Supporting information

Terpene Dispersion Energy Donor Ligands in Borane Complexes

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Abstract: Structural characterization of the complex [B(β-pinane)$_3$] (**1**) reveals non-covalent H···H approaches that are consistent with the generation of London dispersion energies involving the b-pinane ligand frameworks. The homolytic fragmentations of **1**, and camphane and sabinane analogues ([B(camphane)$_3$] (**2**) and [B(sabinane)$_3$] (**3**)) were studied computationally. Isodesmic exchange results showed that London dispersion interactions are highly dependent on the terpene's stereochemistry, with the pinane framework providing the greatest dispersion free energy (ΔG = -7.9 kcal mol^{-1}) with dispersion correction (GD3BJ) employed. PMe_3 was used to coordinate to [B(β-pinane)$_3$], giving the complex [Me_3P–B(b-pinane)$_3$], which displayed a dynamic coordination-equilibrium in solution. The association process was found to be slightly endergonic at 302 K (ΔG = +0.29 kcal mol^{-1}).

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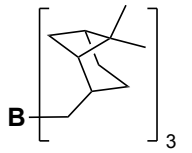
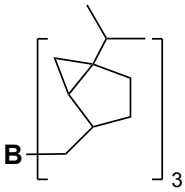
S1. Experimental Procedures

All manipulations were carried out using standard Schlenk-line and glovebox techniques under an inert atmosphere of argon or dinitrogen. A Vacuum Atmospheres OMNI-Lab glovebox was employed, operating at <0.1 ppm O_2 and <0.1 ppm H_2O. Solvents were dried over activated alumina from an SPS (solvent purification system) based upon the Grubbs design and degassed before use. Glassware was dried in an oven overnight at 120 °C prior to use. NMR solvents including C_6D_6 and PhMe-D_8 were dried over 3 Å molecular sieves and were freeze-pump thaw degassed thrice prior to use. [BH_3•THF][1] and complex 1, [B(b-pinane)$_3$][2] were synthesized by a modified literature procedure. b-pinene, camphene and sabinene were procured from Oakwood Chemicals and were purified by distillation before use. NMR spectra (^{1}H, ^{11}B, ^{13}C, ^{31}P and VT-NMR) were recorded on either a 400 MHz Bruker Nanobay AVIIIHD or a 500 MHz Bruker Avance DRX spectrometers and values were recorded in ppm. Data were processed using MNova/Bruker TopSpin software.

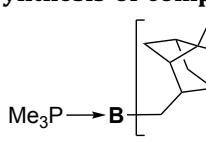
Synthesis of complex 1, [B(β-pinane)$_3$]: In a J-Young's ampoule attached to a Schlenk line, b-pinene (1.15 mL, 21.1 mmol) was dissolved in THF and cooled to -78 °C. BH_3•THF (7.3 mL, 7.33 mmol) was added dropwise to the cooled mixture. The resulting mixture was allowed to warm to room temperature and stirred for 12 hours. After this time, all volatiles were removed yielding a white solid. The solid was taken up in warm hexane, filtered, and the filtrate cooled to -30 °C yielding the product (1) as colorless crystalline blocks, suitable for single crystal X-ray diffraction. Yield = 2.84 g (91%). All spectra match with those previously reported. ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ (ppm): 2.64–2.61 (m, 1H), 2.39–2.36 (m, 1H), 2.11–2.06 (m, 1H), 2.01–1.06 (m, 1H), 1.93–1.86 (m, 2H), 1.80–1.78 (m, 1H), 1.64–1.60 (m, 1H), 1.52–1.42 (m, 2H), 1.23 (s, 3H), 1.16 (s, 3H), 0.97 (d, J_{HH} = 9.5 Hz, 1H). ^{13}C{^{1}H} NMR δ (ppm): 49.6, 41.7, 39.0, 38.9, 34.8, 28.6, 27.2, 25.7, 23.6. ^{11}B NMR (160 MHz, PhMe-D_8) δ (ppm): 89.2.



Synthesis of complex 2, [B(camphane)$_3$]: In a J-Young's ampoule attached to a Schlenk line, camphene (3.00 g, 22.0 mmol) was dissolved in THF and cooled to -78 °C. BH_3•THF (7.3 mL, 7.34 mmol) was added dropwise to the cooled mixture. The resulting mixture was allowed to warm to room temperature and stirred for 12 hours. After this time, all volatiles were removed yielding a colorless gel (2.37 g, yield based 2 = 85%). The gel remained despite many rounds of tituration in hexane. ^{1}H, ^{13}C NMR spectroscopy indicated a mixture of products. ^{11}B NMR showed some formation of the tri-substituted borane (2) with a chemical shift of δ = 87.8 ppm in PhMe-D_8 at 298 K.



Synthesis of complex 3, [B(sabinane)$_3$]: In a J-Young's ampoule attached to a Schlenk line, sabinene (3.00, 22.0 mmol) was dissolved in THF and cooled to -78 °C. BH_3•THF (7.3 mL, 7.33 mmol) was added dropwise to the cooled mixture. The resulting mixture was allowed to warm to room temperature and stirred for 12 hours. After this time, all volatiles were removed yielding a colorless oil (2.12 g, yield based on 3 = 68%). The oil remained despite many rounds of tituration in hexane. ^{1}H, ^{13}C NMR spectroscopy indicated a mixture of products. ^{11}B NMR showed some formation of the tri-substituted borane (3) with a chemical shift of δ = 87.5 ppm in PhMe-D_8 at 298 K.



Synthesis of complex 4, [Me_3P–B(β-pinane)$_3$]: In a J-Young's ampoule attached to a Schlenk line, [B(β-pinane)$_3$] (200 mg, 0.47 mmol) was dissolved in toluene. PMe_3 (0.03 mL, 0.47 mmol) was added to the cooled mixture. The resulting mixture was stirred for 12 hours and all volatiles removed yielding a white solid. The solid was taken up in warm pentane, filtered, and the filtrate cooled to -30 °C yielding the product (4) as colorless crystalline blocks, suitable for single crystal X-ray diffraction. Yield = 152 mg (0.30 mmol, 64%). ^{1}H NMR (400 MHz, PhMe-D_8, 298 K) δ (ppm): 2.37–2.32 (m, 1H), 2.18–2.19 (m, 2H), 2.06–2.01 (m, 1H), 1.94–1.86 (m, 3H), 1.61–1.54 (m, 1H), 1.27 (s, 3H), 1.21 (s, 3H), 0.97 (d, J_{H-H} = 9.3 Hz, 1H), 0.79 (d, $^2J_{PH}$ = 3.4 Hz, 3H, coordinated PMe_3), 0.78 (s, 3H, uncoordinated PMe_3). ^{13}C{^{1}H} NMR: δ (ppm) 51.3, 42.5, 41.0, 39.5, 34.6, 29.2, 28.1, 28.0, 24.4, (d, $^1J_{CP}$ = 4.9 Hz, 15.5). ^{11}B NMR (160 MHz, PhMe-D_8, 209 K)δ (ppm): -14.5. ^{31}P NMR (500 MHz, PhMe-D_8)δ (ppm): -9.5. Melting point: 80–82 °C.

S2. NMR Spectra

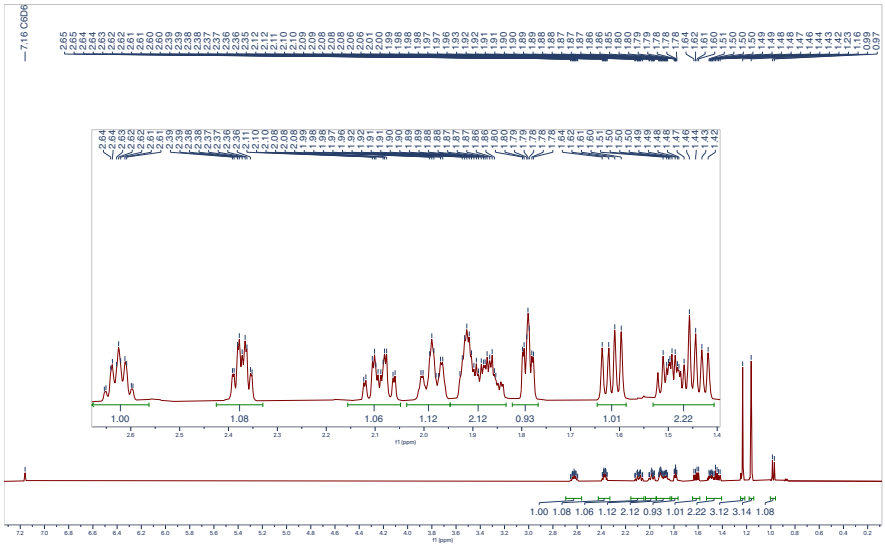


Fig S1. ^{1}H NMR spectrum of complex **1** in C_6D_6 at 298 K.

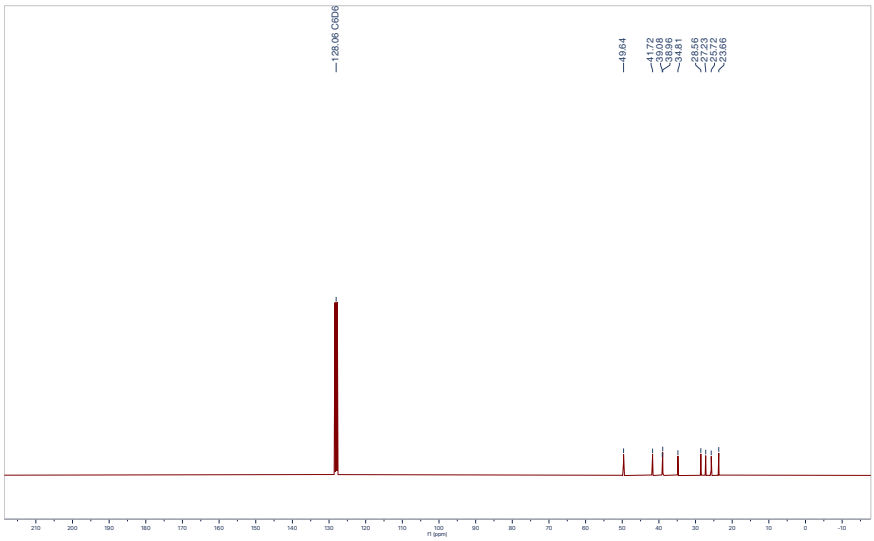


Fig S2. $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** in C_6D_6 at 298 K.

