Supporting Information for

A Comparison of Hydrogen Release Kinetics from 5- and 6-Membered 1,2-BN-Cycloalkanes

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General considerations

Unless otherwise noted, all reagents were obtained from commercial sources and used as received. All materials synthesis was performed in oven-dried glassware under a nitrogen atmosphere using standard syringe techniques. Tetrahydrofuran was passed through an alumina column and dispensed from a solvent purification system under argon. Tetraglyme was vacuum distilled and stored over molecular sieves under an inert atmosphere prior to use. The following compounds were synthesized according to previously reported procedures: 1,2-BN-cyclohexane (**1**),[1] 3-methyl-1,2-BN-cyclopentane (**2**),[2] 4-methyl-1,2-BN-cyclopentane,[3] 5-methyl-1,2-BN-cyclopentane,[4] and 1,2-BN-cyclopentane.[4]

Dichloromethane-d_2 was purchased from Cambridge Isotope Laboratories; it was distilled over CaH_2 and sealed under N_2 in a Schlenk flask prior to use. ^{1}H, ^{13}C, and ^{11}B NMR spectra were measured on either a Varian Gemini 500 MHz, Varian Unity Inova 500 MHz, or Varian Unity Inova 600 MHz spectrometer. All NMR chemical shifts are reported in ppm; coupling constants are reported in Hz. ^{1}H and ^{13}C spectra were internally referenced to residual solvent peaks; ^{11}B spectra were externally referenced to a standard of BF_3•Et_2O (δ = 0.0 ppm). Peaks for carbon atoms adjacent to boron were generally not observed. IR spectra related to characterization of the isomers of 1,2-dimethyl-1,2-BN-cyclohexane (**5**) were measured on a Bruker Alpha-P FT-IR equipped with a single crystal diamond ATR module; peak positions are reported in cm^{-1}. High-resolution mass spectrometry (HRMS) data were generated in Boston College facilities using direct analysis in real-time (DART) on a JEOL AccuTOF DART spectrometer.

Thermogravimetric analysis (TGA) of **1** was performed at Pacific Northwest National Laboratory (Richland, WA) using a TG/DSC STA 449 Jupiter Netzsch instrument under a flow of argon. Temperature-programmed desorption-mass spectrometry (TPD-MS) analysis of **1** was performed using the custom instrumentation available for this purpose at the National Renewable Energy Laboratory (Golden, CO).

IR spectra for *in situ* monitoring of reaction kinetics were measured using either a Mettler Toledo ReactIR iC10 or ReactIR 15 spectrometer with an MCT detector and a DiComp diamond probe connected via a AgX fiber optic cable. Spectra for background subtraction were collected during the experimental runs prior to substrate injection. Peak selection and placement of baseline points for area integration were performed manually within the instrument software (ic IR 4.3). Linear regressions to determine initial rates, reaction orders, and other parameters were performed using Microsoft Excel.

[1] Luo, W.; Zakharov, L. N.; Liu, S.-Y. *J. Am. Chem. Soc.* **2011,** *133,* 13006–13009.
[2] Luo, W.; Campbell, P. G.; Zakharov, L. N.; Liu, S.-Y. *J. Am. Chem. Soc.* **2011,** *133,* 19326–19329.
[3] Liu, S.-Y.; Parab, K.; Luo, W.; Campbell, P. (University of Oregon). Boron-Nitrogen Heterocycles. WO 2012/103251 A1, August, 2, 2012.
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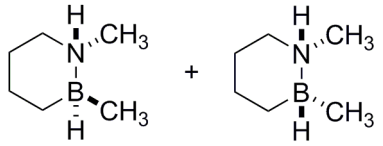
Synthesis of isomers of 1,2-dimethyl-1,2-BN-cyclohexane (**5**)



trans-**5** *cis*-**5**

To a solution of 1,2-dimethyl-1,2-BN-cyclohexene[5] (0.509 g, 4.59 mmol) in THF (11 mL) was added solid lithium aluminum hydride (0.427 g, 11.3 mmol, 2.46 equiv). The mixture was allowed to stir at 22 °C for 90 min, and then the mixture was cooled to –78 °C. Anhydrous methanol was added slowly until gas evolution ceased. Volatiles were removed *in vacuo*, and the residue was extracted with copious amounts of hexanes. The extractions were vacuum-filtered through a glass fritted funnel and concentrated *in vacuo* to afford a mixture of trans and cis diastereomers. (See below for full characterization of a sample of the mixture obtained at this point.) Isolation of the major trans isomer was achieved by recrystallization from a minimal amount of anhydrous pentane at –30 °C (0.3443 g, 66%). Crystals suitable for single-crystal X-ray analysis were grown from a pentane solution at 0 °C assisted by slow evaporation.

Characterization data for mixture of *trans*- and *cis*-**5**.

^{1}H NMR (CD_2Cl_2, 600 MHz) δ 2.95 (app. d, 1H, J = 11.2 Hz), 2.81–2.86 (m, 0.17H), 2.72 (qd, 0.19H, J = 10.7 Hz, 3.0 Hz), 2.60 (td, 1H, 21.8 Hz, 11.1 Hz), 2.44 (d, 3H, J = 4.2 Hz), 2.41 (d, 0.52H, J = 6.1 Hz), 1.73–1.81 (m, 2H), 1.32–1.44 (m, 2H), 0.54 (app. d, 1H, J = 14.4 Hz), 0.32–0.41 (m, 0.39H), –0.07–0.05 (m, 1H), –0.33 (d, 3H, J = 4.8 Hz), –0.36 (d, 0.54H, J = 5.0 Hz); **^{13}C NMR** (CD_2Cl_2, 151 MHz) δ 56.1, 51.6 (minor), 40.4, 38.9 (minor), 29.5, 28.0 (minor), 26.6; **^{11}B NMR** (CD_2Cl_2, 192 MHz) δ –3.6 (d, J = 92.8 Hz), –5.7 (d, J = 94.4 Hz, minor); **IR** 3252, 3191, 2909, 2849, 2799, 2254, 2190, 1463, 1418, 1287, 1238, 1192, 1156, 1139, 1117, 1074, 1039 cm^{-1}; **HRMS** (DART) calcd. for $C_6H_{15}BN$ [M–H]: 112.1298, found 112.1301.

Characterization data for isolated *trans*-**5**:

^{1}H NMR (CD_2Cl_2, 500 MHz) δ 2.94 (app. d, 1H, J = 9.7 Hz), 2.60 (td, 1H, J = 22.1 Hz, 10.9 Hz), 2.37–2.54 (m, 4H), 1.67–1.83 (m, 2H), 1.30–1.44 (m, 2H), 0.53 (app. d, 1H, J = 14.5 Hz), –0.07–0.06 (m, 1H), –0.33 (d, 3H, J = 4.8 Hz), the B-H signal was not clearly observed; **^{13}C NMR** (CD_2Cl_2, 126 MHz) δ 56.1, 40.4, 29.5, 26.6, the signals for the carbon atoms adjacent to the boron atom are not observed; **^{11}B NMR** (CD_2Cl_2, 160 MHz) δ –3.6 (d, J = 92.5 Hz); **IR** 3188, 2896, 2251, 2186, 2134, 1462, 1417, 1286, 1238, 1191, 1158, 1139, 1114, 1074, 992 cm^{-1}; **HRMS** (DART) calcd. for $C_6H_{15}BN$ [M–H]: 112.1298, found 112.1297.

[5] Giustra, Z. X.; Chou, L.-Y.; Tsung, C.-K.; Liu, S.-Y. *Organometallics* **2016,** *35,* 2425–2428.

Isomerization of *trans*-**5**

A 0.2 M solution of *trans*-**5** in CD_2Cl_2 was sealed in J-Young NMR tube and submerged in an oil bath at 37 °C for 6 h. (Note: Heating for longer periods or at higher temperatures resulted in partial dehydrogenation.) After this time, the sample was analyzed by ^{11}B and ^{1}H NMR,[6] which indicated the formation of the minor cis isomer by comparison with spectra of the diastereomeric mixture obtained prior to recrystallization (Figure S1).

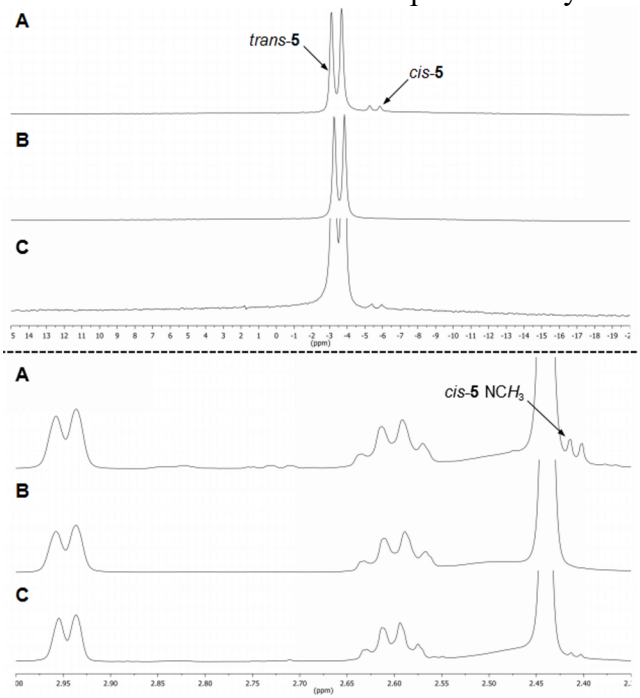


Figure S1. Comparison of ^{11}B (top) and ^{1}H (bottom) NMR spectra of the mixture of *trans*- and *cis*-**5** obtained from hydride/proton addition to **5–H₂** (A), isolated *trans*-**5** (B), and the mixture obtained from heating pure *trans*-**5** (C).

Thermogravimetric analysis of **1**

For TGA measurements of **1**, a neat sample was loaded into an aluminum crucible under an inert atmosphere. The sample was incrementally heated under a stream of argon from 60 °C to 100 °C, with temperature ramping at 10 °C-min^{-1} between isothermal periods of 3 h. As shown in Figure S2, significant weight loss (2–3%) began to occur once the sample was heated to 70 °C. Note that due to the volatility of the **1–H₂** intermediate produced during thermal decomposition, mass loss greater than the effective hydrogen weight capacity of **1** is observed. The evolution of H_2 at 70 °C needed to be confirmed by a separate TPD-MS experiment (*vide infra*) because **1–H₂** (or further decomposition products thereof) consistently blocked the transfer line connecting the TGA instrument to the mass spectrometer.

[6] The concentration of *cis*-**5** at this point proved too low to enable detection by ^{13}C NMR even after more than 18,000 scans.

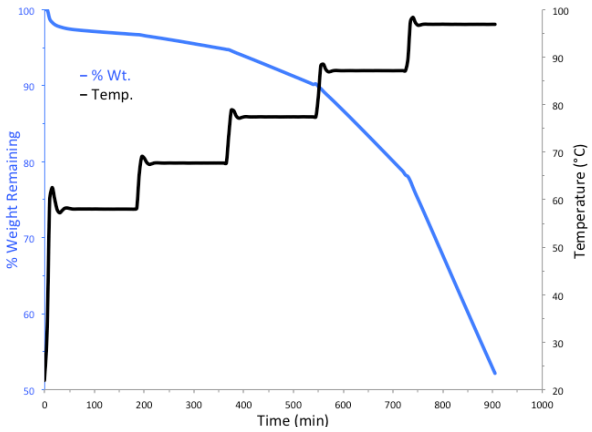


Figure S2. TGA of **1** from 60–100 °C with ramping at 10 °C-min^{-1} between isothermal periods (3 h).

Temperature-programmed desorption-mass spectrometry (TPD-MS) analysis of **1**

For TPD-MS analysis of **1**, a neat sample was loaded into a sample tube inside of a helium-atmosphere dry-box. The sample was then placed on the TPD system, and the head space to the closed valve was evacuated until all signals had reached background levels. The sample was cooled to –196 °C by immersion in a liquid nitrogen dewar. The sample tube was then evacuated until all signals were again at background levels. The sample was incrementally heated from 60 °C to 100 °C, with temperature ramping at 10 °C-min^{-1} between isothermal periods of 1 h. As shown in Figure S3, increasing amounts of H_2 were detected by mass spectrometry after a period at 60 °C, with very small amounts of **1–H$_2$** observed beginning at 80 °C; essentially no significant amount of **1** itself was detected over the indicated temperature range.

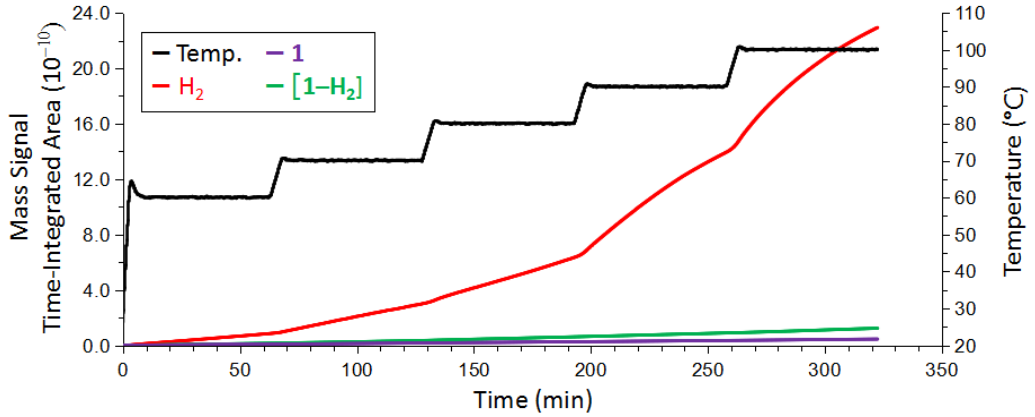


Figure S3. TPD-MS of **1** from 0–100 °C with ramping at 10 °C-min^{-1} between isothermal periods (1 h).

General procedure for ReactIR measurements of **1**

The ReactIR probe was fitted to a two-neck, inverse-pear flask and flushed with nitrogen. Tetraglyme (0.9 mL) was added via syringe and heated to the desired temperature. Upon stabilization of the temperature, the appropriate amount of **1** in 0.3 mL tetraglyme was injected and the disappearance of the starting material peak at 1600 cm^{-1} was monitored based on peak area with a two-point baseline at a sample rate of 1 min^{-1}. The initial rate of the reaction was determined by a linear regression of the disappearance trend up to 20% conversion.

General procedure for ReactIR measurements of **2**

The ReactIR probe was fitted to a two-neck, inverse-pear flask and flushed with nitrogen. Tetraglyme was added via syringe and heated to the desired temperature. Upon stabilization of the temperature, neat **2** was injected via syringe and the disappearance of the starting material peak at 1600 cm^{-1} was monitored based on peak area with a two-point baseline at a sample rate of 4 min^{-1}. The initial rate of the reaction was determined by a linear regression of the disappearance trend up to 20% conversion.

Reaction order determination

All reactions performed at 140 °C in tetraglyme.

