H     -8.415705   -0.708784    0.949236
H     -8.717533    0.510908   -0.288346
H     -7.759997   -0.918450   -0.673119
C     -6.698071    0.550528    0.518508
H     -6.936594    1.307807    1.271684
H     -6.285651    1.090629   -0.337670
C     -5.628264   -0.391040    1.063287
H     -6.026378   -0.947924    1.916848
H     -5.368012   -1.125929    0.299752
C     -4.365224    0.353537    1.477387
H     -4.543912    1.056895    2.298522
H     -4.010878    1.009210    0.663757
C     -3.209695   -0.474646    1.821247
H     -3.249287   -1.538682    1.607118
C     -2.035493    0.013071    2.396111
H     -2.063586    1.029115    2.777291
H     -1.532566   -0.698285    3.055602


B12Br11_1B-CH2-CH-R_3
E(electronic) =     -28851.1980208000
E(zero-point) =           0.2335885447
B      0.299695    0.956144   -1.366239
B      0.389559   -0.935226    1.448020
B      1.761571    0.056025   -0.883227
B      1.221820    1.464158    0.071872
B     -0.557192    1.434453    0.116966
B     -1.103034    0.025483   -0.812749
B      0.317199   -0.832064   -1.432406
B      1.245742   -1.427312   -0.032382
B     -0.531573   -1.436953    0.010429
B     -1.052338   -0.037293    0.949126
B      0.381667    0.847455    1.507866
```

B	1.808988	-0.008566	0.899465
Br	0.256373	-1.800336	-3.125423
Br	-2.800804	0.057048	-1.813867
Br	0.219463	2.044332	-2.983428
Br	-1.668794	3.050679	0.251070
Br	2.210426	3.144279	0.115945
Br	0.351455	1.804165	3.216584
Br	3.482393	-0.033527	1.899396
Br	0.392039	-2.013882	3.082103
Br	2.265587	-3.087321	-0.109379
Br	-1.576101	-3.104434	0.004933
Br	3.393108	0.108026	-1.948467
C	-3.503170	0.044458	1.232442
C	-2.347909	-0.059213	2.013591
C	-7.899017	0.628457	0.309221
C	-6.624071	0.264697	1.062980
C	-5.733544	-0.702440	0.284159
C	-4.446279	-1.055901	1.016610
H	-8.520123	1.317274	0.882965
H	-7.664868	1.104363	-0.644580
H	-2.107499	0.863553	2.550858
H	-3.702026	1.007690	0.773582
H	-6.063800	1.178344	1.285033
H	-6.879446	-0.177408	2.031063
H	-6.284675	-1.623653	0.082982
H	-5.481037	-0.274237	-0.687052
H	-4.643327	-1.514678	1.993713
H	-3.869826	-1.831161	0.487676
H	-8.495040	-0.261502	0.096681
H	-2.254989	-0.956499	2.617997

B12Br11_1B-CH2-CH-R_4
E(electronic) = -28851.1989355000
E(zero-point) = 0.2346241312

B	-0.109604	-0.968722	-1.330668
B	-0.625378	0.956495	1.419464
B	-1.656378	-0.128363	-1.047515
B	-1.180306	-1.495477	0.000049
B	0.568068	-1.386778	0.261292
B	1.140107	0.034512	-0.609159
B	-0.196925	0.820297	-1.434820
B	-1.319902	1.391336	-0.166574
B	0.428449	1.485246	0.093505
B	0.900956	0.122078	1.116493
B	-0.540892	-0.816026	1.519872
B	-1.925049	-0.038761	0.719263

Br	0.057449	1.757162	-3.129030
Br	3.030195	0.099345	-1.182864
Br	0.245010	-2.067224	-2.905298
Br	1.725340	-2.954311	0.541767
Br	-2.095601	-3.216942	-0.048394
Br	-0.660951	-1.743742	3.241267
Br	-3.711996	-0.080692	1.499625
Br	-0.852109	2.058720	3.021976
Br	-2.398807	2.997572	-0.407157
Br	1.432404	3.172726	0.183004
Br	-3.135933	-0.272487	-2.309583
C	3.465969	0.061958	1.450514
C	2.192585	0.273901	2.085629
C	6.392697	-0.506111	0.682501
C	5.772875	0.888544	0.644890
C	4.539297	1.069188	1.524352
H	2.024087	-0.553306	2.788954
H	3.726596	-0.963080	1.224428
H	6.601583	-0.785504	1.720237
H	6.517559	1.624040	0.959483
H	5.507825	1.144015	-0.382706
H	4.839416	0.999911	2.585758
H	4.102394	2.063622	1.417076
H	2.126577	1.240721	2.580337
C	7.674153	-0.592194	-0.141325
H	8.428775	0.104842	0.229122
H	8.100094	-1.595406	-0.109842
H	7.480514	-0.345786	-1.186826
H	5.678353	-1.239391	0.302633

B12Br11_1B-CH2-CH-R_5
E(electronic) = -28851.1979167000
E(zero-point) = 0.2340126539

B	0.413723	0.596625	-1.555692
B	0.191966	-0.564163	1.623592
B	1.811375	-0.130014	-0.719667
B	1.178431	1.453770	-0.195540
B	-0.596985	1.397073	-0.331369
B	-1.050787	-0.205522	-0.951093
B	0.430084	-1.153980	-1.186804
B	1.200453	-1.375852	0.403452
B	-0.573170	-1.414414	0.260578
B	-1.187781	0.159312	0.778540
B	0.189108	1.183633	1.250169
B	1.666779	0.235621	1.020054
Br	0.554226	-2.502340	-2.591535

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Br    -2.596304   -0.458065   -2.151239
Br     0.519847    1.265627   -3.384946
Br    -1.709028    2.974382   -0.705995
Br     2.163634    3.116504   -0.453575
Br    -0.001864    2.525067    2.663820
Br     3.222234    0.486251    2.167890
Br     0.024721   -1.220512    3.460812
Br     2.216208   -2.982941    0.836408
Br    -1.598502   -3.069196    0.543154
Br     3.548101   -0.299685   -1.587416
C     -3.594787    0.238223    0.809238
C     -2.561428    0.415102    1.728426
C     -6.432809    1.465480    1.027810
C     -6.830850    0.029402    0.698612
C     -5.757623   -0.764690   -0.049838
C     -4.459966   -0.938337    0.738120
H     -7.249632    1.997822    1.516455
H     -5.580012    1.507857    1.710128
H     -2.366647    1.455860    1.994603
H     -3.722394    1.013265    0.061352
H     -7.088105   -0.497582    1.622489
H     -7.739242    0.039035    0.091317
H     -6.146196   -1.754885   -0.291128
H     -5.526682   -0.282629   -1.002183
H     -4.625140   -1.335988    1.743240
H     -3.826503   -1.701015    0.255073
H     -6.162941    2.020388    0.127718
H     -2.522347   -0.271808    2.567335


B12Br11_1B-CH2-CH-R_6
E(electronic) =     -28851.1993338000
E(zero-point) =           0.2356965793
B     -1.927885   -0.249082    0.749208
B      1.044578    0.232638   -0.616673
B     -1.720627   -0.053899   -1.021615
B     -1.458251    1.335291    0.073020
B     -0.671862    0.721239    1.560964
B     -0.463575   -1.036404    1.392410
B     -1.120161   -1.526498   -0.201777
B     -0.134096   -0.733746   -1.467809
B      0.618246   -1.340167    0.028978
B      0.901421    0.053198    1.102408
B      0.282764    1.515335    0.304176
B     -0.344707    1.044901   -1.296879
Br    -1.925801   -3.278151   -0.491605
Br    -0.472622   -2.221719    2.949890
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Br	-3.680817	-0.533347	1.555106
Br	-0.921835	1.559023	3.312227
Br	-2.651669	2.877160	0.099233
Br	1.161544	3.250974	0.601214
Br	-0.192258	2.235924	-2.836893
Br	2.969690	0.490652	-1.070019
Br	0.257015	-1.544152	-3.201652
Br	1.891027	-2.838345	0.014821
Br	-3.228048	-0.114154	-2.256928
C	8.418256	0.112753	-0.052330
H	8.237719	0.002021	-1.123285
H	8.601486	1.171356	0.143025
H	9.330740	-0.433573	0.189645
C	7.230546	-0.397320	0.758021
H	7.448020	-0.307615	1.826424
H	7.084491	-1.463718	0.565274
C	5.935492	0.347577	0.443306
H	6.067059	1.414764	0.646971
H	5.729657	0.261715	-0.626961
C	4.746344	-0.180882	1.234772
H	4.974933	-0.130743	2.308296
H	4.558631	-1.234331	1.019508
C	3.465442	0.582691	1.104255
H	3.573065	1.660589	1.094051
C	2.286437	0.101014	1.890570
H	2.489370	-0.889744	2.294784
H	2.162557	0.804978	2.719818

B12Br11_1B-CH2-CH-R_7
E(electronic) = -28851.1995668000
E(zero-point) = 0.2359592151

B	1.118228	-1.529605	-0.071002
Br	1.948319	-3.288590	-0.210713
B	-0.615539	-1.350200	0.209744
Br	-1.838913	-2.881999	0.396673
B	0.512727	-0.889854	1.489010
Br	0.607757	-1.908030	3.158102
B	-0.886086	0.137861	1.143944
C	-2.233128	0.328006	1.975765
C	-3.494604	0.127495	1.200411
C	-4.628181	1.072520	1.448927
H	-4.872398	0.908704	2.507983
H	-4.257877	2.096118	1.380522
C	-5.888871	0.886347	0.607837
H	-6.640323	1.595540	0.964643
H	-5.679143	1.173036	-0.426419

```
C     -6.476114   -0.523504    0.634854
C     -7.784464   -0.624282   -0.143777
H     -7.636726   -0.352176   -1.190656
H     -8.186025   -1.637750   -0.117889
H     -8.540872    0.046863    0.268564
H     -5.759329   -1.234535    0.218271
H     -6.639997   -0.827209    1.673384
H     -3.769370   -0.912923    1.093163
Br    -3.041997    0.343610   -0.981318
B     -1.098604    0.139409   -0.578235
B      0.068303   -0.891321   -1.371509
Br    -0.368610   -1.887033   -2.993617
B      1.655128   -0.141623   -1.061769
Br     3.115628   -0.302279   -2.343583
B      0.245705    0.898445   -1.393856
Br     0.006993    1.917956   -3.042915
B     -0.327957    1.523336    0.172864
Br    -1.245493    3.254797    0.323785
B      1.404690    1.350422   -0.106775
Br     2.566191    2.905869   -0.287468
B      1.933859   -0.146821    0.709935
Br     3.721769   -0.315842    1.470104
B      0.688370    0.879214    1.467275
Br     0.985019    1.897868    3.111951
H     -2.225691    1.312903    2.440098
H     -2.237396   -0.435792    2.761061
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B12Br11_1B-CH2-CH-R_8
E(electronic) =     -28851.1987751000
E(zero-point) =           0.2358697592
B     -0.457193    1.072532   -1.273676
B     -0.310347   -1.065701    1.369074
B     -1.701295   -0.175438   -1.006841
B     -0.056846   -0.668693   -1.487184
B      1.021803    0.402492   -0.628898
B      0.138469    1.574614    0.329885
B     -1.575855    1.210894    0.115598
B     -1.860701   -0.429374    0.761406
B     -0.706283    0.654721    1.579680
B      0.923493    0.172275    1.087103
B      0.778607   -1.220603   -0.013554
B     -0.932405   -1.590750   -0.227666
Br    -2.929317    2.612554    0.190892
Br     0.831959    3.386721    0.656910
Br    -0.457154    2.305220   -2.788250
Br     2.899084    0.879056   -1.101508
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Br	0.395208	-1.395104	-3.243273
Br	2.206692	-2.570831	-0.076601
Br	-1.546559	-3.413434	-0.547136
Br	-0.167675	-2.277567	2.899421
Br	-3.560546	-0.920196	1.581593
Br	-1.020571	1.422919	3.352327
Br	-3.210833	-0.373712	-2.225012
C	7.377334	-1.124265	0.167011
H	7.139850	-1.215871	-0.894666
H	6.697477	-1.779641	0.711457
H	8.388786	-1.503770	0.317102
C	7.262357	0.327834	0.627710
H	8.019881	0.927341	0.117246
H	7.490167	0.394572	1.695968
C	5.890250	0.952583	0.364627
H	5.923058	2.018270	0.606967
H	5.672388	0.884602	-0.704705
C	4.763628	0.296833	1.154534
H	5.008608	0.329321	2.225378
H	4.648157	-0.758291	0.906856
C	3.423150	0.957688	1.069914
H	3.440572	2.040761	1.085728
C	2.304586	0.356830	1.862272
H	2.609606	-0.611931	2.255723
H	2.116345	1.037887	2.698144

B12Br11_1B-CH2-CH-R_9
E(electronic) = -28851.1984308000
E(zero-point) = 0.2358423613

B	-1.675743	-0.725659	0.826466
B	0.901961	0.677533	-0.704127
B	-1.712416	-0.338113	-0.925111
B	-1.725547	0.973844	0.286857
B	-0.652104	0.488537	1.637599
B	0.006064	-1.120349	1.268679
B	-0.656482	-1.643870	-0.313494
B	-0.054723	-0.507490	-1.560699
B	0.981569	-1.001236	-0.199321
B	0.990496	0.326178	0.994628
B	-0.085984	1.616602	0.401992
B	-0.720337	1.119367	-1.187536
Br	-0.985121	-3.521139	-0.724396
Br	0.479891	-2.382392	2.687988
Br	-3.192797	-1.552131	1.730955
Br	-0.938896	1.079986	3.481531
Br	-3.284176	2.111748	0.567044