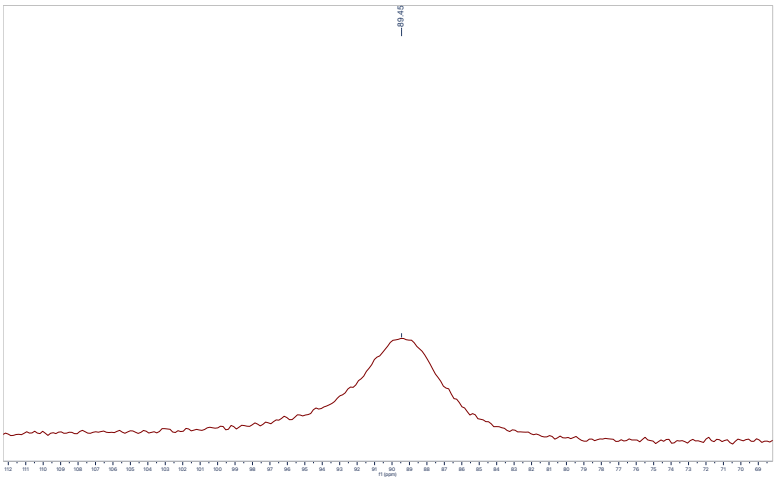


Fig S3. ^{11}B NMR spectrum of complex **1** in C_6D_6 at 298 K.

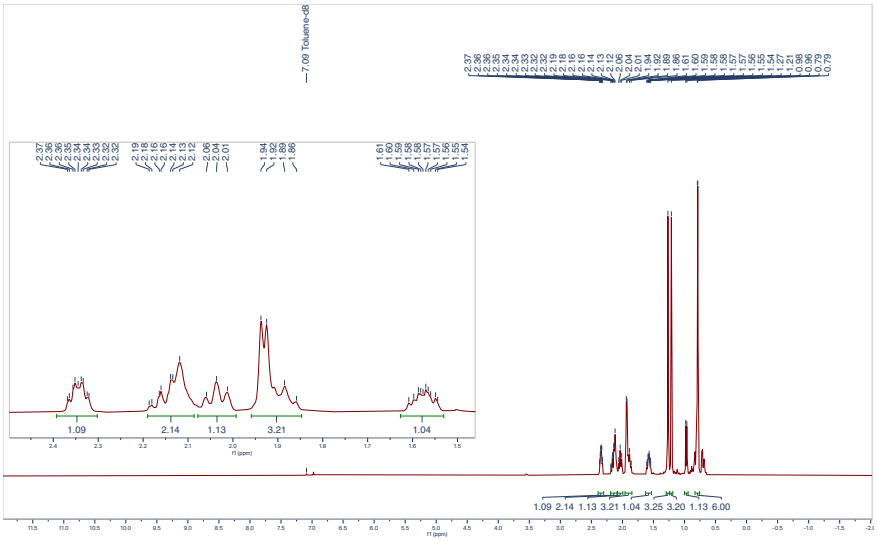


Fig S4. ^{1}H NMR spectrum of complex **4** in PhMe-D_8 at 298 K.

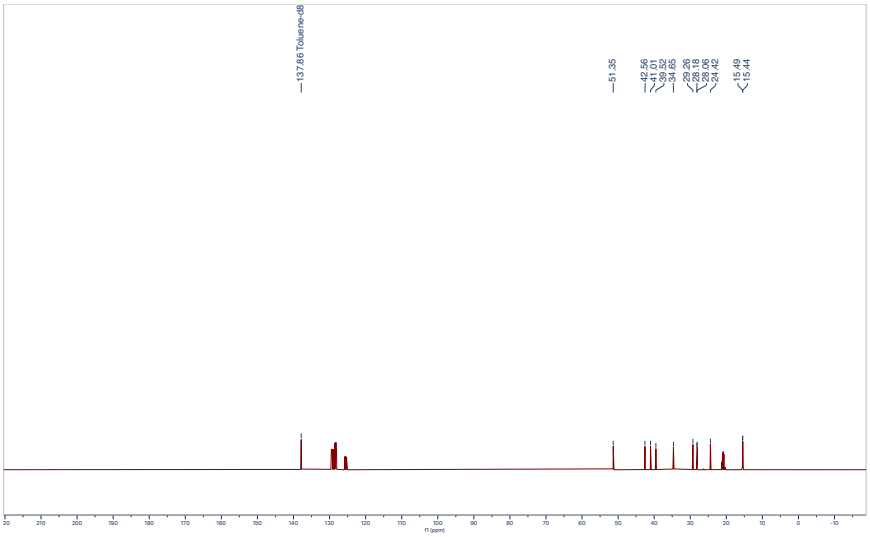


Fig S5. $^{13}C\{^{1}H\}$ NMR spectrum of complex **4** in PhMe-D_8 at 298 K.

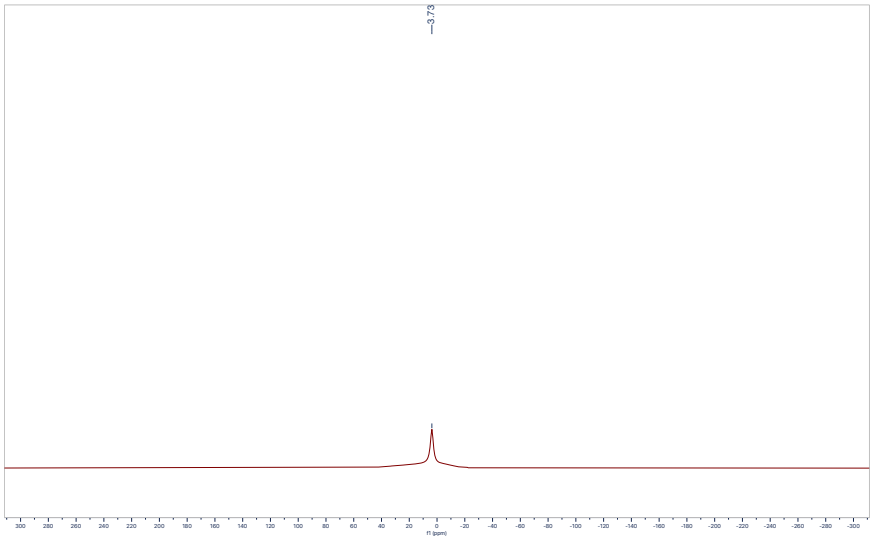


Fig S6. ^{11}B NMR spectrum of complex **4** in PhMe-D_8 at 313 K.

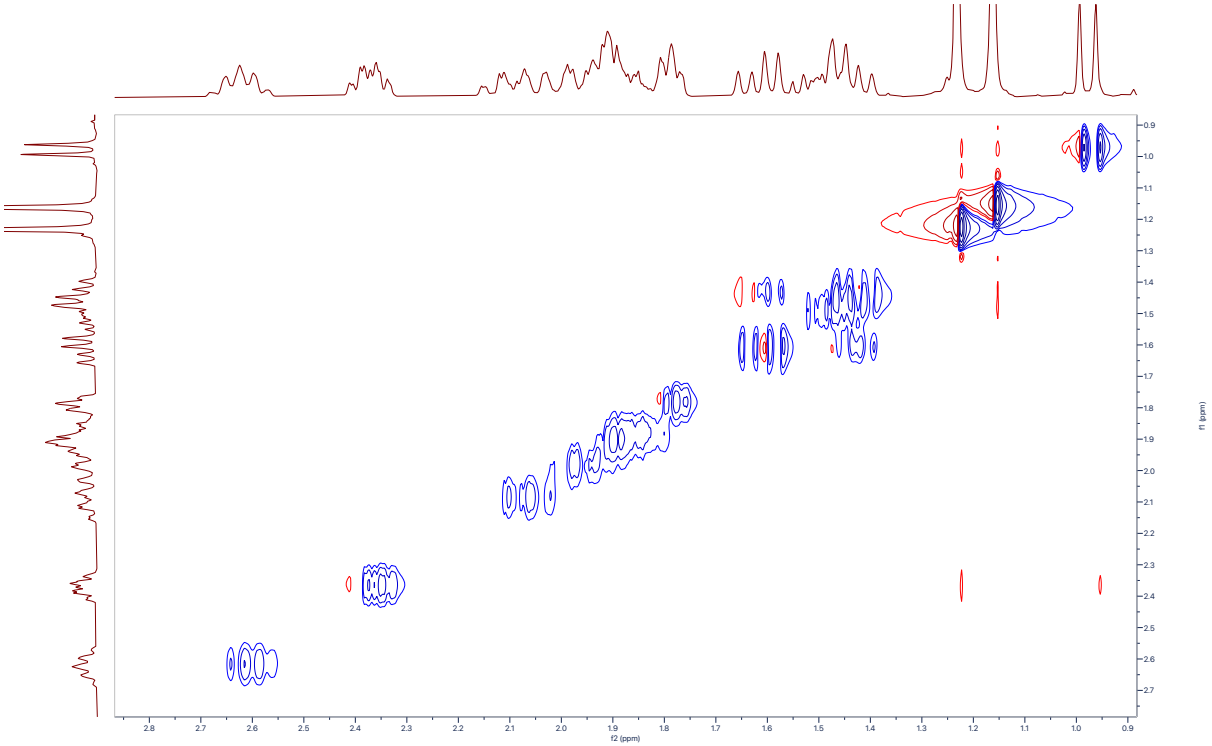


Fig S7. NOESY NMR spectrum of complex **1** in C_6D_6 at 298 K.

