Supporting Information for:

Intramolecular B/N Frustrated Lewis Pairs and the Hydrogenation of Carbon Dioxide

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Contents

S1: General experimental:

Unless otherwise specified, all the manipulations were conducted under an inert atmosphere of dinitrogen, using standard Schlenk and glovebox techniques. Reactions were carried either in a sealed J-Young NMR tube, in which case NMR conversions are indicated, or in standard oven dried Schlenk vessels. Benzene-d_6 was purified by vacuum distillation from Na/K alloy, or by degassing by three subsequent freeze pump thaw cycles followed by standing over activated 3 Å molecular sieves. Acetonitrile-d_3 and bromobenzene-d_5 were dried over 3 Å molecular sieves. Dry CO_2 was purchased from Praxair and used as received. $^{13}CO_2$ (99% isotope label) was purchased from Cambridge Isotope Laboratories or Aldrich. Ultra high purity hydrogen (5.0 grade) was purchased from Praxair and used as received. 5-Bromo,1,2,4-trimethylbenzene, 2-Bromo-1,3,5-trimethylbenzene and $BF_3.Et_2O$ were purchased from Aldrich or TCI and used as received. $FBMes_2$- was synthesized according to a literature procedure[1] and further purified by sublimation. (2-(dimethylamino)phenyl)lithium was synthesized according to a literature procedure.[2] Benzaldehyde was purchased from Aldrich and distilled under reduced pressure before use.

NMR spectra were recorded on Agilent DD2-600 at 600 MHz (^{1}H), 150.84 MHz (^{13}C), 192.45 MHz (^{11}B), Agilent Technologies NMR spectrometer at 500 MHz (^{1}H), 125.758 MHz (^{13}C), 160.462 MHz (^{11}B), a Varian Inova NMR AS400 spectrometer, at 400.0 MHz (^{1}H), 100.580 MHz (^{13}C), 128.378 MHz (^{11}B). ^{1}H NMR and ^{13}C{^{1}H} NMR chemical shifts are referenced to residual protons in deuterated solvent. Multiplicities are reported as singlet (s), broad singlet (s, br) doublet (d), triplet (t), multiplet (m). Chemical shifts are reported in ppm. Coupling constants are reported in Hz. gHSQC experiments were performed in order to confirm C-H correlations. Mass spectroscopy analysis were performed on a JMS T100-LC using AccuTOF DART.

WARNING: Condensation of high pressure of H_2 and CO_2 might lead to an explosion of the glassware. Care should be taken.

S2: Synthesis of compounds 1, 2 and precursors

dimethylbis(2,4,5-trimethylphenyl)stannane

This compound was synthesized with a slightly modified approach from a known procedure.[3]

Ca. 50 mL of THF and 3.48 g (143mmol, 4.0 equivalents) of magnesium turnings were combined in a Schlenk flask. To the resulting mixture, 25.9 g (130 mmol, 3.7 equivalents) of 1-bromo-2,4,5-trimethylbenzene were added and heated at 40°C for 2 hours. Me_2SnCl_2 (7.7g, 35 mmol, 1.0 equivalent) was dissolved in *ca.* 20 mL of THF in a separate Schlenk flask. The solution containing the tin compound was then cannulated into the Schlenk flask containing the Grignard reagent. The resulting mixture was heated at 50°C for 4 hours.

Work-up: The solution was cooled down in an ice bath and 20 mL of a saturated solution of NH_4Cl was added. The contents were transferred to a separatory funnel and extracted three times with a mixture of Et_2O/Hexanes (50/50). The organic layer was then washed with water and with brine. The organic layer was dried with Na_2SO_4 and the solvents removed by rotary evaporation. The compound was then passed through a silica plug using hexanes as an eluent which was then removed by rotary evaporation yielding 11.3 g of white crystals. Yield = 83%.

^{1}H NMR 400 Mhz : δ 7.20 (s, 2H, *m*-Ar); 7.05 (s, 2H, *o*-Ar); 2.35 (s, 6H, m-Me); 2.27 (s, 6H, *p*-Me); 2.25 (s, 6H, *o*-Me); 0.55 (s, 6h, Sn-Me). ^{13}C {^{1}H} (101 MHz): δ 142.3 (m-Ar); 137.8 (m-Ar_{quat}); 137.2 (*p*-Ar); 136.7 (*o*-Ar); 133.3 (o-Ar_{quat}); 130.7 (Sn-Ar); 24.4 (*m*-Me); 19.8 (*p*-Me); 19.3 (*o*-Me); -8.03 (Sn-Me).

chlorobis(2,4,5-trimethylphenyl)borane

This compound was synthesized with a slightly modified approach from a known procedure[4]

In a Schlenk flask, 11.1 g of dimethylbis(2,4,5-trimethylphenyl)stannane (0.029 mol, 1 equivalent) was dissolved in *ca* 10mL of hexanes in a teflon capped Schlenk flask with a magnetic stir bar. 29 mL (0.029 mol, 1 equivalent) of a 1.0 molar solution of BCl_3 in heptane was added at once. The resulting mixture was heated for 40 hours at 100 °C with vigorous stirring. Upon reaction completion, the Schlenk flask was allowed to cool to r.t. naturally after which it was placed in a cold bath. The solution containing the title compound was filtered from the precipitated Me_2SnCl_2. The resulting solution was then evaporated until the title compound started precipitating out. The flask was then stored at -35 °C for 4 hours after which the hexanes were filtered by keeping the solution at -35 °C. The compound was then further purified by sublimation at 80 °C at 0.1 Tor. 6.43 g of white crystals, yield = 80%. Recrystallization from hexanes yielded monocrystals suitable for X-ray crystallography. (The structure is reported in S9).

^{1}H NMR 400MHZ: δ 7.62 (s, 2H, *o*-Ar); 6.8 (s, 2H, *m*-Ar); 2.28 (s, 6H, *o*-Me); 1.98 (s, 6H, *p*-Me); 1.97 (s, 6H, *m*-Me); ^{13}C{^{1}H} (101 MHz): δ 140.8 (*m*-Ar_{quat}); 140.5 (*p*-Ar_{quat}); 139.3(s, br., Ar-B); 136.8 (*m*-Ar); 133.5 (*o*-Ar_{quat}); 132.3 (*o*-Ar); 22.7 (*o*-Me); 19.8 (*p*-Me); 19.1 (m-Me).

1-(dimesitylboryl)-2-NMe_2-C_6H_4 (1)

This compound was synthesized with a slightly modified approach from a known procedure.[5]

1.5 g (5.5 mmol, 1.0 equivalent) of dimesitylboron fluoride was dissolved in toluene and cannulated to a -78°C solution of 700 mg (5.5 mmol, 1.0 equivalent) of (2-(dimethylamino)phenyl)lithium in 10mL of toluene. The resulting mixture was then left to warm to r.t. naturally and to stir for 16 hours. Upon reaction completion the solution was bright, fluorescent green.

Work-up: The salts were left to separate without agitation and the solution was filtered via cannula. The residue was washed once with toluene (10mL). The volatiles were then removed in vacuo. Upon cooling, 1.8 g of a green solid was recovered: yield= 91%. The compound can be further purified by recrystallization from a saturated hexane solution at -35°C. Using this method, 1.46 g of pure compound was recovered. Yield = 72%

The characterization of this compound is conform to that previously reported.[6]

1-(bis(2,4,5-trimethylphenyl)boryl)-2-NMe_2-C_6H_4 (2)

This compound was synthesized with a slightly modified approach from a known procedure[5]

967mg (3.4 mmol, 1.0 equivalent) of chlorobis(2,4,5-trimethylphenyl)borane was dissolved in toluene and cannulated to a -78°C solution of 432 mg (3.4 mmol, 1.0 equivalent) of (2-(dimethylamino)phenyl)lithium in 10mL of toluene. The resulting mixture was then left to warm to r.t. naturally and to stir for 16 hours. Upon reaction completion the solution was bright, fluorescent green.

Work-up: The salts were left to separate without agitation and the solution was filtered via cannula. The residue was washed once with toluene (10 mL). The volatiles were then removed in vacuo and left under vacuum at 110 °C for 2 hours. Upon cooling, 1.1 g of a sticky green solid was recovered: yield= 88 %. The compound can be further purified by recrystallization from a saturated hexane solution at -35°C. Using this method, 807 mg of pure compound was recovered. Yield = 64%

The characterizations of this compound conform to those that were previously reported[6]

S3: HD scrambling with 1

In a glove box, 5.2 mg (0.014 mmol) of **1** was dissolved in benzene-d_6 (0.5 ml) and the green solution transferred to a J Young NMR tube. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The tube was charged with HD (4 atm) and ^{1}H NMR recorded. The reaction was heated at 80 °C for 14 h, cooled and ^{1}H-NMR recorded.

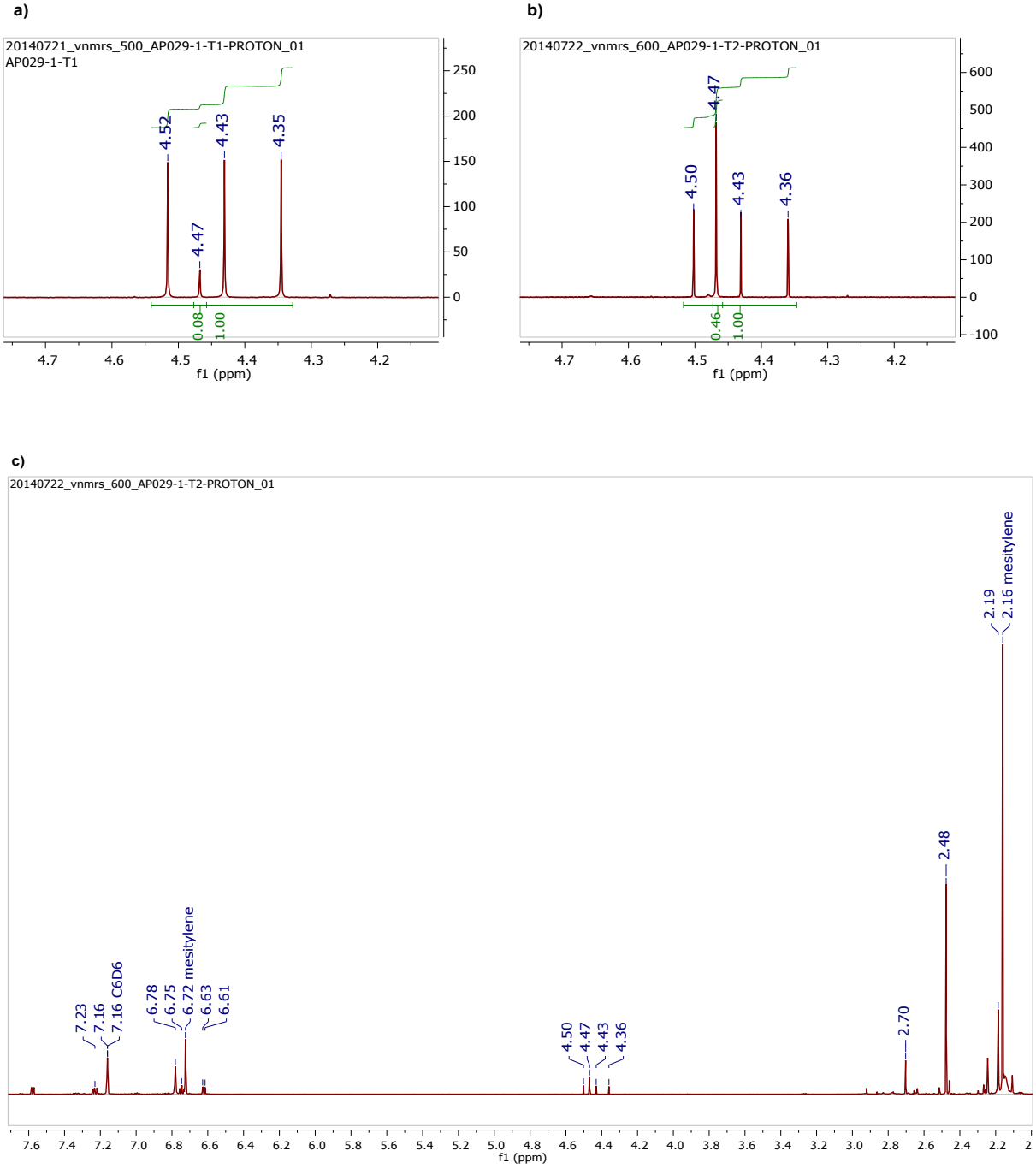
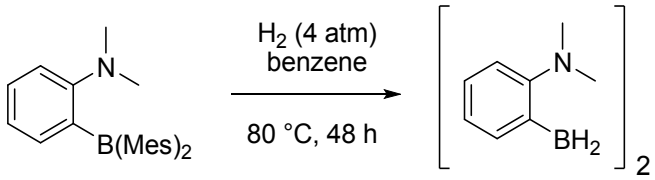