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Br     0.268620    3.511634    0.806556
Br    -1.058032    2.425123   -2.599563
Br     2.640664    1.498803   -1.257551
Br     0.360012   -1.034262   -3.395481
Br     2.581151   -2.103857   -0.481307
Br    -3.265182   -0.717167   -2.041620
C      7.503049   -1.078213    0.276992
H      7.253942   -1.350841   -0.750032
H      8.590245   -1.044372    0.361194
H      7.140818   -1.878969    0.924043
C      6.870081    0.257708    0.655430
H      7.269851    1.048437    0.012716
H      7.156072    0.523187    1.678101
C      5.348400    0.233469    0.543327
H      5.057899   -0.037338   -0.473054
H      4.948178   -0.554740    1.181417
C      4.718597    1.573366    0.907399
H      5.140402    2.370811    0.291367
H      4.981440    1.827749    1.944186
C      3.220447    1.662168    0.890124
H      2.850336    2.676425    0.965457
C      2.389896    0.692334    1.667445
H      2.937639   -0.222434    1.879462
H      2.171955    1.198224    2.615735


B12Br11_1B-CH2-CH-R_10
E(electronic) =     -28851.1985197000
E(zero-point) =           0.2361361342
B     -1.553748   -0.397037    1.186938
B      0.742719    0.369807   -1.064900
B     -1.973892   -0.105164   -0.532234
B     -1.430928    1.247567    0.503145
B     -0.151511    0.626484    1.592597
B      0.083239   -1.100453    1.242591
B     -1.049813   -1.564610   -0.066490
B     -0.599803   -0.642338   -1.533391
B      0.649846   -1.259244   -0.423350
B      1.205549    0.100802    0.585827
B      0.271763    1.547859    0.145738
B     -0.837183    1.105924   -1.178852
Br    -1.808417   -3.356551   -0.187562
Br     0.672709   -2.353487    2.626030
Br    -2.908060   -0.849458    2.515120
Br     0.165459    1.360997    3.379003
Br    -2.627062    2.692124    1.036754
Br     1.097911    3.330913    0.249082
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Br	-1.285499	2.374990	-2.593600
Br	2.390068	0.791046	-2.111354
Br	-0.779893	-1.339881	-3.348986
Br	1.920527	-2.656150	-0.968174
Br	-3.806457	-0.221497	-1.187902
C	8.256489	-0.152390	1.306157
H	8.438119	0.896018	1.551322
H	7.898718	-0.645532	2.211820
H	9.213058	-0.602469	1.037213
C	7.241735	-0.283992	0.174293
H	7.097174	-1.339666	-0.070370
H	7.634613	0.189163	-0.730269
C	5.890007	0.335745	0.522297
H	5.494455	-0.136164	1.423448
H	6.023208	1.395695	0.758976
C	4.876066	0.186182	-0.622518
H	4.706036	-0.870966	-0.829927
H	5.286922	0.646164	-1.522971
C	3.575007	0.832289	-0.243830
H	3.604290	1.914125	-0.198429
C	2.772166	0.212347	0.858011
H	3.153788	-0.782617	1.083049
H	2.904616	0.850603	1.737157

B12Br11_1B-CH2-CH-R_11
E(electronic) = -28851.1980068000
E(zero-point) = 0.2362837909

B	-0.836559	1.147978	-1.133790
B	0.111202	-1.144552	1.195141
B	-1.897189	-0.205194	-0.663699
B	-0.409723	-0.540395	-1.587835
B	0.793605	0.549358	-0.946764
B	0.127166	1.585452	0.301255
B	-1.560944	1.108508	0.501782
B	-1.576681	-0.587774	1.059047
B	-0.310841	0.523074	1.643446
B	1.158755	0.198421	0.712941
B	0.809481	-1.125265	-0.427717
B	-0.875046	-1.607491	-0.227976
Br	-2.923768	2.396116	1.037420
Br	0.775984	3.420075	0.591983
Br	-1.299669	2.475418	-2.488958
Br	2.462241	1.195330	-1.830385
Br	-0.391366	-1.112117	-3.455492
Br	2.243492	-2.358226	-0.964254
Br	-1.449503	-3.445747	-0.531419

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Br     0.715774   -2.440973    2.531330
Br    -2.974459   -1.258595    2.241915
Br    -0.194427    1.145377    3.495570
Br    -3.658351   -0.434629   -1.468347
C      7.327765   -1.191950    0.439024
H      6.896988   -1.784554    1.248327
H      8.368914   -1.494742    0.320465
H      6.802513   -1.459611   -0.477834
C      7.223431    0.301315    0.741606
H      7.642583    0.876899   -0.089164
H      7.837518    0.534885    1.614950
C      5.796266    0.780050    1.019421
H      5.378143    0.210169    1.851244
H      5.820400    1.825635    1.337535
C      4.874967    0.646958   -0.204981
H      4.781792   -0.397835   -0.497894
H      5.315200    1.196701   -1.039112
C      3.511571    1.180672    0.123625
H      3.459569    2.256186    0.241130
C      2.683020    0.429191    1.118772
H      3.133256   -0.542201    1.318493
H      2.686642    1.019371    2.040234


B12Br11_1B-CH2-CH-R_12
E(electronic) =     -28851.1980252000
E(zero-point) =           0.2366141869
B      0.670582    1.028756   -1.289961
B      0.015738   -1.024144    1.344493
B      1.885075   -0.120657   -0.671032
B      1.410516    1.291901    0.319064
B     -0.320544    1.544160    0.098207
B     -0.876718    0.282057   -0.984156
B      0.438265   -0.742428   -1.506034
B      1.035919   -1.556773   -0.028817
B     -0.696650   -1.299435   -0.248457
B     -1.185581    0.112761    0.715617
B      0.245383    0.725565    1.558245
B      1.626610   -0.301698    1.094802
Br     0.470011   -1.560147   -3.278924
Br    -2.619302    0.641255   -1.894846
Br     0.962275    2.204530   -2.822234
Br    -1.184612    3.307976    0.154346
Br     2.622090    2.783702    0.646936
Br     0.072551    1.572475    3.314275
Br     3.103038   -0.646340    2.321223
Br    -0.420597   -2.191681    2.853861
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Br	1.814797	-3.342938	-0.101930
Br	-1.964292	-2.768550	-0.583855
Br	3.653555	-0.253691	-1.481197
C	-7.131652	-0.900054	-0.033802
H	-7.930789	-0.188398	-0.254028
H	-7.585365	-1.883386	0.092205
H	-6.485926	-0.952944	-0.911395
C	-6.359055	-0.489383	1.217673
H	-5.557098	-1.208061	1.402722
H	-7.018861	-0.552993	2.086012
C	-5.784988	0.929224	1.162294
H	-6.604982	1.648981	1.093982
H	-5.260487	1.142589	2.094501
C	-4.836182	1.209050	-0.020395
H	-4.451804	2.225640	0.061444
H	-5.389005	1.134054	-0.957036
C	-3.685501	0.243865	-0.010828
H	-3.941025	-0.770315	-0.288218
C	-2.712290	0.311131	1.125253
H	-2.814719	1.256266	1.656161
H	-2.977870	-0.505493	1.804737

B12Br11_1B-CH2-CH-R_13
E(electronic) = -28851.1976717000
E(zero-point) = 0.2362776209

B	-1.681662	-0.348004	1.058131
B	0.862173	0.325791	-0.943952
B	-1.905166	-0.090648	-0.702815
B	-1.452923	1.277390	0.355777
B	-0.312870	0.661351	1.592803
B	-0.074542	-1.077264	1.309062
B	-1.066008	-1.553737	-0.106101
B	-0.440311	-0.674776	-1.534588
B	0.668154	-1.285551	-0.280510
B	1.135911	0.088864	0.753243
B	0.284168	1.540329	0.181244
B	-0.681324	1.085259	-1.247146
Br	-1.841215	-3.335124	-0.270263
Br	0.335392	-2.306250	2.776345
Br	-3.181834	-0.745528	2.238981
Br	-0.179280	1.433365	3.386528
Br	-2.672193	2.754230	0.722586
Br	1.128954	3.310902	0.335395
Br	-0.947409	2.327220	-2.730304
Br	2.621396	0.694238	-1.812170
Br	-0.433883	-1.412847	-3.343082

Br	1.963790	-2.716219	-0.651144
Br	-3.656764	-0.192057	-1.553344
C	8.059274	0.100838	-0.031239
H	7.629239	-0.038131	-1.023576
H	8.227934	1.170744	0.110608
H	9.032092	-0.392374	-0.027133
C	7.156508	-0.460280	1.065086
H	7.672846	-0.388918	2.025479
H	6.982743	-1.525472	0.890054
C	5.806740	0.249819	1.196006
H	5.280471	-0.141770	2.066989
H	5.970881	1.315675	1.381960
C	4.917077	0.078587	-0.046939
H	4.748487	-0.982675	-0.235324
H	5.419552	0.502326	-0.916023
C	3.597227	0.758153	0.175042
H	3.644713	1.840087	0.198130
C	2.664823	0.181379	1.194846
H	2.999580	-0.813536	1.485398
H	2.710219	0.840456	2.067402

B12Br11_1B-CH2-CH-R_14
E(electronic) = -28851.1973959000
E(zero-point) = 0.2360367297

B	0.599443	1.049484	-1.271731
B	0.063936	-1.040834	1.358833
B	1.565812	-0.429992	-1.038429
B	1.748614	0.937762	0.096390
B	0.151408	1.645842	0.346959
B	-0.976425	0.693306	-0.601506
B	-0.154199	-0.567525	-1.489271
B	0.538532	-1.664395	-0.254054
B	-1.055806	-0.954861	-0.004147
B	-0.896949	0.426606	1.112786
B	0.808178	0.558328	1.574061
B	1.701367	-0.730995	0.725291
Br	-0.778798	-1.166724	-3.240496
Br	-2.734219	1.546971	-1.019592
Br	0.828559	2.271927	-2.776949
Br	-0.105010	3.568630	0.688879
Br	3.363618	2.028970	0.154720
Br	1.305682	1.226438	3.345483
Br	3.277610	-1.569430	1.509421
Br	-0.299561	-2.214445	2.882604
Br	0.759780	-3.570454	-0.598923
Br	-2.713899	-2.007491	-0.057057

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Br     2.979388   -0.920452   -2.288389
C     -3.094968    1.821140    1.174543
C     -2.204286    0.872299    1.908957
C     -5.843619    0.085006   -0.058153
C     -5.340246    0.474585    1.331052
C     -4.580253    1.803310    1.399045
H     -1.870980    1.425592    2.795505
H     -2.691213    2.824819    1.144655
H     -6.447032    0.902640   -0.466129
H     -6.202273    0.550967    1.999473
H     -4.720852   -0.331629    1.724777
H     -5.060432    2.553373    0.766773
H     -4.652181    2.196883    2.422931
H     -2.744743   -0.011452    2.237899
C     -6.665057   -1.199696   -0.024566
H     -7.532289   -1.100900    0.632933
H     -7.025474   -1.465449   -1.018880
H     -6.060518   -2.030845    0.341572
H     -5.001224   -0.055394   -0.732230
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B12Br11_1B-CH2-CH-R_15
E(electronic) =     -28851.1966252000
E(zero-point) =           0.2360790421
B      1.033987   -1.549589   -0.158055
Br     1.793818   -3.329892   -0.394605
B     -0.709144   -1.303874   -0.023113
Br    -2.009964   -2.780762   -0.103761
B      0.308344   -1.028794    1.394907
Br     0.193416   -2.204451    2.955889
B     -1.002268    0.101338    1.025858
C     -2.413978    0.286895    1.742438
C     -3.600395    0.205980    0.839152
C     -4.724344    1.169096    1.075090
H     -5.005313    1.007560    2.124758
H     -4.314911    2.179498    1.037881
C     -5.967751    1.042975    0.191194
H     -6.489765    2.001621    0.212315
H     -5.666339    0.893194   -0.849054
C     -6.964195   -0.050124    0.592442
C     -6.443083   -1.484687    0.513814
H     -5.689232   -1.692393    1.273024
H     -7.253927   -2.197654    0.667944
H     -5.997527   -1.694788   -0.460317
H     -7.319161    0.151094    1.607958
H     -7.839232    0.043085   -0.055789
H     -3.882667   -0.805960    0.590696
```

Br	-2.930631	0.624687	-1.257594
B	-1.045819	0.278188	-0.700423
B	0.145704	-0.734840	-1.480461
Br	-0.174552	-1.547423	-3.227055
B	1.726945	-0.105310	-0.951535
Br	3.296982	-0.222727	-2.101833
B	0.404840	1.036569	-1.307883
Br	0.375073	2.219453	-2.862121
B	-0.290204	1.540268	0.253280
Br	-1.138881	3.297070	0.490019
B	1.451847	1.300828	0.119903
Br	2.694370	2.800937	0.203734
B	1.830856	-0.293564	0.829022
Br	3.526484	-0.630985	1.731284
B	0.564799	0.722039	1.565901
Br	0.744823	1.562294	3.324419
H	-2.415280	1.228208	2.289901
H	-2.526427	-0.537637	2.455696

B12Br11_1B-CH2-CH-R_16
E(electronic) = -28851.1959150000
E(zero-point) = 0.2357707787

B	0.392559	1.093448	1.255403
B	0.344014	-1.084054	-1.358283
B	1.585507	-0.222576	1.108724
B	-0.116072	-0.619970	1.461191
B	-1.065224	0.490316	0.504037
B	-0.045553	1.595438	-0.397906
B	1.624602	1.147267	-0.040286
B	1.872466	-0.518042	-0.636557
B	0.847390	0.609067	-1.561188
B	-0.839648	0.222029	-1.194873
B	-0.859951	-1.154480	-0.066781
B	0.806441	-1.610274	0.290796
Br	3.052639	2.474865	-0.026708
Br	-0.620344	3.431007	-0.810222
Br	0.337913	2.352884	2.746776
Br	-2.940485	1.071343	0.829050
Br	-0.745593	-1.289476	3.184929
Br	-2.359783	-2.426992	-0.099169
Br	1.293520	-3.456516	0.685329
Br	0.258532	-2.315411	-2.877333
Br	3.603703	-1.112640	-1.309131
Br	1.342444	1.325698	-3.314097
Br	2.979960	-0.476444	2.447741
C	-7.100143	-1.091854	-0.302682