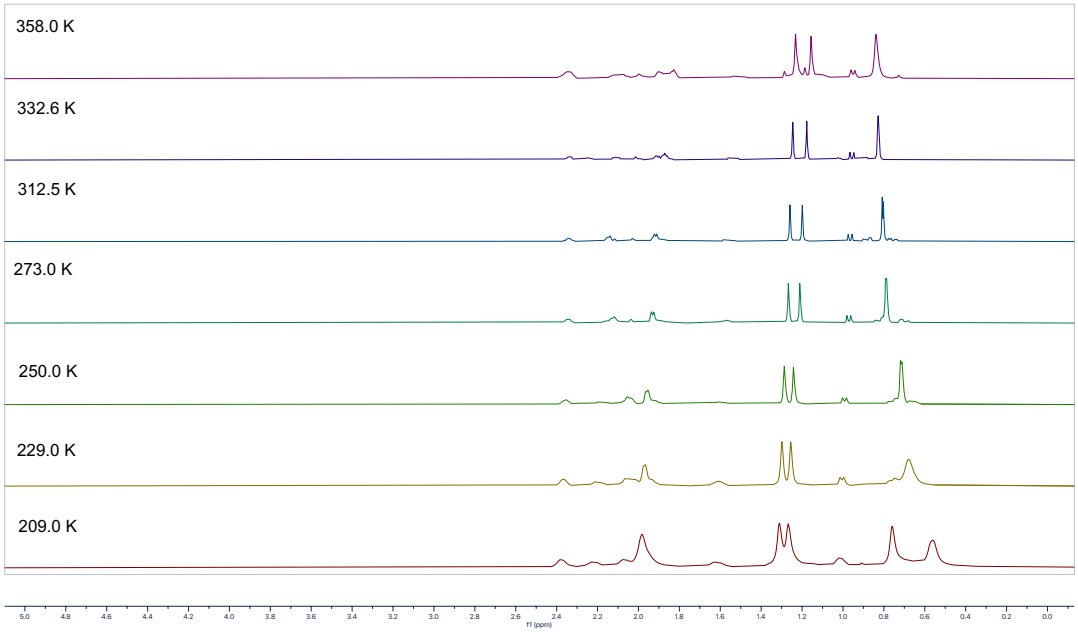


Fig S8. Variable temperature ^{1}H NMR spectra of complex **4** in PhMe-D_8.

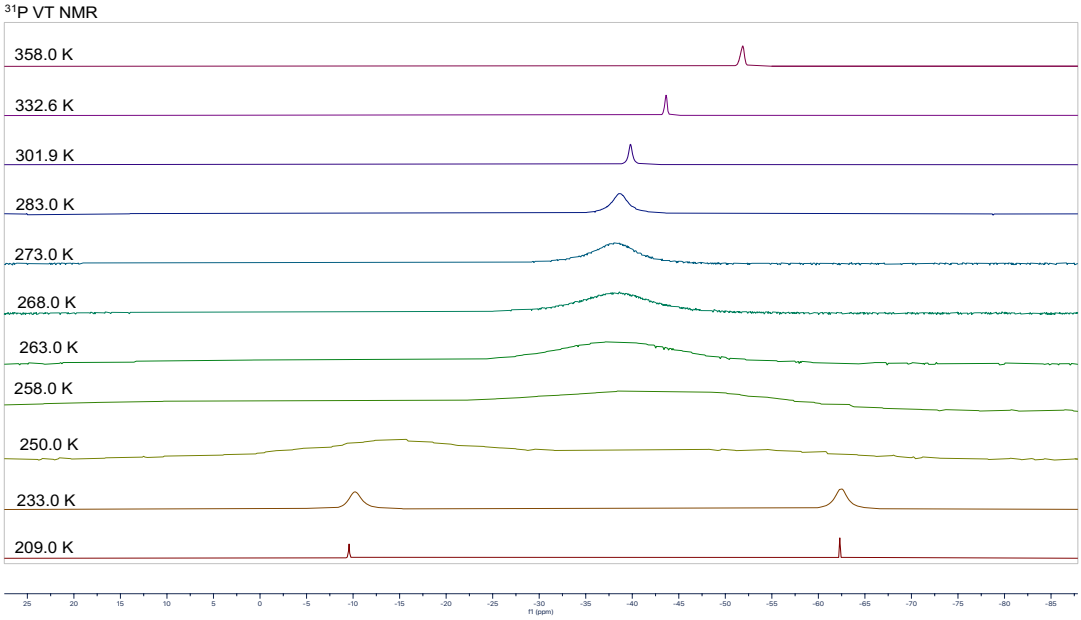


Fig S9. Variable temperature ^{31}P NMR spectra of complex **4** in PhMe-D_8.[3]

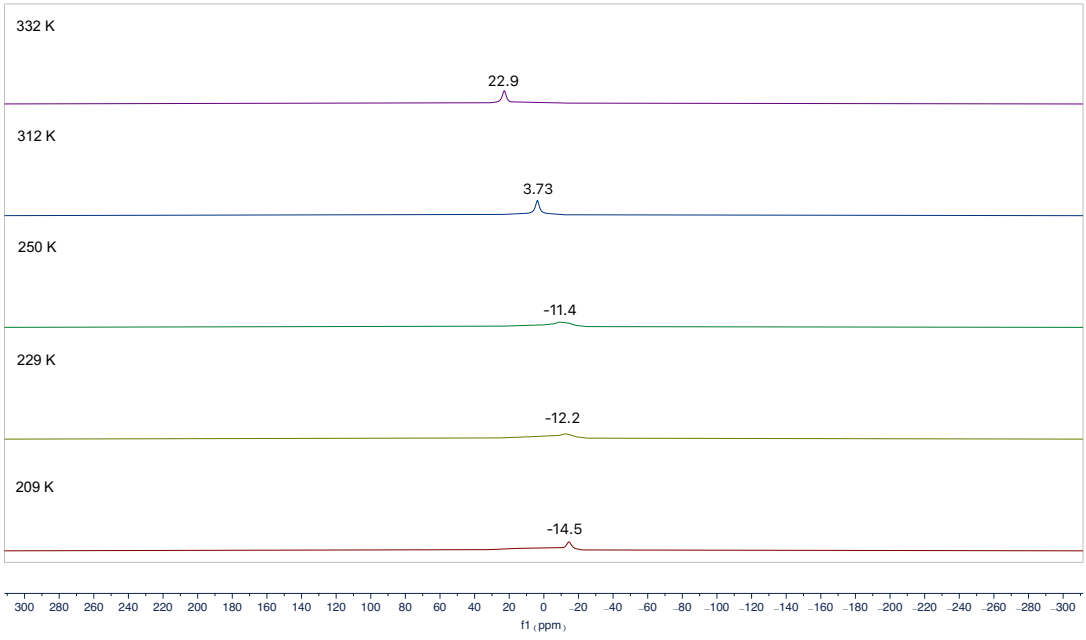


Fig S10. Variable temperature ^{11}B NMR spectra of complex **4** in PhMe-D_8.

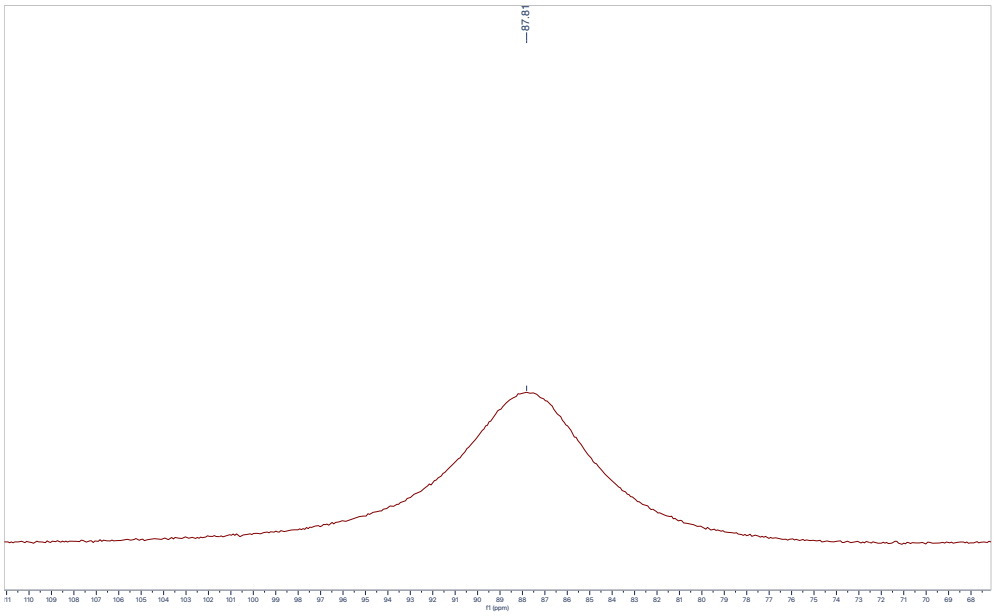


Fig S11. ^{11}B NMR spectrum of complex **2** in PhMe-D_8 at 298 K.

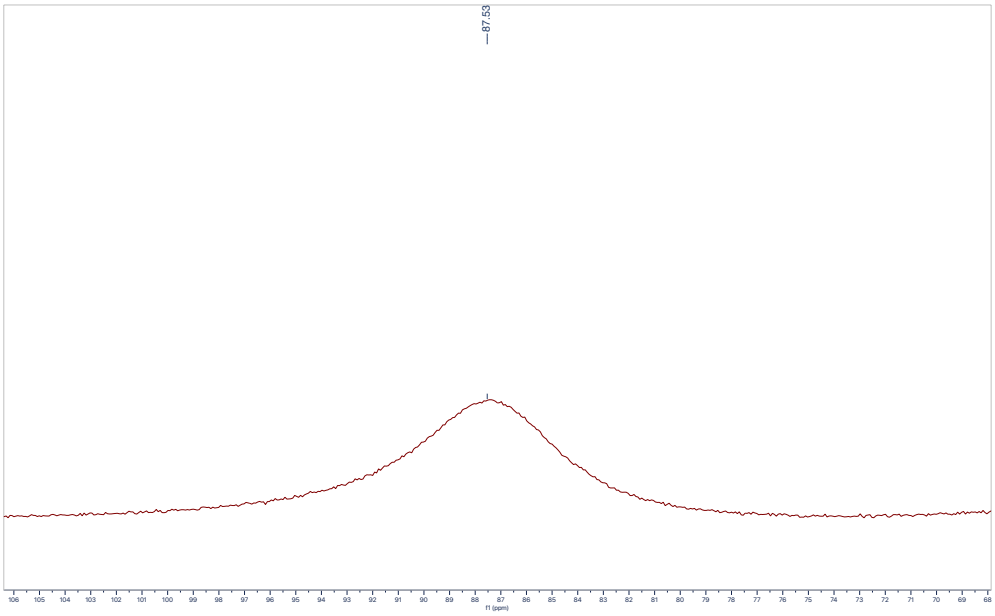


Fig S12. ^{11}B NMR spectrum of complex **3** in PhMe-D_8 at 298 K.