$[\mathbf{1}]_0$ (M)	r_i (M min^{-1})	$\ln([\mathbf{1}]_0)$	$\ln(r_i)$
0.551	0.001036	–0.59602047	–10.9667327
0.743	0.001887	–0.297059234	–10.36711157
0.861	0.002159	–0.149660775	–10.23245469
1.143	0.004804	0.133656385	–9.432650937
1.283	0.005244	0.249201086	–9.345015275

$[\mathbf{2}]_0$ (M)	r_i (M s^{-1})	$\ln([\mathbf{2}]_0)$	$\ln(r_i)$
0.560	0.000545	–0.5798185	–7.51472476
0.742	0.001112	–0.2984060	–6.80159508
0.863	0.000951	–0.1473406	–6.95799650
1.138	0.002032	0.12927324	–6.19873475
1.283	0.002948	0.24920109	–5.82679793

Arrhenius analyses

$[\mathbf{1}]_0$ (M)	Temp. (K)	r_i (M min^{-1})	rate constant (k; M^{-1} s^{-1})	ln(k)
0.745	393.15	0.000423	0.0000127021	–11.27374082
0.742	403.15	0.000993	0.0000299792	–10.41500599
0.742	413.15	0.001887	0.0000569696	–9.772993106
0.742	423.15	0.003109	0.0000936103	–9.276370222
0.744	433.15	0.008073	0.000243074	–8.322146192

$[\mathbf{2}]_0$ (M)	Temp. (K)	r_i (M s^{-1})	rate constant (k; M^{-1} s^{-1})	ln(k)
0.736	373.15	0.000095	0.000175375	–8.648583346
0.742	393.15	0.000536	0.000973547	–6.934564325
0.742	413.15	0.001112	0.002019747	–6.204783012
0.742	423.15	0.001618	0.002938441	–5.829752389
0.530	433.15	0.002315	0.008241367	–4.798589047

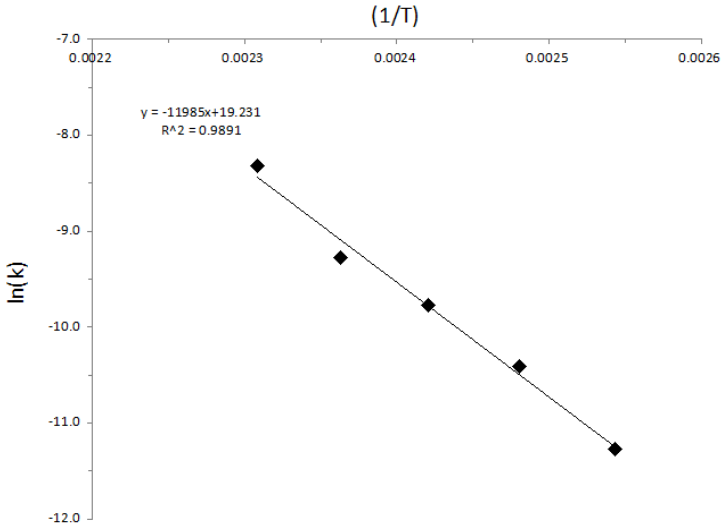


Figure S4. Arrhenius plot for **1**.

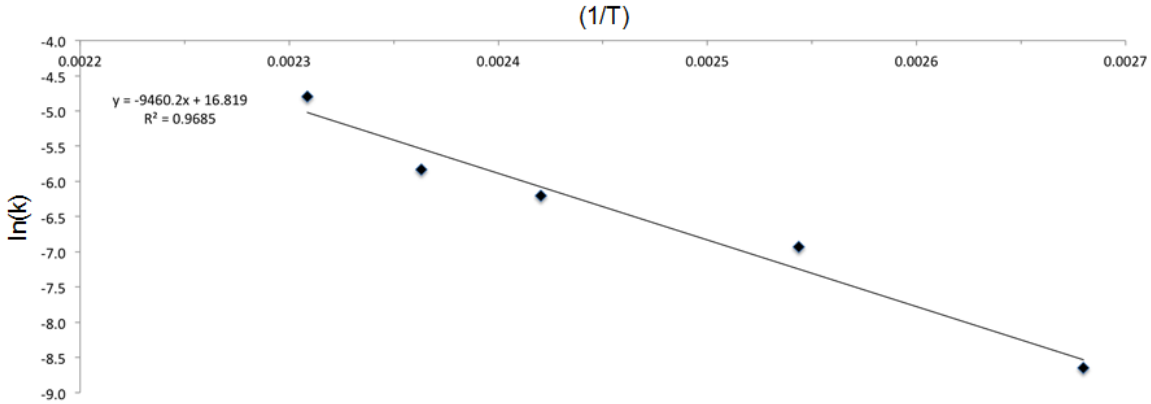


Figure S5. Arrhenius plot for **2**.

Computational details

Methods

The geometries were optimized at the density functional theory (DFT)[7] level with the hybrid M06 exchange-correlation functional[8] and the DZVP2 basis set.[9] Selected points on the potential energy surface were benchmarked at the G3MP2 level and the M06 results are consistent with the G3MP2 composite, correlated molecular orbital theory results. Gas-phase enthalpy and free energy values were calculated using the same method and basis set. Solvent-phase (tetraglyme) free energy values for pathway (C) were calculated using COSMO with the hybrid B3LYP exchange-correlation functional[10,11] and the DZVP2 basis set. Vibrational frequencies were calculated to show that the structures were minima on the potential energy surface and to confirm the identity of transition states. All calculations were done with Gaussian09.[12] The total energies are given in Table S1. The x,y,z coordinates in angstroms at the M06/DZVP2 level for the optimized geometries are given in Table S2. The calculations were performed on a Xeon-based Dell Linux cluster at the University of Alabama, and a local AMD Opteron-based and Intel Xeon-based Linux cluster from Penguin Computing.

[7] Parr, R. G.; Yang, W. *Density-Functional Theory of Atoms and Molecules*; Oxford University Press: New York, 1989.
[8] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008,** *120,* 215–241.
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[11] Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.
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Table S1. Total energies of calculated species in a.u.

Molecule	M06/DZVP2		
	ΔH(0K)	ΔH(298K)	ΔG(298K)
1	−238.98081	−238.97376	−239.00985
1'	−238.93999	−238.93047	−238.97268
[**1-1'**]	−477.942946	−477.926633	−477.987008
TS-1	−477.90722	−477.89084	−477.95096
1−H_2	−237.83178	−237.82497	−237.86068
2	−238.97566	−238.96802	−239.00579
2'	−238.94027	−238.93062	−238.97306
[**2-2'**]	−477.94025	−477.92343	−477.9839
TS-2	−477.90747	−477.89112	−477.9499
2−H_2	−237.82507	−237.81784	−237.85443
TS-S1A	−477.90253	−477.88787	−477.94235
[1−H_2]$_2$(anti)	−475.662972	−475.651089	−475.697843
[1−H_2]$_2$(syn)	−475.68082	−475.66872	−475.71684
TS-S2A	−477.89881	−477.88355	−477.93923
[2−H_2]$_2$	−475.68406	−475.67136	−475.72076
TS-S1B	−477.888427	−477.873665	−477.928080
[1-1'']	−477.946717	−477.932144	−477.986201
TS-S1C	−477.921146	−477.906195	−477.961369
[1-1'']−H_2	−476.768694	−476.753404	−476.810053
TS-S1D	−476.765750	−476.750498	−476.807388
[1-1''']	−476.815076	−476.802093	−476.851717
[1-1''']−H_2	−475.662155	−475.648209	−475.700311
TS-S1E	−475.64106	−475.62841	−475.67735
TS-S2B	−477.90196	−477.88686	−477.94151
[2-2'']	−477.95827	−477.9435	−477.99733
[2-2'']−H_2	−476.77068	−476.75444	−476.8135
TS-S2D	−476.76854	−476.75265	−476.81052
[2-2''']	−476.81273	−476.79855	−476.85146
[2-2''']−H_2	−475.65722	−475.64259	−475.69627
TS-S2E	−475.64429	−475.63053	−475.68255

Table S2. Optimized M06/DZVP2 x,y,z coordinates in Å.

1

0 1

C	-1.160587	-0.838482	0.254223
C	1.255595	0.862608	-0.230913
C	1.359035	-0.590039	0.238363
C	0.160097	-1.409843	-0.236463
H	-0.364531	2.631977	-0.235864
H	-1.342829	0.553228	-1.254520
H	-1.166980	-0.782839	1.346936
H	-2.006747	-1.454937	-0.067119
H	1.337322	0.883278	-1.330416
H	2.114614	1.433408	0.137431
H	2.278921	-1.073653	-0.111381
H	1.387028	-0.616795	1.336113
H	0.147602	-1.443026	-1.336081
H	0.229835	-2.448230	0.102165
H	-0.235534	1.569420	1.480775
N	-1.328582	0.552367	-0.235355
B	-0.109447	1.559819	0.270363
H	-2.216230	0.937050	0.076370

1'

0 1

C	1.736269	-0.540010	0.006330
C	0.540465	0.396342	-0.039875
H	1.660143	-1.176680	0.905321
H	1.695638	-1.216150	-0.856122
C	-0.789361	-0.346424	0.012015
H	0.594177	1.100332	0.802633
H	0.599421	1.002255	-0.951496
C	-1.997513	0.616517	-0.038365
H	-0.838272	-1.054588	-0.826059
H	-0.829894	-0.953957	0.926450
H	-1.918574	1.310387	0.805696
H	-1.937155	1.194876	-0.966447
N	2.980373	0.223860	-0.071751
H	3.060466	0.829939	0.739729
H	3.782442	-0.396836	-0.052855
B	-3.250519	-0.308155	0.038298
H	-3.689518	-0.650078	1.094398
H	-3.728050	-0.774297	-0.951109

[1-1']

0 1

C	4.149685	-1.116797	-0.139877
C	4.467869	0.154230	-0.910968
C	4.034420	1.409075	-0.155467
C	2.528800	1.386833	0.127329
H	5.542187	0.167280	-1.116724
H	4.642676	-1.103806	0.837003
H	4.478932	-2.008887	-0.679735
H	2.163811	-1.243282	-0.760533
H	2.453196	-2.061773	0.620707
H	4.587812	1.457102	0.792052
H	4.324049	2.293937	-0.732149
H	2.240705	2.280524	0.689526
H	1.984975	1.437906	-0.828173
H	2.572575	-0.026332	2.059309
H	0.893122	-0.071997	1.108383
H	3.963084	0.116491	-1.886460
B	2.136270	0.067907	0.936369
N	2.689135	-1.207978	0.118431
H	0.037826	-1.831103	0.613593
H	0.338320	-0.486669	-0.888980
B	-0.054426	-0.682199	0.241045
C	-1.368944	0.115155	0.662805
C	-2.573616	-0.435213	-0.104403
H	-1.273458	1.188549	0.446296
C	-3.880983	0.267622	0.234579
H	-2.678787	-1.510303	0.101285
H	-2.387313	-0.356648	-1.185435
C	-5.067636	-0.284720	-0.536200
H	-3.780042	1.342927	0.024263
H	-4.087633	0.185727	1.308737
H	-4.847505	-0.231268	-1.617094
H	-5.186805	-1.348687	-0.297227
N	-6.298265	0.409182	-0.152900
H	-6.208037	1.398610	-0.366551
H	-7.085054	0.065374	-0.693577
H	-1.571517	0.032247	1.738913

TS-1

0 1

C	3.819397	-0.396142	-0.006009
C	4.780921	0.768776	-0.164295
C	2.358425	0.031027	0.005650
N	6.167539	0.300069	-0.134202
H	4.638623	1.468714	0.668577

H	4.521195	1.323330	-1.083483
H	4.065558	-0.934608	0.917862
H	3.979340	-1.111906	-0.826603
C	1.379143	-1.134130	0.135170
H	2.132279	0.592469	-0.912239
H	2.200595	0.742419	0.831082
H	6.317318	-0.355888	-0.895903
H	6.808830	1.071850	-0.284726
B	-0.154746	-0.685234	0.104984
H	1.620447	-1.710570	1.039292
H	1.547089	-1.826553	-0.703420
H	-0.980515	-1.592922	0.253608
H	-0.470574	0.044562	-0.809953
B	-2.900668	-1.215512	0.584486
C	-3.506517	-1.116336	-0.863139
N	-2.616068	0.037569	1.336582
H	-2.880178	-2.211294	1.232998
C	-4.144099	0.249161	-1.145890
H	-2.695924	-1.294459	-1.579601
H	-4.224110	-1.926768	-1.025883
C	-3.103270	1.352593	0.855563
H	-2.738359	-0.060411	2.338954
C	-3.246223	1.380218	-0.656847
H	-4.348633	0.367787	-2.213909
H	-5.115208	0.322904	-0.637588
H	-2.403448	2.125752	1.191330
H	-4.073758	1.561813	1.320363
H	-2.255545	1.295994	-1.119316
H	-3.653997	2.355310	-0.938321
H	-0.302401	0.055423	1.207037
H	-1.298505	0.026315	1.204606

1–H_2

0 1

C	0.192352	-1.308224	-0.353621
C	-1.106737	-0.860992	0.311450
C	-1.441364	0.579374	-0.085240
C	1.375875	-0.488464	0.139298
H	0.391051	-2.367243	-0.162553
H	-1.919458	-1.547236	0.052061
H	-1.854633	0.600850	-1.104627
H	-0.243838	2.704726	-0.149496
H	1.918974	1.530087	0.082382
H	2.268265	-0.731535	-0.448446
H	1.599957	-0.761666	1.181067
H	-2.235647	0.992304	0.546214

H	0.100741	-1.188015	-1.441066
H	-0.983408	-0.924997	1.400772
N	1.100831	0.941022	0.042146
B	-0.173716	1.515083	-0.064530

2

0 1

B	-0.166209	1.383334	0.227925
N	-1.552783	0.512515	-0.165413
C	0.877114	0.161769	0.537615
H	1.349176	0.286590	1.517810
C	0.007510	-1.106448	0.565498
H	-0.455066	-1.240475	1.552025
C	-1.090367	-0.869241	-0.459279
H	-1.915608	-1.586008	-0.425240
H	0.562216	-2.024172	0.340043
H	-0.676942	-0.860489	-1.471721
C	1.980697	0.037670	-0.512285
H	2.563666	0.960897	-0.575741
H	2.672709	-0.786905	-0.297752
H	1.562202	-0.131714	-1.513133
H	0.099086	2.025483	-0.766092
H	-2.058011	0.929177	-0.940822
H	-2.174595	0.506056	0.638435
H	-0.478022	2.074781	1.171163

2'

0 1

C	-1.372389	0.376161	0.233718
C	-0.214152	-0.531590	-0.164505
H	-1.335498	0.534945	1.325915
H	-1.244967	1.359030	-0.232106
C	1.151862	-0.056253	0.386921
H	-0.433030	-1.545593	0.200651
H	-0.188002	-0.595494	-1.260460
H	1.059734	-0.023226	1.480981
N	-2.630624	-0.187853	-0.246326
H	-2.825414	-1.060636	0.235733
H	-3.403098	0.438362	-0.046817
B	2.085666	-1.218945	-0.068703
H	2.673779	-1.145754	-1.106559
H	2.150060	-2.230822	0.560400
C	1.535846	1.320124	-0.153637
H	1.508814	1.318337	-1.249370
H	0.866413	2.111322	0.199083
H	2.550241	1.598578	0.145368

[2-2']

0 1

C	3.569490	-1.316206	-0.336557
C	3.224266	-0.078833	-1.148933
C	2.801199	0.967452	-0.110041
H	4.065680	0.228490	-1.777062
H	4.504412	-1.166735	0.210438
H	3.646182	-2.241389	-0.911568
H	1.662196	-1.902469	0.282866
H	2.755087	-1.915484	1.511289
H	3.714061	1.361716	0.360421
H	2.079992	0.361866	2.151556
H	0.751335	0.203930	0.713453
H	2.380347	-0.302789	-1.814414
B	1.983487	0.110497	0.982117
N	2.472304	-1.413118	0.675584
H	-0.230882	-1.540713	1.127507
H	0.183658	-1.049798	-0.813577
B	-0.250328	-0.692575	0.261858
C	-1.515598	0.277734	0.262662
C	-2.725762	-0.561464	-0.165474
C	-4.019147	0.225679	-0.314695
H	-2.889920	-1.374480	0.555591
H	-2.505882	-1.049608	-1.127280
H	-3.820816	1.118177	-0.935518
H	-4.346320	0.593146	0.664532
N	-5.076723	-0.637369	-0.843521
H	-5.941085	-0.117176	-0.952669
H	-4.813910	-0.966731	-1.768390
C	2.017331	2.124590	-0.714759
H	1.692693	2.829098	0.057447
H	2.599402	2.685760	-1.454094
H	1.113631	1.751328	-1.212205
C	-1.735060	0.929164	1.628021
H	-1.949525	0.162583	2.383256
H	-0.839753	1.468546	1.958550
H	-2.564714	1.644684	1.631955
H	-1.381038	1.073163	-0.487742