```
H     -7.501937   -1.720668    0.492301
H     -6.424447   -1.711147   -0.893940
H     -7.930189   -0.794370   -0.947875
C     -6.387651    0.130130    0.271877
H     -5.585720   -0.197320    0.935968
H     -7.087031    0.699218    0.889227
C     -5.815487    1.059070   -0.804380
H     -6.616457    1.322025   -1.499204
H     -5.499883    1.999527   -0.346474
C     -4.637549    0.448730   -1.583036
H     -4.812570    0.528243   -2.663710
H     -4.530542   -0.617835   -1.385727
C     -3.302043    1.096636   -1.410886
H     -3.303947    2.179518   -1.430386
C     -2.134312    0.468347   -2.095334
H     -2.431107   -0.485836   -2.529093
H     -1.833460    1.150349   -2.896621
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B12Br11_1B-CH2-CH-R_17
E(electronic) =     -28851.1929518000
E(zero-point) =           0.2360972787
B     -0.021860   -0.951880   -1.306725
B      0.728408    0.957905    1.408015
B      1.588854   -0.220849   -1.091298
B      0.189378    0.829757   -1.434197
B     -1.139520    0.146064   -0.532205
B     -0.659530   -1.309358    0.318957
B      1.059389   -1.540087   -0.007729
B      1.927133   -0.134690    0.668502
B      0.518071   -0.803435    1.534038
B     -0.871226    0.233838    1.179026
B     -0.316052    1.552405    0.113122
B      1.401236    1.326278   -0.212731
Br     1.850094   -3.321274   -0.077149
Br    -1.898280   -2.811301    0.622063
Br    -0.534605   -2.024898   -2.855640
Br    -3.095248    0.366130   -0.858104
Br    -0.086343    1.761390   -3.128934
Br    -1.192542    3.309264    0.193070
Br     2.587405    2.843109   -0.517894
Br     1.100949    2.058551    2.982956
Br     3.735872   -0.300707    1.378205
Br     0.650205   -1.731210    3.252551
Br     3.001197   -0.482809   -2.409740
C     -6.217930   -1.209606   -0.432340
H     -6.822786   -1.853023    0.209746
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H	-5.179786	-1.517444	-0.318086
H	-6.500423	-1.410422	-1.466363
C	-6.444963	0.260316	-0.076034
H	-7.505029	0.483446	-0.215921
H	-5.916827	0.908566	-0.779709
C	-6.058696	0.628095	1.366467
H	-6.735975	1.404996	1.727825
H	-6.230351	-0.239716	2.010413
C	-4.639772	1.150413	1.610766
H	-4.544473	1.375649	2.678736
H	-4.470957	2.105179	1.109072
C	-3.482553	0.230809	1.326127
H	-3.724578	-0.823757	1.292241
C	-2.188358	0.512751	2.027813
H	-2.170114	1.540089	2.388272
H	-2.181112	-0.158580	2.894658

B12Br11_1B-CH-CH2-R_1
E(electronic) = -28851.1857976000
E(zero-point) = 0.2321240076

B	1.531348	0.982465	0.710273
B	-0.864880	-0.992115	-0.662917
B	1.939200	-0.353932	-0.415931
B	1.316698	-0.729815	1.213602
B	0.083291	0.493166	1.619063
B	-0.041142	1.636937	0.211378
B	1.113975	1.097330	-1.027485
B	0.586772	-0.516738	-1.581768
B	-0.613936	0.722681	-1.183395
B	-1.230535	0.337890	0.442586
B	-0.396749	-1.120806	1.056824
B	0.728219	-1.650850	-0.192495
Br	1.988935	2.368584	-2.217619
Br	-0.522150	3.515769	0.484921
Br	2.887800	2.118695	1.520901
Br	-0.299482	1.107877	3.440689
Br	2.424683	-1.534452	2.597978
Br	-1.335016	-2.358277	2.251989
Br	1.149511	-3.533256	-0.453616
Br	-2.314795	-2.071990	-1.420270
Br	0.852991	-1.118564	-3.413846
Br	-1.744818	1.535908	-2.563657
Br	3.776289	-0.753716	-0.914251
C	-3.530039	1.620802	0.520807
C	-2.653553	0.554655	0.913659
C	-7.850062	-0.916025	-0.171267

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C     -7.156594    0.209070    0.591970
C     -5.699230    0.390288    0.182041
C     -4.988506    1.513427    0.936699
H     -7.841452   -0.723147   -1.245782
H     -7.344657   -1.869178   -0.005915
H     -3.026441   -0.152117    1.655314
H     -3.001772    2.508165    0.946132
H     -3.388916    1.827099   -0.551283
H     -7.695617    1.148369    0.433370
H     -7.205351    0.008298    1.666480
H     -5.156983   -0.548386    0.338136
H     -5.639501    0.586945   -0.892576
H     -5.491908    2.463993    0.747449
H     -5.049444    1.335188    2.014015
H     -8.889587   -1.029817    0.139859
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B12Br11_1B-CH-CH2-R_2
E(electronic) =     -28851.1849717000
E(zero-point) =           0.2322749171
B     -1.392127   -0.400181    1.268749
B      0.742206    0.432212   -1.237029
B     -1.984545    0.120100   -0.343375
B     -1.187726    1.302411    0.729707
B      0.133191    0.458821    1.580908
B      0.134441   -1.269964    1.018644
B     -1.180585   -1.455411   -0.162899
B     -0.788456   -0.420537   -1.564747
B      0.500160   -1.280569   -0.706377
B      1.290142   -0.092661    0.359354
B      0.477808    1.490759    0.178239
B     -0.808504    1.290753   -1.010348
Br    -2.139538   -3.141283   -0.353505
Br     0.718816   -2.711604    2.208856
Br    -2.595627   -0.868725    2.724854
Br     0.755461    0.922469    3.381227
Br    -2.153929    2.765364    1.576947
Br     1.501897    3.148796    0.384019
Br    -1.333194    2.740163   -2.199106
Br     2.046303    0.879999   -2.629907
Br    -1.295380   -0.904764   -3.380853
Br     1.490852   -2.749022   -1.547448
Br    -3.882548    0.242070   -0.750625
C      3.630437   -1.198162    0.850365
C      2.765526   -0.063155    0.700667
C      7.555532    1.066872    0.595096
C      7.194806   -0.112284   -0.307039
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C	5.699796	-0.426670	-0.350366
C	5.120903	-0.925282	0.975223
H	7.009876	1.964512	0.297164
H	7.316217	0.867827	1.640309
H	3.194311	0.920805	0.891993
H	3.185229	-1.695647	1.746082
H	3.377374	-1.948763	0.085970
H	7.534294	0.100066	-1.323667
H	7.741852	-1.003648	0.016385
H	5.150224	0.465761	-0.668907
H	5.507193	-1.179757	-1.118703
H	5.635391	-1.839237	1.280856
H	5.285443	-0.191624	1.767088
H	8.621656	1.291937	0.541563

B12Br11_1B-CH-CH2-R_3

E(electronic) = -28851.1848669000

E(zero-point) = 0.2322631995

B	-0.711481	-0.310600	-1.612636
B	0.026038	0.284680	1.646281
B	-1.991507	-0.107873	-0.373543
B	-0.948011	-1.559736	-0.339960
B	0.698643	-1.055228	-0.816242
B	0.649748	0.722960	-1.148156
B	-1.010445	1.287922	-0.873668
B	-1.379069	1.041206	0.861311
B	0.245441	1.547054	0.357265
B	1.268328	0.094878	0.399281
B	0.277751	-1.307384	0.901625
B	-1.365762	-0.728082	1.178401
Br	-1.757347	2.775962	-1.886611
Br	1.827434	1.533584	-2.490307
Br	-1.114712	-0.676982	-3.481560
Br	1.972551	-2.218116	-1.747135
Br	-1.613682	-3.337799	-0.769663
Br	1.091839	-2.770252	1.920012
Br	-2.518411	-1.533220	2.525515
Br	0.546206	0.651044	3.500487
Br	-2.551964	2.242424	1.846070
Br	0.968513	3.314020	0.795546
Br	-3.880560	-0.224266	-0.821951
C	3.709563	1.075777	0.499692
C	2.723165	0.085207	0.821719
C	8.188478	0.295631	0.118223
C	7.132788	-0.787935	0.332317
C	5.712311	-0.353048	-0.026035

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C       5.155437    0.767745    0.854249
H       8.176401    0.651933   -0.914207
H       8.022914    1.157086    0.766351
H       3.030558   -0.738711    1.466115
H       3.567998    1.393103   -0.545775
H       3.298807    1.978123    1.013501
H       7.390791   -1.662260   -0.269957
H       7.154616   -1.119578    1.374912
H       5.677613   -0.034891   -1.072485
H       5.044596   -1.217203    0.040986
H       5.220341    0.478343    1.907276
H       5.751299    1.674077    0.740484
H       9.189814   -0.083210    0.327847


B12Br11_1B-CH-CH2-R_4
E(electronic) =     -28851.1848841000
E(zero-point) =           0.2323847607
B       0.466076   -1.319557   -1.023417
B       0.180722    1.319590    1.095132
B       1.841238   -0.214773   -0.698918
B       0.443767    0.365663   -1.631640
B      -1.018286   -0.356587   -0.931733
B      -0.514019   -1.404765    0.458717
B       1.262565   -1.310609    0.586827
B       1.691333    0.372388    0.982476
B       0.249920   -0.365465    1.681237
B      -1.157132    0.219796    0.749368
B      -0.594106    1.308449   -0.539228
B       1.168637    1.417543   -0.384588
Br      2.303783   -2.830181    1.217437
Br     -1.579769   -2.975972    0.956797
Br      0.609171   -2.847819   -2.221047
Br     -2.598184   -0.800646   -2.007140
Br      0.557948    0.778962   -3.532963
Br     -1.678178    2.822093   -1.155998
Br      2.128157    3.048219   -0.843399
Br     -0.069767    2.828261    2.317788
Br      3.239647    0.820090    2.074367
Br      0.063692   -0.766132    3.589813
Br      3.578108   -0.466780   -1.537691
C      -3.717208    0.740126    0.902760
C      -2.485979    0.299354    1.479926
C      -6.637518   -1.255915    0.080857
C      -6.511934    0.229011   -0.252740
C      -6.228027    1.122543    0.960234
C      -4.974971    0.748904    1.755879
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H	-6.929058	-1.829151	-0.799487
H	-5.695415	-1.674291	0.436482
H	-2.501208	-0.069953	2.505280
H	-3.521792	1.686898	0.366266
H	-3.805054	0.081762	0.004365
H	-5.731477	0.364692	-1.005245
H	-7.436556	0.575265	-0.721220
H	-6.137150	2.158576	0.621709
H	-7.087953	1.093735	1.635442
H	-4.845457	1.456011	2.577981
H	-5.099816	-0.235331	2.211943
H	-7.390070	-1.424043	0.855107

B12Br11_1B-CH-CH2-R_5
E(electronic) = -28851.1845821000
E(zero-point) = 0.2341553615

B	1.443916	1.280201	0.169407
B	-0.762933	-1.286740	-0.085391
B	1.736390	-0.111998	-0.922159
B	1.803907	-0.345334	0.845883
B	0.537670	0.676254	1.574916
B	-0.307896	1.557040	0.227720
B	0.444573	1.053481	-1.298803
B	0.142227	-0.691090	-1.499759
B	-1.104656	0.349232	-0.781299
B	-1.027778	0.105531	0.976472
B	0.272445	-1.066051	1.350129
B	1.000833	-1.558729	-0.178179
Br	0.551371	2.267725	-2.819248
Br	-1.054332	3.346159	0.499077
Br	2.701902	2.753436	0.348656
Br	0.659769	1.475664	3.365063
Br	3.463731	-0.711070	1.796051
Br	0.098138	-2.260454	2.894310
Br	1.728800	-3.346896	-0.432711
Br	-2.063057	-2.745298	-0.212950
Br	-0.102918	-1.496703	-3.254930
Br	-2.795378	0.721517	-1.705948
Br	3.336081	-0.234994	-2.022232
C	-3.375101	0.976998	1.866747
C	-2.149083	0.232612	1.991342
C	-7.989283	0.075790	-0.047897
C	-6.703033	-0.551419	0.483475
C	-5.690781	0.494988	0.943522
C	-4.403091	-0.151767	1.447439
H	-8.479519	0.680155	0.718461