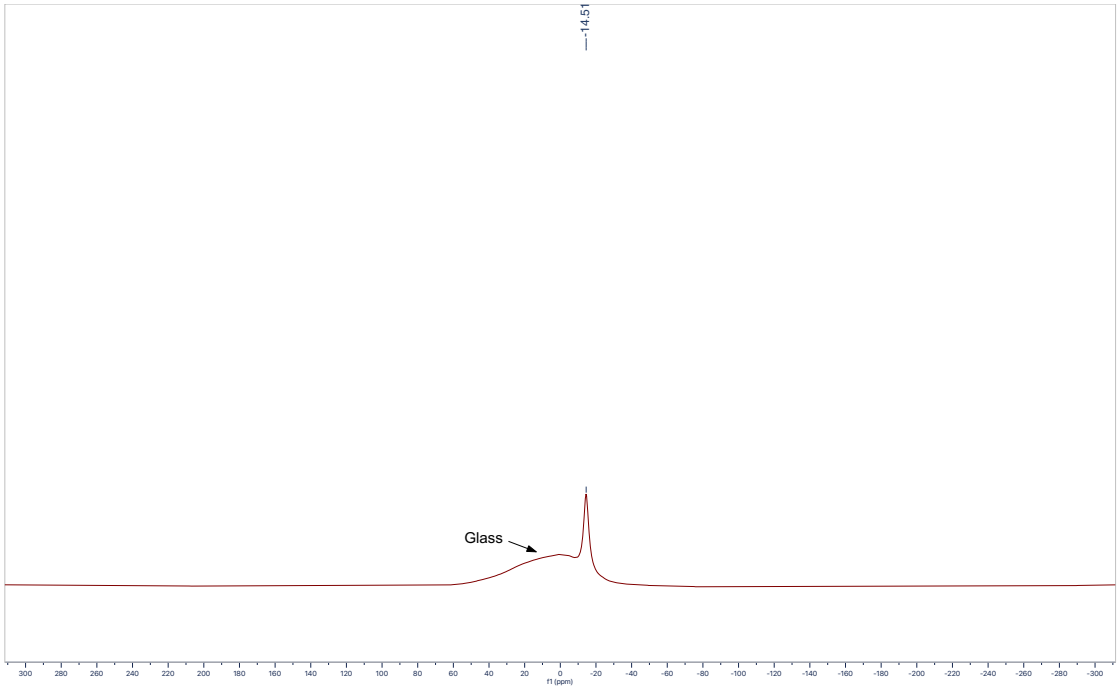
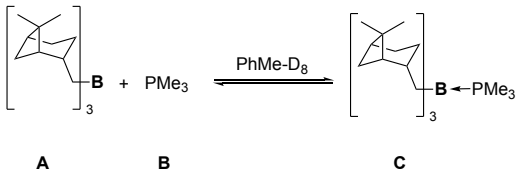


Fig S13. ^{11}B NMR spectrum of complex **4** in PhMe-D_8 at 209 K.

S3. Van't Hoff Analysis

Using variable temperature ^{31}P NMR spectra to calculation the thermodynamic parameters of the following equilibrium:



The equilibrium constant (K_{eq}) was calculated according to **Equation 1**:

$$K_{eq} = \frac{[\mathbf{C}]}{[\mathbf{A}]\ [\mathbf{B}]}$$

The concentrations of the species for broad peaks were calculated according to their relative populated states using **Equation 2:**

$$\delta_{obs} = \delta_{\mathbf{B}} P_{\mathbf{B}} + \delta_{\mathbf{C}}(1 - P_{\mathbf{B}})$$

A Van't Hoff plot of Ln(K_{eq}) against 1/T was constructed for the above reaction. ΔS and ΔH were calculated using the gradient and intercept of the plot according to **equation 3**:

$$\ln(K_{eq}) = \frac{-\Delta H}{R} \cdot \frac{1}{T} + \frac{\Delta S}{R}$$

$$y = m \cdot x + c$$

The free energy ΔG was then calculated using **equation 4:**

$$\Delta G = \Delta H - T\Delta S$$

Table S1. Calculated concentrations, equilibrium constants and natural logs used for Fig S9.

Temperature (K)	$P_{[C]}$	$P_{[B]}$	K_{eq}	$\ln(K_{eq})$	1/T
209.0	2.32E+09	1.71E+09	1.361	0.308	4.78E-03
233.0	3.41E+09	2.17E+09	1.572	0.452	4.29E-03
250.0	4.66E+09	5.08E+09	0.916	-0.086	3.95E-03
258.0		9.36E+09[a]	0.982	-0.018	3.86E-03
263.0		7.44E+09[a]	0.896	-0.109	3.80E-03
268.0		8.02E+09[a]	0.859	-0.152	3.73E-03
273.0		4.21E+09[a]	0.860	-0.150	3.66E-03
283.0		2.23E+09[a]	0.813	-0.206	3.53E-03
301.9		5.44E+09[a]	0.745	-0.294	3.31E-03
332.6		3.72E+09[a]	0.548	-0.601	3.01E-03
358.0		2.72E+09[a]	0.248	-1.394	2.79E-03

[a] **Equation 2** used for these data points to determine relative populations of **B** and C, where δ_B = -62.3 ppm, δ_C = -9.5 ppm.[8]

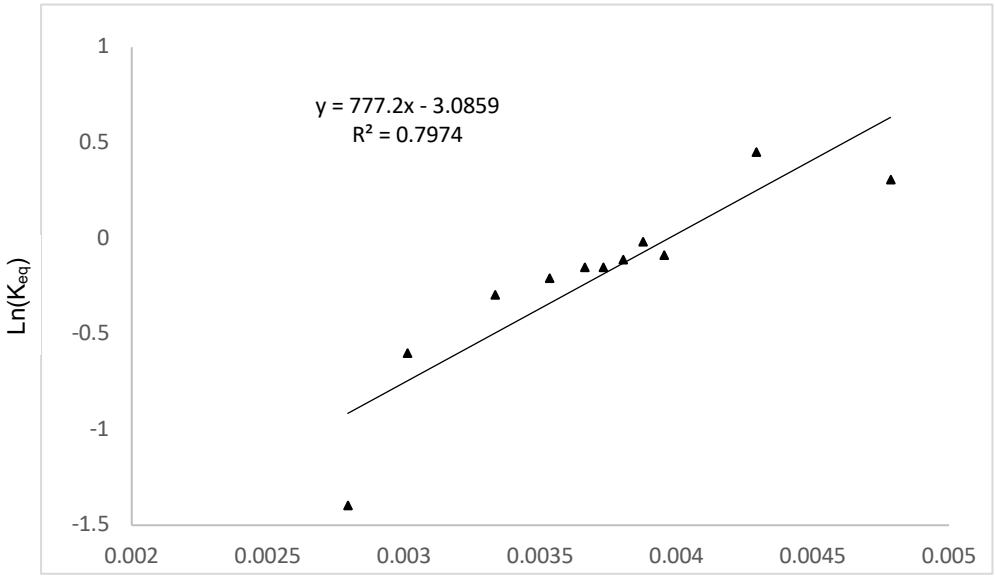


Fig S14. Van't Hoff plot of $\ln(K_{eq})$ against 1/T.

Table S2. Calculated thermodynamic parameters of the association reaction of complex **4**.

Gradient = 777.2	ΔS (kJ mol^{-1} K^{-1})	ΔS (kcal mol^{-1} K^{-1})	ΔH (kJ mol^{-1})	ΔH (kcal mol^{-1})
Intercept = -3.0859	-25.66E-03	-6.14E-03	-6.466	-1.55

Table S3. Temperature dependence on free energy (ΔG) used to make **Fig 7** in main text.

Temperature (K)	ΔG
209.0	-0.267
233.0	-0.119
250.0	-0.015
258.0	0.003
263.0	0.034
268.0	0.065
273.0	0.096
283.0	0.126
301.9	0.188
332.6	0.292
358.0	0.372

Estimate of Error: The uncertainty in the integration was estimated to be 10% due to broadening. The VT apparatus indicated an uncertainty in the temperature of 1 °C.

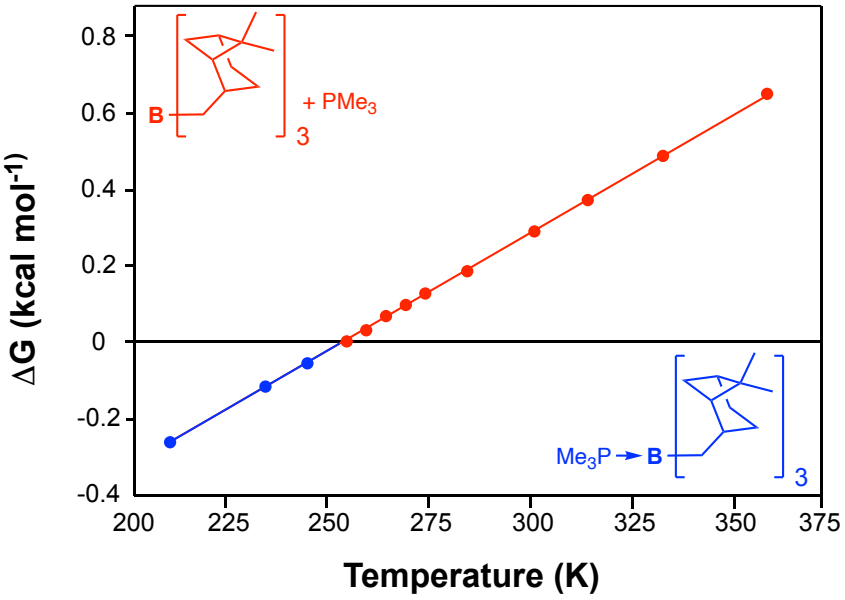


Figure S15. Plot of free energy (kcal mol^{-1}) of association against temperature (K) for the formation of [Me_3P–B(β-pinane)$_3$].