TS-2

0 1

C	-4.160539	0.189437	0.111509
C	-2.773510	0.185651	-0.512269
H	-4.234503	-0.607836	0.869346
H	-4.309941	1.139939	0.639623

C	-1.621222	0.468704	0.455996
H	-2.766960	0.925729	-1.321139
H	-2.605179	-0.793162	-0.994994
B	-0.238935	0.582634	-0.331612
H	0.744825	0.800485	0.391412
H	-0.204741	1.240734	-1.339401
B	2.090374	-0.121315	1.024826
C	3.254564	0.574649	0.216590
N	1.820880	-1.418409	0.348727
H	1.763190	0.063869	2.151360
C	3.240338	-0.211662	-1.103596
H	4.167799	0.291371	0.770112
C	2.826096	-1.629844	-0.718959
H	1.584966	-2.233461	0.901767
H	2.481191	0.225115	-1.765446
H	4.193052	-0.195546	-1.639192
H	2.398657	-2.195034	-1.553459
H	3.679518	-2.195371	-0.327422
H	-0.036657	-0.666446	-0.865495
H	0.652613	-0.942523	-0.317376
N	-5.181484	0.080659	-0.934409
H	-5.035880	-0.780500	-1.454698
H	-6.106300	0.015382	-0.521558
C	3.231092	2.085090	0.044645
H	3.213146	2.597322	1.010520
H	4.103822	2.445120	-0.509780
H	2.334816	2.389695	-0.506609
C	-1.555563	-0.562165	1.586101
H	-1.486429	-1.578297	1.170048
H	-0.675367	-0.402713	2.219271
H	-2.433118	-0.543451	2.240758
H	-1.803023	1.458076	0.905954

2–H_2

0 1

B	-0.135347	1.272614	-0.394671
C	0.848335	0.041175	-0.569981
C	-0.126625	-1.147760	-0.462594
H	0.338628	-2.049203	-0.049921
C	-1.294533	-0.662039	0.404976
H	-1.122062	-0.873434	1.469576
H	-0.507317	-1.398370	-1.457822
H	0.058849	2.427537	-0.604377
H	1.389256	0.023954	-1.520752
H	-2.241224	-1.137594	0.128977
N	-1.321938	0.780904	0.162893

H	-2.106345	1.316694	0.499935
C	1.864266	0.051821	0.580222
H	2.511778	-0.831339	0.552434
H	2.504205	0.938398	0.546936
H	1.355878	0.054779	1.552384

TS-S1A

0 1

C	-2.371572	-1.027329	1.178247
C	-2.822224	-1.259482	-0.255829
C	-3.426185	0.005279	-0.858889
C	-2.371087	1.116277	-0.909877
H	-1.933367	-1.947103	1.587363
H	-2.310513	2.177254	1.250718
H	-1.959928	-1.573112	-0.859751
H	-3.542888	-2.083131	-0.267247
H	-3.827228	-0.205627	-1.855814
H	-4.277894	0.323079	-0.240041
H	-1.580002	0.795194	-1.602936
H	-2.800134	2.037174	-1.316717
H	-3.253540	-0.789932	1.793963
C	2.215031	1.310549	0.318105
H	1.261233	1.261963	-1.509072
C	3.573687	0.637163	0.167146
H	1.848816	1.132925	1.343208
H	2.304704	2.397621	0.211965
C	2.514948	-1.480021	-0.670775
C	3.460341	-0.872339	0.364962
H	4.275178	1.073217	0.886832
H	3.972645	0.846667	-0.834977
H	2.367400	-2.551260	-0.496275
H	2.984096	-1.404943	-1.664549
H	4.452905	-1.333819	0.322593
H	3.073863	-1.065285	1.377035
B	1.135717	-0.685061	-0.782965
B	-1.796102	1.330359	0.559571
N	-1.369670	0.052957	1.258235
N	1.183106	0.813996	-0.599984
H	0.325105	-1.055286	-1.587755
H	-1.168592	0.223178	2.239719
H	0.580056	-1.260555	0.503368
H	-0.168120	1.647248	0.064382
H	-0.046168	-0.723737	0.666144
H	-0.607386	2.202532	0.498512

[1–H_2]$_2$(syn)

0 1

C	-1.732407	1.446764	-0.587330
C	-2.834419	0.896209	0.304269
C	-3.140615	-0.565969	-0.006826
C	-1.943648	-1.450108	0.351164
H	-1.448922	2.459121	-0.272441
H	-0.512567	-1.546121	-1.559115
H	-2.544365	0.992483	1.357011
H	-3.720800	1.522443	0.160902
H	-4.041040	-0.875768	0.534623
H	-3.372070	-0.665276	-1.077733
H	-1.776716	-1.367039	1.435648
H	-2.181317	-2.501360	0.154198
H	-2.114103	1.516577	-1.613626
C	1.946926	-1.388298	-0.359023
H	0.641027	-1.624383	1.223554
C	3.137221	-0.515396	0.003904
H	1.727481	-1.259496	-1.425886
H	2.168506	-2.450433	-0.219369
C	1.726446	1.451729	0.652571
C	2.832352	0.952994	-0.279671
H	4.003324	-0.856840	-0.572527
H	3.390337	-0.640756	1.065345
H	1.435429	2.479550	0.394490
H	2.141813	1.513898	1.667558
H	3.741519	1.555025	-0.176935
H	2.527646	1.045172	-1.334534
B	0.430035	0.512462	0.681369
B	-0.645091	-1.010390	-0.481944
N	-0.530763	0.594516	-0.598641
N	0.713244	-1.054410	0.388163
H	-0.242393	0.607839	1.677180
H	0.023988	0.836710	-1.416471

[1–H_2]$_2$(anti)

0 1

C	-1.437810	1.969211	0.458527
C	-0.748848	3.204135	-0.125411
C	0.778514	3.217857	0.047957
C	1.492126	1.953821	-0.481612
H	-2.513234	1.982612	0.250963
H	-0.847165	0.885895	-1.140653
H	0.872744	0.817618	1.480386
H	-0.988546	3.251431	-1.198441
H	-1.181221	4.105543	0.320465

H	1.168851	4.121696	-0.433485
H	1.004927	3.316599	1.117468
H	1.377111	1.900781	-1.576850
H	2.565412	2.039647	-0.282098
H	-1.303915	1.909331	1.543258
C	1.437810	-1.969211	0.458527
H	0.847165	-0.885895	-1.140653
C	0.748848	-3.204135	-0.125411
H	1.303915	-1.909331	1.543258
H	2.513234	-1.982612	0.250963
C	-1.492126	-1.953821	-0.481612
H	-0.872744	-0.817618	1.480386
C	-0.778514	-3.217857	0.047957
H	1.181221	-4.105543	0.320465
H	0.988546	-3.251431	-1.198441
H	-2.565412	-2.039647	-0.282098
H	-1.377111	-1.900781	-1.576850
H	-1.168851	-4.121696	-0.433485
H	-1.004927	-3.316599	1.117468
B	-0.778514	-0.746943	0.279373
B	0.778514	0.746943	0.279373
N	-0.792073	0.790338	-0.124949
N	0.792073	-0.790338	-0.124949

TS-S2A

0 1

C	1.891743	1.662423	-0.630860
C	3.096586	0.724236	-0.639268
C	2.576926	-0.584519	-0.023997
H	1.852023	-0.123555	2.268896
H	2.006777	-1.113972	-0.804550
C	-1.701272	-1.770396	-0.538736
H	-0.233292	-0.700054	-1.595141
C	-3.098749	0.186056	-0.250596
C	-2.823696	-1.207462	0.327097
H	-3.625471	0.054622	-1.209905
B	-1.624480	0.655808	-0.648909
B	1.581378	-0.004131	1.102281
N	1.160231	1.381890	0.625491
N	-0.808493	-0.611949	-0.764890
H	-1.389515	1.565985	-1.386893
H	1.354958	2.095378	1.318293
H	-1.311315	1.246002	0.710000
H	0.093138	-0.694028	0.444178
H	-0.484306	1.351411	0.578192
H	0.434193	-0.840578	1.244410

H	1.237484	1.449128	-1.487768
H	2.162054	2.719289	-0.701329
H	3.531352	0.600567	-1.637595
H	3.881003	1.135302	0.011507
H	-2.101522	-2.144749	-1.488852
H	-1.161412	-2.593861	-0.054697
H	-3.697616	-1.865224	0.348404
H	-2.467863	-1.102385	1.363166
C	3.686919	-1.497004	0.477727
H	3.285490	-2.416627	0.914911
H	4.384183	-1.783151	-0.318318
H	4.265616	-0.994639	1.261443
C	-3.932764	1.079909	0.652518
H	-4.068222	2.074551	0.217786
H	-4.926300	0.660929	0.844222
H	-3.442242	1.212234	1.625268

[2–H_2]$_2$

0 1

B	0.712086	0.370653	-0.759598
N	0.075240	-1.080529	-0.438837
C	2.278132	0.125469	-0.463604
C	2.285812	-1.103188	0.454751
H	2.050997	-0.801706	1.485228
C	1.175208	-2.001262	-0.073349
H	0.832485	-2.742290	0.655746
H	3.246230	-1.627563	0.485218
B	-0.712086	-0.370654	0.759598
C	-2.278132	-0.125469	0.463604
N	-0.075240	1.080528	0.438837
C	-2.285812	1.103189	-0.454751
C	-1.175207	2.001262	0.073350
H	-3.246230	1.627563	-0.485217
H	-2.050997	0.801707	-1.485228
H	-0.832484	2.742291	-0.655745
H	0.391734	0.828209	-1.828387
H	0.535074	1.479544	1.143757
H	-0.391734	-0.828210	1.828387
H	-0.535074	-1.479545	-1.143757
H	-1.511864	2.527989	0.973365
H	1.511865	-2.527990	-0.973365
H	2.729363	-0.174784	-1.420845
H	-2.729363	0.174784	1.420845
C	-3.074623	-1.297167	-0.091855
H	-3.024475	-2.168901	0.568011
H	-4.132576	-1.048354	-0.231084

H	-2.700656	-1.609787	-1.076765
C	3.074622	1.297167	0.091854
H	4.132576	1.048355	0.231083
H	3.024474	2.168901	-0.568012
H	2.700656	1.609788	1.076764

TS-S1B

0 1

C	-2.553202	1.581338	-0.060226
C	-1.764198	-1.463128	0.053989
C	-3.172903	-0.920020	-0.151348
C	-3.234946	0.446748	-0.834130
C	1.425264	-1.384888	0.055544
C	3.143439	0.810164	0.485681
C	2.254218	-0.919466	-1.143013
H	2.078208	-1.944993	0.741033
H	0.685383	-2.111783	-0.290998
C	3.467020	-0.085036	-0.711285
H	3.286149	0.273266	1.429414
H	3.784320	1.695706	0.510944
H	2.601582	-1.764635	-1.744712
H	1.613328	-0.324296	-1.808356
H	3.820515	0.524384	-1.549406
H	4.296611	-0.742096	-0.433295
B	0.741894	-0.169342	0.871829
B	-0.949990	1.761243	-0.255183
H	-0.341095	0.637599	-0.151507
N	-1.026745	-0.871187	1.196485
H	1.449324	1.551073	-0.480016
N	1.720388	1.190353	0.438035
H	1.486568	1.934420	1.090874
H	0.920287	-0.084857	2.069388
H	-0.620504	2.120161	-1.379663
H	-1.525512	-0.051134	1.539607
H	-0.963942	-1.530259	1.968945
H	-3.721078	-1.648426	-0.759435
H	-3.692133	-0.880358	0.817320
H	-4.294940	0.673385	-1.006368
H	-2.775720	0.360197	-1.829674
H	-3.000654	2.533101	-0.375006
H	-2.839991	1.497680	1.003654
H	-0.483954	2.507581	0.598363
H	-1.180667	-1.266726	-0.855048
H	-1.785270	-2.546932	0.197805

[1-1"]

0 1

C	-2.888246	1.345096	0.008646
C	-1.453176	-1.601128	0.124215
C	-2.936140	-1.264455	0.127771
C	-3.329035	0.010997	-0.633862
H	-2.913682	1.217060	1.104926
H	-3.675160	2.081763	-0.182569
H	-1.091321	-1.697790	-0.903131
H	-1.239987	-2.538667	0.646703
H	-3.458580	-2.125372	-0.303792
H	-3.286520	-1.187298	1.167744
H	-2.934447	-0.054883	-1.658177
H	-4.420669	-0.018605	-0.732558
C	1.529051	-1.222888	-0.572412
H	-0.809878	2.480013	0.429462
C	2.451082	1.348521	-0.139022
C	3.056333	-1.070037	-0.631796
H	1.276106	-2.285961	-0.648781
H	1.078243	-0.743324	-1.454548
C	3.544008	0.296477	-0.112314
H	2.832354	2.340697	0.113401
H	1.971653	1.419670	-1.118678
H	3.524722	-1.858375	-0.034584
H	3.407515	-1.216789	-1.658097
H	4.396291	0.655980	-0.694148
H	3.901412	0.206000	0.921943
B	0.932989	-0.594535	0.768958
B	-1.471096	2.028049	-0.529426
H	-0.757265	1.199548	-1.133592
N	-0.661281	-0.513609	0.752762
H	0.566621	1.611029	0.660608
N	1.383095	0.985324	0.837608
H	1.721151	1.190701	1.774881
H	1.305292	-1.122022	1.791375
H	-1.658992	2.934076	-1.312381
H	-0.901673	0.328069	0.182362
H	-1.038610	-0.340590	1.684017

TS-S1C

0 1

C	-2.853565	1.367518	-0.045638
C	-1.491570	-1.713636	0.200789
C	-2.942779	-1.261633	0.115212
C	-3.167356	0.006654	-0.724653
H	-2.875093	1.247634	1.046577

H	-3.692160	2.044072	-0.241157
H	-1.115491	-2.007900	-0.784172
H	-1.362365	-2.568150	0.870352
H	-3.525853	-2.085240	-0.308598
H	-3.336764	-1.099153	1.128084
H	-2.597284	-0.085729	-1.660556
H	-4.218411	0.005972	-1.027214
C	1.582594	-1.217887	-0.635974
H	-0.747633	2.546226	0.761030
C	2.275860	1.346954	0.033476
C	3.096319	-0.969622	-0.686003
H	1.388482	-2.284265	-0.807305
H	1.097709	-0.685145	-1.473547
C	3.487539	0.470555	-0.277199
H	2.607722	2.340024	0.359572
H	1.697017	1.514402	-0.885667
H	3.577674	-1.678816	-0.003243
H	3.494064	-1.195250	-1.681317
H	4.084304	0.948692	-1.061989
H	4.123170	0.445690	0.616424
B	1.013482	-0.711890	0.778781
B	-1.538355	2.153217	-0.541563
H	-0.729731	1.572216	-1.219929
N	-0.634075	-0.615705	0.672781
H	-0.181748	1.976403	0.754706
N	1.390910	0.762364	1.045587
H	1.821818	0.877619	1.957129
H	1.242500	-1.448735	1.719813
H	-1.608460	3.328655	-0.749926
H	-0.766454	0.161479	0.022160
H	-0.972757	-0.277378	1.574054

[1-1'']–H_2

0 1

C	-3.277500	1.290764	-0.089805
C	-1.388136	-1.454957	0.096761
C	-2.880738	-1.228487	0.285578
C	-3.522440	-0.140734	-0.580657
H	-3.506002	1.383073	0.979489
H	-4.012564	1.965605	-0.570160
H	-1.157327	-1.660417	-0.953475
H	-1.059679	-2.327321	0.670598
H	-3.371676	-2.183403	0.071504
H	-3.084981	-1.020027	1.345433
H	-3.167224	-0.244727	-1.614703
H	-4.599940	-0.332312	-0.607446