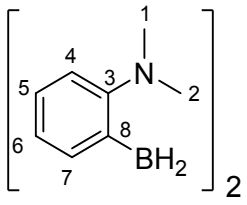
Figure S3. 600 MHz ^{1}H-NMR during isotope scrambling of HD by **1**. a) Expansion of reaction mixture at t = 0 h. b) Expansion reaction mixture after 14 h at 80 °C. c) Full spectra of reaction mixture after 14 h at 80 °C.

S4: Synthesis of 3 from 1



1 **3**

In a glove box, **1** (46 mg, 0.13 mmol) was dissolved in benzene (4 ml) and the green solution transferred to a J Young flask (bomb) equipped with a teflon coated magnetic stir bar. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The flask was charged with H_2 (4 atm) and the mixture was stirred and heated at 80 °C for 48 h. The volatiles were removed *in vacuo* to give a pale green solid. The product was crystallised from hot *n*-hexane (2 ml), which after decantation of the supernatant and washing the solid with *n*-hexane (0.5 ml) gave **3** as white feathery crystals (9 mg, 54%).



3

*The H atoms are numbered based on the carbon atom to which they are attached

^{1}H NMR (600 MHz, benzene-d_6): δ 7.76 (dd, *J* = 7.3, 1.5 Hz, 1H, H7), 7.16 (td, *J* = 7.3, 1.0 Hz, 1H, H5), 6.99 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H, H6), 6.62 (dd, *J* = 8.0, 1.0 Hz, 1H, H4), 3.54 (app. br. d, *J* = 96 Hz, 1H, BH), 2.77 (s, 3H, C2), 2.55 (s, 3H, C1).

^{13}C{^{1}H} NMR (151 MHz, benzene-d6): δ 158.1 (C3), 137.3 (C7), 126.6 (H5), 126.5 (H6), 116.9 (C4), 59.3 (C1), 48.2 (C2).

^{11}B{^{1}H} NMR (193 MHz, benzene-d6): δ +2.5.

HRMS (DART-TOF+): mass [M−H] calc'd for $C_{16}H_{23}B_2N_2$ 265.20473 *Da*, measured 265.20539 *Da*.

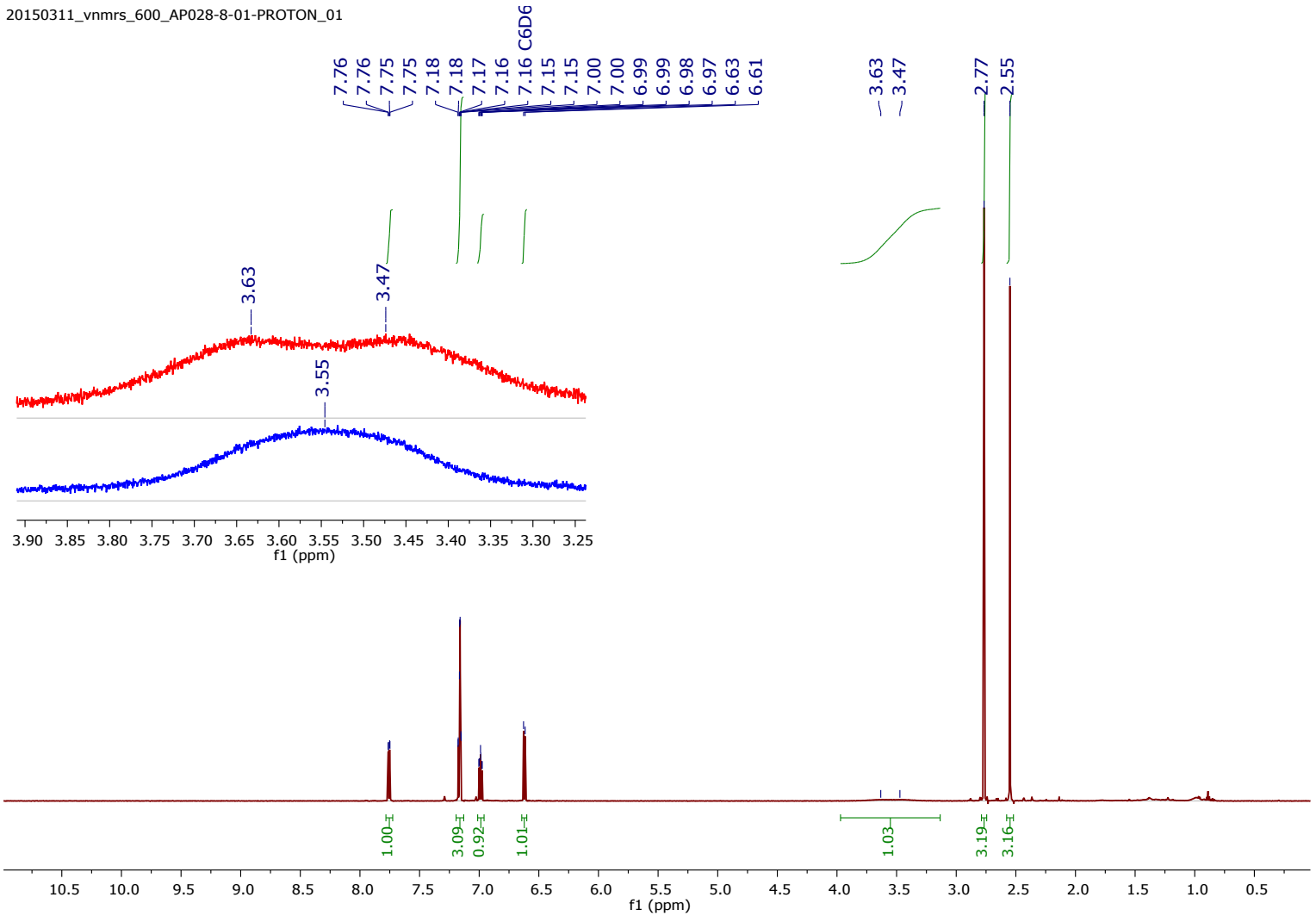


Figure S4-1. 600Mz ^{1}H-NMR of isolated **3** in C_6D_6 showing an expansion of the BH signal (top, red) superimposed on the ^{11}B decoupled spectra (bottom, blue).

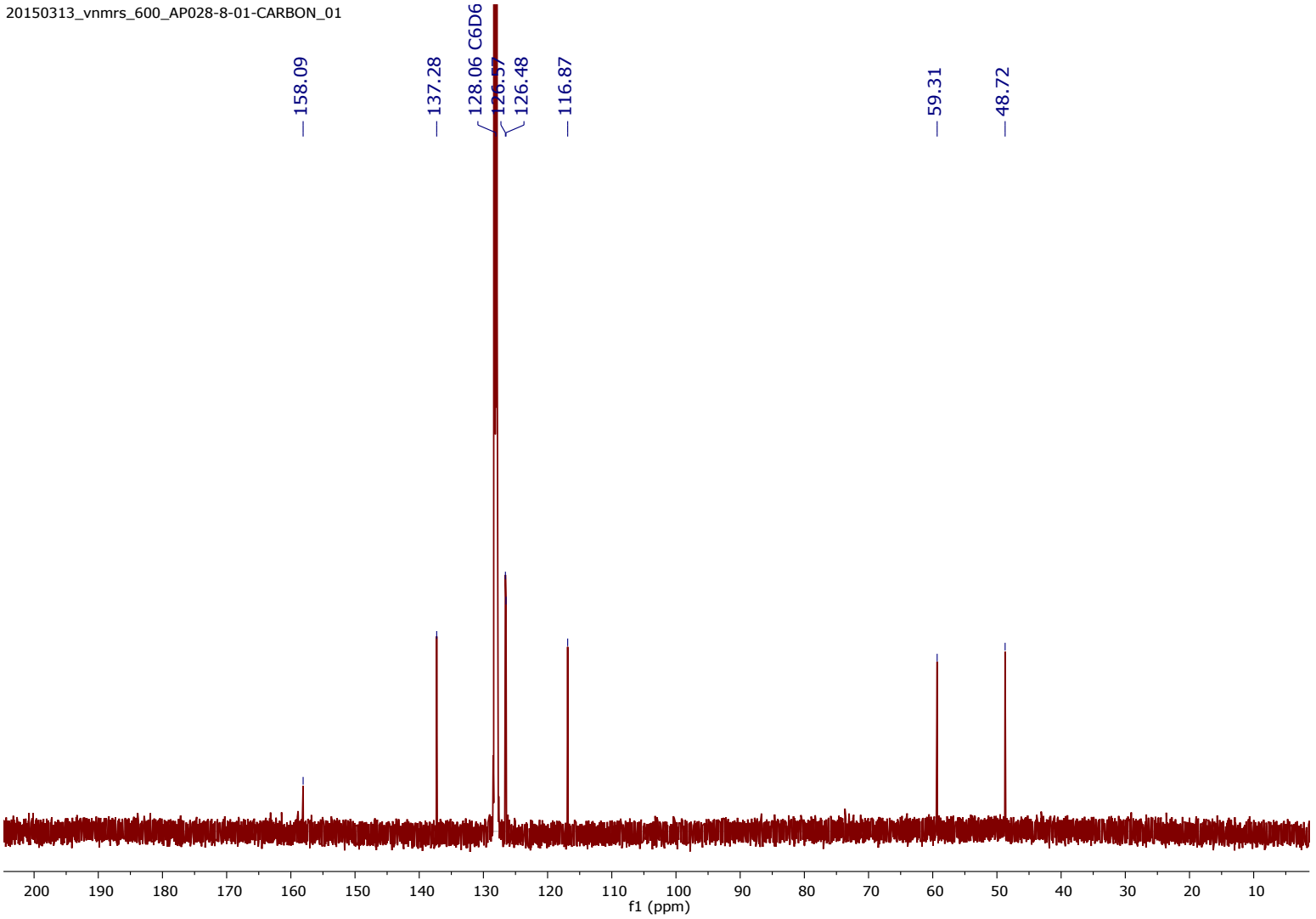


Figure S4-2. 151 MHz ^{13}C-NMR of isolated **3** in C_6D_6.