S4. Crystallographic Details

Complex	[B(β-pinane)$_3$] (1)	[Me$_3$P–B(β-pinane)$_3$] (4)
Chemical Formula	$C_{30}H_{51}B$	$C_{33}H_{60}BP$
F.w. (g mol^{-1})	422.55	498.63
Crystal System	Trigonal	Trigonal
a (Å)	16.8436(6)	18.5902(2)
b (Å)	16.8436(6)	18.5902(2)
c (Å)	8.0192(4)	7.7698(9)
a (°)	90	90
b (°)	90	90
g (°)	120	120
V (Å^3)	1970.30(17)	2325.5(6)
Z	3	3
$F_{calc'd}$ (g cm^{-3})	1.068	1.068
μ (mm^{-1})	0.058	0.108
Reflns. collected	10930	5548
Uniq. Reflns.	2414	2144
R_{int}	0.0230	0.0195
R_1 and $wR_{2\ [I>=2s\ (I)]]}$	0.0302, 0.0823	0.0251, 0.0608
R_1 and $wR_{2\ [all\ data]}$	0.0309, 0.0827	0.0258, 0.0614
CCDC Number	2180015	2180016

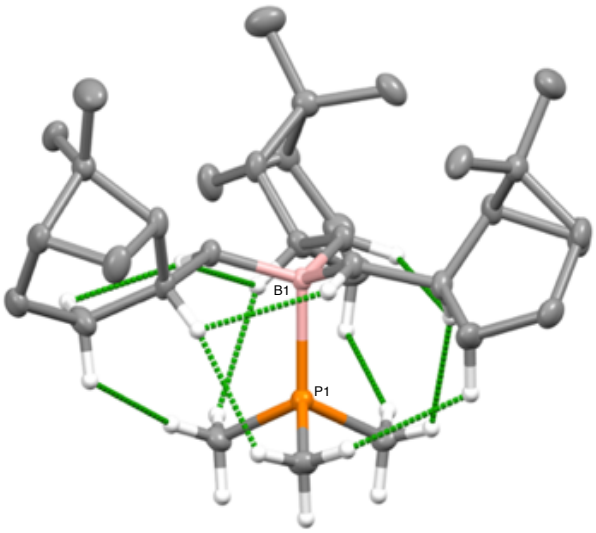
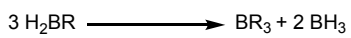


Figure S16. Molecular structure of complex [Me$_3$P–B(b-pinane)$_3$] with inter-ligand H···H close contacts shown in green.

S5. Computational Methods

The geometry optimizations of compounds **1**-**4** were performed with Gaussian16 (Revision C.01) program[4] using the PBE1PBE hybrid exchange functional[5a–c] and Def2-TZVP basis sets.[6a,b] In addition, Grimme's empirical dispersion correction with Becke-Johnson damping (D3BJ)[7] was used as well as an ultrafine integration grid. Full analytical frequency calculations were performed for the optimized structures to ensure the nature of the stationary points found (minima, no imaginary frequencies). For species **2** and **3**, 3 and 4 different organic ligand orientations respectively were considered to find the global minimum conformation. Here we report only the energetically most favoured structures: for **2**, the reported structure is at least 6.3 kcal/mol (Gibbs free energy) more stable than the other conformers and for **3** the value is 2.5 kcal/mol. The three structures **1**-**3** along with the species BH_3 and H_2BR (R = pinane, camphane or sabinane) were optimized with and without dispersion correction to calculate the isodesmic exchange reaction and evaluate the effects of stabilizing dispersion effects brought about by the organic substituents. Finally, the association reaction of **1** + PMe_3 to form **4** was calculated at the same level of theory (results are given in the gas phase and at 298 K).

Table S4. Calculated ΔE reaction energies of the heterolytic cleavage of a terpane ligand from H_2B(terpane) (terpane = β-pinane, camphane, sabinane) to form B(terpane)$_3$ using PBE1PBE/Def2-TZVP basis set with and without Grimme's dispersion correction (D3BJ) applied (kcal mol^{-1}).



	[B(β-pinane)$_3$]	[B(camphane)$_3$]	[B(sabinane)$_3$]
ΔE	7.618	7.799	7.649
$\Delta E_{(D3BJ)}$	-3.056	1.055	1.122
ΔG	9.791	10.320	10.571
$\Delta G_{(D3BJ)}$	1.415	3.715	5.201

Optimized xyz-coordinates

1 (with dispersion)

82

C	-1.57095	-0.14444	-2.06808
H	-2.08357	0.79685	-1.85347
H	-1.75073	-0.32048	-3.14421
C	-2.22978	-1.28285	-1.28957
H	-1.72945	-2.21152	-1.58635
C	-3.73463	-1.43285	-1.62237
H	-4.06619	-0.51161	-2.10597
H	-3.85833	-2.21027	-2.38012
C	-4.65928	-1.72599	-0.41789
H	-5.52658	-1.05987	-0.45274
H	-5.05510	-2.74433	-0.48240
C	-3.95072	-1.58464	0.92110
H	-4.63998	-1.74781	1.75494
C	-2.65657	-2.41420	0.87080
H	-2.68092	-3.32584	0.26783
H	-2.25294	-2.65390	1.85332
C	-2.01132	-1.17731	0.21674
H	-0.95989	-0.97167	0.44125
C	-3.06647	-0.30967	0.97083
C	-2.59282	-0.00289	2.38612
H	-3.41757	0.39133	2.98721
H	-1.80534	0.75613	2.36577
H	-2.19413	-0.87688	2.90241
C	-3.61245	0.97593	0.37777
H	-4.01027	0.85913	-0.62792
H	-2.83968	1.74758	0.34563
H	-4.42127	1.35586	1.01025
B	-0.00149	-0.00280	-1.98528
C	0.90562	-1.29141	-2.06755

H	0.34717	-2.20535	-1.84916
H	1.14483	-1.36181	-3.14422
C	2.22311	-1.29135	-1.29290
H	2.77691	-0.39507	-1.59431
C	3.10332	-2.52143	-1.62442
H	2.46904	-3.27036	-2.10324
H	3.83615	-2.24315	-2.38561
C	3.82293	-3.17195	-0.42004
H	3.67908	-4.25616	-0.45087
H	4.90262	-3.00633	-0.48853
C	3.35082	-2.62419	0.91869
H	3.83915	-3.13709	1.75263
C	3.42308	-1.08891	0.86303
H	4.22314	-0.65671	0.25611
H	3.43233	-0.61632	1.84400
C	2.02716	-1.14978	0.21354
H	1.32441	-0.34098	0.43753
C	1.80486	-2.49446	0.97321
C	1.30738	-2.23206	2.38928
H	1.37975	-3.14126	2.99348
H	0.25645	-1.92890	2.37147
H	1.86720	-1.44829	2.90084
C	0.96141	-3.61167	0.38730
H	1.25758	-3.90181	-0.61838
H	-0.09313	-3.32762	0.35795
H	1.03841	-4.49981	1.02281
C	0.66083	1.42713	-2.06806
H	1.73203	1.40020	-1.85204
H	0.59969	1.67025	-3.14441
C	0.00381	2.56759	-1.29108
H	-1.05052	2.59775	-1.58824
C	0.62609	3.94558	-1.62556
H	1.59010	3.77168	-2.10823
H	0.01498	4.44013	-2.38441
C	0.83358	4.89475	-0.42232
H	1.84396	5.31314	-0.45721
H	0.14928	5.74636	-0.48838
C	0.60135	4.21221	0.91754
H	0.80402	4.89193	1.75055
C	-0.76371	3.50540	0.86764
H	-1.54108	3.98108	0.26377
H	-1.17337	3.27682	1.85030
C	-0.01422	2.32768	0.21543
H	-0.36123	1.31441	0.44126
C	1.26415	2.80948	0.96926
C	1.29301	2.24763	2.38528
H	2.04629	2.76602	2.98593
H	1.55740	1.18632	2.36623
H	0.33662	2.33915	2.90133
C	2.65100	2.63962	0.37712
H	2.74886	3.04002	-0.62959
H	2.93415	1.58483	0.34791
H	3.38356	3.15258	1.00864

1 (without dispersion)

82

C	-1.45626	0.61178	-1.61709
H	-1.51548	1.57207	-1.09460
H	-1.52862	0.89749	-2.68350
C	-2.66670	-0.25103	-1.26318
H	-2.52891	-1.22243	-1.75296
C	-3.99388	0.35118	-1.78916

H	-3.82929	1.41307	-1.98526
H	-4.22287	-0.08303	-2.76599
C	-5.21288	0.19919	-0.85010
H	-5.75344	1.14950	-0.79763
H	-5.92041	-0.52941	-1.25913
C	-4.82699	-0.26013	0.54968
H	-5.69854	-0.29334	1.21088
C	-3.96017	-1.52567	0.42060
H	-4.18564	-2.19180	-0.41663
H	-3.91134	-2.11564	1.33460
C	-2.76751	-0.56615	0.23080
H	-1.79468	-0.86978	0.63176
C	-3.56520	0.48019	1.07499
C	-3.35211	0.24018	2.56660
H	-4.08819	0.80019	3.15159
H	-2.35906	0.58707	2.86902
H	-3.43475	-0.80989	2.84915
C	-3.43441	1.97475	0.83343
H	-3.59485	2.27103	-0.20098
H	-2.44394	2.33132	1.13223
H	-4.16546	2.51165	1.44699
B	-0.00191	0.00058	-1.52887
C	0.19560	-1.56436	-1.61797
H	-0.60650	-2.09541	-1.09522
H	-0.01675	-1.76932	-2.68427
C	1.54851	-2.18139	-1.26594
H	2.31970	-1.57740	-1.75894
C	1.68814	-3.63318	-1.78940
H	0.68539	-4.02070	-1.98262
H	2.17674	-3.61689	-2.76724
C	2.43006	-4.61192	-0.85008
H	1.87633	-5.55444	-0.79456
H	3.41360	-4.86241	-1.26075
C	2.63874	-4.04570	0.54795
H	3.10377	-4.78314	1.20960
C	3.30281	-2.66339	0.41460
H	3.99026	-2.52805	-0.42481
H	3.79231	-2.32479	1.32649
C	1.87573	-2.10871	0.22721
H	1.65481	-1.11325	0.62673
C	1.36874	-3.32040	1.07470
C	1.47366	-3.01300	2.56553
H	1.35833	-3.92933	3.15261
H	0.67718	-2.32613	2.86847
H	2.42482	-2.55864	2.84515
C	0.00748	-3.95253	0.83809
H	-0.17208	-4.24365	-0.19470
H	-0.79449	-3.27008	1.13574
H	-0.09258	-4.85122	1.45574
C	1.25456	0.95383	-1.62062
H	2.11761	0.52320	-1.10238
H	1.53382	0.87564	-2.68835
C	1.11377	2.43301	-1.26399
H	0.20302	2.80078	-1.75146
C	2.29847	3.28228	-1.79034
H	3.13502	2.60898	-1.99019
H	2.03492	3.70036	-2.76549
C	2.77899	4.41150	-0.84954
H	3.87232	4.40347	-0.79873
H	2.50192	5.38970	-1.25590
C	2.19044	4.30416	0.55082
H	2.59886	5.07390	1.21307