C	1.723464	-1.165492	-0.651059
C	2.351279	1.403495	0.153472
C	3.227158	-0.875741	-0.595139
H	1.552957	-2.233382	-0.835459
H	1.290170	-0.633828	-1.518325
C	3.508655	0.633783	-0.507848
H	2.706830	2.371352	0.525240
H	1.608094	1.650732	-0.621210
H	3.630835	-1.369585	0.298588
H	3.766279	-1.304249	-1.447407
H	3.674483	1.046643	-1.511032
H	4.436130	0.804156	0.050876
B	1.115022	-0.666828	0.762670
B	-1.959609	2.015971	-0.482207
H	-1.361910	1.684489	-1.468861
N	-0.524033	-0.336008	0.520125
N	1.666591	0.668171	1.207302
H	2.225120	0.626372	2.049882
H	1.108170	-1.503987	1.646093
H	-1.550701	2.945950	0.137802
H	-0.513944	0.404333	-0.185215
H	-0.838531	0.083887	1.395672

TS-S1D

0 1

C	-3.538097	1.214792	-0.090952
C	-1.448877	-1.241161	-0.003512
C	-2.917793	-1.218734	0.403152
C	-3.822690	-0.263197	-0.371826
H	-3.630525	1.426409	0.981900
H	-4.321544	1.828491	-0.568094
H	-1.356446	-1.373574	-1.087220
H	-0.966424	-2.111757	0.458564
H	-3.298831	-2.239054	0.286684
H	-2.985132	-0.997639	1.478316
H	-3.715258	-0.460264	-1.446730
H	-4.862403	-0.495096	-0.116789
C	1.794498	-1.167121	-0.537618
C	2.661144	1.391625	0.141726
C	3.317630	-0.979492	-0.580892
H	1.536589	-2.223973	-0.663914
H	1.353578	-0.636647	-1.397743
C	3.715317	0.506314	-0.549640
H	3.135473	2.288796	0.549722
H	1.952192	1.754948	-0.622100
H	3.749957	-1.484370	0.291192

H	3.761039	-1.458535	-1.460771
H	3.859874	0.879809	-1.570241
H	4.679082	0.613244	-0.041157
B	1.305535	-0.566817	0.864644
B	-2.219717	1.781231	-0.702652
H	-1.859507	1.401905	-1.781163
N	-0.650030	-0.066756	0.374802
N	1.949653	0.678969	1.185489
H	1.990305	1.067816	2.112108
H	0.973203	-1.282629	1.773771
H	-1.618502	2.678629	-0.193919
H	-0.478669	0.593880	-0.378921
H	-0.991293	0.413902	1.201871

[1-1'''']

0 1

C	-1.928261	-1.362267	0.473027
C	-3.164194	-0.726256	-0.148409
C	-3.219819	0.787738	0.046814
C	-1.936332	1.454779	-0.459965
H	-1.907152	-2.442309	0.302187
H	-0.758002	-0.886802	-1.088314
H	-0.690700	0.893778	1.468138
H	-3.174594	-0.955249	-1.224533
H	-4.055441	-1.201800	0.273307
H	-4.111322	1.190752	-0.446230
H	-3.328471	1.001401	1.118110
H	-1.887686	1.344497	-1.557865
H	-1.978899	2.533659	-0.259020
H	-1.900657	-1.203947	1.556667
C	1.877131	1.358658	0.675852
H	0.988409	0.838466	-1.106536
C	3.131355	0.806945	0.019985
H	1.585431	0.741705	1.528055
H	2.016371	2.383517	1.025480
C	1.918539	-1.403489	-0.660030
H	0.873887	-1.389848	1.510278
C	3.162142	-0.719837	-0.066760
H	3.998535	1.153690	0.591158
H	3.237998	1.251820	-0.981023
H	2.243243	-2.395624	-0.992773
H	1.646487	-0.908758	-1.615612
H	4.062163	-0.992012	-0.632178
H	3.308610	-1.115332	0.946272
B	0.634760	-1.666854	0.347450
B	-0.691407	0.749547	0.268930

N	-0.673649	-0.784475	-0.072879
N	0.712786	1.366414	-0.275960
H	0.532716	2.316783	-0.590525
H	0.264981	-2.823046	0.251848

[1-1'''] –H_2

0 1

C	2.136944	1.468880	0.449737
C	3.164621	0.542315	-0.192159
C	3.011416	-0.949488	0.098835
C	1.740261	-1.606805	-0.449656
H	2.537345	2.491847	0.443565
H	0.907989	1.451741	-1.222877
H	0.468598	-1.181598	1.566590
H	3.155102	0.706892	-1.280363
H	4.157342	0.860434	0.146394
H	3.893720	-1.455457	-0.310633
H	3.053252	-1.100145	1.186000
H	1.603118	-1.339884	-1.508544
H	1.895719	-2.696500	-0.448455
H	1.981028	1.198971	1.500753
C	-2.138347	-1.468159	0.477160
C	-3.155047	-0.545447	-0.190826
H	-1.961421	-1.152162	1.511924
H	-2.565079	-2.479130	0.528518
C	-1.739293	1.609393	-0.475047
C	-3.004647	0.949602	0.086166
H	-4.153310	-0.855547	0.139585
H	-3.132213	-0.721876	-1.276616
H	-1.922993	2.693697	-0.530738
H	-1.577767	1.291580	-1.515988
H	-3.890335	1.447470	-0.325743
H	-3.045443	1.111087	1.172001
B	-0.426602	1.469906	0.387214
B	0.419496	-1.377122	0.384272
N	0.841808	1.442328	-0.211085
N	-0.850935	-1.514468	-0.196462
H	-0.925361	-1.697126	-1.190621
H	-0.475311	1.465013	1.585384

TS-S1E

0 1

C	1.992759	1.407129	0.475930
C	3.198963	0.697460	-0.124698
C	3.165060	-0.821039	0.058426
C	1.875115	-1.463076	-0.468341

H	2.080312	2.492497	0.351133
H	0.857431	0.934740	-1.172070
H	0.672076	-0.842541	1.476904
H	3.243820	0.936705	-1.197886
H	4.110055	1.113639	0.316961
H	4.052068	-1.251202	-0.421140
H	3.253794	-1.043733	1.129888
H	1.818442	-1.336540	-1.562664
H	1.910428	-2.545414	-0.293621
H	1.909308	1.201683	1.548723
C	-2.001046	-1.416200	0.532023
C	-3.190075	-0.681795	-0.087399
H	-1.849672	-1.090912	1.568680
H	-2.227481	-2.492456	0.576178
C	-1.858567	1.489308	-0.541310
C	-3.136205	0.843131	0.023099
H	-4.117377	-1.039174	0.374850
H	-3.251211	-0.966946	-1.148266
H	-1.979559	2.582864	-0.497692
H	-1.732001	1.233634	-1.602043
H	-4.017428	1.259621	-0.477586
H	-3.226267	1.121156	1.081782
B	-0.608570	1.118230	0.327633
B	0.592718	-0.857271	0.271637
N	0.767186	0.904719	-0.157833
N	-0.784159	-1.149814	-0.210688
H	-0.695217	1.197379	1.517049
H	-0.889473	-1.383645	-1.192265

TS-S2B

0 1

C	2.405864	-0.496110	0.121517
C	1.480777	1.861417	0.568155
C	2.640608	1.013499	0.081082
C	-2.144796	0.425175	-0.456669
C	-2.994800	-0.789670	-0.081235
H	-1.928875	0.356991	-1.534714
C	-2.063048	-1.985880	0.002866
B	-0.759584	0.340717	0.364091
B	1.298704	-0.985284	-0.964793
H	0.154940	-0.520940	-0.690233
N	0.219354	1.605998	-0.189929
N	-0.965942	-1.562552	0.882116
H	1.543843	-0.552292	-2.084636
H	2.092700	-0.752351	1.150828
H	1.126471	-2.198929	-0.958929

H	2.892816	1.304014	-0.950847
H	3.508864	1.295283	0.694982
H	1.726709	2.925138	0.489394
H	1.253382	1.646586	1.617943
C	-2.916658	1.719471	-0.197834
H	-2.401201	2.611517	-0.575710
H	-3.898149	1.707132	-0.684428
H	-3.082042	1.865140	0.876154
C	3.728579	-1.204780	-0.160619
H	3.612031	-2.291528	-0.112312
H	4.071536	-0.965918	-1.175588
H	4.526056	-0.913916	0.536848
H	-0.776957	0.653923	1.538084
H	-1.222116	-1.634012	1.863039
H	-0.107939	-2.084550	0.702854
H	-2.556385	-2.897919	0.353793
H	-1.624694	-2.194776	-0.978523
H	-3.452202	-0.617986	0.905155
H	-3.814324	-0.965307	-0.785703
H	-0.376495	2.431977	-0.126293
H	0.443390	1.452694	-1.176531

[2-2'']

0 1

C	2.720207	0.234900	-0.035887
C	0.663432	1.780122	0.037079
C	1.519005	0.831822	-0.780940
H	3.244406	1.074413	0.453161
H	-0.119490	2.252177	-0.563708
H	1.298149	2.572090	0.449477
H	0.893996	0.020432	-1.188767
H	1.857372	1.407617	-1.654793
C	-2.061333	0.347626	-0.461063
H	1.728530	-0.564217	2.062387
C	-2.549789	-1.075002	-0.749155
H	-1.373902	0.619773	-1.277220
C	-1.350127	-1.959001	-0.447476
B	-1.263350	0.137003	0.919963
B	2.388240	-0.931467	1.069278
H	1.761702	-1.845113	0.490222
N	-0.001545	1.094013	1.186864
H	0.281764	-1.527775	0.808605
N	-0.759441	-1.404189	0.810020
H	-1.102295	-1.920241	1.614983
H	-1.966721	0.215230	1.901176
H	3.407610	-1.416581	1.516906

H	0.743852	0.528317	1.653867
H	-0.302352	1.794058	1.859462
H	-3.377135	-1.325235	-0.070435
H	-2.910951	-1.221247	-1.771431
H	-1.577423	-3.019816	-0.331004
H	-0.586457	-1.861591	-1.225971
C	-3.187061	1.369912	-0.400166
H	-2.809257	2.374793	-0.177742
H	-3.746764	1.433346	-1.339670
H	-3.895164	1.110434	0.395183
C	3.667606	-0.358780	-1.077491
H	4.563361	-0.766467	-0.601646
H	3.177792	-1.191896	-1.599919
H	3.980185	0.371465	-1.836919

[2-2'']−H_2

0 1

C	3.247682	-0.070868	0.282052
C	0.950915	1.029766	0.224891
C	2.342266	0.961736	-0.382377
H	3.266401	0.090146	1.367270
H	2.267227	0.738505	-1.456405
H	2.790087	1.960728	-0.306507
C	-2.251173	0.732667	-0.297306
C	-3.476013	-0.163362	-0.528065
H	-1.722910	0.817819	-1.267180
C	-2.914919	-1.584321	-0.481861
B	-1.386435	-0.180095	0.739107
B	3.009560	-1.560923	-0.105916
H	2.653107	-1.824381	-1.216744
N	0.208766	-0.243359	0.186775
N	-1.899950	-1.593948	0.579898
H	-2.262765	-2.008769	1.427113
H	-1.260721	0.229006	1.878796
H	3.277669	-2.448151	0.642169
H	0.179484	-0.625942	-0.760368
H	0.648230	-0.955400	0.771015
H	-4.175006	-0.027945	0.309925
H	-4.021924	0.060747	-1.453450
H	-3.682033	-2.348007	-0.318602
H	-2.445735	-1.821298	-1.451419
H	0.990191	1.332923	1.275994
H	0.333168	1.767535	-0.294663
C	-2.621678	2.132752	0.176375
H	-1.739001	2.767666	0.322333
H	-3.289957	2.652549	-0.521324

H	-3.132336	2.077889	1.144954
C	4.698361	0.082481	-0.242510
H	5.078689	1.076494	0.011240
H	5.383680	-0.653320	0.188742
H	4.734484	-0.017656	-1.332753

TS-S2D

C	3.345692	-0.110634	0.239016
C	1.066082	0.977832	0.462753
C	2.418485	1.013926	-0.232099
H	3.491311	-0.013764	1.322897
H	2.274573	0.928222	-1.319130
H	2.887066	1.991097	-0.056965
C	-2.206938	0.751147	-0.327286
C	-3.281363	-0.212546	-0.870862
H	-1.452137	0.905033	-1.117601
C	-2.821867	-1.618082	-0.481853
B	-1.581719	-0.092148	0.902534
B	2.747533	-1.506325	-0.147864
N	0.332839	-0.285886	0.320220
N	-2.176541	-1.404454	0.804111
H	-2.080769	-2.181902	1.435571
H	-1.298135	0.384545	1.971085
H	-4.227539	-0.004204	-0.355157
H	-3.461817	-0.108016	-1.946045
H	-3.657074	-2.323795	-0.412105
H	-2.127092	-2.021505	-1.242482
H	1.176269	1.158285	1.536901
H	0.415375	1.772029	0.081315
C	-2.785186	2.111481	0.048798
H	-2.009077	2.799471	0.402701
H	-3.301987	2.592566	-0.790594
H	-3.510607	2.002669	0.863419
C	4.712391	0.011172	-0.455756
H	5.175658	0.976166	-0.225637
H	5.410034	-0.771636	-0.145951
H	4.599697	-0.054631	-1.543534
H	0.298304	-0.611568	-0.644682
H	0.696737	-1.029544	0.913301
H	2.479822	-1.707932	-1.297408
H	2.614463	-2.402610	0.630173

[2-2'''']

0 1

C	-1.275726	-1.967441	0.178490
C	-2.643853	-1.255173	0.072387

C	-2.364260	0.214621	-0.310546
H	-0.296368	-1.027882	-1.309698
H	-0.711855	0.512771	1.375670
H	-2.404052	0.293732	-1.412924
H	0.224832	1.184959	-1.503842
C	1.195113	2.076669	0.080346
C	2.331562	-0.230545	-0.270433
H	1.293612	-1.664195	1.265497
C	2.124838	1.003560	0.624207
H	2.283804	0.086213	-1.332413
B	1.279465	-1.435040	0.067002
B	-0.841346	0.351013	0.185821
N	-0.238310	-1.012008	-0.288489
N	-0.036477	1.528651	-0.578663
H	-0.691789	2.291968	-0.741167
H	1.511700	-2.436488	-0.591890
H	-3.148396	-1.284341	1.044009
H	-3.308404	-1.752820	-0.640336
H	-1.205002	-2.895955	-0.393034
H	-1.024827	-2.204439	1.215276
H	0.847585	2.731641	0.883167
H	1.709029	2.696054	-0.662399
H	1.763946	0.668446	1.603638
H	3.080008	1.515768	0.808000
C	-3.370038	1.191536	0.280973
H	-3.153765	2.230170	-0.003183
H	-4.398649	0.984184	-0.034439
H	-3.341759	1.145063	1.375467
C	3.737821	-0.779561	-0.033022
H	4.522565	-0.041449	-0.244115
H	3.843021	-1.085421	1.015222
H	3.924936	-1.666341	-0.644960

[2-2'''] − H_2

0 1

C	-1.340928	-2.093403	-0.364175
C	-2.291487	-1.138633	0.365390
C	-2.258247	0.305469	-0.156361
H	0.034118	-1.092889	-1.560653
H	-0.551917	0.890466	1.406430
H	-2.390090	0.294527	-1.251174
C	1.331464	2.092953	-0.329891
C	2.240866	-0.327724	-0.133959
C	2.161823	1.089130	0.468889
H	2.289525	-0.224050	-1.231120
B	0.984300	-1.206591	0.275033