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H     -7.782575    0.725976   -0.899863
H     -2.037654   -0.353688    2.902326
H     -3.715078    1.400411    2.812317
H     -3.337175    1.728789    1.085904
H     -6.936077   -1.224677    1.313531
H     -6.244712   -1.167652   -0.293657
H     -5.446864    1.156039    0.109838
H     -6.126302    1.118573    1.730292
H     -4.593893   -0.797600    2.304614
H     -3.977967   -0.769350    0.658649
H     -8.697203   -0.687160   -0.374684
```

```
B12Br11_1B-CH-CH2-R_6
E(electronic) =     -28851.1838413000
E(zero-point) =           0.2336420471
B      0.645428    0.864484   -1.379407
B     -0.164603   -0.904433    1.398300
B      1.762354   -0.301966   -0.634039
B      1.370083    1.225497    0.208079
B     -0.337847    1.587217   -0.096955
B     -1.025283    0.302316   -1.094785
B      0.266318   -0.878689   -1.432662
B      0.807827   -1.608694    0.107653
B     -0.923992   -1.247837   -0.160168
B     -1.312989    0.283695    0.658823
B      0.170129    0.853587    1.474077
B      1.476718   -0.314598    1.128468
Br     0.302910   -1.880414   -3.102217
Br    -2.438174    0.628889   -2.413355
Br     1.116576    1.870985   -2.981357
Br    -0.958776    3.444984   -0.210206
Br     2.673190    2.649210    0.461037
Br     0.072665    1.861061    3.157970
Br     2.898646   -0.631675    2.419840
Br    -0.671572   -1.899951    3.010433
Br     1.458097   -3.443389    0.204834
Br    -2.240973   -2.678048   -0.377293
Br     3.528516   -0.630693   -1.380839
C     -3.315668    1.795064    1.677611
C     -2.506773    0.589363    1.572070
C     -5.882849   -1.543436    0.598369
C     -4.892010   -0.429213    0.296128
C     -5.420239    0.973870    0.532394
C     -4.319725    2.026938    0.517420
H     -5.431323   -2.519118    0.424909
H     -6.222303   -1.503906    1.635500
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H     -2.595827   -0.110347    2.400948
H     -3.840491    1.836406    2.631676
H     -2.599743    2.628504    1.616415
H     -3.998644   -0.593709    0.934262
H     -4.510331   -0.519067   -0.718596
H     -6.148690    1.217717   -0.247177
H     -5.958476    1.017935    1.485522
H     -3.784498    2.014729   -0.429078
H     -4.732668    3.027311    0.648781
H     -6.762813   -1.458428   -0.043715
```

```
B12Br11_1B-CH-CH2-R_7
E(electronic) =     -28851.1837925000
E(zero-point) =           0.2341580917
B      0.496479   -1.011722   -1.316355
B      0.182662    1.008748    1.386408
B      1.851393    0.008083   -0.737509
B      0.426073    0.760364   -1.493515
B     -1.015612   -0.144605   -0.979145
B     -0.467426   -1.488733    0.104277
B      1.310615   -1.381186    0.245263
B      1.712041    0.161793    1.035093
B      0.292716   -0.757696    1.542964
B     -1.142155   -0.001284    0.786470
B     -0.617803    1.388071   -0.202433
B      1.144679    1.495725   -0.027803
Br     2.397105   -2.980238    0.478690
Br    -1.436888   -3.187534    0.193920
Br     0.661522   -2.193591   -2.854149
Br    -2.599745   -0.350984   -2.117775
Br     0.511335    1.631176   -3.234753
Br    -1.726955    2.986613   -0.419413
Br     2.057036    3.213403   -0.072519
Br    -0.103753    2.164697    2.947839
Br     3.260344    0.370732    2.197243
Br     0.134770   -1.619015    3.296298
Br     3.584025    0.015890   -1.621807
C     -3.717425    0.496062    1.217776
C     -2.403523    0.070606    1.624345
C     -8.086881    0.404585    0.134025
C     -6.779686    0.293291    0.915003
C     -5.781964   -0.646008    0.246584
C     -4.488236   -0.873969    1.027532
H     -8.786387    1.085189    0.621186
H     -7.906119    0.778011   -0.875606
H     -2.318174   -0.287645    2.649457
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H     -4.226920    1.058030    2.001278
H     -3.715994    1.040970    0.279831
H     -6.339724    1.288258    1.016708
H     -6.986084   -0.058329    1.930900
H     -6.246033   -1.626993    0.103446
H     -5.528905   -0.275811   -0.748868
H     -4.690000   -1.302010    2.010010
H     -3.861043   -1.576900    0.483040
H     -8.574457   -0.568210    0.043353
```

```
B12Br11_1B-CH-CH2-R_8
E(electronic) =     -28851.1836346000
E(zero-point) =           0.2341206024
B     -0.311741    0.716670   -1.504648
B     -0.356769   -0.698078    1.575058
B     -1.757397   -0.135419   -0.876695
B     -0.293247   -1.053209   -1.303780
B      1.122459   -0.085882   -0.835810
B      0.523913    1.462871   -0.118063
B     -1.262879    1.419499   -0.147959
B     -1.806680    0.082323    0.892685
B     -0.410206    1.060878    1.352533
B      1.064022    0.140674    0.925931
B      0.590115   -1.415495    0.194192
B     -1.185191   -1.454151    0.197163
Br    -2.301286    3.051846   -0.366341
Br     1.549235    3.123388   -0.271596
Br    -0.274483    1.554272   -3.261199
Br     2.815505   -0.158917   -1.822843
Br    -0.235650   -2.268962   -2.825395
Br     1.659190   -3.037168    0.433931
Br    -2.153361   -3.128011    0.408504
Br    -0.278921   -1.508965    3.361907
Br    -3.473157    0.148897    1.897620
Br    -0.396791    2.267219    2.897227
Br    -3.389829   -0.297793   -1.921720
C      3.572601   -0.259158    1.728885
C      2.221128    0.214008    1.900526
C      7.761123   -0.402153   -0.024195
C      6.253325   -0.204073    0.103942
C      5.887713    0.724903    1.257866
C      4.395945    1.042846    1.381343
H      8.003240   -1.069271   -0.852173
H      8.269795    0.547918   -0.201993
H      2.017030    0.721714    2.842028
H      3.979974   -0.657130    2.661073
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H       3.665457   -0.974791    0.920050
H       5.849899    0.204512   -0.824447
H       5.771981   -1.174737    0.237033
H       6.253642    0.306753    2.200996
H       6.405660    1.679798    1.122331
H       4.238282    1.788102    2.161061
H       4.015015    1.458058    0.451207
H       8.181219   -0.835799    0.886303


B12Br11_1B-CH-CH2-R_9
E(electronic) =     -28851.1837349000
E(zero-point) =           0.2342844174
B       1.080051    1.357101   -0.636318
B      -0.455272   -1.376495    0.668932
B       1.734924   -0.288544   -0.826514
B       1.727394    0.486289    0.792081
B       0.232681    1.438782    0.923744
B      -0.692050    1.243392   -0.568743
B       0.220923    0.181566   -1.658972
B       0.368625   -1.439487   -0.888349
B      -1.141707   -0.496863   -0.732072
B      -1.115142    0.274358    0.860726
B       0.370711   -0.202749    1.705251
B       1.306607   -1.251106    0.611911
Br      0.111608    0.381962   -3.592002
Br     -1.864540    2.659465   -1.252918
Br      1.971462    2.922194   -1.378804
Br      0.133651    3.068689    2.000209
Br      3.357820    1.047710    1.691763
Br      0.367185   -0.373846    3.661521
Br      2.451881   -2.661254    1.313400
Br     -1.416007   -2.900854    1.442830
Br      0.424431   -3.072465   -1.946620
Br     -2.817842   -1.047501   -1.578795
Br      3.385837   -0.610963   -1.802875
C      -3.190881    1.558352    1.932663
C      -2.304984    0.429814    1.784459
C      -6.554303   -0.318864   -0.691449
C      -6.594867   -0.146499    0.825872
C      -5.214287   -0.034268    1.476649
C      -4.461112    1.220179    1.047748
H      -7.560930   -0.425830   -1.098381
H      -6.086027    0.532629   -1.185099
H      -2.538393   -0.439018    2.396109
H      -3.534454    1.664122    2.963482
H      -2.755597    2.480919    1.561162
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H     -7.183162    0.741321    1.081167
H     -7.118833   -0.996620    1.270079
H     -5.332587   -0.032703    2.564573
H     -4.627773   -0.921412    1.225137
H     -4.141268    1.155890    0.011757
H     -5.097505    2.102613    1.141880
H     -5.981607   -1.205191   -0.965690
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B12Br11_1B-CH-CH2-R_10
E(electronic) =     -28851.1836493000
E(zero-point) =           0.2343409066
B      0.077483   -0.722607   -1.482016
B      0.543625    0.713969    1.552733
B      1.684753   -0.149860   -0.941491
B      0.399203    1.020528   -1.328222
B     -1.146190    0.345840   -0.772142
B     -0.820345   -1.267816   -0.041175
B      0.938271   -1.568295   -0.145866
B      1.781163   -0.338977    0.827573
B      0.246538   -1.021507    1.381654
B     -1.045172    0.149429    0.993363
B     -0.325895    1.572533    0.199284
B      1.425953    1.273627    0.120493
Br     1.634399   -3.373345   -0.360755
Br    -2.146395   -2.706446   -0.109662
Br    -0.200000   -1.571891   -3.211609
Br    -2.837644    0.716164   -1.691401
Br     0.495676    2.199577   -2.875893
Br    -1.072221    3.363577    0.448873
Br     2.699035    2.739444    0.236977
Br     0.715572    1.561206    3.315718
Br     3.453462   -0.706165    1.755534
Br     0.073059   -2.172734    2.958655
Br     3.264538   -0.321281   -2.063004
C     -3.435543    0.957231    1.870851
C     -2.137960    0.344129    2.023153
C     -6.217915   -0.568156   -0.731510
C     -6.210083    0.614444    0.234215
C     -5.878929    0.221255    1.674981
C     -4.441061   -0.257330    1.905168
H     -6.484097   -0.245761   -1.738555
H     -5.240360   -1.043357   -0.797799
H     -1.932060   -0.061938    3.012363
H     -3.674775    1.588131    2.730828
H     -3.535853    1.509017    0.943448
H     -5.503793    1.367887   -0.119614
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H     -7.193109    1.093021    0.229042
H     -6.087233    1.057315    2.347971
H     -6.543097   -0.594687    1.977570
H     -4.359496   -0.745711    2.876140
H     -4.152461   -0.988902    1.153422
H     -6.943468   -1.322439   -0.417054


B12Br11_1B-CH-CH2-R_11
E(electronic) =     -28851.1836646000
E(zero-point) =           0.2345000754
B      0.661999    0.365431   -1.591171
B     -0.143093   -0.378290    1.611230
B      1.856429   -0.338774   -0.457740
B      1.287470    1.334360   -0.233501
B     -0.442492    1.390415   -0.648659
B     -0.941627   -0.270385   -1.150229
B      0.488681   -1.332896   -1.027621
B      0.983541   -1.398820    0.681659
B     -0.728827   -1.353064    0.248044
B     -1.301946    0.325078    0.475200
B      0.057555    1.330229    1.044222
B      1.462079    0.255873    1.185754
Br     0.728240   -2.843678   -2.234323
Br    -2.348151   -0.564859   -2.481626
Br     1.100203    0.786080   -3.441679
Br    -1.300531    2.979984   -1.415818
Br     2.449672    2.874173   -0.510078
Br    -0.203818    2.840291    2.263692
Br     2.819534    0.547269    2.549759
Br    -0.712771   -0.752497    3.455753
Br     1.789445   -2.983587    1.477152
Br    -1.956772   -2.853470    0.544285
Br     3.686827   -0.719561   -0.998262
C     -3.439330    1.704520    1.274987
C     -2.682066    0.500463    1.102051
C     -5.682349   -1.367013   -0.068645
C     -6.000695   -0.234937    0.905520
C     -5.802806    1.164091    0.315587
C     -4.365514    1.532791   -0.025300
H     -5.861119   -2.338483    0.392297
H     -6.310226   -1.295759   -0.959323
H     -3.172855   -0.415575    1.422903
H     -4.080610    1.705196    2.153715
H     -2.851776    2.610331    1.198247
H     -7.038970   -0.322120    1.234853
H     -5.398182   -0.342679    1.812654
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H     -6.384176    1.238192   -0.608869
H     -6.207253    1.912639    1.001858
H     -3.945054    0.816313   -0.736712
H     -4.282944    2.490660   -0.533449
H     -4.644820   -1.359066   -0.399200


B12Br11_1B-CH-CH2-R_12
E(electronic) =     -28851.1833618000
E(zero-point) =           0.2344730262
B      1.747464    0.764231    0.517556
B     -1.123925   -0.767612   -0.445913
B      1.635888   -0.154287   -1.016884
B      1.588375   -1.022021    0.537237
B      0.674391   -0.022049    1.683675
B      0.149667    1.487106    0.829334
B      0.756445    1.387407   -0.840148
B     -0.035446    0.002866   -1.627074
B     -0.943077    1.011735   -0.483738
B     -0.986786    0.139998    1.066715
B     -0.108138   -1.396964    0.894413
B      0.474869   -1.492714   -0.771130
Br     1.257640    2.993834   -1.822069
Br    -0.078283    3.176686    1.793909
Br     3.381632    1.653323    1.090015
Br     1.009840   -0.002716    3.619599
Br     3.034511   -2.179317    1.141372
Br    -0.695404   -2.956706    1.929259
Br     0.636181   -3.199243   -1.696424
Br    -2.785245   -1.647991   -0.994832
Br    -0.452574   -0.001335   -3.530552
Br    -2.402849    2.177868   -1.090435
Br     3.152993   -0.322497   -2.224307
C     -3.121673    1.150226    2.322805
C     -1.991429    0.276854    2.212067
C     -7.313375   -0.004838   -0.345170
C     -6.280580   -0.514871    0.656168
C     -5.244264    0.549780    1.005717
C     -4.183530    0.008855    1.958704
H     -7.852729    0.859609    0.048311
H     -6.831014    0.299850   -1.275096
H     -1.848652   -0.406758    3.046424
H     -3.324517    1.510812    3.327374
H     -3.145301    1.945934    1.588493
H     -6.782596   -0.855380    1.567037
H     -5.764935   -1.383237    0.240394
H     -4.751325    0.893493    0.096517
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H     -5.729530    1.420451    1.456475
H     -4.596061   -0.360148    2.896082
H     -3.711188   -0.850278    1.467367
H     -8.047156   -0.775560   -0.585059