C	0.66082	4.18767	0.42340
H	0.19619	4.71774	-0.41247
H	0.12662	4.43924	1.33840
C	0.89388	2.67530	0.23075
H	0.14436	1.98479	0.63177
C	2.20043	2.84006	1.07281
C	1.88869	2.77253	2.56486
H	2.74294	3.12837	3.14903
H	1.69262	1.73855	2.86551
H	1.02139	3.36894	2.85028
C	3.42804	1.97900	0.82706
H	3.76465	1.97439	-0.20744
H	3.24019	0.94178	1.12087
H	4.25911	2.33979	1.44212

2 (with dispersion)

82

B	-0.00084	0.00244	-0.80232
C	-2.49159	0.88150	-0.49234
C	-2.72690	0.61434	1.00348
C	-2.38158	1.85578	1.83818
C	-3.56883	2.80926	1.56251
C	-4.37163	2.05136	0.50290
C	-3.58076	1.96784	-0.82948
C	-4.48935	1.46564	-1.94710
C	-3.01277	3.31185	-1.26696
C	-4.25491	0.62541	1.05073
C	0.48254	-2.59274	-0.48791
C	0.81701	-2.66396	1.01111
C	-0.43793	-2.98981	1.83334
C	-0.66423	-4.49483	1.55329
C	0.40460	-4.80740	0.50358
C	0.09259	-4.07964	-0.83099
C	0.99374	-4.61198	-1.94063
C	-1.35062	-4.26203	-1.28289
C	1.57382	-3.99126	1.06394
C	2.00919	1.71702	-0.48746
C	1.90198	2.04783	1.01030
C	2.80597	1.12246	1.83724
C	4.22525	1.67239	1.55843
C	3.96814	2.75212	0.50495
C	3.49421	2.11580	-0.82842
C	3.51154	3.15829	-1.94196
C	4.37047	0.95201	-1.27376
C	2.67811	3.36385	1.06072
C	1.53936	0.32892	-0.88561
C	-0.48598	-1.49433	-0.88987
C	-1.05413	1.17236	-0.88627
H	-2.79392	-0.03063	-1.01920
H	-2.23976	-0.29538	1.35918
H	-2.31380	1.60001	2.89786
H	-1.42138	2.29223	1.55827
H	-3.25793	3.80419	1.24509
H	-4.17957	2.93844	2.45958
H	-5.38532	2.43514	0.36496
H	-3.90573	1.24832	-2.84706
H	-5.24102	2.21578	-2.21070
H	-5.01256	0.54961	-1.66388
H	-2.56143	3.23581	-2.25946
H	-3.81078	4.05783	-1.32695
H	-2.24753	3.69598	-0.59227
H	-4.70655	-0.13844	0.41466

H	-4.66212	0.52898	2.06060
H	1.42839	-2.39648	-1.00525
H	1.35592	-1.78628	1.37305
H	-0.26048	-2.80451	2.89500
H	-1.29481	-2.37809	1.54654
H	-1.67764	-4.72458	1.22542
H	-0.47846	-5.08918	2.45142
H	0.58296	-5.87658	0.36597
H	0.89809	-3.99638	-2.84044
H	0.72420	-5.63797	-2.20876
H	2.04579	-4.60593	-1.64695
H	-1.50086	-3.83412	-2.27731
H	-1.59568	-5.32647	-1.34466
H	-2.07329	-3.79168	-0.61600
H	2.46734	-3.99759	0.43653
H	1.85173	-4.29643	2.07615
H	1.36990	2.43822	-1.00915
H	0.87207	2.08118	1.37038
H	2.55489	1.18768	2.89820
H	2.70066	0.07405	1.55322
H	4.92842	0.90576	1.23418
H	4.64727	2.13133	2.45601
H	4.80809	3.43720	0.36691
H	3.02734	2.76609	-2.84169
H	4.53660	3.43307	-2.20835
H	2.98282	4.06943	-1.65335
H	4.07659	0.60527	-2.26772
H	5.41618	1.26789	-1.33375
H	4.31946	0.09367	-0.60365
H	2.24132	4.14072	0.43009
H	2.80285	3.75968	2.07201
H	2.12819	-0.44813	-0.39195
H	1.75556	0.16719	-1.95715
H	-1.45545	-1.61897	-0.40153
H	-0.72732	-1.59986	-1.96305
H	-0.67856	2.07077	-0.39029
H	-1.02022	1.44174	-1.95745

2 (without dispersion)

82

B	0.00004	-0.00020	-0.64071
C	2.67050	-0.11968	-0.43265
C	2.93257	0.22325	1.04587
C	3.02394	-1.05105	1.89912
C	4.40832	-1.63244	1.52051
C	4.87938	-0.68878	0.40975
C	4.00272	-0.85086	-0.86223
C	4.64698	-0.11937	-2.03810
C	3.82170	-2.30772	-1.27527
C	4.39968	0.65102	0.97820
C	-1.23169	2.37227	-0.43331
C	-1.66228	2.42732	1.04444
C	-0.60488	3.14197	1.89971
C	-0.79128	4.63196	1.52149
C	-1.84256	4.56987	0.40937
C	-1.26294	3.89195	-0.86224
C	-2.21715	4.08560	-2.03920
C	0.09017	4.46307	-1.27325
C	-2.76496	3.48507	0.97586
C	-1.43858	-2.25320	-0.43321
C	-1.27240	-2.65214	1.04527
C	-2.42073	-2.09259	1.89897

C	-3.61770	-2.99918	1.52043
C	-3.03734	-3.87991	0.40979
C	-2.73860	-3.04050	-0.86257
C	-2.42802	-3.96504	-2.03811
C	-3.90906	-2.15457	-1.27603
C	-1.63727	-4.13597	0.97789
C	-1.38114	-0.76158	-0.73119
C	0.03150	1.57674	-0.72954
C	1.35034	-0.81574	-0.73117
H	2.66070	0.83572	-0.97038
H	2.23522	0.96233	1.44630
H	2.97481	-0.80365	2.96224
H	2.20706	-1.74800	1.70185
H	4.36865	-2.67855	1.21698
H	5.09868	-1.57450	2.36619
H	5.94807	-0.76751	0.19426
H	3.96492	-0.09015	-2.89381
H	5.56252	-0.62439	-2.36147
H	4.90386	0.91224	-1.78643
H	3.30803	-2.37739	-2.23782
H	4.79668	-2.79077	-1.39243
H	3.24514	-2.89235	-0.55777
H	4.56679	1.50527	0.31879
H	4.83517	0.87224	1.95653
H	-2.05331	1.88650	-0.97276
H	-1.95531	1.45393	1.44385
H	-0.79627	2.97541	2.96247
H	0.40701	2.78192	1.70372
H	0.13551	5.11973	1.21948
H	-1.18721	5.20096	2.36684
H	-2.30745	5.53537	0.19385
H	-1.90107	3.48043	-2.89486
H	-2.23626	5.13116	-2.36212
H	-3.23953	3.79310	-1.78880
H	0.40826	4.05362	-2.23573
H	0.02186	5.54908	-1.38965
H	0.88375	4.25494	-0.55495
H	-3.58766	3.20391	0.31510
H	-3.17543	3.75139	1.95376
H	-0.60652	-2.72238	-0.97141
H	-0.28328	-2.41893	1.44539
H	-2.18179	-2.17421	2.96202
H	-2.61445	-1.03635	1.70189
H	-4.50311	-2.44062	1.21692
H	-3.91350	-3.62557	2.36616
H	-3.64098	-4.76540	0.19469
H	-2.06090	-3.38972	-2.89399
H	-3.32365	-4.50459	-2.36144
H	-1.66391	-4.70403	-1.78601
H	-3.71237	-1.67579	-2.23901
H	-4.81544	-2.75669	-1.39249
H	-4.12621	-1.36215	-0.55915
H	-0.98188	-4.70868	0.31838
H	-1.66370	-4.62357	1.95629
H	-2.15515	-0.21480	-0.18445
H	-1.66224	-0.59529	-1.78733
H	0.89110	1.97277	-0.18073
H	0.31837	1.73789	-1.78494
H	1.26359	-1.75952	-0.18469
H	1.34737	-1.14205	-1.78738

3 (with dispersion)