B	-0.880542	0.965896	0.254514
N	-0.033154	-1.510995	-0.640926
N	-0.032418	1.655717	-0.623838
H	-0.298119	1.750088	-1.594153
H	0.886968	-1.629950	1.393954
H	1.322573	3.053095	0.202092
H	1.839212	2.275703	-1.284342
H	3.175623	1.506952	0.540258
H	1.791849	1.031502	1.500652
H	-1.209359	-3.004717	0.227747
H	-1.787787	-2.400325	-1.316266
H	-3.310004	-1.545294	0.302656
H	-2.032938	-1.121468	1.433584
C	3.519941	-1.016006	0.351108
H	4.417092	-0.463640	0.049392
H	3.521960	-1.080465	1.445368
H	3.609116	-2.036810	-0.033493
C	-3.406937	1.100722	0.472311
H	-4.381277	0.656340	0.240086
H	-3.304399	1.116308	1.563994
H	-3.420896	2.139995	0.130723

TS-S2E

0 1

B	-0.818967	-0.114403	-0.959148
N	-0.366161	1.222096	-0.598780
C	-2.317402	-0.222085	-0.453604
C	-2.407001	0.932700	0.554666
H	-2.067833	0.575426	1.536201
C	-1.435715	1.996993	0.042087
H	-1.046269	2.628013	0.849831
H	-3.418002	1.330059	0.684890
B	0.818942	0.114371	0.959135
C	2.317382	0.222105	0.453600
N	0.366199	-1.222153	0.598784
C	2.407016	-0.932677	-0.554667
C	1.435763	-1.997005	-0.042088
H	3.418029	-1.330005	-0.684894
H	2.067837	-0.575412	-1.536203
H	1.046338	-2.628022	-0.849847
H	-0.328925	-0.740529	-1.847794
H	-0.304409	-1.744028	1.145292
H	0.328911	0.740481	1.847800
H	0.304433	1.743954	-1.145322
H	1.930257	-2.653830	0.686708
H	-1.930190	2.653822	-0.686719

H	-2.888147	0.072003	-1.352556
H	2.888132	-0.071968	1.352554
C	2.878666	1.541749	-0.052141
H	2.676648	2.360795	0.644882
H	3.961755	1.494181	-0.206938
H	2.438623	1.813783	-1.019416
C	-2.878725	-1.541705	0.052156
H	-3.961797	-1.494068	0.207052
H	-2.676826	-2.360744	-0.644910
H	-2.438605	-1.813796	1.019380

[1-1']N

0 1

C	2.827108	1.837441	0.073097
C	4.176837	1.208111	0.426460
C	4.423007	-0.060974	-0.387944
C	3.334231	-1.100322	-0.175813
H	5.010900	1.902152	0.266935
H	2.869419	2.196092	-0.968589
H	2.662062	2.730358	0.685843
H	1.520848	0.401970	1.437485
H	0.539438	1.154983	-0.163708
H	4.470499	0.191808	-1.457590
H	5.387026	-0.513640	-0.134768
H	3.542444	-2.016535	-0.738421
H	3.260977	-1.362113	0.884940
H	2.013006	-0.341348	-1.557559
H	1.271170	-1.257370	-0.384029
H	4.186651	0.944456	1.493055
H	-0.117823	-1.034252	1.225355
H	-0.730768	-2.545026	1.103882
C	-1.478846	-1.225600	-0.276354
C	-2.610389	-0.561816	0.493593
H	-1.869208	-2.040886	-0.896906
C	-3.703586	-0.016177	-0.414034
H	-2.188779	0.256702	1.094671
H	-3.042706	-1.279609	1.206076
C	-4.832529	0.667196	0.351418
H	-4.114861	-0.831084	-1.024633
H	-3.263094	0.693267	-1.126509
H	-5.268418	-0.016757	1.097030
H	-4.429885	1.480168	0.979343
H	-5.984052	1.286605	-1.671819
H	-6.918642	1.793824	0.081389
H	-1.043707	-0.488682	-0.965196
B	-5.993662	1.289034	-0.477587

B	1.614680	0.795322	0.282251
N	2.011331	-0.559162	-0.562351
N	-0.394557	-1.757125	0.557760

TS-S1F

0 1

C	3.635537	-0.188156	0.312160
C	4.634073	0.746692	-0.363079
C	2.382527	-0.421635	-0.519237
H	4.152199	1.712862	-0.592726
H	4.911731	0.371784	-1.360202
H	3.350669	0.225078	1.287960
H	4.118864	-1.150381	0.527299
C	1.395329	-1.343581	0.172914
H	2.661622	-0.841619	-1.496443
H	1.888108	0.537559	-0.722465
H	6.098383	0.735169	1.547141
H	6.777198	1.761194	-0.094247
H	1.082385	-0.904918	1.126340
H	1.861054	-2.312734	0.393254
H	-0.591937	-1.902318	-0.065691
H	0.333598	-2.049249	-1.475887
C	-3.332462	-1.051263	0.090263
H	-2.246781	-0.781883	1.801133
C	-4.351408	0.085687	0.043908
H	-3.067064	-1.309096	-0.950455
H	-3.787376	-1.952968	0.518530
C	-2.529430	1.814100	0.154213
H	-0.522662	0.892850	1.108198
C	-3.758706	1.327995	-0.616341
H	-5.250208	-0.248110	-0.488640
H	-4.659558	0.330568	1.070408
H	-2.063788	2.666512	-0.355047
H	-2.858703	2.193395	1.134188
H	-3.468135	1.068633	-1.646451
H	-4.522413	2.110508	-0.701180
H	-0.458029	-0.321001	-0.774336
H	-0.982874	0.488323	-0.854012
B	-1.487618	0.617996	0.424585
B	5.931239	1.098747	0.422428
N	0.175086	-1.511299	-0.630347
N	-2.093248	-0.734831	0.798839

[2-2']N

0 1

C	3.199599	0.879313	0.176402

C	2.171925	0.411063	1.207510
C	2.307667	-1.102218	1.231470
H	2.298611	0.838064	2.208979
H	4.197745	0.753838	0.624651
H	2.066691	0.165264	-1.773499
H	3.968127	-0.510782	-1.664063
H	3.232656	-1.386877	1.740982
H	3.016153	-2.314461	-0.317189
H	1.480446	-1.729746	-0.554032
H	1.162382	0.684191	0.859433
H	-0.794355	-1.859412	-1.884995
H	0.051068	-0.498480	-1.590903
C	-1.392904	-0.885188	-0.189421
C	-2.478717	0.002027	-0.788159
C	-3.478882	0.555589	0.232663
H	-3.020407	-0.568669	-1.556412
H	-1.996332	0.837188	-1.312744
H	-2.886476	1.136103	0.977604
H	-5.382139	2.006678	0.259004
H	-3.962322	2.436325	-1.164225
H	-0.896455	-0.344419	0.629345
B	-4.353250	1.735716	-0.281043
B	2.987046	-0.171801	-1.042332
N	-0.363999	-1.316791	-1.140311
N	2.422639	-1.500569	-0.201794
C	3.013564	2.338342	-0.210349
H	3.115852	3.021468	0.642418
H	3.740291	2.643765	-0.969118
H	2.016275	2.489389	-0.643241
H	1.474217	-1.626687	1.709425
C	-4.230645	-0.536206	0.999022
H	-4.739696	-1.211882	0.303099
H	-3.567870	-1.146469	1.619431
H	-4.993004	-0.105668	1.653240
H	-1.830567	-1.783102	0.259602

TS-S2F

0 1

C	3.703144	0.385164	0.312328
C	2.472314	0.321875	-0.595585
C	1.515083	-0.807679	-0.250955
H	2.797128	0.211711	-1.640442
H	1.925512	1.271012	-0.537955
H	-0.419806	-1.398952	-0.722394
H	0.441159	-0.734440	-2.046437
C	-3.128308	-1.558145	0.134677

H	-1.593522	-1.758671	1.511193
C	-3.603243	-0.278741	-0.544758
H	-3.838171	-1.828358	0.931513
C	-3.198973	0.837792	0.423000
H	-1.272255	0.671033	1.957610
H	-3.058681	-0.141631	-1.493835
H	-4.671781	-0.307661	-0.786366
H	-3.879518	0.789406	1.288270
H	-0.384138	0.270096	-0.552442
H	-0.901506	0.926123	0.018674
H	4.019337	2.702957	-0.208136
H	5.651027	1.742334	0.592244
H	1.984354	-1.788033	-0.386342
N	0.283835	-0.710680	-1.045014
N	-1.803912	-1.213082	0.684488
B	4.526112	1.702789	0.198314
B	-1.761645	0.300601	0.916352
C	-3.269376	2.227889	-0.186139
H	-4.280948	2.493084	-0.517126
H	-2.940492	2.993665	0.523698
H	-2.610114	2.295148	-1.062014
H	-3.083581	-2.411309	-0.556258
H	1.208972	-0.730220	0.800326
H	3.329183	0.534525	1.350411
C	4.531867	-0.902733	0.306223
H	3.982387	-1.759122	0.708285
H	4.836521	-1.159506	-0.714242
H	5.442080	-0.786339	0.899374

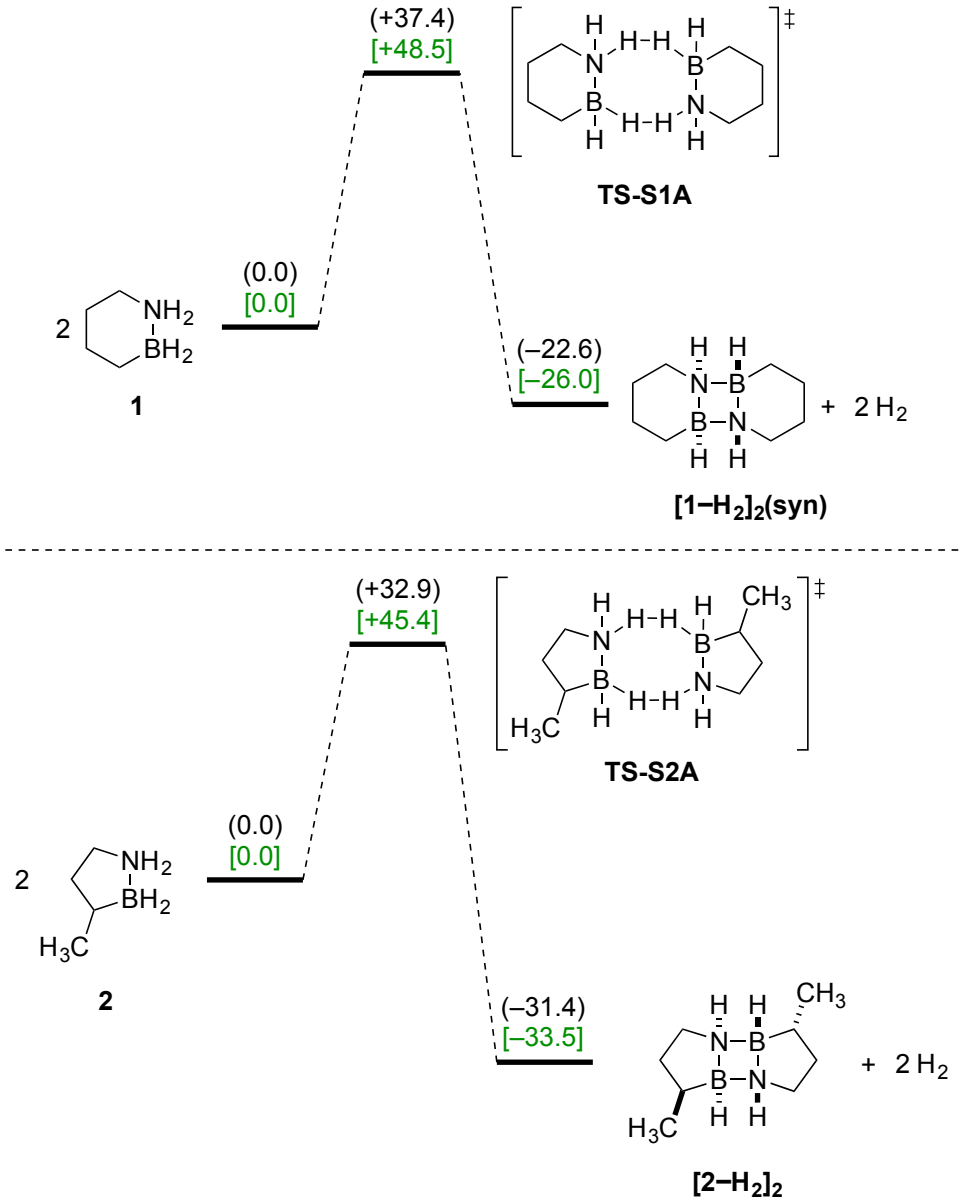


Figure S6. Potential energy surfaces for pathway (A): bimolecular release of two H_2 equivalents from **1** (top) or **2** (bottom) based on a "head-to-tail" interaction. Gas-phase enthalpy (black) and free energy [green] values (kcal-mol^{-1}) were calculated at 298 K using DFT at the M06/DZVP2 level of theory.

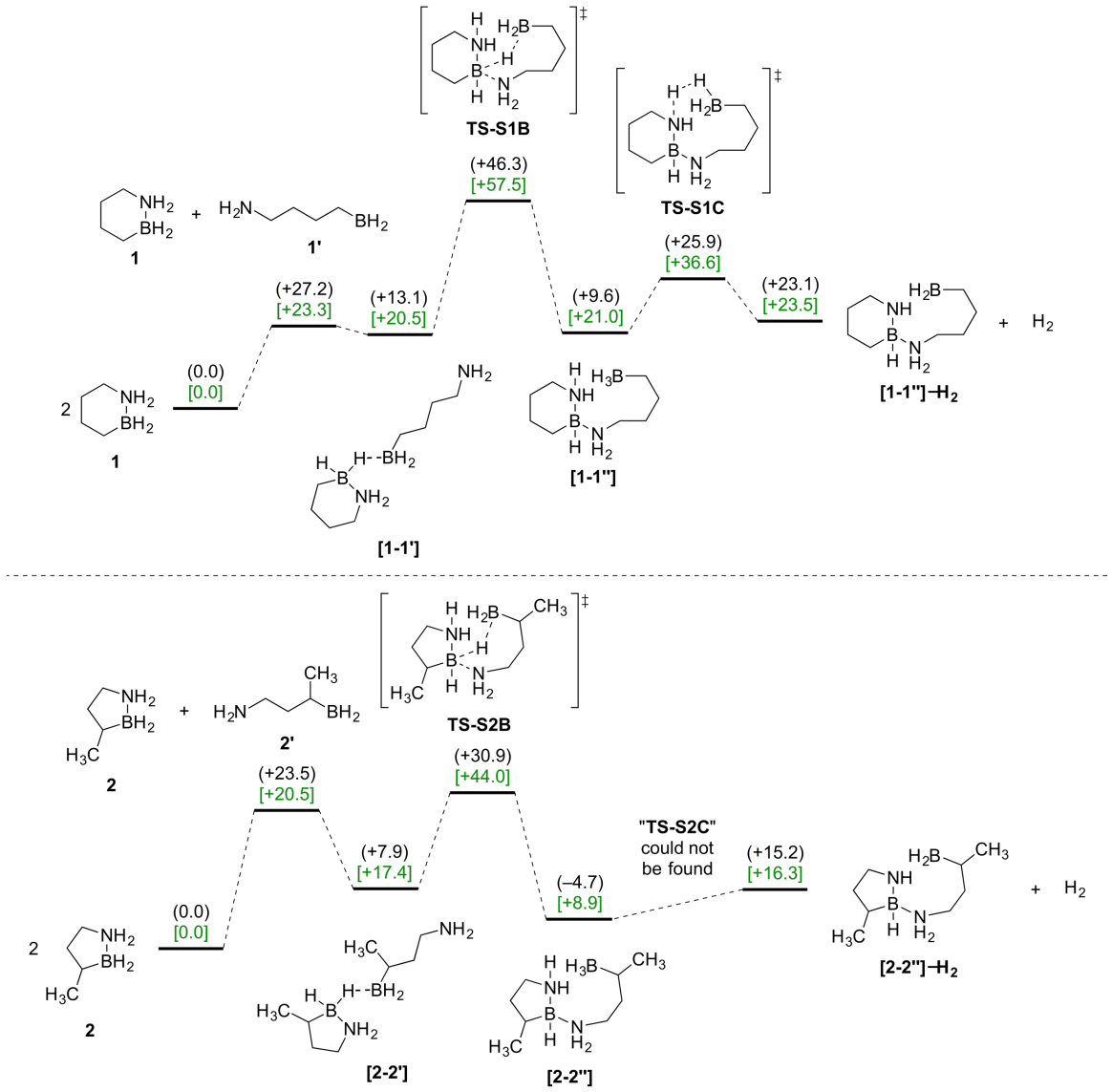


Figure S7. Potential energy surfaces for pathway (B): bimolecular release of one H_2 equivalent from **1** (top) or **2** (bottom) through a DADB-like intermediate. Gas-phase enthalpy (black) and free energy [green] values (kcal-mol^{-1}) were calculated at 298 K using DFT at the M06/DZVP2 level of theory.