B12Br11_1B-CH-CH2-R_13
E(electronic) =     -28851.1831617000
E(zero-point) =           0.2343721779
B     -0.309512    0.578452   -1.565262
B     -0.324995   -0.554999    1.628227
B     -1.772290   -0.141451   -0.824330
B     -0.366268   -1.164899   -1.206844
B      1.105457   -0.230501   -0.865284
B      0.606350    1.400617   -0.274856
B     -1.180849    1.445069   -0.251154
B     -1.756443    0.232655    0.918407
B     -0.300379    1.176358    1.252123
B      1.114203    0.151401    0.868385
B      0.544983   -1.437654    0.294144
B     -1.229962   -1.387592    0.347653
Br    -2.146480    3.102294   -0.585336
Br     1.704415    2.987309   -0.602219
Br    -0.288218    1.254420   -3.390585
Br     2.759563   -0.476637   -1.890728
Br    -0.412202   -2.512213   -2.613628
Br     1.549099   -3.079032    0.650460
Br    -2.268200   -2.986869    0.732772
Br    -0.228994   -1.208929    3.477909
Br    -3.385801    0.471670    1.957723
Br    -0.179066    2.511544    2.682260
Br    -3.442479   -0.314228   -1.806398
C      3.633099   -0.275036    1.655169
C      2.296170    0.238640    1.813453
C      6.569562   -0.293786   -0.776103
C      6.590021   -0.396089    0.746729
C      5.950936    0.798336    1.454628
C      4.455122    0.997758    1.195110
H      7.080360   -1.142962   -1.231360
H      5.552662   -0.277173   -1.164723
H      2.121897    0.796156    2.732208
H      4.047805   -0.605234    2.609690
H      3.709361   -1.050663    0.900989
H      6.095075   -1.319267    1.059476
H      7.623774   -0.480822    1.092667
H      6.112643    0.712877    2.532518
H      6.455782    1.716102    1.136445
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H       4.115822    1.884552    1.731370
H       4.236582    1.166383    0.144590
H       7.069972    0.617307   -1.111882


B12Br11_1B-CH-CH2-R_14
E(electronic) =     -28851.1777058000
E(zero-point) =           0.2335890195
B       1.259818    1.311336    0.247311
B      -0.830392   -1.326082   -0.201710
B       1.778184   -0.156598   -0.636874
B       1.498806   -0.242837    1.119955
B       0.103228    0.802343    1.496937
B      -0.473464    1.542257   -0.061994
B       0.571303    0.933883   -1.357919
B       0.336559   -0.828256   -1.456782
B      -1.048840    0.231469   -1.096293
B      -1.336734    0.142116    0.662270
B      -0.093598   -0.962740    1.374305
B       0.926416   -1.556584    0.069742
Br      0.965579    2.021446   -2.926781
Br     -1.248657    3.340040   -0.097351
Br      2.440328    2.830174    0.542264
Br     -0.079122    1.762942    3.203582
Br      2.941281   -0.477865    2.405765
Br     -0.531148   -2.036188    2.956003
Br      1.715785   -3.336848    0.119443
Br     -2.038309   -2.835959   -0.474225
Br      0.464873   -1.783372   -3.148552
Br     -2.459937    0.447665   -2.438838
Br      3.565503   -0.319437   -1.386395
C      -3.532133    1.417194    1.625588
C      -2.510433    0.392640    1.611990
C      -4.921584   -1.527881    1.292578
C      -5.385847   -0.748451    0.064212
C      -5.637658    0.747344    0.290709
C      -4.411509    1.656492    0.387068
H      -4.973427   -2.601189    1.115356
H      -3.876450   -1.338680    1.546166
H      -2.411470   -0.158156    2.544668
H      -4.129415    1.375064    2.536484
H      -2.870704    2.311773    1.702990
H      -4.665848   -0.882242   -0.744698
H      -6.322490   -1.191163   -0.284319
H      -6.233021    1.122179   -0.546091
H      -6.258805    0.876827    1.184768
H      -3.807723    1.569088   -0.510639
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H     -4.749937    2.692395    0.435352
H     -5.528341   -1.292403    2.170342


B12Br11_Cyclohexan_Sessel-a
E(electronic) =     -28851.1973402000
E(zero-point) =           0.2373681975
B     -1.078721   -1.446271    0.277010
B      0.611814    1.453593   -0.275353
B     -1.870797    0.000000   -0.401985
B     -1.328135   -0.000001    1.297878
B      0.204634   -0.900471    1.380499
B      0.611814   -1.453593   -0.275354
B     -0.670393   -0.893114   -1.373931
B     -0.670393    0.893115   -1.373930
B      0.867537    0.000001   -1.297058
B      1.326486    0.000000    0.392648
B      0.204634    0.900470    1.380499
B     -1.078721    1.446271    0.277012
Br    -1.156381   -1.920419   -2.955647
Br     1.601727   -3.107569   -0.604661
Br    -2.038191   -3.110986    0.598375
Br     0.758096   -1.917334    2.957514
Br    -2.573149   -0.000001    2.796284
Br     0.758096    1.917332    2.957515
Br    -2.038191    3.110985    0.598377
Br     1.601727    3.107570   -0.604658
Br    -1.156381    1.920422   -2.955645
Br     2.190602    0.000001   -2.736975
Br    -3.761522    0.000000   -0.868817
C      4.106069   -1.274222    1.226321
C      3.298107   -0.000001    1.375627
C      4.106070    1.274221    1.226322
C      4.957229    1.266721   -0.041423
C      5.810732    0.000000   -0.145665
C      4.957229   -1.266722   -0.041424
H      3.454571    2.142585    1.267557
H      2.657788    0.000000    0.352607
H      2.669385   -0.000001    2.256430
H      4.745247   -1.310841    2.115532
H      3.454571   -2.142587    1.267555
H      4.295787    1.335751   -0.907910
H      5.587642    2.157174   -0.060993
H      6.360583    0.000000   -1.088621
H      6.559219   -0.000001    0.654813
H      4.295787   -1.335750   -0.907911
H      5.587641   -2.157174   -0.060995
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H      4.745248    1.310839    2.115533