82

C	1.25148	-0.99471	0.30242
C	1.49082	-0.89262	-1.20905
C	2.56070	-1.93161	-1.46220
C	2.40569	-3.27393	-0.80648
C	3.27370	-2.22584	-0.17393
C	2.59876	-1.39477	0.90303
C	0.22071	-1.02655	-2.05042
B	-0.82621	0.14083	-1.88815
C	-0.34095	1.62685	-2.11491
C	-1.09442	2.74078	-1.39058
C	-0.60058	4.14810	-1.76684
C	0.55260	4.45305	-0.80425
C	0.22475	3.68398	0.46108
C	-0.81776	2.66204	0.09529
C	-1.18490	3.83653	0.95235
C	1.31018	3.39153	1.47180
C	1.76905	4.66222	2.17511
C	4.76776	-2.44677	-0.12523
C	5.17064	-3.24824	1.10546
C	-2.36544	-0.09271	-1.65991
C	-2.92160	-1.50691	-1.52198
C	-2.49364	-2.11739	-0.20606
C	-3.59801	-1.95193	0.80320
C	-4.76939	-1.33094	0.06407
C	-4.45695	-1.51871	-1.42468
C	-3.22562	-3.32008	0.30877
C	-3.35096	-1.50061	2.23177
C	-2.82113	-0.07081	2.26604
C	-2.41513	-2.40951	3.01419
C	2.49204	2.65080	0.85998
C	5.54572	-1.14012	-0.21139
H	-2.59007	-2.11120	-2.37433
H	-4.91074	-0.74529	-2.04806
H	-4.85078	-2.47553	-1.77488
H	-4.83168	-0.26667	0.31002
H	-5.72634	-1.77933	0.34809
H	-3.91020	-3.84585	-0.34712
H	-2.67687	-3.96797	0.97924
H	-1.46286	-1.99762	0.10200
H	1.94762	0.08313	-1.41580
H	1.45798	-3.53954	-0.35175
H	2.91666	-4.10662	-1.27580
H	3.11139	-1.88546	-2.39619
H	0.85424	-0.06934	0.72651
H	2.48894	-1.92757	1.85187
H	0.51068	-1.77261	0.50253
H	-2.16438	2.64960	-1.60518
H	-0.29687	4.20700	-2.81417
H	-1.40382	4.87614	-1.63109
H	1.49728	4.08540	-1.21526
H	0.67306	5.52664	-0.63386
H	-1.81882	4.61411	0.54154
H	-1.35493	3.63614	2.00418
H	-0.80811	1.68448	0.56561
H	-2.25040	-2.00911	4.01733
H	-2.81800	-3.41816	3.11979
H	-1.43613	-2.48268	2.52934
H	-2.75616	0.29908	3.29240
H	-1.81732	-0.03261	1.83340
H	-3.45128	0.62096	1.70380
H	-4.32402	-1.51391	2.74123

H	5.02299	-3.04169	-1.01165
H	6.24022	-3.47303	1.09781
H	4.95788	-2.68885	2.02108
H	4.62377	-4.19287	1.15594
H	6.61889	-1.33155	-0.28876
H	5.24126	-0.55625	-1.08357
H	5.38904	-0.52236	0.67692
H	0.86091	2.73309	2.22684
H	2.50460	4.44010	2.95253
H	2.23633	5.35108	1.46545
H	0.92712	5.18079	2.63959
H	3.18521	2.31847	1.63683
H	2.16437	1.77203	0.30065
H	3.05430	3.29261	0.17670
H	-0.21180	-2.01953	-1.89343
H	0.51714	-0.99565	-3.11204
H	0.73536	1.74265	-1.94452
H	-0.46689	1.76494	-3.20338
H	-2.87183	0.42079	-2.49324
H	-2.66503	0.50070	-0.78374
H	3.20048	-0.50198	1.09943

3 (without dispersion)

82

C	2.35812	0.09513	0.71373
C	2.43721	-0.22422	-0.78759
C	3.77400	-0.92661	-0.92206
C	4.10783	-1.99200	0.08395
C	4.63643	-0.59808	0.26364
C	3.80543	0.28949	1.17486
C	1.23905	-1.00549	-1.31400
B	-0.15512	-0.29348	-1.50104
C	-0.20389	1.27501	-1.67703
C	-1.54918	1.98526	-1.82577
C	-1.40840	3.45873	-2.25581
C	-1.31175	4.26896	-0.95763
C	-2.10468	3.47428	0.06324
C	-2.26610	2.08359	-0.49342
C	-3.45120	3.00095	-0.40349
C	-1.90991	3.72777	1.54350
C	-2.36077	5.13168	1.93068
C	6.12645	-0.36544	0.13106
C	6.85232	-0.62474	1.44612
C	-1.45522	-1.15200	-1.74625
C	-1.43837	-2.65447	-1.46981
C	-1.43821	-2.93735	0.02008
C	-2.83118	-3.30677	0.46593
C	-3.69330	-3.32830	-0.78443
C	-2.71175	-3.37006	-1.96085
C	-1.73782	-4.33682	0.47053
C	-3.47702	-2.80047	1.74683
C	-3.72253	-1.29530	1.68895
C	-2.70802	-3.14639	3.01444
C	-0.48145	3.46596	2.00498
C	6.45686	1.01929	-0.41368
H	-0.55826	-3.09399	-1.95325
H	-3.11931	-2.90365	-2.86063
H	-2.48342	-4.40587	-2.22306
H	-4.29934	-2.41800	-0.82416
H	-4.38942	-4.17316	-0.79506
H	-1.76027	-5.13399	-0.26448
H	-1.33025	-4.63591	1.42723

H	-0.80103	-2.33477	0.65976
H	2.51859	0.72194	-1.33855
H	3.33256	-2.36579	0.74363
H	4.82344	-2.74629	-0.22338
H	4.21159	-1.01450	-1.91186
H	1.73320	0.96515	0.92574
H	3.93617	0.05864	2.23638
H	1.90253	-0.74952	1.24000
H	-2.15620	1.44428	-2.56092
H	-0.54592	3.61242	-2.90842
H	-2.28839	3.76944	-2.82425
H	-0.26977	4.34199	-0.63035
H	-1.67903	5.29154	-1.08516
H	-3.87932	3.40056	-1.31611
H	-4.18148	2.78322	0.36791
H	-2.24239	1.22751	0.17279
H	-3.21106	-2.72380	3.88772
H	-2.63181	-4.22462	3.16563
H	-1.69416	-2.73373	2.99281
H	-4.29386	-0.96021	2.55861
H	-2.77150	-0.75427	1.68748
H	-4.27648	-0.99864	0.79604
H	-4.45562	-3.29542	1.81656
H	6.48947	-1.09987	-0.59988
H	7.93488	-0.53475	1.32312
H	6.54724	0.09614	2.21037
H	6.63572	-1.62629	1.82591
H	7.52898	1.11409	-0.60479
H	5.92857	1.21367	-1.35056
H	6.18383	1.80533	0.29572
H	-2.55864	3.01358	2.06736
H	-2.29936	5.28102	3.01188
H	-1.72983	5.88972	1.45734
H	-3.39255	5.31449	1.62051
H	-0.40141	3.56518	3.09064
H	-0.15635	2.45794	1.73539
H	0.22117	4.17719	1.56201
H	1.14216	-1.94410	-0.75548
H	1.46084	-1.34487	-2.34349
H	0.38644	1.75942	-0.88768
H	0.39675	1.45324	-2.58630
H	-1.67071	-0.98803	-2.81737
H	-2.31510	-0.68847	-1.24550
H	4.10607	1.33274	1.03318

BH_3 (with dispersion)

4

B	-0.00044	-0.00003	0.00041
H	0.56287	-1.05232	-0.00068
H	0.63214	1.01248	-0.00068
H	-1.19282	0.04000	-0.00068

BH_3 (without dispersion)

4

B	-0.00044	-0.00003	0.00041
H	0.56335	-1.05206	-0.00068
H	0.63167	1.01276	-0.00067
H	-1.19283	0.03945	-0.00068

H_2B(pinane) (with dispersion)

30

B	3.20407	-1.13639	-0.40748

H	3.21763	-1.13237	-1.60764
C	2.33044	-0.13743	0.38847
H	3.09315	0.61405	0.68147
H	2.00512	-0.54854	1.35000
C	1.19211	0.56204	-0.34807
H	1.62424	0.97037	-1.27008
C	0.58558	1.73364	0.46251
H	0.90273	1.62508	1.50213
H	1.03425	2.67167	0.12718
C	-0.95592	1.84846	0.42014
H	-1.25395	2.74659	-0.12953
H	-1.34150	1.97221	1.43657
C	-1.61913	0.65167	-0.24372
H	-2.70946	0.73761	-0.21904
C	-0.93575	0.40930	-1.60082
H	-0.56524	1.29143	-2.12937
H	-1.53199	-0.18830	-2.28810
C	0.10803	-0.40618	-0.81419
H	0.55528	-1.27813	-1.30400
C	-1.00431	-0.68979	0.24115
C	-0.67426	-0.85336	1.71327
H	-0.09542	-0.02984	2.12661
H	-1.59977	-0.92860	2.29287
H	-0.11255	-1.77657	1.88350
C	-1.85423	-1.88251	-0.17830
H	-2.76838	-1.92829	0.42106
H	-2.14692	-1.84962	-1.22817
H	-1.30556	-2.81520	-0.01636
H	3.94262	-1.88668	0.16579

H_2B(pinane) (without dispersion)

30

B	3.23151	-1.13746	-0.40646
H	3.26105	-1.11909	-1.60634
C	2.33885	-0.15672	0.39228
H	3.09789	0.59647	0.69347
H	2.01487	-0.57740	1.35048
C	1.19892	0.54748	-0.34036
H	1.63144	0.95578	-1.26257
C	0.60002	1.72186	0.47376
H	0.90347	1.60045	1.51631
H	1.06623	2.65660	0.15210
C	-0.93980	1.85878	0.41438
H	-1.21937	2.75813	-0.14360
H	-1.33400	1.99566	1.42613
C	-1.61444	0.66732	-0.25080
H	-2.70396	0.76848	-0.23372
C	-0.92561	0.41428	-1.60381
H	-0.54273	1.29115	-2.13284
H	-1.52458	-0.17776	-2.29395
C	0.10513	-0.41221	-0.80933
H	0.54543	-1.28935	-1.29681
C	-1.02055	-0.68373	0.23874
C	-0.70629	-0.85683	1.71488
H	-0.11852	-0.04427	2.13797
H	-1.63808	-0.92031	2.28633
H	-0.16115	-1.78972	1.88806
C	-1.88392	-1.86608	-0.18898
H	-2.80349	-1.90028	0.40326
H	-2.16888	-1.83046	-1.24104
H	-1.35007	-2.80683	-0.02274
H	3.97297	-1.88491	0.16729

H_2B(camphane) (with dispersion)