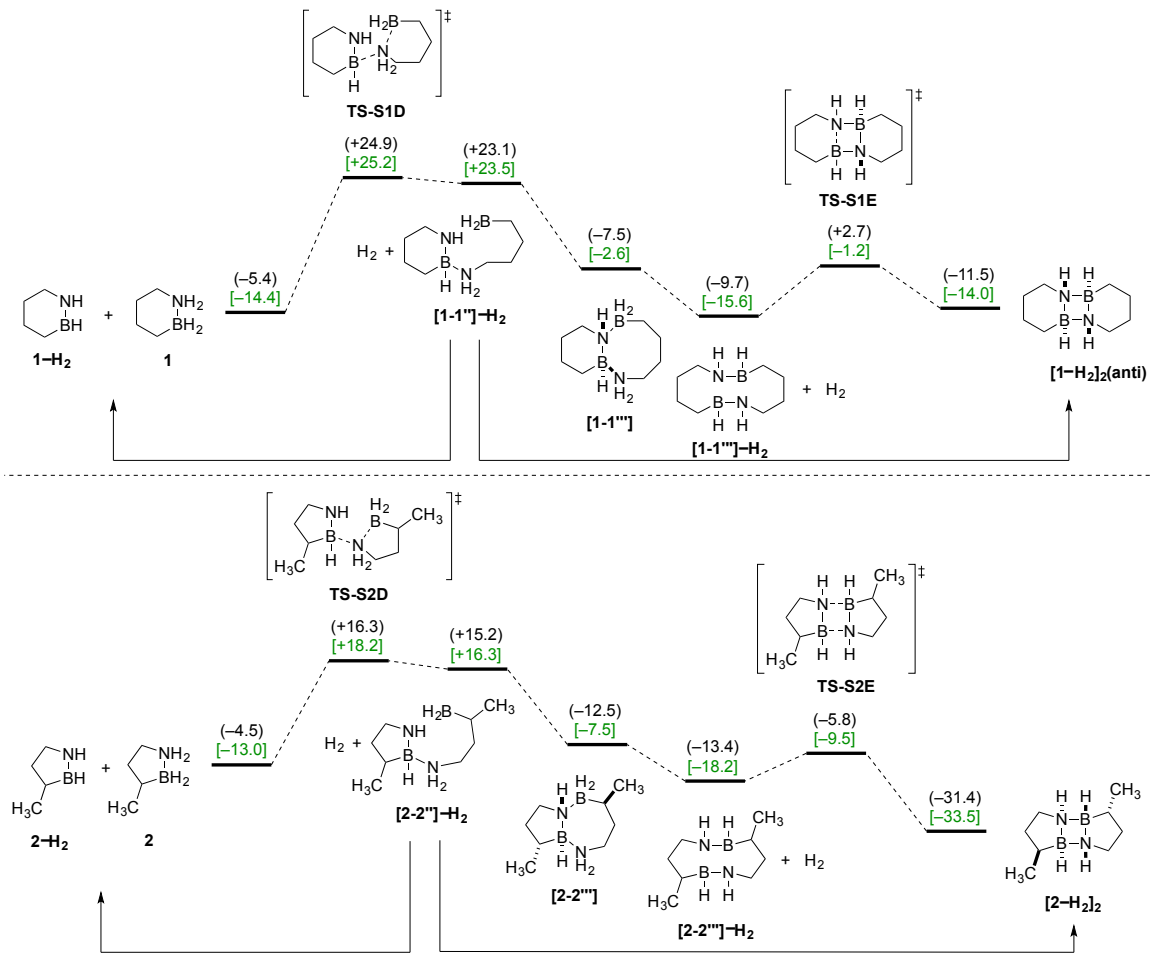


Figure S8. Potential energy surfaces for continued decomposition of **[1-1"]−H₂** (top) or **[2-2"]−H₂** (bottom) to thermodynamically stable species. Gas-phase enthalpy (black) and free energy [green] values (kcal-mol^{-1}) were calculated at 298 K using DFT at the M06/DZVP2 level of theory.

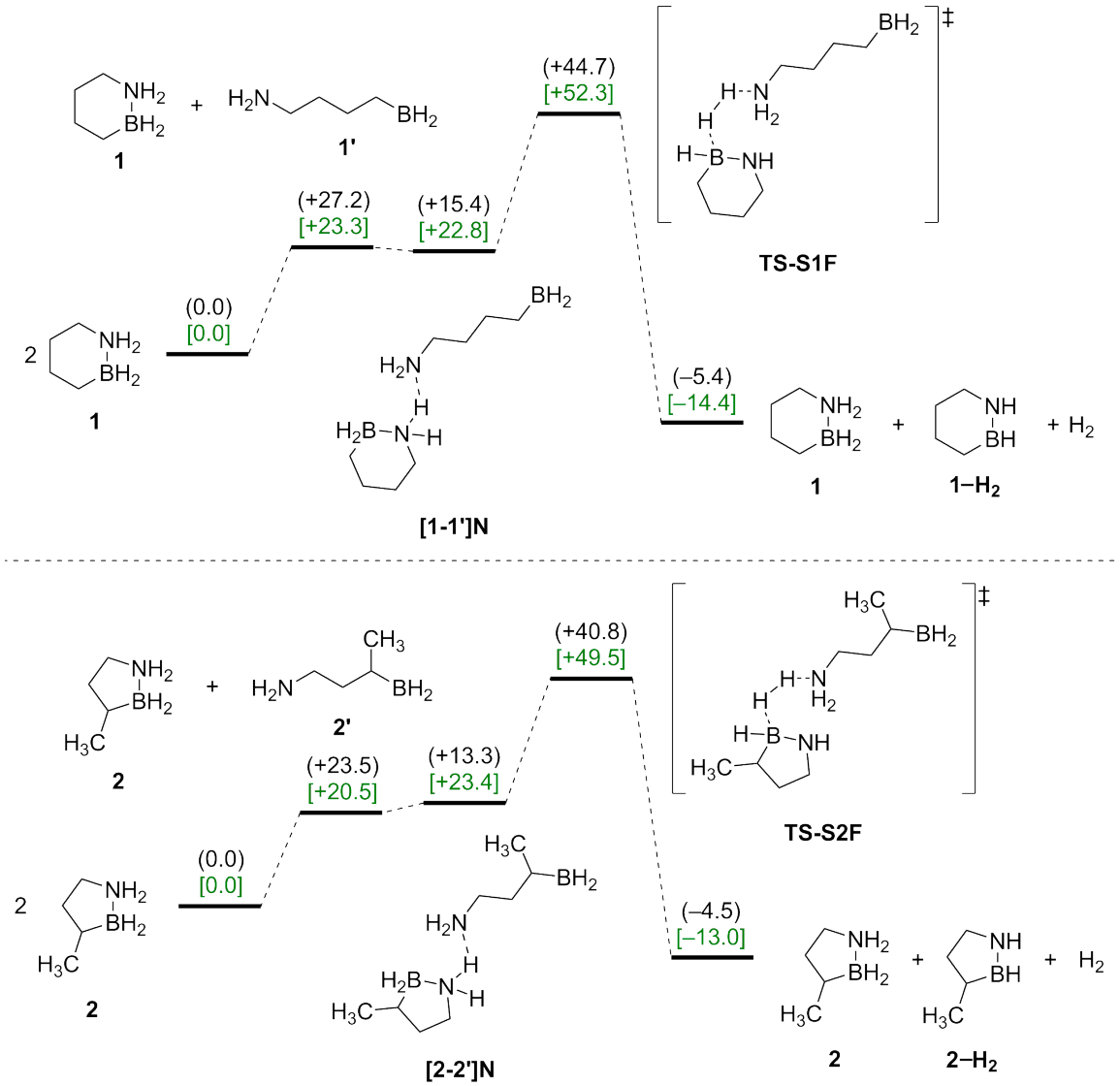


Figure S9. Potential energy surfaces for pathway (D): bimolecular H_2 release from **1** (top) or **2** (bottom) involving proton transfer mediated by a ring-opened intermediate. Gas-phase enthalpy (black) and free energy [green] values (kcal-mol^{-1}) were calculated at 298 K using DFT at the M06/DZVP2 level of theory.

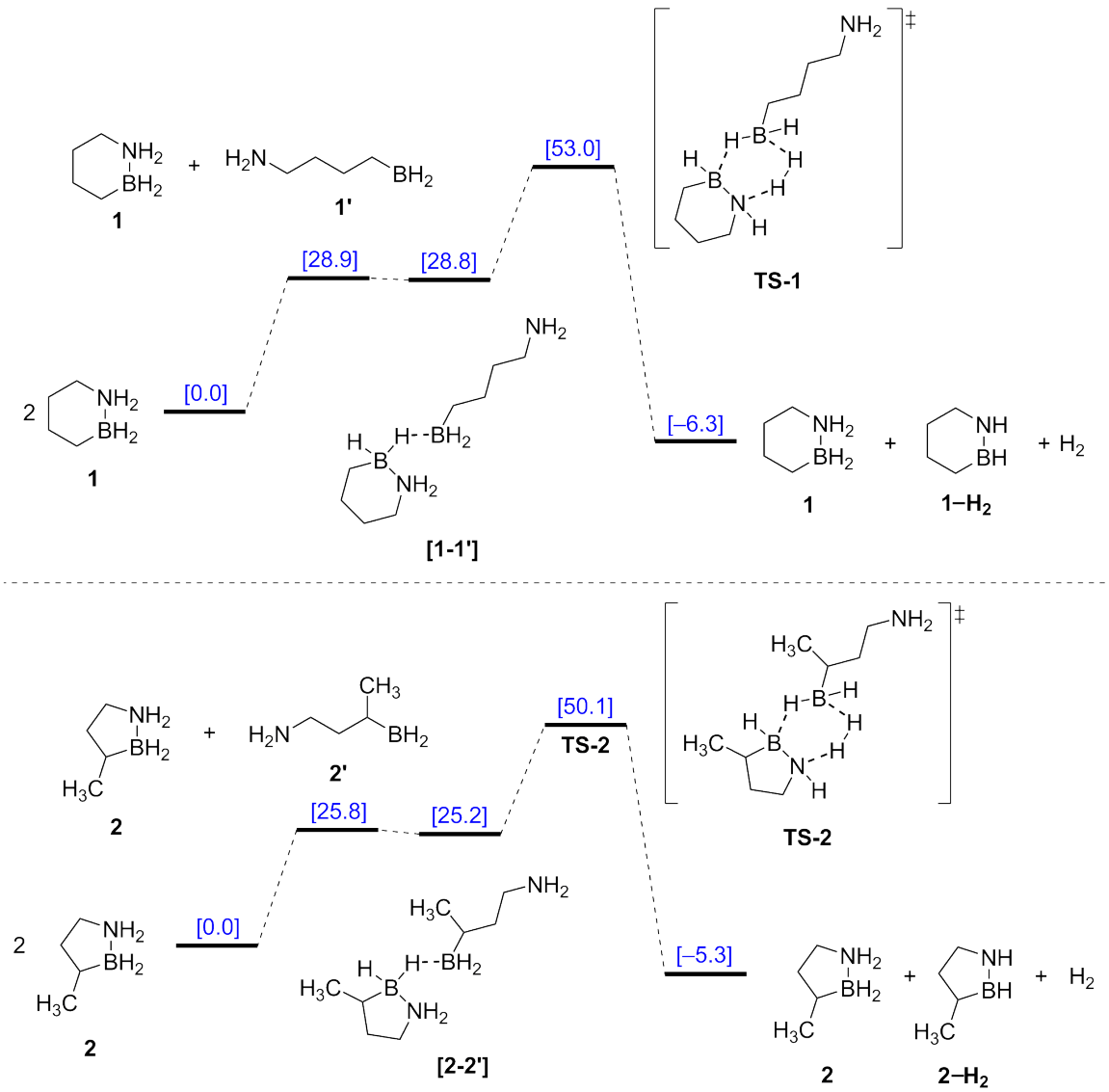


Figure S10. Potential energy surfaces for pathway (C) in *tetraglyme*. Solvent-phase free energy values (kcal-mol^{-1}) were calculated at 298 K using COSMO at the B3LYP/DZVP2 level of theory.

Calculation of strain energies

The strain energies of **1** and **2** were calculated using the homodesmotic reactions shown in Table S3; strain energy was interpreted as the opposite value of the forward reaction enthalpy (ΔH_{rxn}). The heats of formation (ΔH_f) of the required species were calculated at the G3MP2 level of theory[13] and are listed in Table S4. The method was validated by calculation of the strain energy of cyclopentane and comparison with experimental values.[14] Cyclohexane was assumed to be strain free.

Table S3. Enthalpies of homodesmotic reactions (ΔH_{rxn}; kcal-mol^{-1}) to determine the strain energies of **1** and **2** based on the calculated heats of formation listed in Table S4.

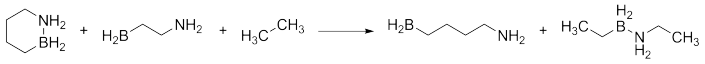
Reaction	ΔH_{rxn} (0K,calc.)	ΔH_{rxn} (298K,calc.)	ΔH_{rxn} (298K,exp.)
	−6.2	−5.9	−6.2
 **1**	+1.1	+1.3	
 **2**	−2.9	−1.8	

Table S4. Calculated (G3MP2) heats of formation (ΔH_f; kcal-mol^{-1}) of the individual species in the reactions in Table S3, and comparison to experimental values when available.

Molecule	ΔH_f (0K,calc.)	ΔH_f (298K,calc.)	ΔH_f (298K,exp.)
CH_3CH_3	−16.4	−20.1	−20.0
$CH_3CH_2CH_3$	−19.8	−25.1	−25.0
c-C_5H_{10}	−10.4	−18.4	−18.3
c-C_6H_{12}	−20.0	−29.3	−29.5
1	−13.5	−23.3	
2	−5.9	−14.0	
$BH_2(CH_2)_2NH_2$	+20.4	+15.0	
$BH_2(CH_2)_4NH_2$	+14.9	+6.2	
$BH_2CH(CH_3)CH_2CH_2NH_2$	+14.9	+6.6	
$CH_3CH_2BH_2NH_2CH_2CH_3$	−23.3	−33.2	

[13] Curtiss, L. A.; Redfern, P. C.; Raghavachari, K.; Rassolov, V.; Pople, J. A. *J. Chem. Phys.* **1999**, *110*, 4703–4709.
[14] Wiberg, K. B. *Angew. Chem. Int. Ed. Engl.* **1986,** *25,* 312–322.

Predicted IR spectra

The IR spectra of **1**, **1**−$\mathbf{H_2}$, **2**, and **2**−$\mathbf{H_2}$ were calculated (B3LYP/6-31G*) based on the above optimized geometries for those structures. As shown in Figures S11−S14, none of the predicted IR peaks for either **1**−$\mathbf{H_2}$ or **2**−$\mathbf{H_2}$ overlap with the frequency of the NH_2 bending mode in **1** and **2**.