B12Br11_Cyclohexan_Sessel-e
E(electronic) =     -28851.1939944000
E(zero-point) =           0.2376929435
B     -0.583441   -0.932367    1.446211
B      0.600901    0.391887   -1.454810
B     -0.279009   -1.930374    0.000000
B     -1.618201   -0.749543    0.000000
B     -1.077664    0.686736    0.901018
B      0.600901    0.391887    1.454810
B      1.094193   -1.221618    0.892551
B      1.094193   -1.221618   -0.892551
B      1.637859    0.219008    0.000000
B      0.278176    1.316931    0.000000
B     -1.077664    0.686736   -0.901018
B     -0.583441   -0.932367   -1.446211
Br     2.349265   -2.301058    1.918493
Br     1.300978    1.160008    3.110474
Br    -1.264532   -1.682858    3.110016
Br    -2.297164    1.835073    1.912489
Br    -3.491215   -1.285687    0.000000
Br    -2.297164    1.835073   -1.912489
Br    -1.264532   -1.682858   -3.110016
Br     1.300978    1.160008   -3.110474
Br     2.349265   -2.301058   -1.918493
Br     3.468925    0.906663    0.000000
Br    -0.612502   -3.849117    0.000000
C      0.237979    3.442495    0.000000
C      0.639143    4.161229   -1.277735
C      0.010601    5.559633   -1.260391
C      0.387570    6.338285    0.000000
C      0.010601    5.559633    1.260391
C      0.639143    4.161229    1.277735
H      0.321528    6.099172   -2.156550
H      1.726780    4.235572   -1.333117
H      0.303954    3.601105   -2.144991
H     -0.825229    3.226787    0.000000
H      0.944538    2.488860    0.000000
H      1.466348    6.525174    0.000000
H     -0.100920    7.315058    0.000000
H      0.321528    6.099172    2.156550
H     -1.077043    5.457126    1.315411
H      1.726780    4.235572    1.333117
H      0.303954    3.601105    2.144991
H     -1.077043    5.457126   -1.315411
```

B12Br11_Cyclohexan_Twist-a
E(electronic) = -28851.1876522000
E(zero-point) = 0.2371636967

B	1.289299	0.581929	1.193177
B	-0.833101	-0.577698	-1.195725
B	1.873390	-0.028941	-0.376867
B	1.165393	-1.159559	0.807522
B	-0.178319	-0.329341	1.620471
B	-0.304338	1.327800	0.930174
B	0.964500	1.504582	-0.303537
B	0.639825	0.331711	-1.613110
B	-0.707221	1.171179	-0.810156
B	-1.338239	0.040078	0.365378
B	-0.509249	-1.501732	0.306113
B	0.763760	-1.313206	-0.925960
Br	1.793815	3.232866	-0.650348
Br	-0.961562	2.824661	2.004617
Br	2.493457	1.248388	2.572056
Br	-0.687854	-0.710194	3.471359
Br	2.229344	-2.498942	1.740121
Br	-1.376410	-3.221474	0.644647
Br	1.361962	-2.829669	-1.991761
Br	-2.089687	-1.238725	-2.538188
Br	1.092904	0.709273	-3.469284
Br	-1.823630	2.480301	-1.743931
Br	3.770957	-0.067721	-0.813522
C	-3.325404	0.260155	1.321915
C	-4.129824	-1.012012	1.466912
C	-4.873730	-1.382806	0.173873
C	-5.234272	-0.147641	-0.673811
C	-5.450764	1.088753	0.197497
C	-4.154866	1.477260	0.925853
H	-4.247672	-2.054960	-0.412994
H	-2.674795	0.025039	0.327910
H	-3.503645	-1.828231	1.815442
H	-4.840579	-0.790015	2.269609
H	-2.683810	0.453111	2.170142
H	-4.428888	0.058063	-1.380987
H	-6.119380	-0.355092	-1.276317
H	-5.787735	1.930820	-0.407668
H	-6.243503	0.889561	0.924501
H	-3.556254	2.151156	0.319769
H	-4.368990	2.016023	1.850737
H	-5.775426	-1.938439	0.437237

B12Br11_Cyclohexan_Twist-ae
E(electronic) = -28851.1861199000
E(zero-point) = 0.2374944073

B	1.001112	-1.464768	0.435432
B	-0.481772	1.472631	-0.437973
B	1.926761	-0.094130	-0.231171
B	0.790718	-0.986442	-1.278109
B	-0.617514	-1.429625	-0.289828
B	-0.362756	-0.801259	1.369504
B	1.212910	0.024289	1.401542
B	1.140498	1.420460	0.287555
B	-0.274794	0.994311	1.277283
B	-1.328159	0.087052	0.222153
B	-0.700532	-0.022347	-1.403667
B	0.876931	0.795356	-1.368411
Br	2.296696	0.054276	3.020139
Br	-1.129943	-1.690077	2.933160
Br	1.839164	-3.149268	0.939893
Br	-1.666234	-3.044384	-0.636505
Br	1.380528	-2.120324	-2.747614
Br	-1.914711	-0.043942	-2.939295
Br	1.570669	1.709353	-2.942133
Br	-1.334113	3.157397	-0.941168
Br	2.144925	3.055609	0.623503
Br	-0.945159	2.120605	2.728967
Br	3.853268	-0.201149	-0.495907
C	-4.158578	1.436333	0.217552
C	-3.384275	0.272488	0.850261
C	-4.180057	-1.020275	0.990386
C	-5.126468	-1.194385	-0.191352
C	-6.159713	-0.047976	-0.258811
C	-5.658445	1.228914	0.436762
H	-3.508998	-1.865916	1.101166
H	-2.634602	-0.018849	-0.025856
H	-2.891123	0.547704	1.774521
H	-3.811125	2.375066	0.639747
H	-3.955004	1.484058	-0.851491
H	-4.529614	-1.220066	-1.105456
H	-5.627085	-2.160544	-0.130451
H	-6.385932	0.172153	-1.303660
H	-7.098679	-0.360559	0.202698
H	-6.198708	2.100167	0.064484
H	-5.863513	1.178628	1.508886
H	-4.735593	-0.943418	1.928638

B12Br11_Cyclohexan_Twist-e
E(electronic) = -28851.1847776000
E(zero-point) = 0.2377772851

B	-0.900894	1.262010	-0.931763
B	0.368534	-1.269050	0.949647
B	-1.918904	-0.064589	-0.310510
B	-0.708144	-0.392287	-1.581019
B	0.722890	0.609068	-1.240543
B	0.397936	1.553929	0.246646
B	-1.233388	1.132717	0.821868
B	-1.249632	-0.599777	1.254426
B	0.184952	0.395385	1.599203
B	1.316521	0.060380	0.309733
B	0.708227	-1.138240	-0.804562
B	-0.926740	-1.544675	-0.232156
Br	-2.332545	2.435010	1.764581
Br	1.160515	3.330126	0.531526
Br	-1.621949	2.712922	-2.013655
Br	1.909783	1.291973	-2.637977
Br	-1.201713	-0.844231	-3.410645
Br	1.875706	-2.412414	-1.722016
Br	-1.674432	-3.322324	-0.507135
Br	1.125002	-2.698607	2.047858
Br	-2.364422	-1.288730	2.695042
Br	0.833499	0.836696	3.391825
Br	-3.829408	-0.139238	-0.680486
C	3.405485	0.079740	0.356868
C	4.103365	1.410747	0.658657
C	5.630240	1.201559	0.668774
C	6.041219	0.124461	-0.334267
C	5.471699	-1.250545	0.071391
C	4.157728	-1.137679	0.870939
H	6.118696	2.150959	0.446907
H	3.818689	2.133704	-0.101252
H	3.767513	1.808149	1.614434
H	2.452048	0.115127	1.047131
H	3.214776	-0.028338	-0.705231
H	5.666297	0.403629	-1.322324
H	7.127176	0.069970	-0.421825
H	5.293587	-1.853125	-0.819676
H	6.196864	-1.791621	0.681511
H	3.562718	-2.036957	0.754833
H	4.355516	-1.014682	1.935880
H	5.959667	0.907741	1.668466

B12Cl11_1B-CH2-CH-R_1

E(electronic) = -5597.7098679700
E(zero-point) = 0.2418423741

B	2.044685	-0.266865	0.952906
B	-0.712374	0.284807	-0.955826
B	2.054291	0.887069	-0.409659
B	1.932945	-0.861798	-0.734992
B	0.930917	-1.579546	0.539871
B	0.404577	-0.264520	1.660061
B	1.116230	1.253646	1.062316
B	0.421492	1.591450	-0.540940
B	-0.596084	0.880230	0.736503
B	-0.704478	-0.864388	0.406437
B	0.221542	-1.237470	-1.057901
B	0.928310	0.280300	-1.652940
Cl	1.577352	2.563029	2.186491
Cl	0.120227	-0.573218	3.403840
Cl	3.482616	-0.565951	1.967790
Cl	1.202819	-3.255548	1.115689
Cl	3.251245	-1.790143	-1.503750
Cl	-0.313222	-2.576088	-2.136287
Cl	1.183432	0.569984	-3.397328
Cl	-2.109450	0.634999	-2.044064
Cl	0.145292	3.259835	-1.118045
Cl	-1.896930	1.834869	1.531459
Cl	3.514795	1.817317	-0.840502
C	-6.234818	1.153162	-0.293625
H	-6.127522	1.079300	-1.377489
H	-7.125667	1.746722	-0.084229
H	-5.375663	1.708017	0.082870
C	-6.342112	-0.231570	0.340726
H	-7.264258	-0.714564	0.007000
H	-6.423392	-0.133803	1.427107
C	-5.169894	-1.156573	0.005823
H	-5.359883	-2.149764	0.420327
H	-5.094555	-1.273346	-1.078567
C	-3.832708	-0.612577	0.540643
H	-3.871114	-0.449335	1.616532
H	-3.638565	0.349329	0.068771
C	-2.736192	-1.531911	0.186137
H	-2.685904	-1.850685	-0.850060
C	-1.807679	-2.057110	1.057667
H	-1.903147	-1.862931	2.118885
H	-1.289180	-2.968471	0.785473

B12Cl11_1B-CH-CH2-R_1
E(electronic) = -5597.6964010300

E(zero-point) = 0.2392907464

B	-1.962888	-1.145604	0.045924
B	0.503606	1.194311	-0.013323
B	-2.293552	0.570314	-0.368631
B	-1.842597	0.142267	1.306018
B	-0.629176	-1.164245	1.225138
B	-0.334601	-1.534638	-0.545002
B	-1.378560	-0.456205	-1.498777
B	-0.835423	1.218326	-1.191061
B	0.348613	-0.095764	-1.296629
B	0.791542	-0.513871	0.380020
B	-0.129852	0.519443	1.517018
B	-1.145752	1.590807	0.549421
Cl	-2.046249	-0.963426	-3.075689
Cl	0.118093	-3.191421	-1.063471
Cl	-3.247285	-2.380665	0.097954
Cl	-0.472208	-2.440149	2.472954
Cl	-3.002857	0.234699	2.658623
Cl	0.600624	0.994332	3.087773
Cl	-1.557140	3.241196	1.087794
Cl	1.834719	2.394562	-0.053026
Cl	-0.928268	2.485301	-2.441941
Cl	1.528072	-0.191277	-2.647452
Cl	-3.931097	1.144884	-0.768601
C	3.082148	-1.784502	0.052598
C	2.167729	-0.943524	0.794783
C	7.031832	1.361202	-0.142829
C	6.539810	-0.014523	0.298771
C	5.071611	-0.250670	-0.036262
C	4.558480	-1.623094	0.399776
H	6.924890	1.486571	-1.221949
H	6.454947	2.153903	0.336589
H	2.507652	-0.617753	1.778580
H	2.698479	-2.794440	0.319881
H	2.883480	-1.723624	-1.019550
H	7.147966	-0.792387	-0.173993
H	6.686026	-0.127827	1.377400
H	4.459171	0.527622	0.431994
H	4.913848	-0.134967	-1.112365
H	5.136076	-2.410989	-0.088653
H	4.699385	-1.748857	1.477330
H	8.082736	1.511109	0.109506

The following geometries were obtained by DFT geometry optimization (B3LYP-GD3BJ/6-311++G(2d,2p)).

B12Br11_CH2_H2O
E(electronic) = -28730.5036221000
E(zero-point) = 0.1181318100

B	-0.346975	1.053459	1.282827
B	0.394891	-0.925759	-1.413412
B	-1.555751	0.599697	0.054182
B	-0.185337	1.612332	-0.357298
B	1.261354	1.122976	0.478276
B	0.781232	-0.325378	1.405400
B	-0.955250	-0.634351	1.136085
B	-1.196403	-0.994991	-0.614419
B	0.253334	-1.589413	0.238429
B	1.625576	-0.523693	-0.154292
B	1.035403	0.711334	-1.239368
B	-0.710331	0.449840	-1.507097
Br	-0.796607	2.235388	2.771748
Br	0.803709	-2.024496	-2.981762
Br	-3.398272	1.304584	0.172615
Br	-0.836619	3.196594	-1.526528
Br	2.634268	2.386541	1.056117
Br	1.643372	-0.771866	3.099688
Br	-2.095076	-1.424783	2.511932
Br	-2.609541	-2.216253	-1.231819
Br	0.513364	-3.491791	0.598869
Br	3.459017	-1.186249	-0.263325
Br	2.145972	1.531399	-2.642601
C	-1.285991	1.397370	-2.645950
H	-0.688640	1.549608	-3.535961
H	-2.353526	1.471117	-2.810280
O	-4.275571	0.247925	-3.015094
H	-3.874389	-0.617931	-2.859858
H	-4.397210	0.581936	-2.116756

B12Br11_CH2
E(electronic) = -28654.0220112000
E(zero-point) = 0.0907585279

B	1.168101	0.920589	0.624713
B	-1.167079	-0.934189	-1.020847
B	0.468612	1.476043	-0.893552
B	1.544145	0.020636	-0.867402
B	1.192081	-0.889301	0.624458
B	-0.094349	-0.001395	1.495170
B	-0.532390	1.443147	0.550246
B	-1.191426	0.903029	-1.020619

B	-1.560952	-0.020791	0.455750
B	-0.493862	-1.456933	0.549922
B	0.507641	-1.462826	-0.893907
B	0.082431	0.001288	-1.853703
Br	2.561746	1.939693	1.525297
Br	-2.501317	-1.954017	-2.021582
Br	1.049972	3.120326	-1.789320
Br	3.307290	0.044264	-1.777602
Br	2.612493	-1.871083	1.524868
Br	-0.189531	-0.002840	3.440935
Br	-1.147547	3.090491	1.398986
Br	-2.552455	1.887174	-2.021131
Br	-3.361313	-0.045001	1.200236
Br	-1.064601	-3.120242	1.398492
Br	1.132834	-3.090927	-1.789697
C	0.650323	0.009031	-3.232635
H	0.921303	-0.907703	-3.743760
H	0.896991	0.932684	-3.743476

B12Br11_H2O
E(electronic) = -28691.2456475000
E(zero-point) = 0.0935170964

B	1.185586	0.891943	-0.968794
B	-0.095599	-0.000680	-1.748744
B	-0.511315	-1.431340	-0.860512
B	0.094088	0.000571	1.543293
B	0.507713	1.450921	0.578374
B	-1.191395	0.896678	0.690261
B	-1.560696	-0.001617	-0.777790
B	1.187073	-0.890560	-0.968127
B	1.557880	0.001480	0.521428
B	0.510193	-1.449718	0.579402
B	-1.189871	-0.898287	0.690908
B	-0.513786	1.429848	-0.861638
Br	2.496793	1.901800	-2.014760
Br	-1.101662	-2.972689	-1.941106
Br	0.210962	0.001392	3.493321
Br	1.089895	3.130656	1.389387
Br	-2.563975	1.937394	1.612898
Br	-3.300367	-0.003378	-1.700307
Br	2.499922	-1.898916	-2.013548
Br	3.359189	0.003386	1.277064
Br	1.095376	-3.127882	1.391534
Br	-2.560636	-1.940857	1.614178
Br	-1.106919	2.969956	-1.942303
O	-0.302368	-0.002283	-3.244647

H	-0.813082	-0.809069	-3.477009
H	-0.817590	0.800982	-3.478652

[B12Br11H][H3O]_MIN1
E(electronic) = -28692.4303968000
E(zero-point) = 0.1117706003

B	0.471730	-1.444819	0.475831
B	-0.212879	1.435800	-1.171505
B	1.449987	-0.889480	-0.904711
B	-0.214991	-1.435485	-1.171571
B	-1.189938	-0.885264	0.201863
B	-0.129515	0.000232	1.312078
B	1.508226	-0.001120	0.636980
B	1.451166	0.887278	-0.904730
B	0.473931	1.444305	0.475992
B	-1.188485	0.887370	0.201959
B	-1.247160	0.000959	-1.335314
B	0.388123	-0.000250	-2.013628
Br	0.837018	-3.104957	1.449693
Br	-0.632128	3.107079	-2.113558
Br	2.982671	-1.927563	-1.550492
Br	-0.636789	-3.106175	-2.113454
Br	-2.740526	-2.012478	0.778585
Br	-0.329748	0.000224	3.304606
Br	3.082722	-0.002206	1.799994
Br	2.985509	1.923145	-1.550332
Br	0.841758	3.104015	1.449490
Br	-2.737884	2.016216	0.778686
Br	-2.864422	0.002063	-2.451818
H	0.564523	-0.000368	-3.176156
H	-3.343938	0.792785	2.333918
O	-3.358005	0.002341	2.977398
H	-3.344567	-0.788171	2.333630
H	-2.399253	0.001713	3.324242

[B12Br11H][H3O]_MIN2
E(electronic) = -28692.4290559000
E(zero-point) = 0.1113058910

B	-0.320338	-1.445381	0.535986
B	0.519108	1.435719	-1.039632
B	0.517795	-1.436265	-1.039756
B	-1.151998	-0.880965	-0.927162
B	-1.347250	0.000723	0.598122
B	0.209472	-0.000007	1.440181
B	1.369054	-0.893014	0.426990

B	1.554985	-0.000675	-1.106515
B	1.369972	0.891830	0.427070
B	-0.319149	1.445738	0.535885
B	-1.151133	0.882215	-0.927234
B	-0.008221	0.000034	-1.940554
Br	-0.848312	-3.104574	1.433243
Br	0.972378	3.105258	-1.968956
Br	0.969270	-3.106022	-1.969380
Br	-2.583665	-2.004851	-1.778981
Br	-3.018140	0.001071	1.701984
Br	0.301714	-0.000105	3.395754
Br	2.826135	-1.931236	1.213196
Br	3.237618	-0.001571	-2.112235
Br	2.828020	1.928767	1.213023
Br	-0.845474	3.105350	1.433385
Br	-2.581666	2.007218	-1.779518
H	-0.104557	-0.000180	-3.113025
H	-4.173613	-0.786982	-1.245719
O	-4.680534	0.002259	-0.847579
H	-4.173607	0.791949	-1.245071
H	-4.341156	0.001727	0.114495

[B12Br11H][H3O]_MIN3
E(electronic) = -28692.4096522000
E(zero-point) = 0.1105258551

B	0.946970	1.240823	0.000000
B	-1.303734	-1.299058	0.000000
B	-0.588192	1.311974	0.877166
B	-0.588192	1.311974	-0.877166
B	0.676222	0.223611	-1.443203
B	1.461249	-0.461870	0.000000
B	0.676222	0.223611	1.443203
B	-1.035867	-0.293878	1.435444
B	0.237768	-1.411178	0.891489
B	0.237768	-1.411178	-0.891489
B	-1.035867	-0.293878	-1.435444
B	-1.813468	0.397476	0.000000
Br	2.198207	2.750667	0.000000
Br	-2.624290	-2.749934	0.000000
Br	-1.081367	2.921268	1.984770
Br	-1.081367	2.921268	-1.984770
Br	1.639410	0.563585	-3.114711
Br	3.356366	-0.946218	0.000000
Br	1.639410	0.563585	3.114711
Br	-2.051026	-0.548324	3.099489
Br	0.718422	-2.996895	1.929735

Br	0.718422	-2.996895	-1.929735
Br	-2.051026	-0.548324	-3.099489
H	-2.949772	0.713655	0.000000
H	-3.390541	4.450002	0.000000
O	-3.260368	3.489738	0.000000
H	-2.635903	3.271947	-0.813397
H	-2.635903	3.271947	0.813397

[B12Br11H][H3O]_TS1

E(electronic) = -28692.4121766000

E(zero-point) = 0.1102370162

B	-0.522938	1.439680	0.507244
B	0.194380	-1.432766	-1.135733
B	-1.472625	0.886116	-0.891636
B	0.194372	1.432770	-1.135731
B	1.134182	0.884661	0.257341
B	0.081173	0.000000	1.371280
B	-1.552678	-0.000004	0.658788
B	-1.472620	-0.886123	-0.891638
B	-0.522930	-1.439682	0.507243
B	1.134186	-0.884653	0.257340
B	1.233966	0.000005	-1.273541
B	-0.390297	0.000001	-1.987401
Br	-0.906281	3.109899	1.457785
Br	0.630115	-3.099819	-2.081160
Br	-2.993536	1.923271	-1.568509
Br	0.630097	3.099826	-2.081156
Br	2.598166	2.104537	0.899107
Br	0.442683	0.000000	3.303862
Br	-3.149815	-0.000010	1.787363
Br	-2.993525	-1.923286	-1.568511
Br	-0.906263	-3.109905	1.457782
Br	2.598175	-2.104525	0.899107
Br	2.913485	0.000010	-2.308680
H	-0.549519	0.000001	-3.152633
H	4.043033	-0.812619	1.088500
O	4.665762	0.000004	1.321660
H	4.043038	0.812621	1.088482
H	4.730951	0.000013	2.289926

[B12Br11H][H3O]_TS2

E(electronic) = -28692.4084889000

E(zero-point) = 0.1099508171

B	0.245800	1.439457	0.624119
B	-0.381026	-1.432747	-1.054040

B	-0.381026	1.432747	-1.054039
B	1.253322	0.879184	-0.715861
B	1.281142	0.000000	0.821928
B	-0.385810	0.000000	1.451169
B	-1.412632	0.889975	0.291162
B	-1.399507	0.000000	-1.256512
B	-1.412631	-0.889975	0.291161
B	0.245801	-1.439457	0.624118
B	1.253323	-0.879183	-0.715861
B	0.263663	0.000000	-1.882477
Br	0.634465	3.108917	1.573377
Br	-0.709727	-3.102360	-2.039433
Br	-0.709729	3.102360	-2.039432
Br	2.765126	2.101713	-1.267726
Br	2.887874	0.000000	1.951373
Br	-0.740116	-0.000001	3.374835
Br	-2.963543	1.928445	0.873721
Br	-2.935777	0.000000	-2.476529
Br	-2.963542	-1.928447	0.873720
Br	0.634467	-3.108918	1.573375
Br	2.765128	-2.101711	-1.267726
H	0.507468	0.000000	-3.035256
H	4.629114	0.000002	-3.087277
O	4.691472	0.000002	-2.119790
H	4.108828	-0.813813	-1.788946
H	4.108827	0.813817	-1.788946

[B12Br11H][H3O]_TS3

E(electronic) = -28692.3549267000

E(zero-point) = 0.1036293270

B	0.380941	1.446289	0.614655
B	-0.410488	-1.445654	-0.989752
B	-0.410175	1.445732	-0.989760
B	1.290940	0.895920	-0.799770
B	1.422762	-0.000156	0.729780
B	-0.173354	0.000018	1.504563
B	-1.306104	0.894924	0.464861
B	-1.472908	0.000152	-1.043979
B	-1.306292	-0.894649	0.464863
B	0.380634	-1.446373	0.614654
B	1.290749	-0.896204	-0.799768
B	0.140349	-0.000020	-1.784242
Br	0.837503	3.119368	1.513362
Br	-0.841672	-3.068479	-1.990771
Br	-0.841011	3.068648	-1.990783
Br	2.792054	1.960660	-1.507861

Br	3.090290	-0.000323	1.746808
Br	-0.354059	0.000040	3.448276
Br	-2.790503	1.939087	1.184195
Br	-3.135262	0.000337	-2.076983
Br	-2.790923	-1.938487	1.184197
Br	0.836834	-3.119550	1.513370
Br	2.791631	-1.961254	-1.507881
H	-1.097573	-0.000046	-3.362008
H	-0.353382	-0.000211	-3.538942
O	1.541300	-0.000133	-3.659245
H	2.082216	-0.768353	-3.406536
H	2.082219	0.768113	-3.406624

B12Br11_n-hexane_primary
E(electronic) = -28851.9175063000
E(zero-point) = 0.2521667236

B	0.736134	-1.406334	0.896297
B	0.057099	1.321078	-0.864395
B	-0.798815	-1.227350	-0.000112
B	-0.490431	-0.227417	1.435235
B	1.259431	0.198313	1.448479
B	2.010687	-0.535126	0.000372
B	0.736528	-1.406659	-0.895863
B	-0.489765	-0.227872	-1.435597
B	1.260036	0.197872	-1.448273
B	1.595579	1.178046	0.000039
B	0.056729	1.321287	0.863720
B	-1.270210	0.496424	-0.000450
Br	1.138155	-3.009989	1.937857
Br	-0.355330	3.122617	-1.680581
Br	-2.089757	-2.707030	-0.000139
Br	-1.516358	-0.390564	3.103070
Br	2.223057	0.506586	3.123630
Br	3.873824	-1.123392	0.000849
Br	1.139008	-3.010605	-1.936742
Br	-1.515198	-0.391453	-3.103715
Br	2.224370	0.505742	-3.123095
Br	2.924694	2.620339	0.000117
Br	-0.355924	3.123021	1.679443
C	-2.730154	1.134685	-0.001125
H	-2.815812	1.789857	0.869786
H	-2.815679	1.788132	-0.873337
C	-3.933118	0.190622	-0.000306
H	-3.890672	-0.462696	-0.871627
H	-3.890444	-0.461573	0.871848
C	-5.257069	0.953008	-0.000636

H	-5.296339	1.610004	-0.876281
H	-5.296254	1.610920	0.874325
C	-6.482107	0.040927	-0.000109
H	-6.441705	-0.616319	0.873900
H	-6.441811	-0.617163	-0.873486
C	-7.808765	0.799850	-0.000401
H	-7.846246	1.456473	-0.874604
H	-7.846202	1.457232	0.873232
C	-9.029036	-0.120241	0.000022
H	-9.030831	-0.766040	0.880214
H	-9.962041	0.445852	-0.000204
H	-9.030864	-0.766798	-0.879612
H	-0.437539	3.543274	-0.000391

B12Br11_n-hexane_secondary
E(electronic) = -28851.9065952000
E(zero-point) = 0.2525089804

B	-0.841206	-1.160330	-1.104120
B	0.410946	1.027329	1.054406
B	0.811907	-1.333371	-0.447400
B	0.448757	-0.011601	-1.577415
B	-1.223331	0.565282	-1.218226
B	-1.865119	-0.403196	0.140313
B	-0.601979	-1.564422	0.621646
B	0.821833	-0.656223	1.198000
B	-0.842354	-0.084861	1.570767
B	-1.240598	1.215707	0.436071
B	0.180792	1.415193	-0.612326
B	1.516925	0.298712	-0.166315
Br	-1.584761	-2.439476	-2.380326
Br	1.125940	2.558123	2.158691
Br	1.850645	-2.911362	-0.988999
Br	1.154665	0.053206	-3.410306
Br	-2.352641	1.339313	-2.617912
Br	-3.770747	-0.798815	0.307991
Br	-1.059497	-3.317217	1.355580
Br	1.963309	-1.294370	2.669117
Br	-1.534626	-0.071495	3.401272
Br	-2.381840	2.725678	0.952984
Br	0.564365	3.356210	-1.057066
H	0.954266	3.367971	0.601267
C	3.083134	0.706305	-0.172913
H	3.228747	1.206726	0.789213
C	4.039793	-0.501052	-0.153209
H	3.667253	-1.268341	0.518212
H	4.062237	-0.952231	-1.146250

C	3.537548	1.708639	-1.271463
H	4.260475	1.209050	-1.918195
H	2.721254	1.976314	-1.932711
C	4.170150	2.983895	-0.713490
H	5.044305	2.757851	-0.102207
H	4.483218	3.656667	-1.514701
H	3.469448	3.529840	-0.079967
C	5.463485	-0.151532	0.281415
H	5.898643	0.594108	-0.388142
H	5.428376	0.308112	1.273765
C	6.369986	-1.381790	0.321149
H	6.440739	-1.845242	-0.664692
H	7.381082	-1.128759	0.645886
H	5.974060	-2.132708	1.006666

B12Br11
E(electronic) = -28614.6841851000
E(zero-point) = 0.0648983746

B	1.479128	0.459309	-0.989911
B	-0.000184	-0.000113	-1.687820
B	-0.926863	-1.241139	-0.989727
B	0.000206	-0.000039	1.441677
B	0.913604	1.223428	0.519530
B	-0.881286	1.246952	0.519696
B	-1.466790	0.497785	-0.989718
B	0.893899	-1.264931	-0.989907
B	1.446094	-0.490857	0.519447
B	-0.019862	-1.526953	0.519584
B	-1.458221	-0.452844	0.519693
B	0.020183	1.548729	-0.989774
Br	3.085078	0.958076	-1.972849
Br	-1.933555	-2.588601	-1.972107
Br	0.000482	0.000056	3.394102
Br	1.963785	2.629829	1.367907
Br	-1.894151	2.680470	1.367997
Br	-3.059367	1.038304	-1.972431
Br	1.864435	-2.638296	-1.972754
Br	3.108469	-1.054817	1.367338
Br	-0.042715	-3.281993	1.368086
Br	-3.134421	-0.973213	1.368341
Br	0.041972	3.230280	-1.972597

H2O
E(electronic) = -76.4626145156
E(zero-point) = 0.0213879589