30

C	-1.07163	-0.96913	-1.31877
C	0.29733	-1.21942	-0.68677
C	0.76990	0.22469	-0.45545
C	-0.53937	0.95637	0.02070
C	-1.59965	-0.16707	-0.12478
C	-1.44444	-1.20864	0.98629
C	-0.09252	-1.88054	0.64264
C	2.01943	0.36316	0.39855
B	3.34583	-0.16969	-0.19400
H	3.47457	-0.32836	-1.37666
C	-0.86569	2.11063	-0.92215
C	-0.46337	1.52395	1.43205
H	4.29535	-0.35914	0.51266
H	1.02374	0.62740	-1.44327
H	1.00396	-1.80472	-1.27974
H	-0.20769	-2.95910	0.51461
H	0.65994	-1.73501	1.41998
H	-1.47230	-0.78336	1.98911
H	-2.26255	-1.93063	0.92580
H	-2.61514	0.22536	-0.21710
H	-0.04511	2.83443	-0.94127
H	-1.76765	2.63868	-0.59867
H	-1.02588	1.76678	-1.94621
H	0.22104	2.37547	1.47010
H	-1.44760	1.88165	1.74829
H	-0.12086	0.79932	2.17088
H	-1.01516	-0.40314	-2.25042
H	-1.64310	-1.88381	-1.49638
H	1.87377	0.04520	1.43475
H	2.28163	1.43744	0.49960

H_2B(camphane) (without dispersion)

30

C	-1.08653	-0.95280	-1.32126
C	0.27616	-1.22923	-0.68472
C	0.77612	0.20731	-0.45113
C	-0.52322	0.96477	0.02114
C	-1.60357	-0.14137	-0.12776
C	-1.47193	-1.18813	0.98312
C	-0.13264	-1.88761	0.64148
C	2.02990	0.32498	0.40308
B	3.35783	-0.20184	-0.19334
H	3.49310	-0.34353	-1.37754
C	-0.82752	2.12542	-0.92421
C	-0.44329	1.53543	1.43280
H	4.30508	-0.39915	0.51457
H	1.03842	0.60475	-1.43924
H	0.97308	-1.82755	-1.27681
H	-0.27062	-2.96314	0.50767
H	0.61973	-1.76336	1.42297
H	-1.49388	-0.76438	1.98711
H	-2.30489	-1.89320	0.92013
H	-2.61212	0.26877	-0.22325
H	0.00420	2.83680	-0.94119
H	-1.72162	2.66886	-0.60356
H	-0.99084	1.78591	-1.94946
H	0.25474	2.37616	1.47190
H	-1.42246	1.91169	1.74418
H	-0.11648	0.80839	2.17679

H	-1.01764	-0.38856	-2.25343
H	-1.67429	-1.85706	-1.50102
H	1.88412	-0.00129	1.43701
H	2.30241	1.39645	0.51478

H_2B(sabinane) (with dispersion)

30

B	3.14846	1.57812	0.46683
H	3.51462	2.64954	0.07286
C	2.38976	0.61940	-0.48396
H	1.68755	1.17273	-1.12154
H	3.18598	0.31544	-1.19181
C	1.72809	-0.61861	0.11455
H	2.48112	-1.17759	0.68143
C	1.07152	-1.51494	-0.94776
H	1.02688	-2.54712	-0.59347
H	1.63965	-1.52776	-1.88048
C	-0.34587	-0.95950	-1.13125
H	-1.04730	-1.72801	-1.46752
H	-0.35100	-0.16874	-1.88758
C	-0.71526	-0.36968	0.21678
C	-0.42963	-1.25701	1.39238
H	-0.19083	-2.30261	1.23493
H	-1.00097	-1.06500	2.29328
C	0.56504	-0.20803	0.99091
H	0.69887	0.63945	1.65650
C	-1.83967	0.63490	0.32057
H	-1.90074	0.92491	1.37742
C	-1.56349	1.89781	-0.48444
H	-0.60390	2.34127	-0.20745
H	-2.34258	2.64490	-0.31392
H	-1.54165	1.69085	-1.55779
C	-3.17435	0.01396	-0.06985
H	-3.37778	-0.88345	0.51935
H	-3.17688	-0.27108	-1.12586
H	-3.99697	0.71688	0.08396
H	3.43689	1.25503	1.58594

H_2B(sabinane) (without dispersion)

30

B	3.22649	1.54120	0.47797
H	3.60965	2.61128	0.09579
C	2.42440	0.61883	-0.47385
H	1.74270	1.19683	-1.11137
H	3.21668	0.29676	-1.17996
C	1.73030	-0.60896	0.11176
H	2.46862	-1.18123	0.68540
C	1.07266	-1.49825	-0.95854
H	1.03206	-2.53370	-0.61270
H	1.64012	-1.50326	-1.89206
C	-0.34801	-0.94780	-1.13919
H	-1.04566	-1.71990	-1.47642
H	-0.35743	-0.15683	-1.89569
C	-0.72013	-0.35938	0.21015
C	-0.42643	-1.24417	1.38700
H	-0.18185	-2.28908	1.23177
H	-0.99663	-1.05454	2.28948
C	0.56313	-0.19107	0.98193
H	0.69643	0.65666	1.64773
C	-1.85842	0.63296	0.32022
H	-1.90390	0.93494	1.37477
C	-1.62252	1.89324	-0.50370

H	-0.66503	2.35799	-0.25514
H	-2.41042	2.62818	-0.31970
H	-1.62473	1.67834	-1.57588
C	-3.19428	-0.01030	-0.03419
H	-3.37665	-0.90142	0.57148
H	-3.21765	-0.30998	-1.08604
H	-4.02153	0.68568	0.12780
H	3.53858	1.18668	1.58136

4 (with dispersion)

95

P	-0.00361	-0.00276	-2.75905
B	-0.00139	-0.00174	-0.74683
C	-1.47106	0.55735	-0.30879
H	-1.42629	0.72722	0.77428
H	-1.62135	1.55815	-0.73373
C	-2.71865	-0.28688	-0.60847
H	-2.51949	-0.88778	-1.50779
C	-3.02920	-1.31688	0.47647
H	-2.12984	-1.86111	0.76480
C	-3.90663	-0.77387	1.64623
C	-5.10668	-1.04648	0.70016
H	-6.05407	-1.33875	1.16358
C	-5.30344	0.08792	-0.29203
H	-5.80963	0.92693	0.19512
H	-5.98146	-0.26308	-1.07668
C	-3.97315	0.57824	-0.90780
H	-3.77254	1.59035	-0.55196
H	-4.09441	0.68055	-1.99035
C	-4.25494	-2.13428	0.02355
H	-4.38700	-2.25753	-1.05526
H	-4.33331	-3.11014	0.50024
C	-3.88669	-1.74308	2.82166
H	-4.66838	-1.48542	3.54286
H	-2.92513	-1.68805	3.34078
H	-4.04047	-2.78023	2.52161
C	-3.71491	0.62578	2.20127
H	-4.53141	0.86255	2.89149
H	-3.68662	1.40164	1.43968
H	-2.78276	0.69079	2.76989
C	1.58927	0.39766	-3.53233
H	2.34143	-0.32691	-3.21845
H	1.91305	1.38517	-3.20283
H	1.50778	0.38581	-4.62116
C	0.25016	-1.55413	-0.30952
H	0.08243	-1.60060	0.77379
H	-0.54211	-2.18477	-0.73309
C	1.60420	-2.21317	-0.61144
H	2.02149	-1.74379	-1.51429
C	2.65599	-1.96258	0.46814
H	2.67814	-0.91068	0.75274
C	2.63075	-2.98998	1.64155
C	3.46288	-3.89571	0.69455
H	4.19223	-4.56806	1.15686
C	2.57534	-4.63700	-0.29183
H	2.10581	-5.49494	0.19908
H	3.21548	-5.04886	-1.07874
C	1.48095	-3.73338	-0.90385
H	0.50688	-4.06473	-0.53975
H	1.44524	-3.89399	-1.98554
C	3.97525	-2.61602	0.01150
H	4.14338	-2.67226	-1.06787

H	4.86133	-2.19382	0.48297
C	3.46611	-2.48382	2.81097
H	3.63747	-3.28709	3.53414
H	2.94036	-1.67673	3.32993
H	4.43965	-2.09958	2.50454
C	1.32570	-3.52188	2.20521
H	1.53236	-4.34438	2.89796
H	0.63607	-3.88858	1.44843
H	0.80601	-2.74474	2.77306
C	-1.14826	1.17621	-3.53079
H	-0.89571	2.19009	-3.21859
H	-2.16478	0.96365	-3.19885
H	-1.09965	1.11059	-4.61966
C	1.21710	0.99378	-0.31226
H	1.34517	0.87007	0.77041
H	2.15897	0.62662	-0.73981
C	1.10334	2.49620	-0.61139
H	0.47474	2.62236	-1.50495
C	0.37357	3.27754	0.48014
H	-0.54297	2.76746	0.77657
C	1.29155	3.76848	1.64171
C	1.64258	4.94570	0.69296
H	1.86406	5.91283	1.15482
C	2.71553	4.55308	-0.30942
H	3.69967	4.57547	0.16856
H	2.74041	5.31608	-1.09415
C	2.47465	3.15506	-0.92336
H	3.25688	2.47818	-0.57516
H	2.61333	3.21011	-2.00725
C	0.26920	4.74757	0.02874
H	0.21805	4.92379	-1.04959
H	-0.53424	5.30048	0.51298
C	0.45149	4.23237	2.82514
H	1.07019	4.78253	3.54077
H	0.02631	3.37040	3.34797
H	-0.37491	4.88121	2.53280
C	2.41603	2.90602	2.18530
H	3.03447	3.49646	2.86944
H	3.06720	2.49596	1.41667
H	2.01473	2.06477	2.75773
C	-0.45333	-1.58368	-3.52988
H	-1.45659	-1.87285	-3.21517
H	0.24060	-2.35695	-3.19972
H	-0.42340	-1.50866	-4.61881

PMe_3 (with dispersion)

13

P	0.00003	0.00009	-0.59704
C	-0.13338	-1.61293	0.27613
C	-1.33036	0.92187	0.27620
C	1.46369	0.69092	0.27622
H	1.60574	1.73299	-0.01795
H	1.35860	0.64109	1.36433
H	2.35853	0.13846	-0.01821
H	-1.29934	1.97313	-0.01794
H	-2.30376	0.52387	-0.01826
H	-1.23489	0.85540	1.36431
H	0.69803	-2.25698	-0.01812
H	-0.12374	-1.49679	1.36421
H	-1.05930	-2.11166	-0.01810

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