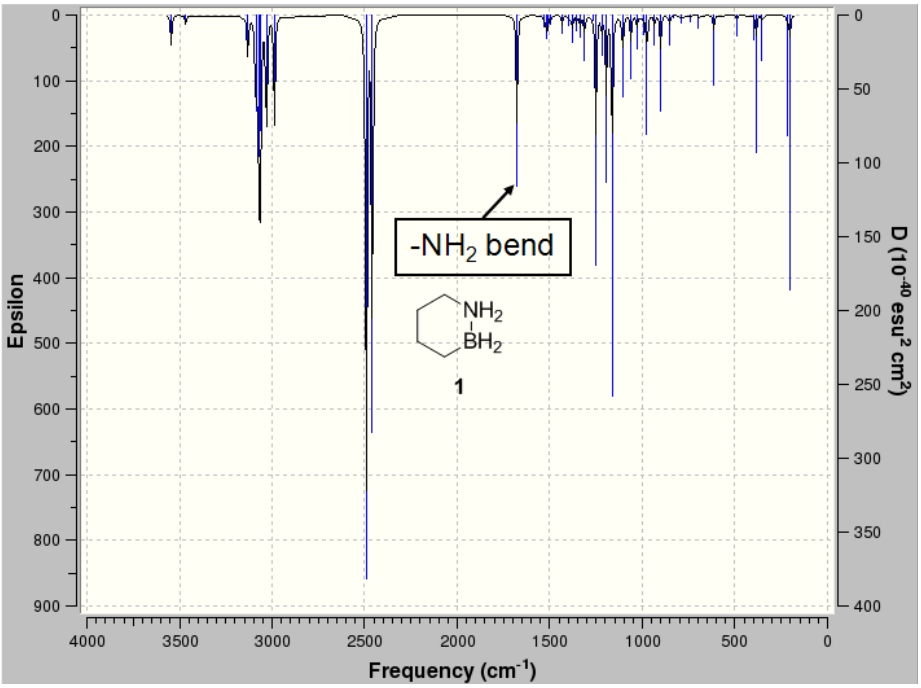


Figure S11. Predicted (B3LYP/6-31G*) IR spectrum for **1**.

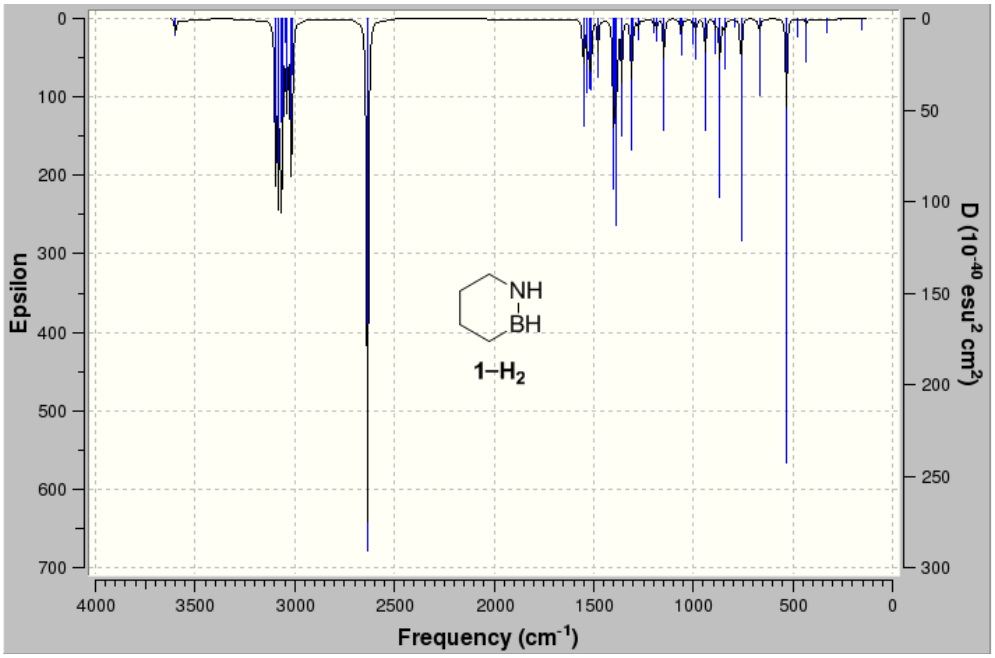


Figure S12. Predicted (B3LYP/6-31G*) IR spectrum for **1**−$\mathbf{H_2}$.

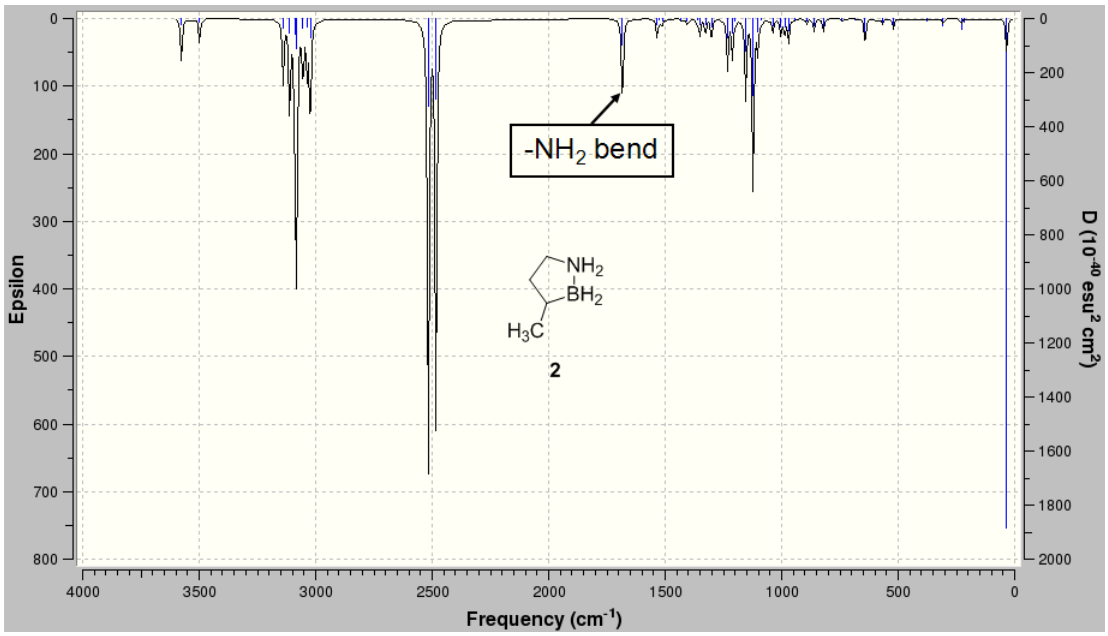


Figure S13. Predicted (B3LYP/6-31G*) IR spectrum for **2**.

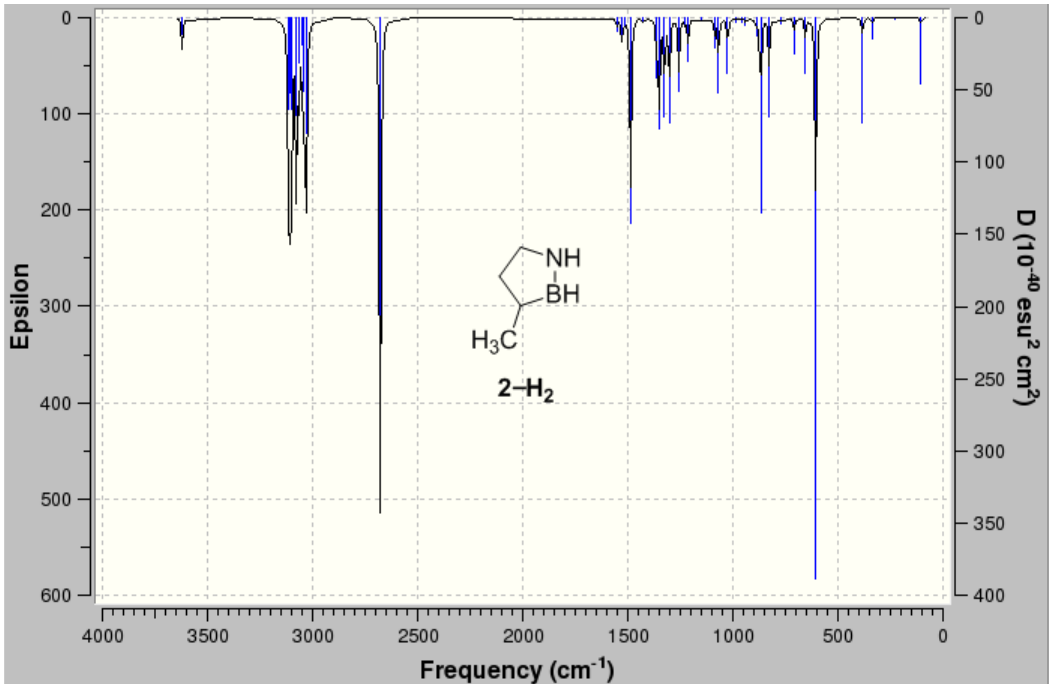


Figure S14. Predicted (B3LYP/6-31G*) IR spectrum for **2**−H_2.

NMR spectra of new compounds

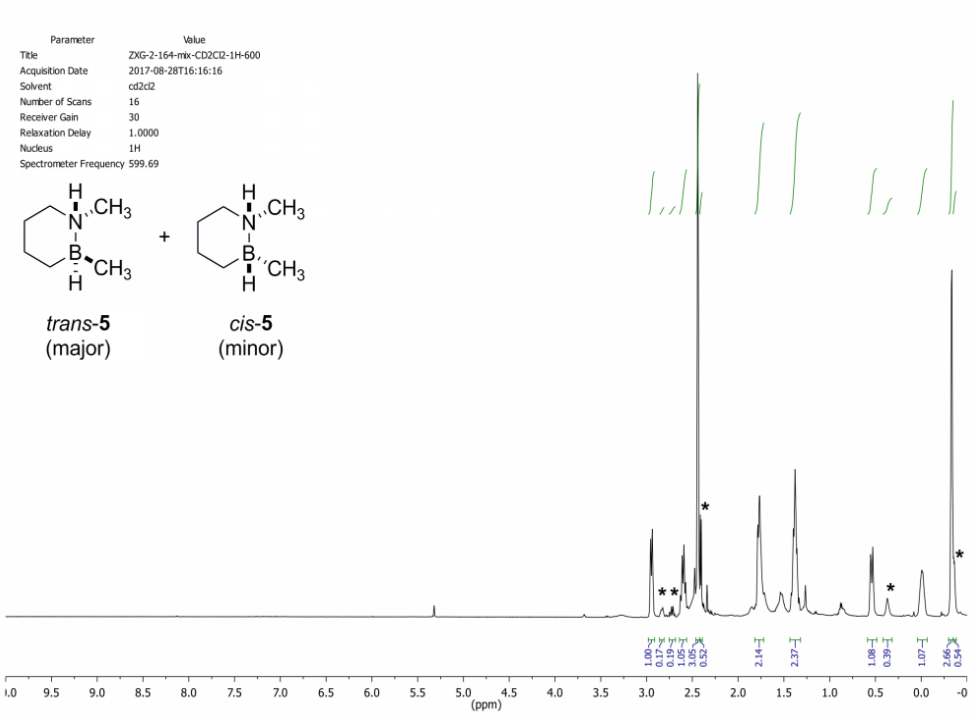


Figure S15. ^{1}H NMR spectrum of the initial mixture of *trans*- and *cis*-**5**. Identifiable peaks assigned to *cis*-**5** are marked with an asterisk.

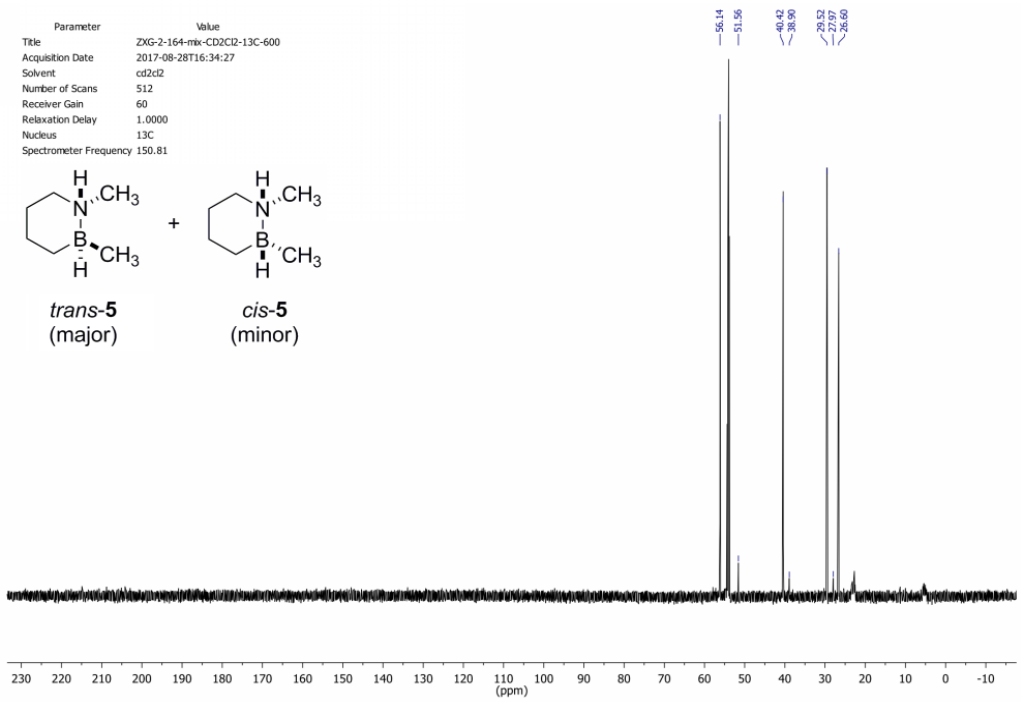


Figure S16. ^{13}C NMR spectrum of the initial mixture of *trans*- and *cis*-**5**.

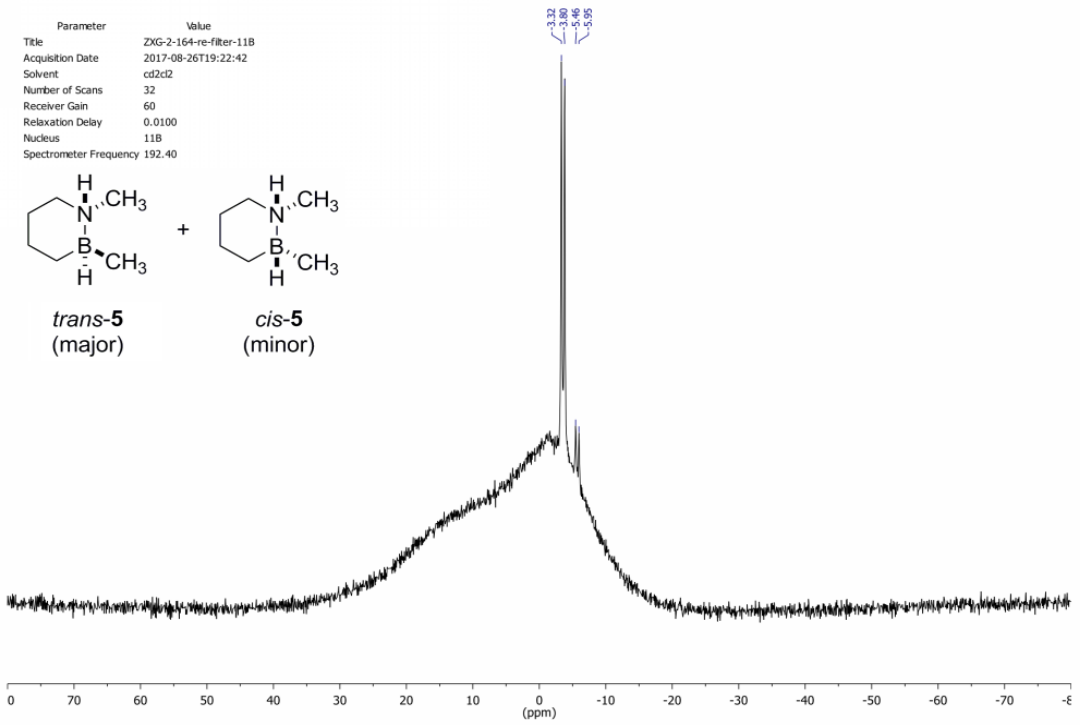


Figure S17. ^{11}B NMR spectrum of the initial mixture of *trans*- and *cis*-**5**.