```
O       0.000000    0.000000    0.116775
H       0.000000    0.762889   -0.467102
H       0.000000   -0.762889   -0.467102


H2
E(electronic) =         -1.1801541784
E(zero-point) =          0.0100609279
H       0.000000    0.000000    0.371415
H       0.000000    0.000000   -0.371415


n-hexane
E(electronic) =       -237.1894628190
E(zero-point) =          0.1887842665
C       3.211333   -0.208327    0.000033
H       3.297182   -0.847935    0.880524
H       3.297208   -0.848010   -0.880400
H       4.062719    0.473254    0.000017
C       1.884556    0.549525   -0.000020
H       1.838026    1.205606    0.873756
H       1.838056    1.205537   -0.873848
C       0.666426   -0.373407   -0.000007
H       0.712665   -1.030764   -0.874194
H       0.712661   -1.030726    0.874207
C      -0.666426    0.373407   -0.000028
H      -0.712669    1.030754    0.874165
H      -0.712657    1.030735   -0.874236
C      -1.884556   -0.549525   -0.000030
H      -1.838064   -1.205533   -0.873862
H      -1.838018   -1.205610    0.873742
C      -3.211333    0.208327    0.000043
H      -3.297199    0.848042   -0.880368
H      -4.062719   -0.473254   -0.000009
H      -3.297191    0.847902    0.880555


2_4_Dimethylbutan.out
E(electronic) =       -237.1898264210
E(zero-point) =          0.1880734190
C       1.508587   -1.250910    0.053684
H       1.610237   -1.334673    1.138562
H       1.045730   -2.166063   -0.310263
H       2.513004   -1.200660   -0.367957
C       0.704205    0.000004   -0.318521
H       0.564985   -0.000003   -1.405984
C      -0.704199    0.000006    0.318540
H      -0.565043   -0.000017    1.406016
C       1.508580    1.250914    0.053673
```

```
H      2.512973    1.200712   -0.368037
H      1.045685    2.166078   -0.310209
H      1.610304    1.334653    1.138547
C     -1.508574   -1.250879   -0.053696
H     -1.045728   -2.166002    0.310334
H     -2.513020   -1.200601    0.367893
H     -1.610180   -1.334685   -1.138574
C     -1.508587    1.250862   -0.053681
H     -1.045772    2.166010    0.310333
H     -1.610213    1.334687   -1.138561
H     -2.513035    1.200580    0.367908
```

```
B12Br11_H_2_4_Dimethylbutan_A.out
E(electronic) =     -28851.9180939000
E(zero-point) =          0.2513726243
B     -1.306788    1.277267    0.209524
B      0.805904   -1.338323   -0.193347
B      0.279078    1.403172   -0.590107
B      0.201309    1.075452    1.108666
B     -1.147094    0.015589    1.454104
B     -1.913833   -0.348736   -0.115101
B     -1.030925    0.547608   -1.384467
B      0.656268   -0.075383   -1.434636
B     -0.708915   -1.185640   -1.129048
B     -0.780029   -1.513034    0.622999
B      0.533969   -0.602812    1.396109
B      1.467190    0.285349    0.127455
Br    -2.464129    2.841112    0.458484
Br     2.003220   -2.874970   -0.422242
Br     0.910390    3.266454   -1.032234
Br     0.775625    2.632671    2.266807
Br    -2.137159    0.130300    3.138859
Br    -3.829975   -0.703835   -0.258108
Br    -1.902858    1.264648   -2.983403
Br     1.596390   -0.125662   -3.159863
Br    -1.246174   -2.523674   -2.448463
Br    -1.388678   -3.227953    1.335376
Br     1.431580   -1.208514    3.036871
C      2.996682    0.624971    0.435078
H      3.071590    1.667852    0.752013
H      3.225577    0.049761    1.331528
H      0.967171    3.344143    0.740760
C      4.094412    0.366648   -0.617447
H      3.793672   -0.476780   -1.237912
C      4.279738    1.574924   -1.538175
H      4.577593    2.460528   -0.972998
H      5.048405    1.378447   -2.288328
H      3.361174    1.811951   -2.066348
C      5.443356   -0.036159    0.033690
H      6.174698   -0.060493   -0.781695
C      5.948089    0.974092    1.070610
H      6.019138    1.981891    0.661032
```