S5: Hydrogenation of CO_2 - J Young NMR Tube Experiments

General procedure

In a glove box, the solvent (0.5 ml) and cyclohexane (~1 μl) was added to 0.014 mmol of aminoborane. The bright green solution was transferred to a J Young NMR tube and the mixture was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The tube was charge with the stated pressure of CO_2 or ^{13}C labelled CO_2 (99% ^{13}C). The mixture was frozen in liquid nitrogen and the tube charged with H_2 (4 atm). The ^{1}H NMR was recorded and the tube heated at the stated temperature. The reaction was periodically monitored by ^{1}H-, ^{13}C- and ^{11}B-NMR. When stated, at the end of the reaction, the reaction solution was colourless and contained a white precipitate. The mixture was homogenised by cooling to −20 °C and then adding acetonitrile-d_3 (0.15 ml) followed by shaking of the tube. The final ^{1}H-, ^{13}C- and ^{11}B-NMRs were then recorded. For the experiments involving **2**, the solution remained homogeneous throughout the entire process.

Table S5. Hydrogenation of CO_2 with **1** and **2**

Entry	Amino borane	$^{13}CO_2$ pressure / atm	H_2 pressure / atm	Temp / °C	Time / h	Solvent	Number of CO_2 equiv. hydrogenated				Number of H_2 equiv. activated	Yield of **4**	^{11}B shifts / ppm * = <10%
							HCOO	H_2CO	CH_3O	CH_4			
1	**1**	1	4	80	24	C_6D_6	0.24	0.02	0	0	0.28	0	+72*, +44*, +7.2
2					72		0.31	0.02	Trace	0	0.36	0	+44*, +7.2, 5.2
3					216		0.30	0.00	Trace	0	0.32	0	+7.2*, +5.2, +2.5
4[a]					216		0.89	0.00	Trace	0	1.51	0	+5.2, +2.5
5	**1**	0.5	4	80	24	C_6D_6	0.21	0.04	Trace	0	0.29	0	+72*, +44*, +7.2
6					72		0.29	0.03	Trace	0	0.36	0	+44*, +7.2
7					216		0.29	0	0.01	0	0.33	0	+7.2*, +5.2, +2.5*
8[a]					216		0.84	0.34	0.01	0	1.54	0	+7.2*, +5.2, +2.5
9	**1**	0.1	4	80	24	C_6D_6	0	Trace	0.065	Trace	0.21	14	+72, +6.7*, +2.5*
10					72		0	0	0.075	0.002	0.24	14	+6.7, +2.5
11					216		0	0	0.083	0.004	0.26	43	+6.7, +2.5
(12[a]					216		0	0	0.083	Trace	0.25	43	+6.7, +2.5
13	**1**	1	4	130	24	BrC_6D_5	0.41	0	0.079	0	0.64	0	+5.2*, +2.2
14[a]					24		0.75	0.21	0.079	0	1.39	0	+5.2, +2.2
15	**2**	1	4	80	6	C_6D_6	0.19	0.28	0	0	0.74	0	+46*, +7.0
16[a]					6		0.22	0.31	0	0	0.84	0	+46*, +7.0
17	**2**	1	1	23	72	C_6D_6	0.37	0	0	0	0.74	0	+46*
[a] After addition of acetonitrile-d_3													

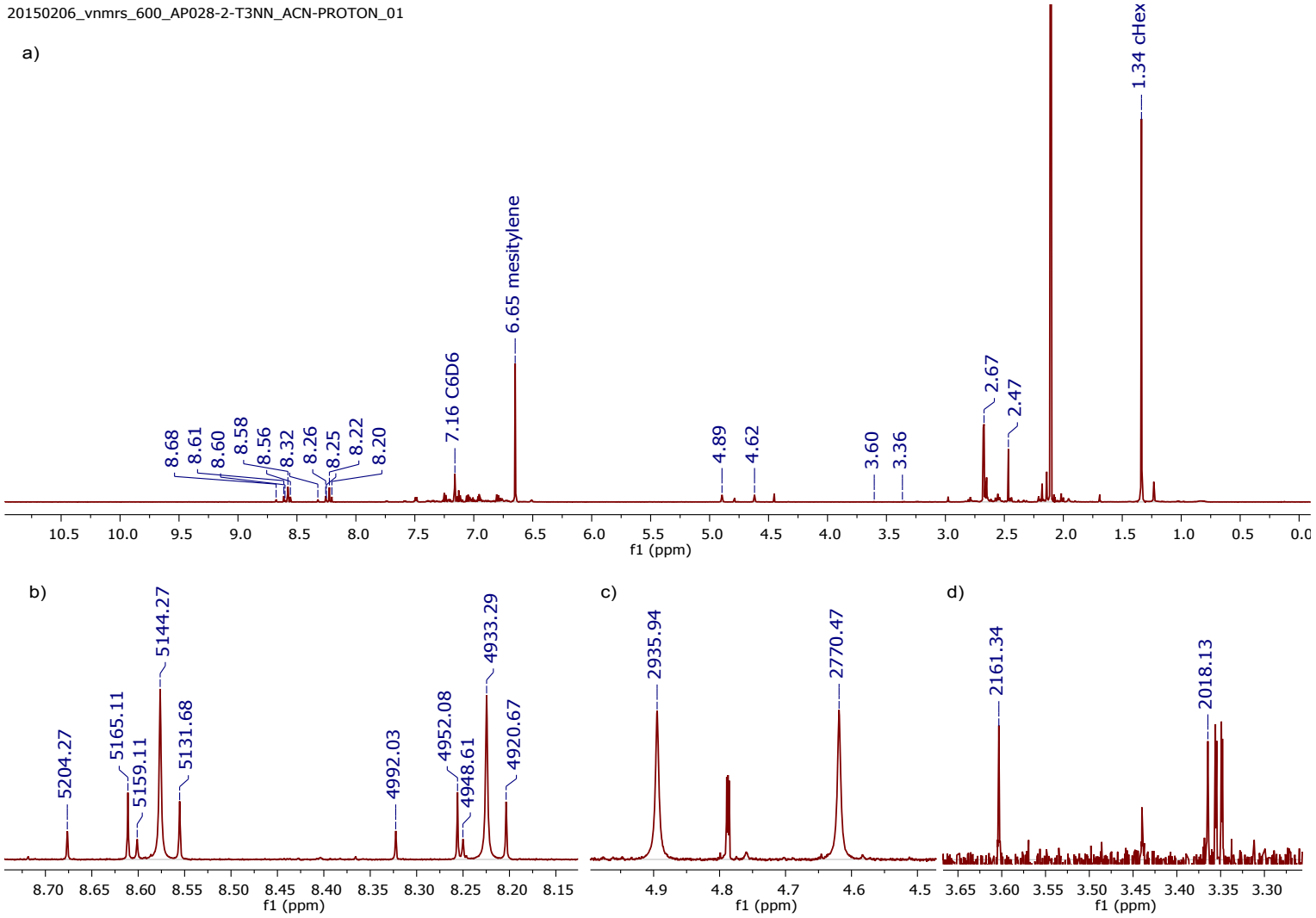


Figure S5-1. 600Mz ^{1}H-NMR of the reaction between **1**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in benzene-d_6 after 9 days at 80 °C, after the addition of acetonitrile-d_3. a) Full spectra. b) Formate region [J_{CH} = 211-213 Hz]. c) (OCH_2O) region [J_{CH} = 165 Hz]. d) Methoxide region [J_{CH} = 143 Hz].

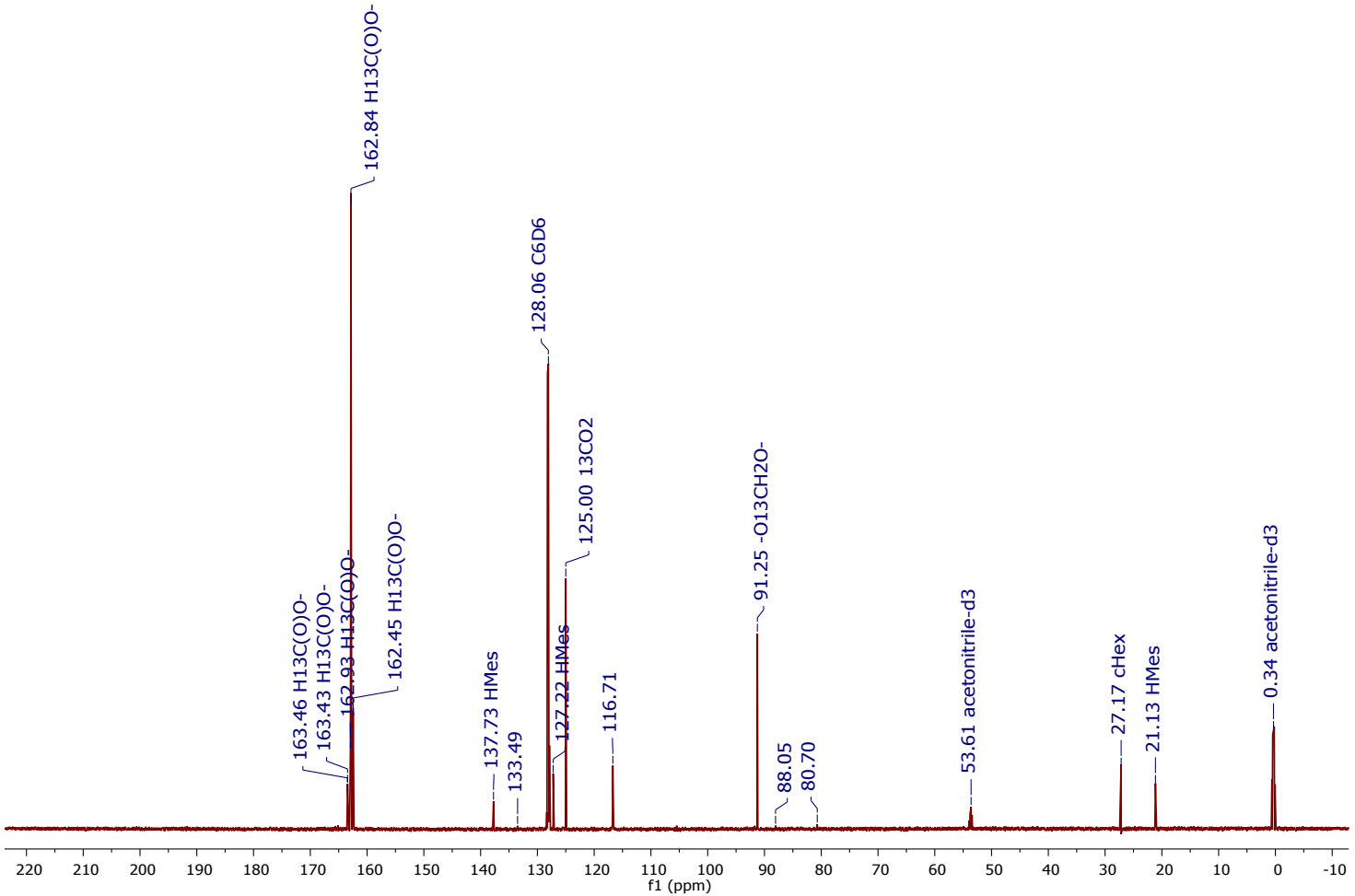


Figure S5-2. 151 MHz ^{13}C-NMR of the reaction between **1**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in benzene-d_6 after 9 days at 80 °C, after the addition of acetonitrile-d3.