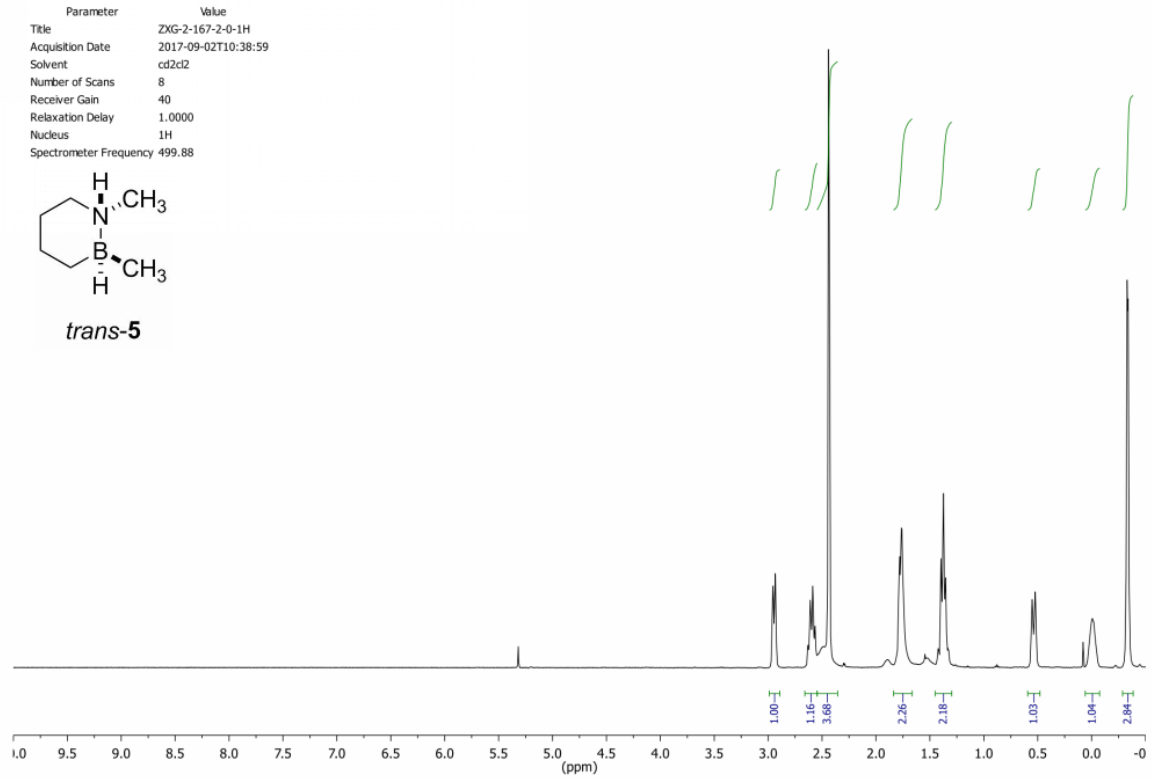


Figure S18. ^{1}H NMR spectrum of isolated of *trans*-**5**.

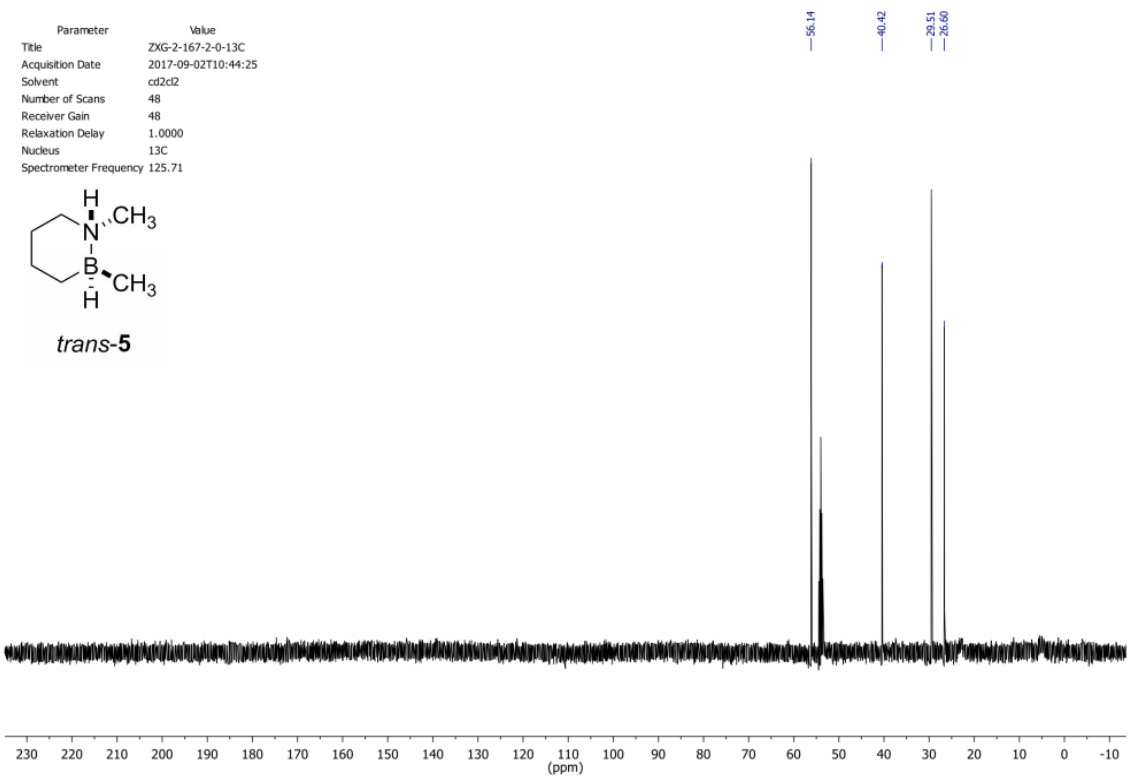


Figure S19. ^{13}C NMR spectrum of isolated of *trans*-**5**.

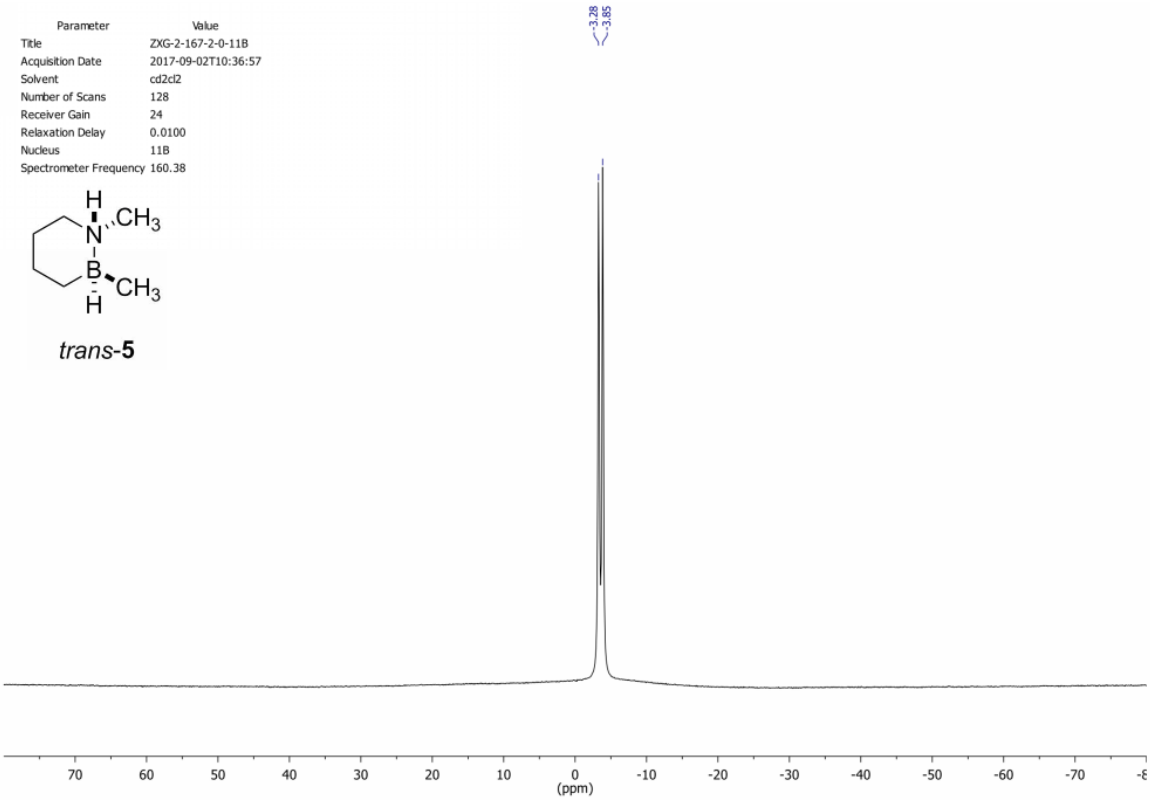
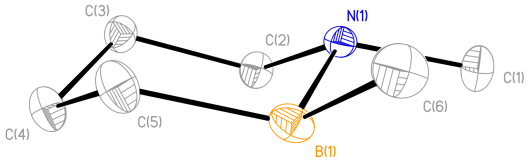


Figure S20. ^{11}B NMR spectrum of isolated of *trans*-**5**.

X-ray crystallographic data

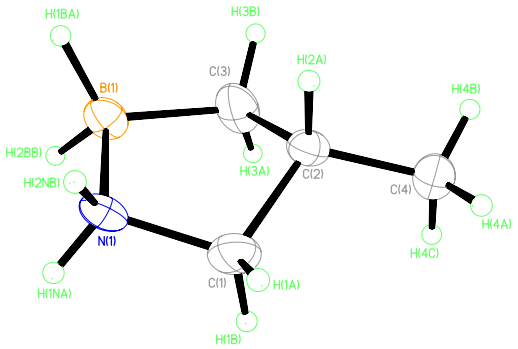
Crystal data and structure refinement for *trans*-1,2-dimethyl-1,2-BN-cyclohexane (*trans*-**5**).



Identification code	C6H16BN	
Empirical formula	C6 H16 B N	
Formula weight	113.01	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 9.5116(14) Å	α = 90°
	b = 12.6484(18) Å	β = 90°
	c = 6.5253(9) Å	γ = 90°
Volume	785.04(19) $Å^3$	
Z	4	
Density (calculated)	0.956 Mg/m^3	
Absorption coefficient	0.054 mm^{-1}	
F(000)	256	
Crystal size	0.450 x 0.380 x 0.320 mm^3	
Theta range for data collection	2.679 to 28.513°.	
Index ranges	-12<=h<=12, -16<=k<=16, -8<=l<=8	
Reflections collected	14886	
Independent reflections	1988 [R(int) = 0.0228]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6957	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1988 / 1 / 79	
Goodness-of-fit on F2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0899	
R indices (all data)	R1 = 0.0338, wR2 = 0.0912	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.301 and -0.126 $e.Å^{-3}$	

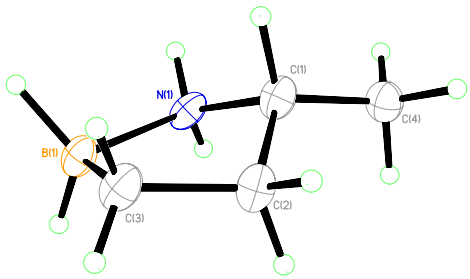
Crystal data and structure refinement for 4-methyl-1,2-BN-cyclopentane.

Identification code	liu107a
Empirical formula	C4 H12 B N
Formula weight	84.96
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c



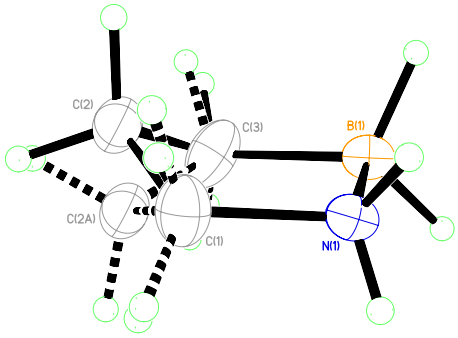
Unit cell dimensions	a = 10.60(4) Å	α = 90°
	b = 6.32(2) Å	β = 96.06(3)°
	c = 9.48(3) Å	γ = 90°
Volume	631(4) Å^3	
Z	4	
Density (calculated)	0.894 Mg/m^3	
Absorption coefficient	0.051 mm^{-1}	
F(000)	192	
Crystal size	0.60 x 0.24 x 0.01 mm^3	
Theta range for data collection	1.93 to 24.99°.	
Index ranges	-12<=h<=12, -7<=k<=7, -11<=l<=11	
Reflections collected	5074	
Independent reflections	1116 [R(int) = 0.0454]	
Completeness to theta = 24.99°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9995 and 0.9703	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1116 / 0 / 80	
Goodness-of-fit on F2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0710, wR2 = 0.1778	
R indices (all data)	R1 = 0.0960, wR2 = 0.1964	
Largest diff. peak and hole	0.198 and -0.184 e.Å^{-3}	

Crystal data and structure refinement for 5-methyl-1,2-BN-cyclopentane.



Identification code	liu167	
Empirical formula	C4 H12 B N	
Formula weight	84.96	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 7.078(7) Å	α = 90°
	b = 9.187(9) Å	β = 90°
	c = 18.233(18) Å	γ = 90°
Volume	1186(2) $Å^3$	
Z	8	
Density (calculated)	0.952 Mg/m^3	
Absorption coefficient	0.054 mm^{-1}	
F(000)	384	
Crystal size	0.27 x 0.14 x 0.02 mm^3	
Theta range for data collection	2.23 to 24.99°.	
Index ranges	-8<=h<=8, -10<=k<=10, -21<=l<=21	
Reflections collected	7701	
Independent reflections	1046 [R(int) = 0.1638]	
Completeness to theta = 24.99°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9989 and 0.9856	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1046 / 0 / 103	
Goodness-of-fit on F2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0853, wR2 = 0.1888	
R indices (all data)	R1 = 0.1547, wR2 = 0.2279	
Largest diff. peak and hole	0.168 and -0.183 $e.Å^{-3}$	

Crystal data and structure refinement for 1,2-BN-cyclopentane.



Identification code	liu104a	
Empirical formula	C3 H10 B N	
Formula weight	70.93	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 8.519(3) Å	α = 90°
	b = 6.850(2) Å	β = 90°
	c = 8.309(3) Å	γ = 90°
Volume	484.9(3) Å3	
Z	4	
Density (calculated)	0.972 Mg/m^3	
Absorption coefficient	0.055 mm^{-1}	
F(000)	160	
Crystal size	0.42 x 0.19 x 0.03 mm^3	
Theta range for data collection	2.97 to 26.99°.	
Index ranges	-10<=h<=10, -8<=k<=8, -10<=l<=10	
Reflections collected	4991	
Independent reflections	1065 [R(int) = 0.0286]	
Completeness to theta = 26.99°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9983 and 0.9772	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1065 / 5 / 66	
Goodness-of-fit on F2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1187	
R indices (all data)	R1 = 0.0599, wR2 = 0.1291	
Absolute structure parameter	?	
Largest diff. peak and hole	0.156 and -0.144 $e.Å^{-3}$	