```
H      5.287271    1.010336    1.937673
H      6.940038    0.690912    1.427249
C      5.392384   -1.441594    0.638047
H      4.669484   -1.504700    1.451920
H      5.099293   -2.178890   -0.107935
H      6.368154   -1.724975    1.038524
```

```
B12Br11_H_2_4_Dimethylbutan_C.out
E(electronic) =     -28851.9139655000
E(zero-point) =          0.2546617771
B      1.236512   -1.443140    0.257948
B     -0.357833    1.444397   -0.526953
B      1.056170   -0.890202   -1.429580
B     -0.358008   -1.444411   -0.526748
B     -0.193077   -0.895345    1.161518
B      1.334784    0.000055    1.302760
B      2.114996   -0.000109   -0.303959
B      1.056280    0.889937   -1.429707
B      1.236663    1.443112    0.257737
B     -0.192984    0.895573    1.161372
B     -1.189650    0.000046    0.015807
B     -0.471093   -0.000057   -1.569342
Br     2.146531   -3.113115    0.714923
Br    -1.289816    3.129649   -0.948712
Br     1.755704   -1.921017   -2.946543
Br    -1.290009   -3.129738   -0.948150
Br    -0.987465   -1.906248    2.645615
Br     2.358737    0.000120    2.969055
Br     4.059851   -0.000227   -0.504538
Br     1.755904    1.920432   -2.946843
Br     2.146833    3.113066    0.714478
Br    -0.987259    1.906773    2.645338
Br    -3.185807    0.000655    0.425143
H     -1.092730   -0.000029   -2.569029
C     -4.399939    0.000094   -1.363923
C     -5.826966   -0.000152   -0.794456
H     -6.423004    0.000426   -1.716665
C     -4.027115    1.252403   -2.116153
H     -4.117067    2.153644   -1.522600
H     -3.012445    1.198643   -2.494333
H     -4.706212    1.324752   -2.971539
C     -4.026693   -1.252287   -2.115772
H     -3.012206   -1.198097   -2.494377
H     -4.115931   -2.153310   -1.521789
H     -4.706098   -1.325389   -2.970857
C     -6.208486    1.259471   -0.009220
H     -7.263914    1.213158    0.256874
H     -5.638912    1.341276    0.915771
H     -6.049849    2.169951   -0.581237
C     -6.208375   -1.260768   -0.010778
H     -6.051635   -2.170349   -0.584756
H     -5.637190   -1.344808    0.913022
```

```
H     -7.263286   -1.213930    0.257267


B12Br11_H_Neohexan_A.out
E(electronic) =     -28851.9214779000
E(zero-point) =          0.2509247805
B     -1.144272    1.408547   -0.287910
B      0.538109   -1.468650    0.318121
B      0.524819    1.104905   -0.830447
B      0.188304    1.265788    0.860135
B     -1.345234    0.522178    1.245041
B     -1.970019   -0.154419   -0.281796
B     -0.809010    0.242290   -1.581375
B      0.742774   -0.582126   -1.208754
B     -0.809866   -1.384944   -0.850620
B     -1.138179   -1.211254    0.894515
B      0.206002   -0.297757    1.611060
B      1.405477    0.080543    0.325594
Br    -2.042155    3.118663   -0.627778
Br     1.526461   -3.125678    0.677117
Br     1.549320    2.653203   -1.614296
Br     0.873841    2.994068    1.665026
Br    -2.495063    1.217867    2.668470
Br    -3.888598   -0.286456   -0.628701
Br    -1.361393    0.603542   -3.423737
Br     1.855216   -1.195451   -2.709845
Br    -1.400760   -2.952276   -1.857765
Br    -2.099139   -2.574797    1.912261
Br     0.802461   -0.532933    3.468677
C      2.931019    0.263512    0.745275
H      3.091829    1.307751    1.018595
H      3.055970   -0.296742    1.671848
H      1.383779    3.220008    0.083541
C      4.003320   -0.166137   -0.254313
H      3.847145   -1.211944   -0.516667
H      3.887800    0.394564   -1.183113
C      5.464404   -0.004168    0.221885
C      6.379920   -0.490787   -0.911470
H      7.432517   -0.402066   -0.633226
H      6.179165   -1.536470   -1.149327
H      6.219294    0.092962   -1.819704
C      5.784597    1.467629    0.520452
H      5.574515    2.094667   -0.348603
H      5.196925    1.844527    1.357263
H      6.839363    1.589729    0.776043
C      5.727974   -0.853305    1.473495
H      5.140801   -0.509402    2.324160
H      5.470130   -1.898005    1.293685
H      6.782127   -0.806831    1.755787


B12Br11_H_Neohexan_C_2.out
E(electronic) =     -28851.9288913000
```

E(zero-point) =   0.2548472477
B   0.515581   0.554317   1.182443
B   -1.328021   -0.542038   -1.438145
B   0.622471   1.307819   -0.433736
B   1.187192   -0.324609   -0.183264
B   0.138499   -1.176578   0.951354
B   -1.148141   -0.041248   1.397668
B   -0.851514   1.492264   0.544190
B   -0.957291   1.172263   -1.212331
B   -2.062208   0.347727   -0.082832
B   -1.447225   -1.304503   0.168754
B   0.025102   -1.478163   -0.811466
B   0.347331   0.049589   -1.687198
Br   1.643173   1.165108   2.671584
Br   -2.384458   -1.181512   -2.963584
Br   1.758771   2.886088   -0.788053
Br   3.095731   -1.080395   -0.120880
Br   0.828111   -2.545199   2.181496
Br   -1.981276   -0.098688   3.166622
Br   -1.347523   3.219459   1.320184
Br   -1.577521   2.536275   -2.481818
Br   -3.974668   0.753123   -0.030765
Br   -2.628310   -2.824547   0.515845
Br   0.588973   -3.195803   -1.595884
C   1.040906   0.083729   -3.107520
H   1.860356   -0.632786   -3.173169
H   0.319657   -0.176136   -3.881076
C   4.731009   0.219716   -0.594862
C   5.859615   -0.804719   -0.523367
H   5.672255   -1.599778   -1.245099
H   5.873273   -1.258142   0.467920
C   4.460456   0.746987   -1.980594
H   4.406539   -0.055834   -2.711931
H   3.549526   1.334259   -2.014865
H   5.286512   1.409518   -2.251202
C   4.764445   1.257073   0.497525
H   3.853407   1.844541   0.525630
H   4.927407   0.806004   1.473208
H   5.591738   1.938446   0.282128
H   1.426170   1.077304   -3.335122
C   7.232253   -0.179332   -0.807326
H   7.480075   0.594129   -0.082405
H   7.999040   -0.950568   -0.746794
H   7.277971   0.257372   -1.803682

B12Br11_nHexan_A_sek.out
E(electronic) =   -28851.9082295000
E(zero-point) =   0.2529262578
B   0.011015   -1.468648   -0.843939
B   0.469146   1.325083   0.863502
B   -1.245132   -0.198857   -0.781820
B   -0.862158   -1.137573   0.674713

```
B      0.898368   -1.446419    0.701115
B      1.609581   -0.695458   -0.752697
B      0.286113    0.085493   -1.668951
B     -0.413500    1.331416   -0.625571
B      1.353601    1.044924   -0.642454
B      1.729920    0.114971    0.829520
B      0.190999   -0.162031    1.715513
B     -1.175458    0.625061    0.833218
Br    -0.258168   -3.123064   -1.849666
Br     0.809859    3.186136    1.625237
Br    -2.881038   -0.443933   -1.849037
Br    -2.129997   -2.432786    1.428575
Br     1.653372   -3.065810    1.492770
Br     3.184052   -1.432866   -1.644247
Br     0.325020    0.282994   -3.615446
Br    -1.042953    3.143627   -1.220639
Br     2.605551    2.359918   -1.387418
Br     3.418654    0.381907    1.785952
Br     0.178384   -0.283054    3.677676
C     -2.460670    1.153816    1.659054
H     -2.726379    0.281729    2.260976
C     -2.205970    2.283597    2.669048
H     -1.361786    2.084082    3.323139
H     -2.043181    3.238752    2.169365
H     -3.090387    2.401930    3.299429
C     -3.717594    1.514570    0.822343
H     -4.103186    2.478962    1.165810
H     -3.474046    1.655504   -0.226916
C     -4.835106    0.480139    0.936134
H     -5.141082    0.395991    1.984715
H     -4.449416   -0.499270    0.652900
C     -6.049409    0.812494    0.073281
H     -6.445131    1.792290    0.359781
H     -5.725607    0.904630   -0.966367
C     -7.154471   -0.238406    0.171432
H     -8.011456    0.015444   -0.455114
H     -6.785922   -1.215411   -0.145300
H     -7.510380   -0.339467    1.199080
H     -0.050936    3.620397    0.348479


B12Br11_nHexan_C.out
E(electronic) =     -28851.9267693000
E(zero-point) =          0.2559059831
B      0.899141   -0.411510    0.706793
B     -1.897734    0.391362   -1.027873
B      0.899834    0.503603   -0.789500
B      0.493638   -1.187564   -0.853725
B     -0.480681   -1.522699    0.595685
B     -0.625058   -0.011012    1.530940
B      0.262121    1.256455    0.663852
B     -0.530833    1.496761   -0.925005
B     -1.504170    1.176373    0.525558
```

B	-1.966409	-0.544544	0.484892
B	-1.267250	-1.262441	-0.989452
B	-0.376999	-0.004840	-1.888123
Br	2.551977	-0.839921	1.683379
Br	-3.509024	0.864243	-2.042064
Br	2.592546	1.422828	-1.499978
Br	1.622080	-2.594067	-1.663657
Br	-0.438973	-3.276403	1.462552
Br	-0.746612	-0.007426	3.483040
Br	1.210493	2.724927	1.560496
Br	-0.482362	3.246194	-1.830010
Br	-2.643861	2.555842	1.314619
Br	-3.659834	-1.172676	1.233611
Br	-2.141744	-2.724056	-1.964823
C	-0.232057	0.006408	-3.462098
H	0.087224	-0.967314	-3.832650
H	-1.188849	0.242115	-3.926122
H	0.484552	0.757395	-3.798736
C	3.797352	0.030419	-2.355797
H	4.344166	0.666554	-3.045763
H	3.096227	-0.612678	-2.871849
C	4.656453	-0.680685	-1.348402
H	4.026931	-1.288190	-0.703134
H	5.256255	-1.382752	-1.941831
C	5.569354	0.208432	-0.511504
H	6.198456	0.825541	-1.162090
H	4.955325	0.892623	0.076776
C	6.447300	-0.601259	0.441053
H	7.081918	-1.280778	-0.135275
H	5.802452	-1.230026	1.058347
C	7.313329	0.280822	1.337687
H	6.693192	0.936613	1.950351
H	7.929740	-0.317572	2.009199
H	7.979980	0.911951	0.746178

Neohexan.out

E(electronic) = -237.1917278860

E(zero-point) = 0.1877701946

C	-0.518646	-0.881298	-1.254867
H	-0.438766	-0.279066	-2.161777
H	0.273351	-1.629448	-1.276772
H	-1.472131	-1.410674	-1.288525
C	-0.434611	-0.000295	0.000008
C	-1.617884	0.978704	0.000750
H	-1.594861	1.620010	0.883561
H	-1.594606	1.621651	-0.880862
H	-2.568636	0.443217	0.000113
C	-0.518911	-0.883531	1.253293
H	0.272922	-1.631888	1.273901
H	-0.438964	-0.282953	2.161294
H	-1.472511	-1.412761	1.285935
C	0.870293	0.827641	0.000846

```
H      0.853245    1.486081   -0.872136
H      0.853244    1.484378    0.875112
C      2.179154    0.037398    0.000063
H      2.269445   -0.597526   -0.881111
H      3.032312    0.716279    0.000564
H      2.269590   -0.599012    0.880146
```

```
nHexan.out
E(electronic) =       -237.1894378780
E(zero-point) =          0.1886977816
C      3.211341   -0.208343    0.000037
H      3.297110   -0.847962    0.880537
H      3.297127   -0.848112   -0.880352
H      4.062869    0.473054   -0.000013
C      1.884656    0.549591   -0.000041
H      1.838078    1.205664    0.873732
H      1.838099    1.205520   -0.873923
C      0.666449   -0.373331    0.000018
H      0.712833   -1.030657   -0.874180
H      0.712839   -1.030550    0.874294
C     -0.666449    0.373331   -0.000018
H     -0.712860    1.030602    0.874219
H     -0.712813    1.030606   -0.874255
C     -1.884656   -0.549591   -0.000061
H     -1.838115   -1.205511   -0.873949
H     -1.838061   -1.205672    0.873707
C     -3.211341    0.208343    0.000054
H     -3.297099    0.848202   -0.880274
H     -4.062869   -0.473053   -0.000097
H     -3.297138    0.847872    0.880615
```