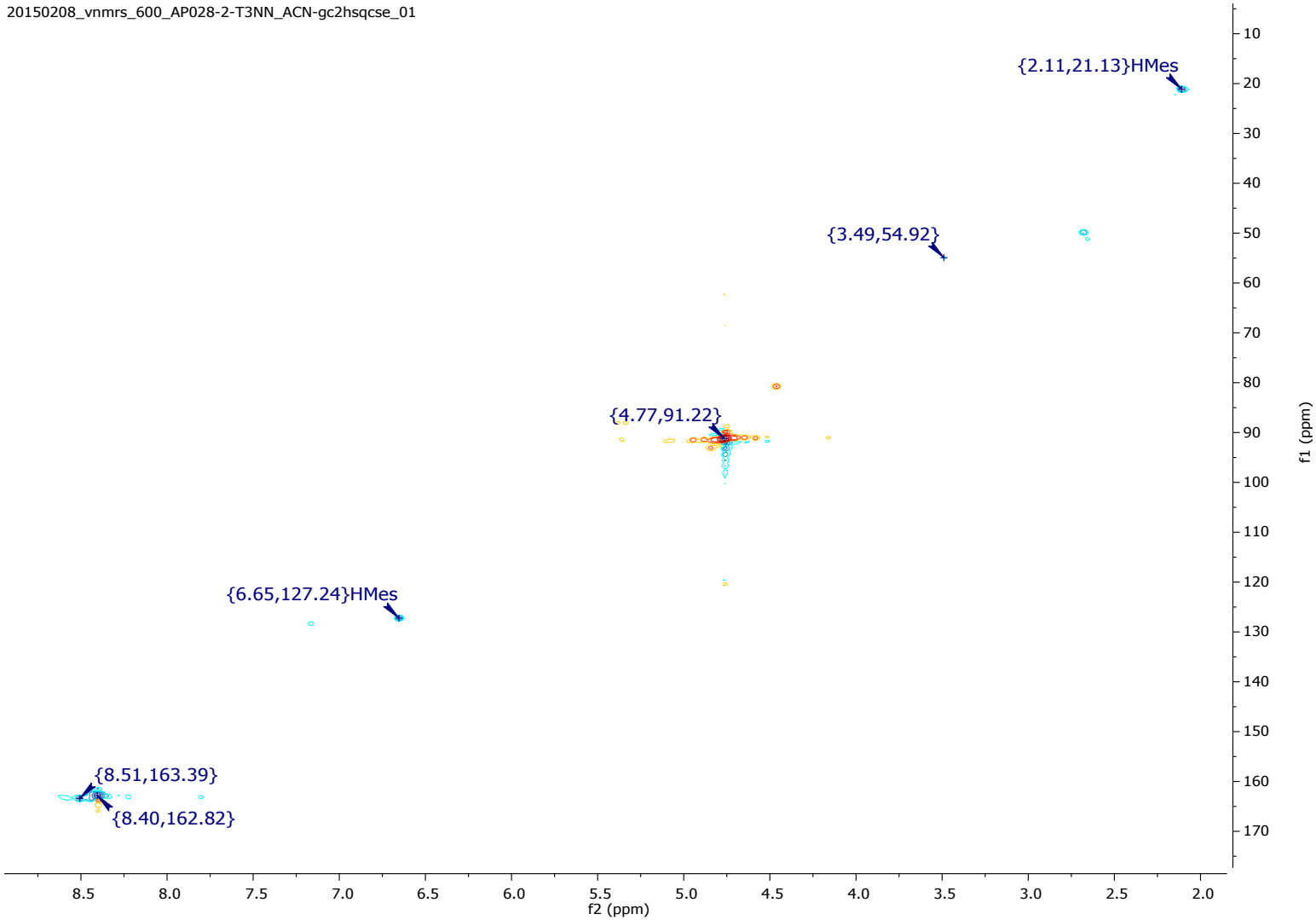


Figure S5-3. HSQC-NMR of the reaction between **1**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in benzene-d_6 after 9 days at 80 °C, after the addition of acetonitrile-d3.

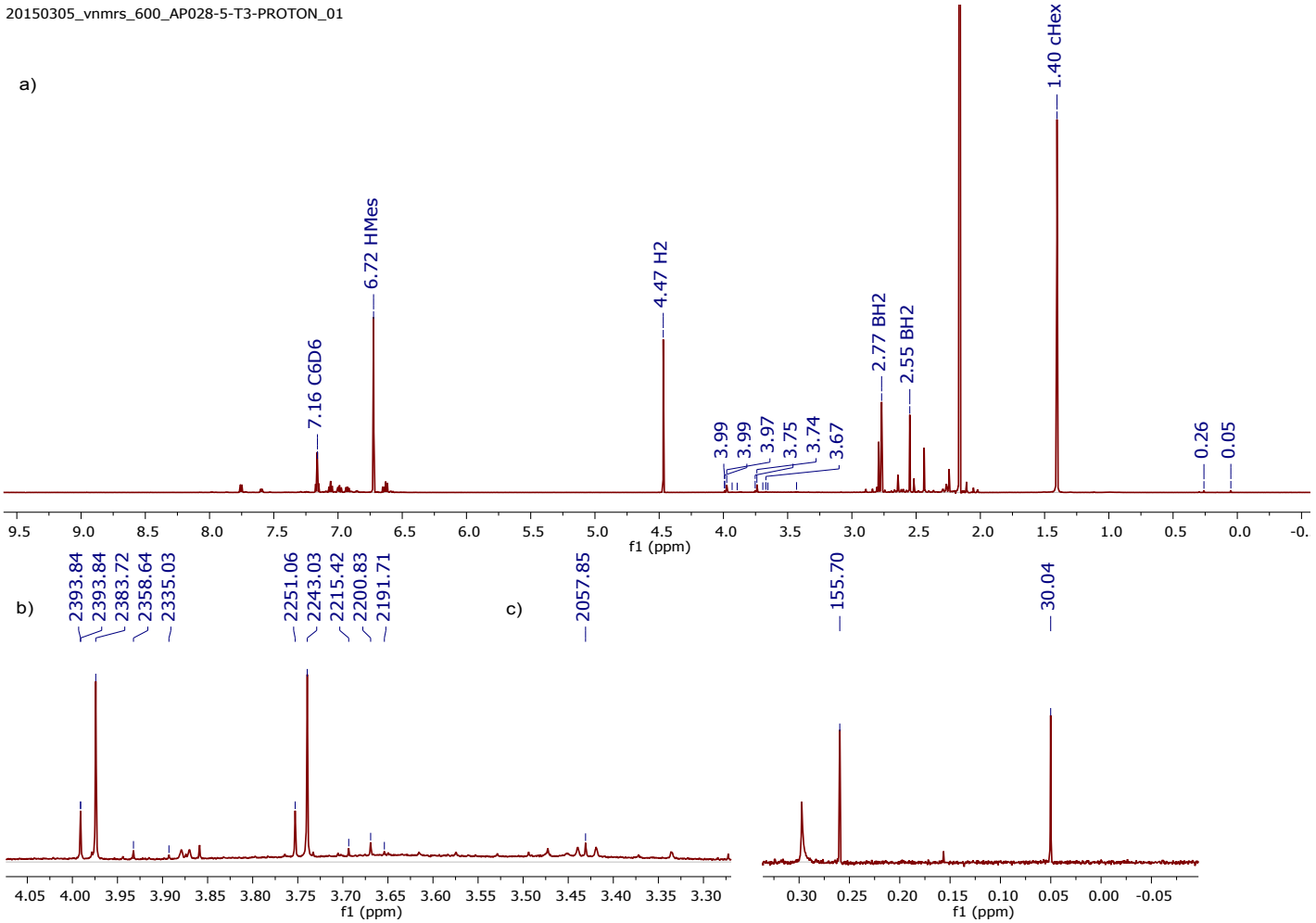


Figure S5-4. 600Mz ^{1}H-NMR of the reaction between **1**, $^{13}CO_2$ (0.1 atm) and H_2 (4 atm) in benzene-d_6 after 9 days at 80 °C. a) Full spectra. b) Methoxide region [J_{CH} = 141-143 Hz]. c) Methane [J_{CH} = 126 Hz].

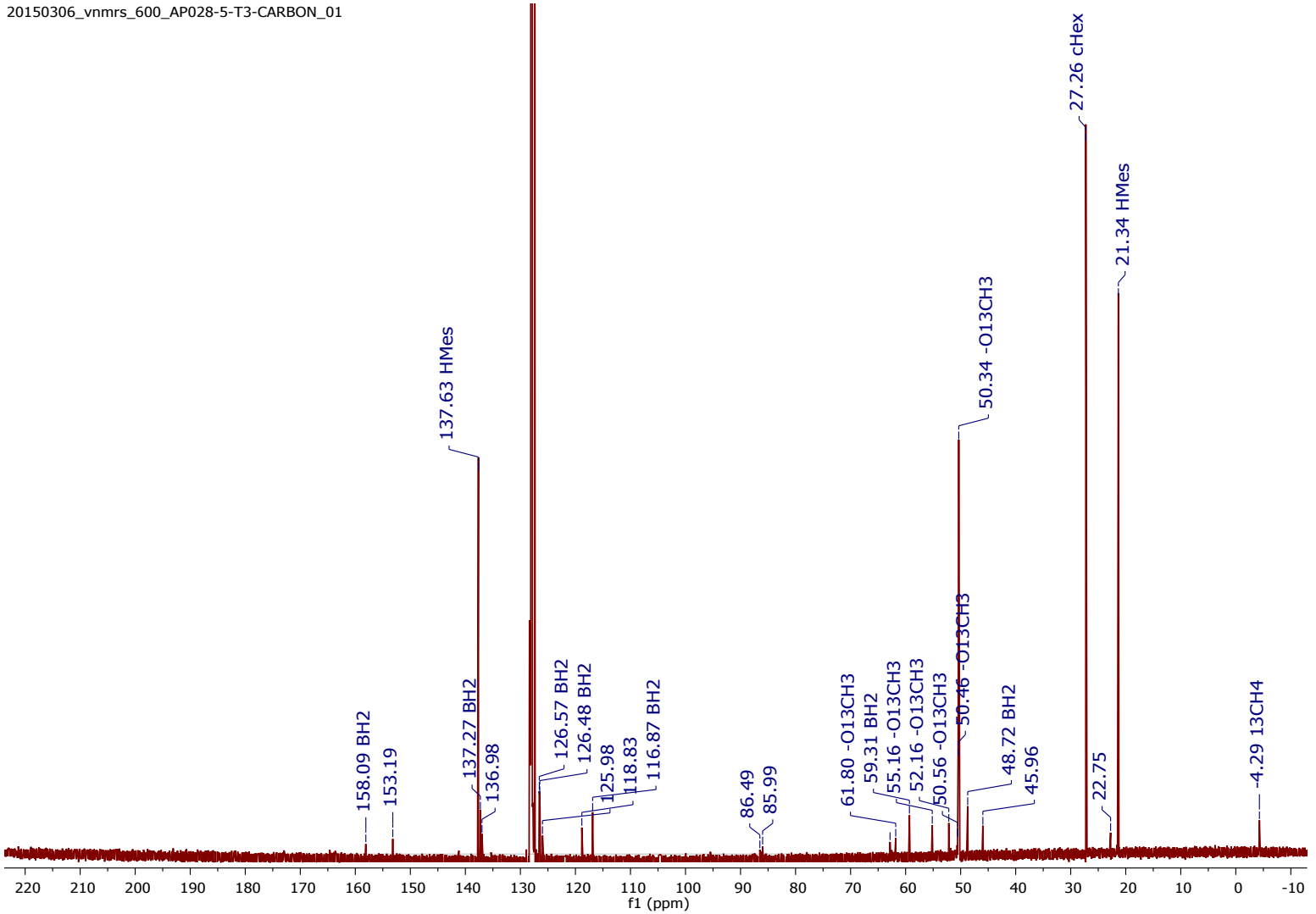


Figure S5-5. 151 MHz ^{13}C-NMR of the reaction between **1**, $^{13}CO_2$ (0.1 atm) and H_2 (4 atm) in benzene-d_6 after 9 days at 80 °C.

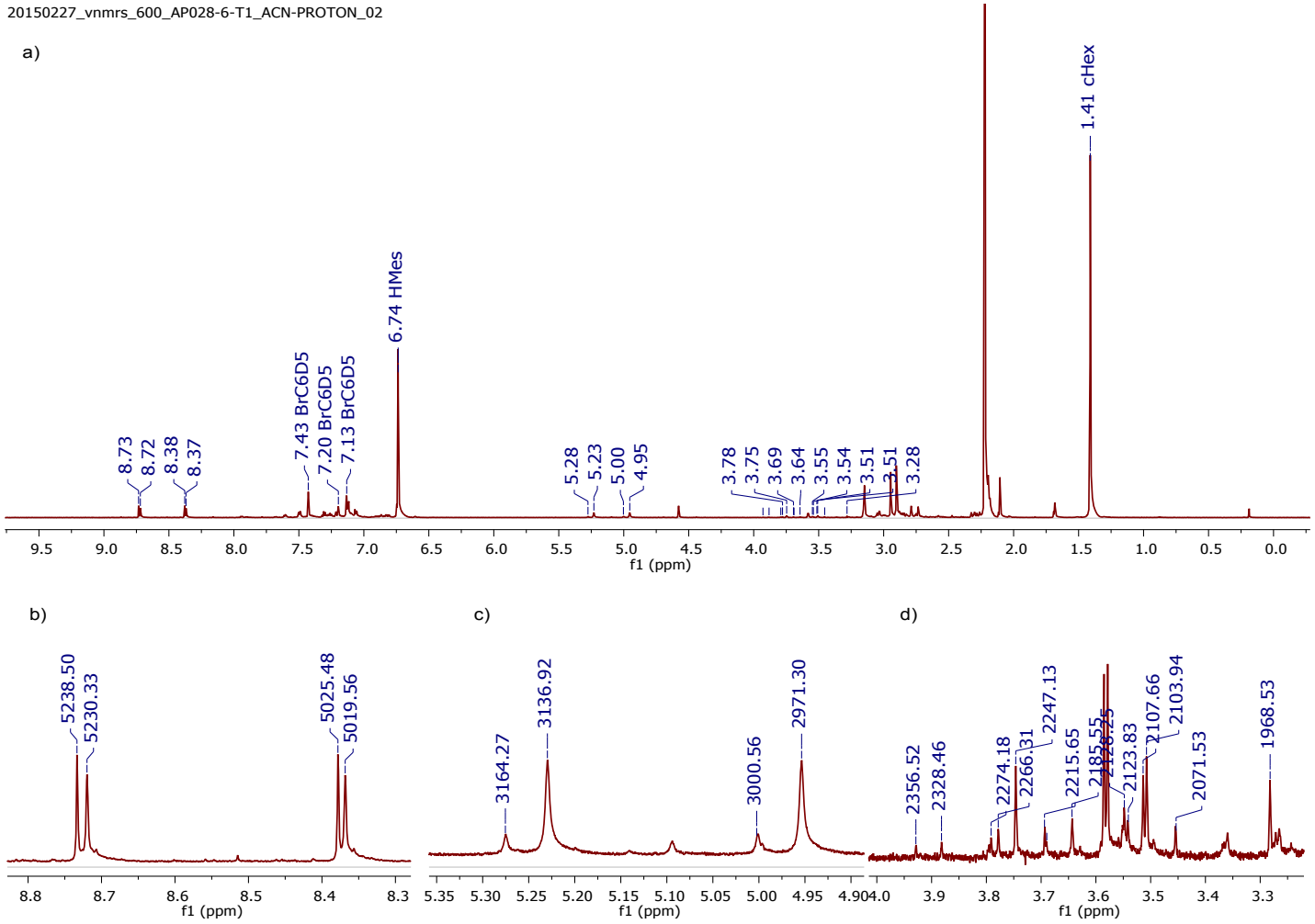


Figure S5-6. 600Mz ^{1}H-NMR of the reaction between **1**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in BrC_6D_5 after 1 day at 130 °C, after the addition of acetonitrile-d3. a) Full spectra. b) Formate region [J_{CH} = 212-213 Hz]. c) (OCH_2O) region [J_{CH} = 165-167 Hz]. d) Methoxide region [J_{CH} = 140-143 Hz].

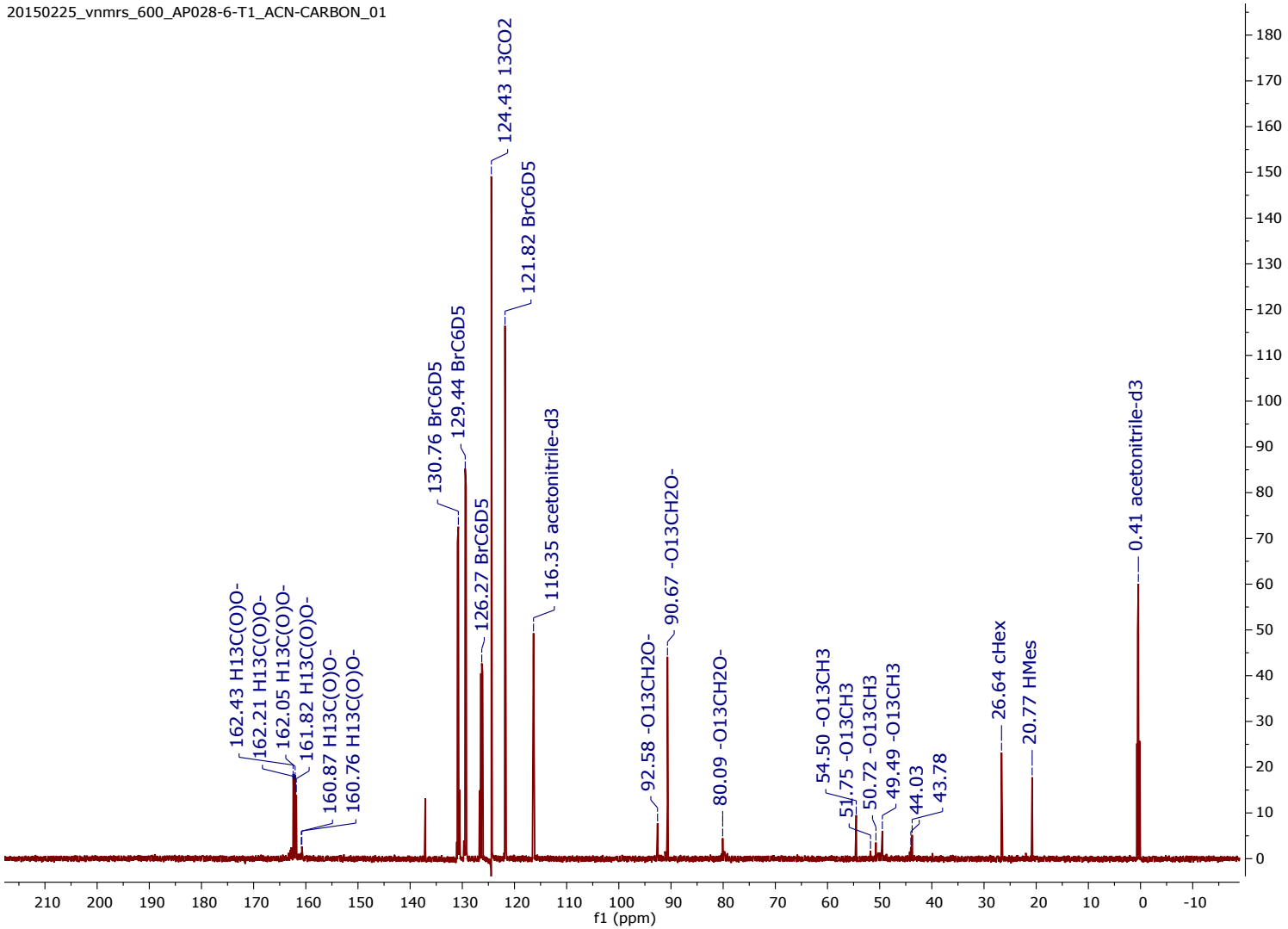


Figure S5-7. 151 MHz ^{13}C-NMR of the reaction between **1**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in BrC_6D_5 after 1 day at 130 °C, after the addition of acetonitrile-d3.

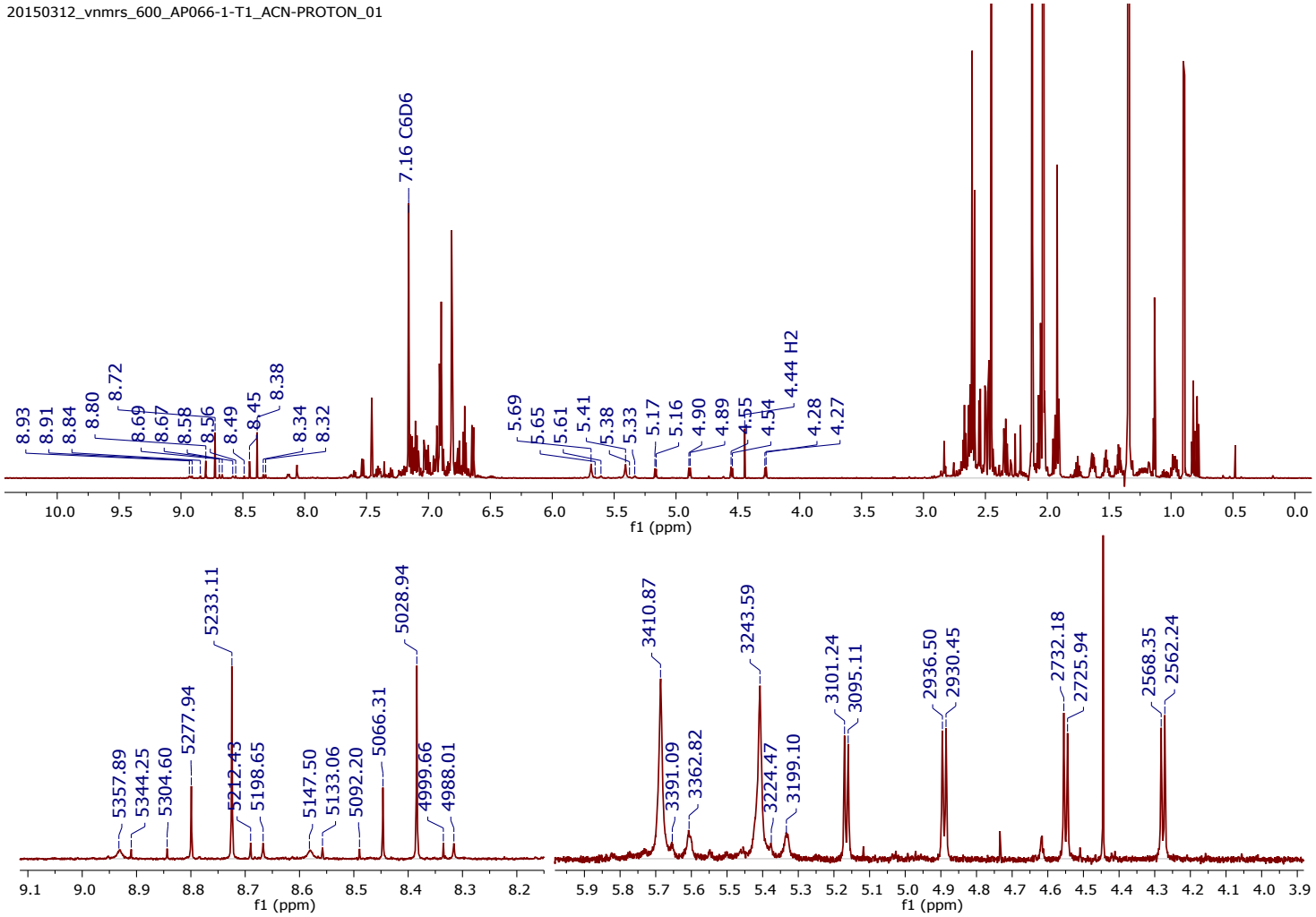


Figure S5-8. 600Mz ^{1}H-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in C_6D_6 after 6 h at 80 °C after the addition of acetonitrile-d3. a) Full spectra. b) Formate region [J_{CH} = 204-212 Hz]. c) (OCH_2O) region [J_{CH} = 163-165 Hz].

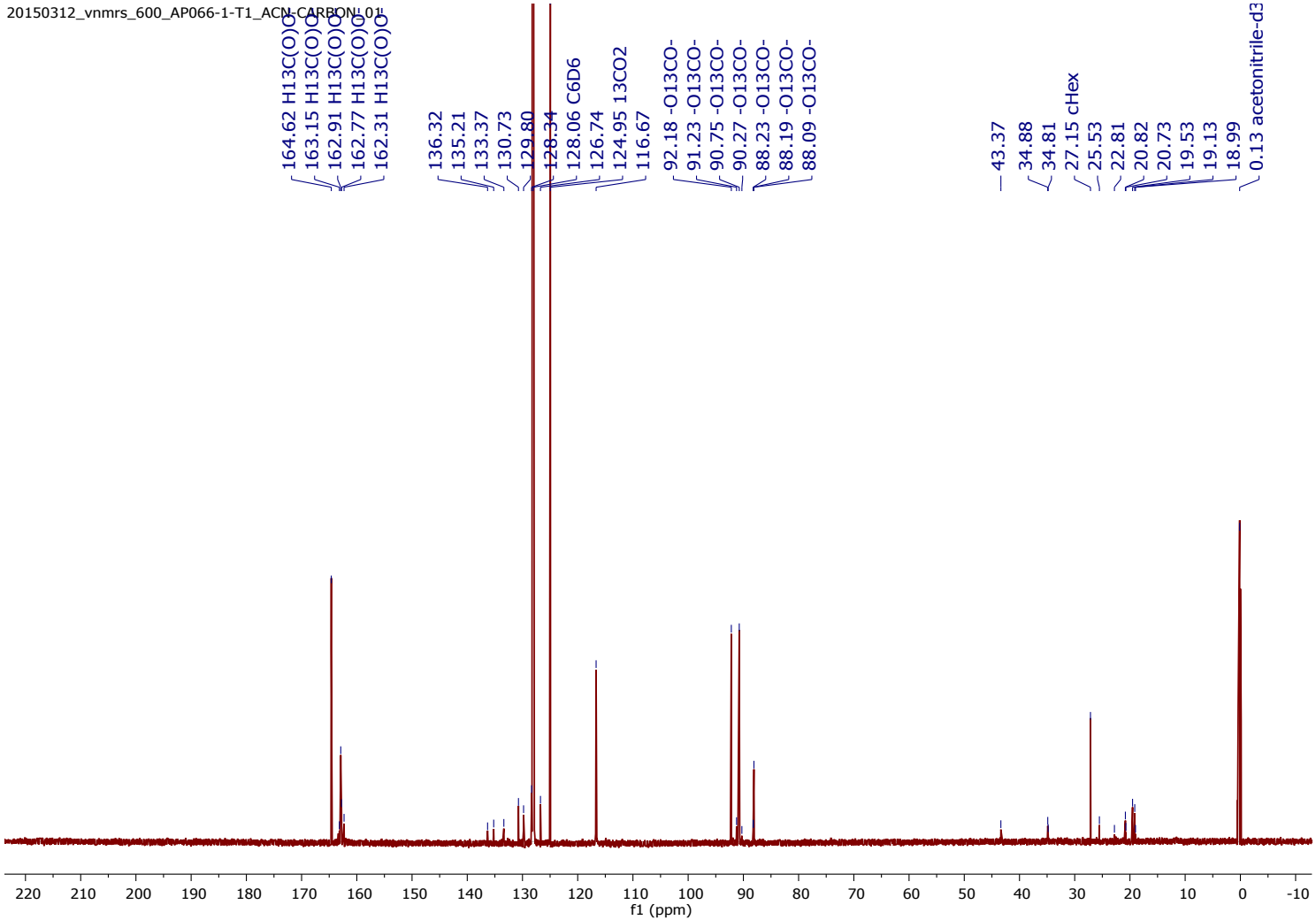


Figure S5-9. 151 MHz ^{13}C-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in C_6D_6 after 6 h at 80 °C after the addition of acetonitrile-d3.

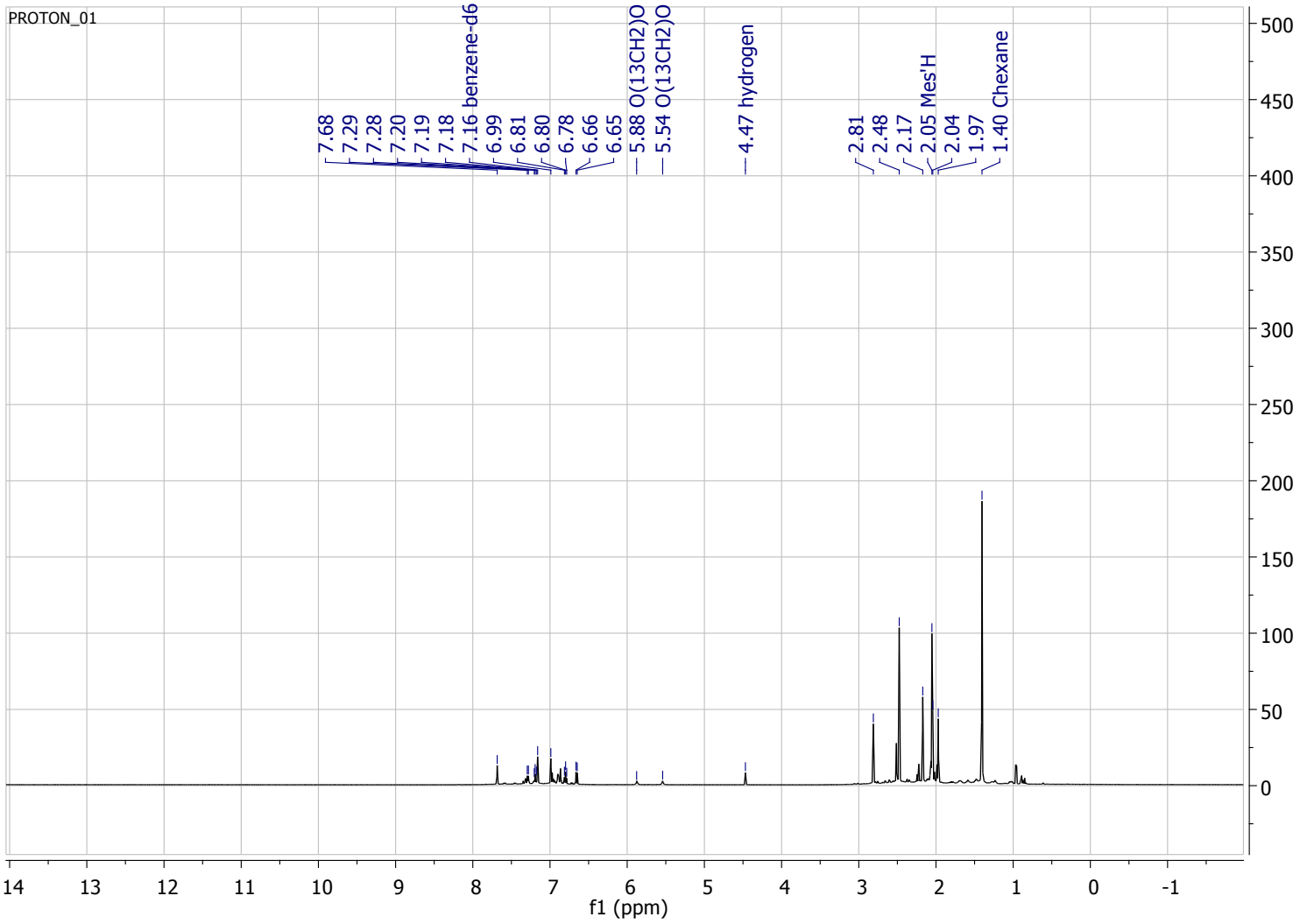


Figure S5-10 ^{1}H-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in benzene-d_6 after 72 h at r.t. in benzene-d6

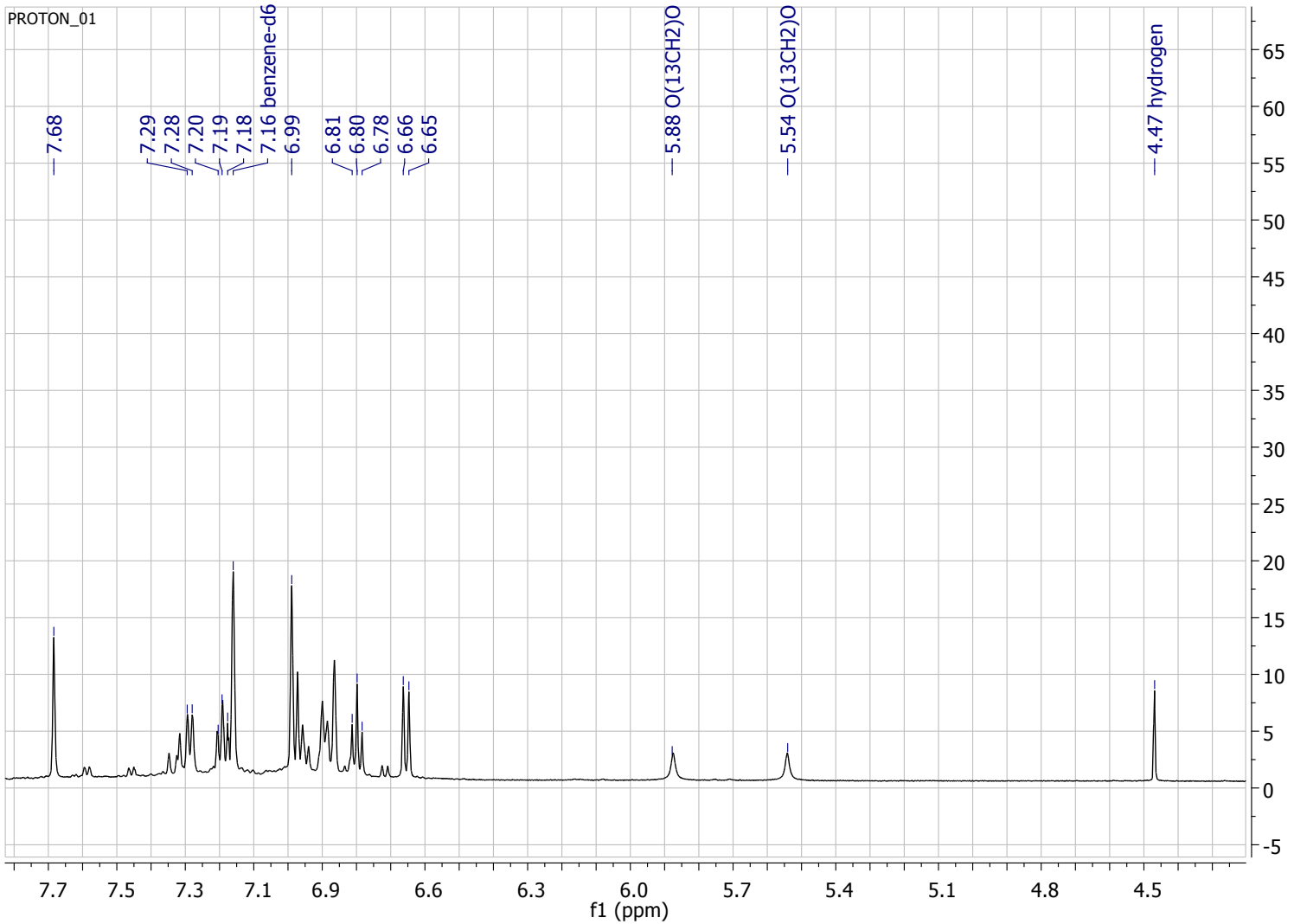


Figure S5-11 ^{1}H-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in C_6D_6 after 72 h at r.t. in benzene-d6. Zoom on aromatic region.

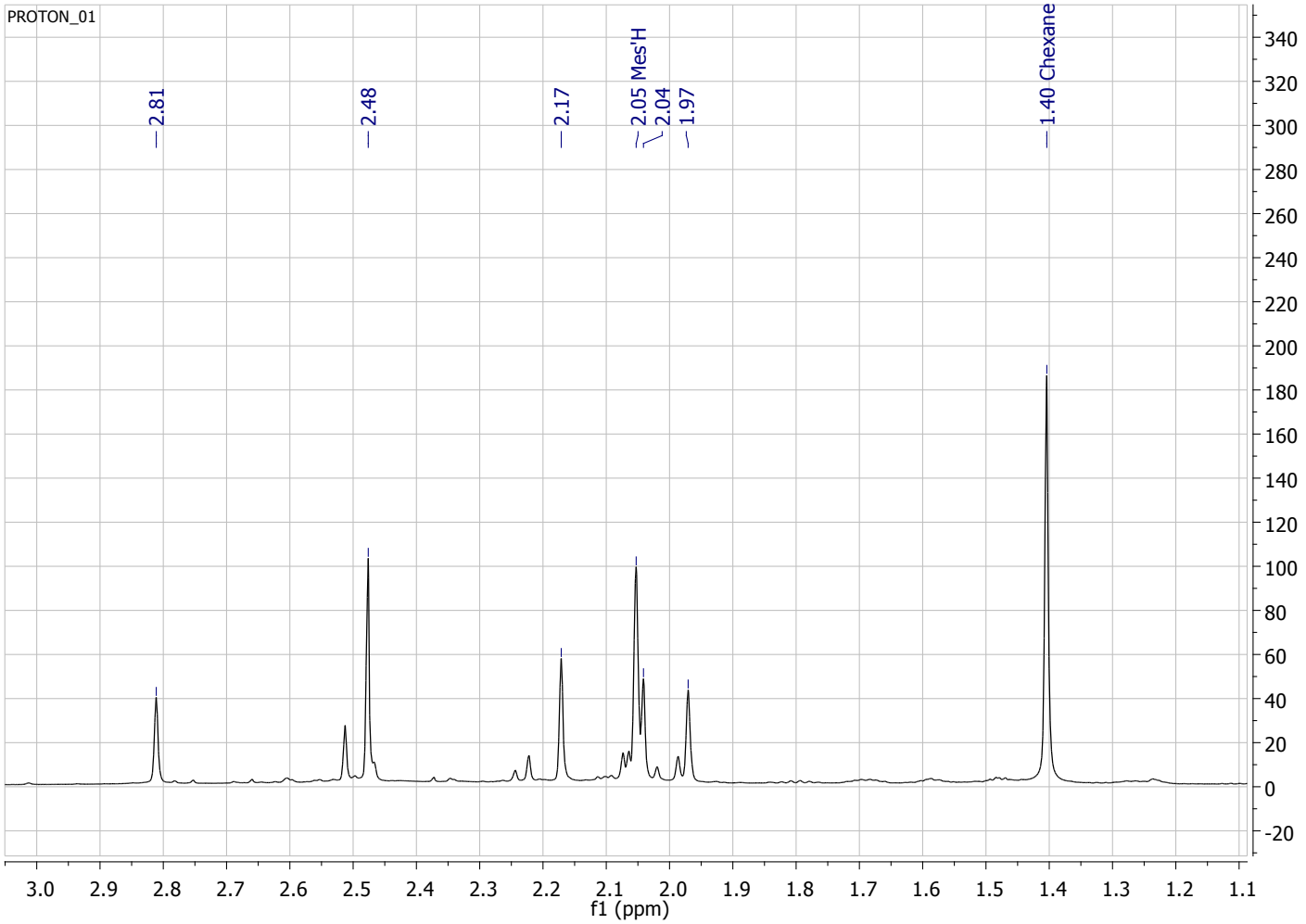


Figure S5-12 ^{1}H-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in C_6D_6 after 72 h at r.t. in benzene-d6. Zoom on aliphatic region.

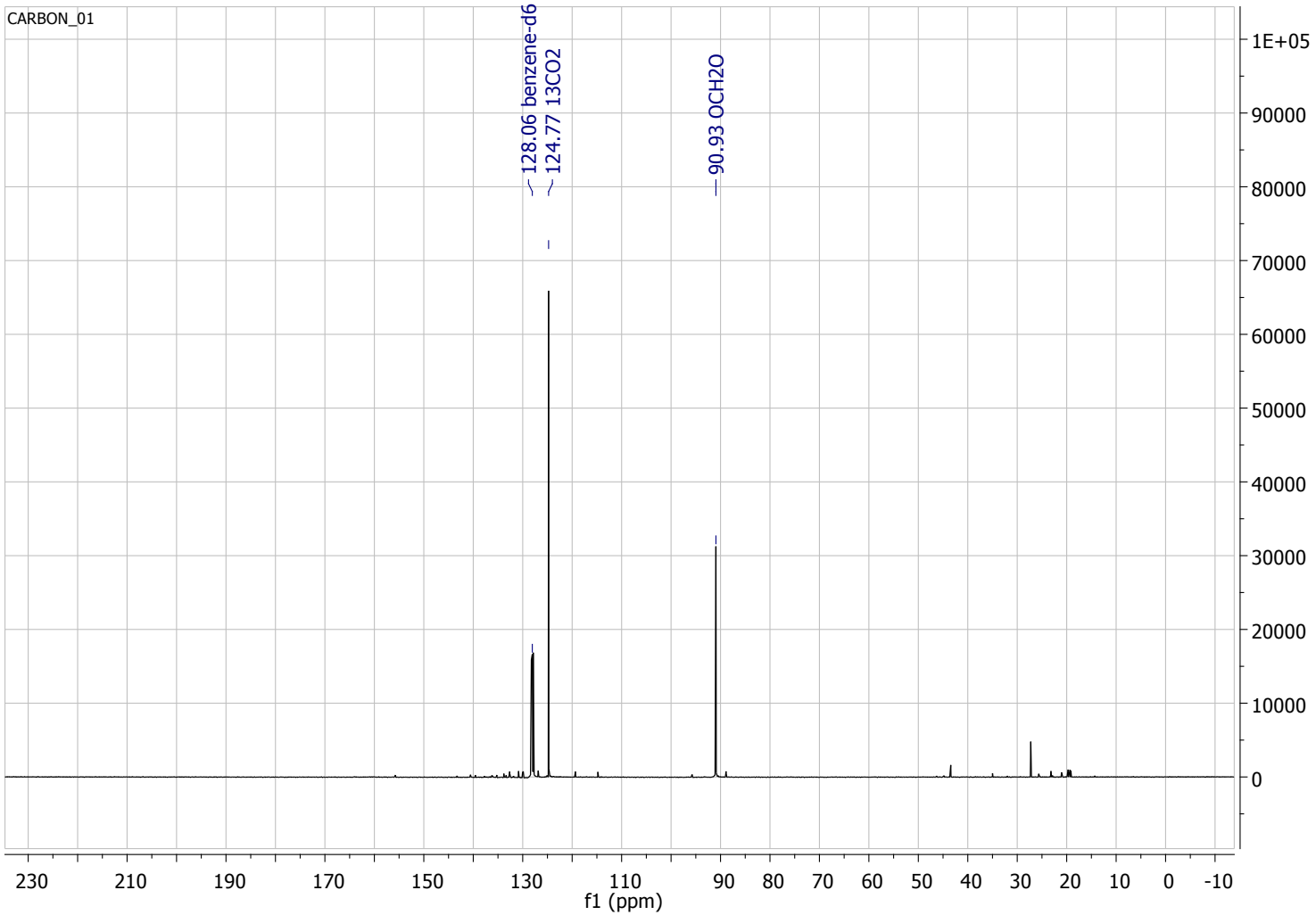
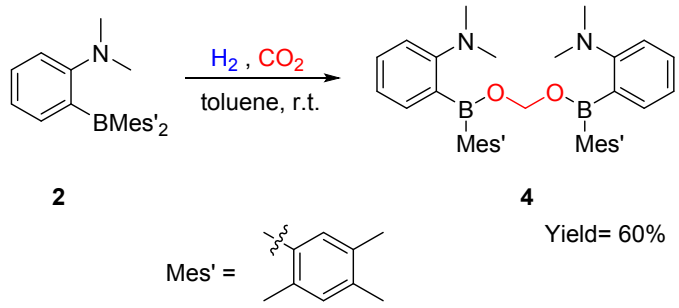
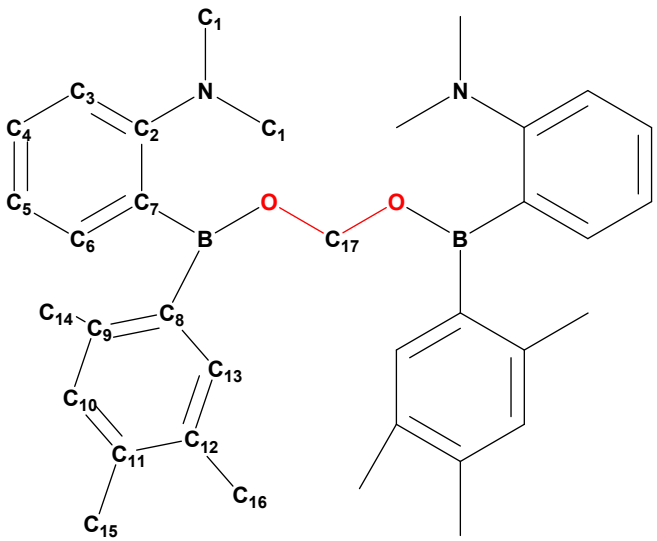


Figure S5-13 ^{13}C-NMR of the reaction between **2**, $^{13}CO_2$ (1 atm) and H_2 (4 atm) in benzene-d_6 after 72 h at r.t. in benzene-d6. Zoom on aliphatic region.

S6: Synthesis of 4 from 2 (Bigger scale hydrogenation)



In a glove box, **2** (200 mg, 0.54 mmol) was dissolved in toluene (4 ml) and the green solution transferred to a teflon capped Schlenk flask equipped with a teflon coated magnetic stir bar. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The flask was charged with CO_2 (1atm) and H_2 (1 atm) and the mixture was stirred at r.t. for 72 h after which the bright green coloration had almost completely disappeared and white precipitate had formed. The volatiles were removed in vacuo and left under vacuum at 60°C for one hour to ensure complete removal of 1,2,4-trimethylbenzene. The residue was dissolved in hot hexanes (*ca* 4mL) and filtered hot. The hexane solution was stored at -35°C for 72 hours, yielding the title compound as colorless crystals (90 mg, 60%). Note that the crystals readily re-dissolve upon warming of the hexanes solution. The crystals were isolated by cold filtration at -35°C followed by rapid evacuation of the remaining traces of hexanes *in vacuo*.



*The H atoms are numbered based on the carbon atom to which they are attached

11: ^{1}H NMR (500 MHz, benzene-d6) δ 7.69 (s, 2H, H13), 7.29 (d, *J* = 7.2 Hz, 2H, H6), 7.19 (t, *J* = 7.8 Hz, 2H, H4), 6.99 (s, 2H, H10), 6.80 (t, *J* = 7.3 Hz, 2H, H5), 6.66 (m, 2H,H3), 5.72 (s, 2H, H17), 2.82 (s, 6H, H14), 2.48 (s, 12H, H1), 2.04 (s, 6H, H15), 1.97 (s, 6H, H16).

^{13}C {^{1}H} NMR (126 MHz, benzene-d6) δ (155.7, C8), (143.3, C7), (140.5, C9), (139.6, C13), (133.8, C6), (132.7, C11) (132.6, C10) (130.0, C4), (128.4, C12), (119.3,C5), (114.8, C3), (90.9, C17), (43.4, C1), (23.2, C14), (19.7,C15),(19.2, C16).

^{11}B {^{1}H} NMR (193 MHz, benzene-d6): δ +46.1.

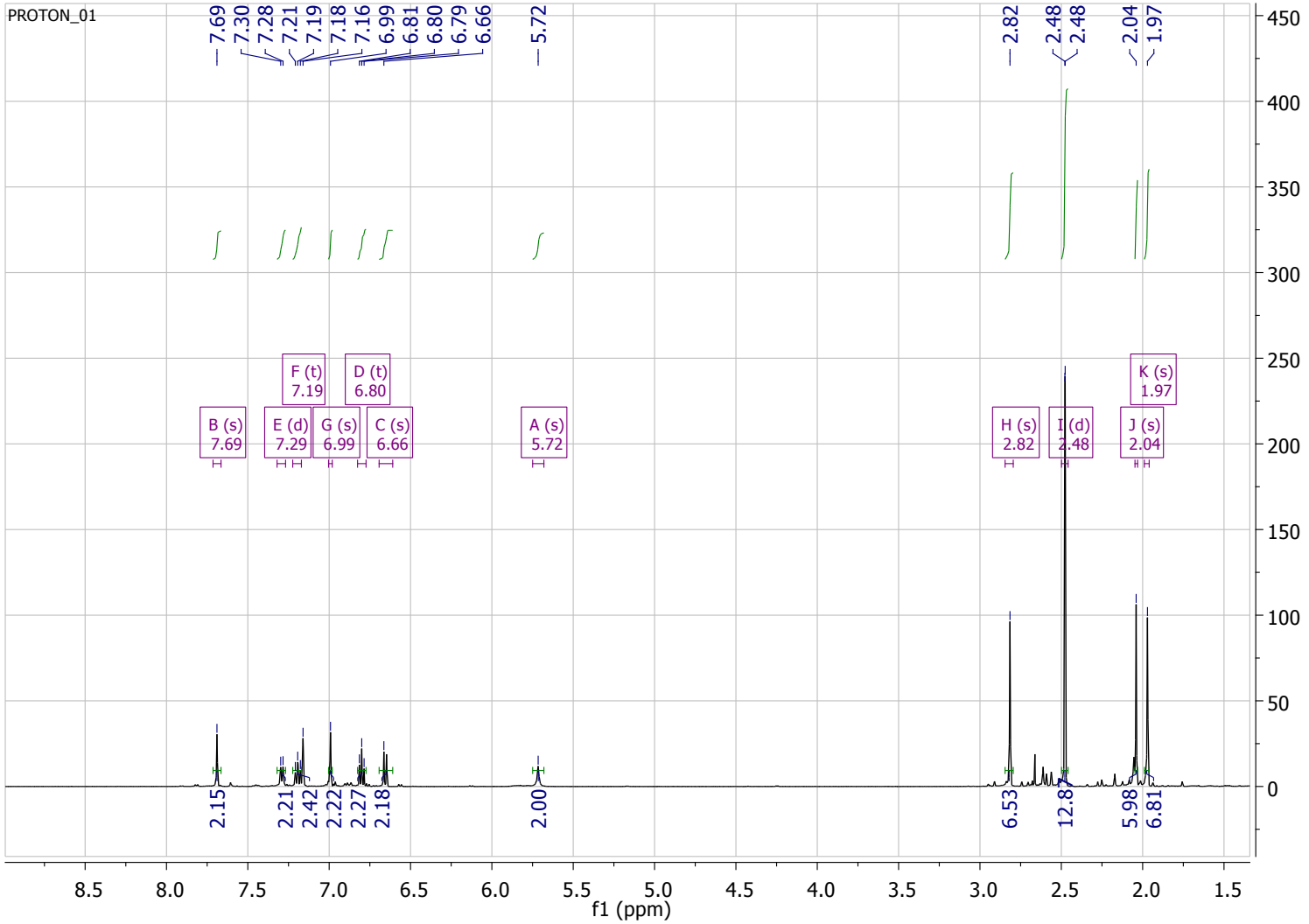


Figure S6-1: ^{1}H NMR spectra of the crystals of **4** in benzene-d6

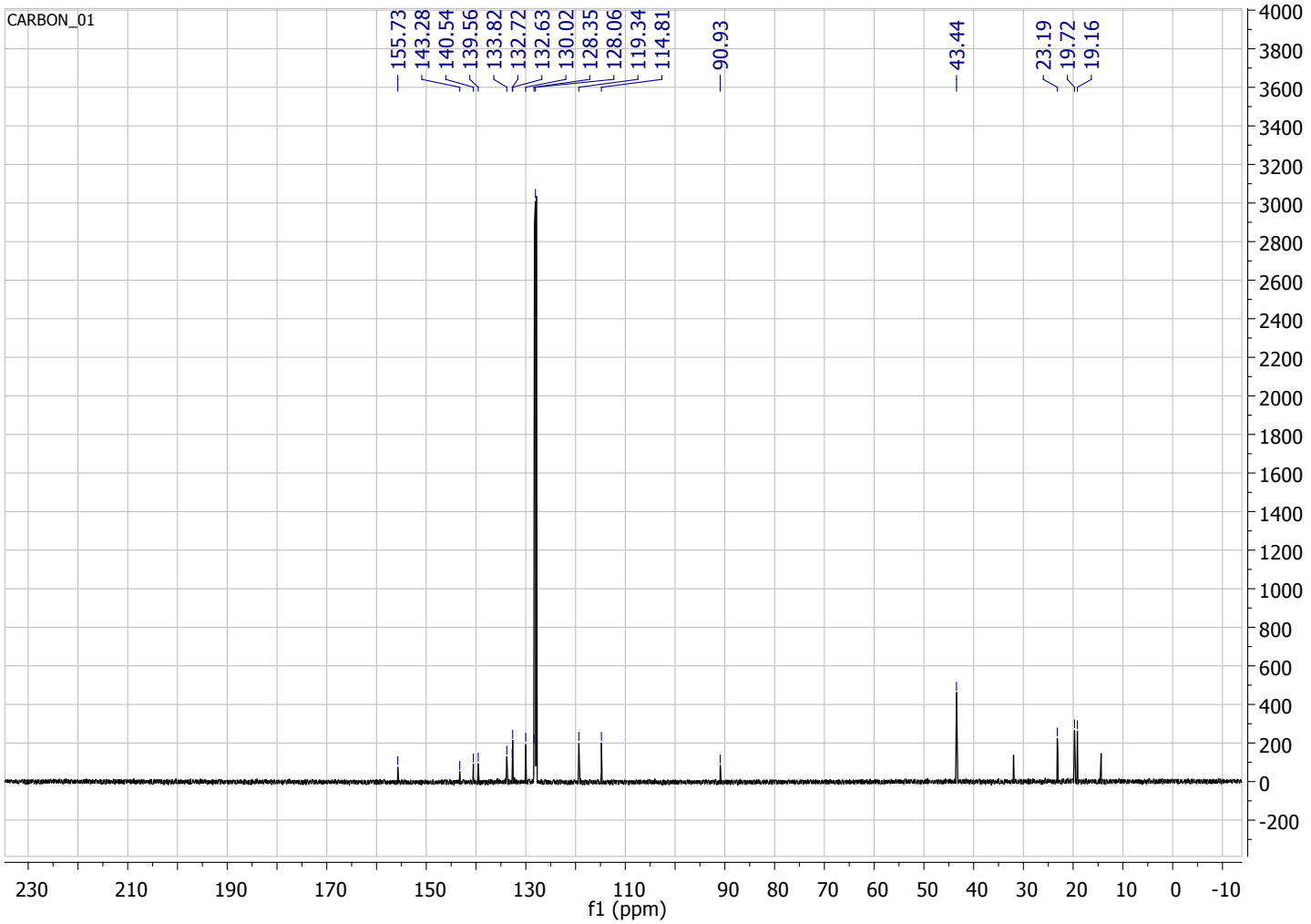


Figure S6-2: ^{13}C {^{1}H} NMR spectra of the crystals of **4** in benzene-d6. *n*-hexane was found to co-crystallize with the product, explaining the presence of small amounts of n-hexane in the product

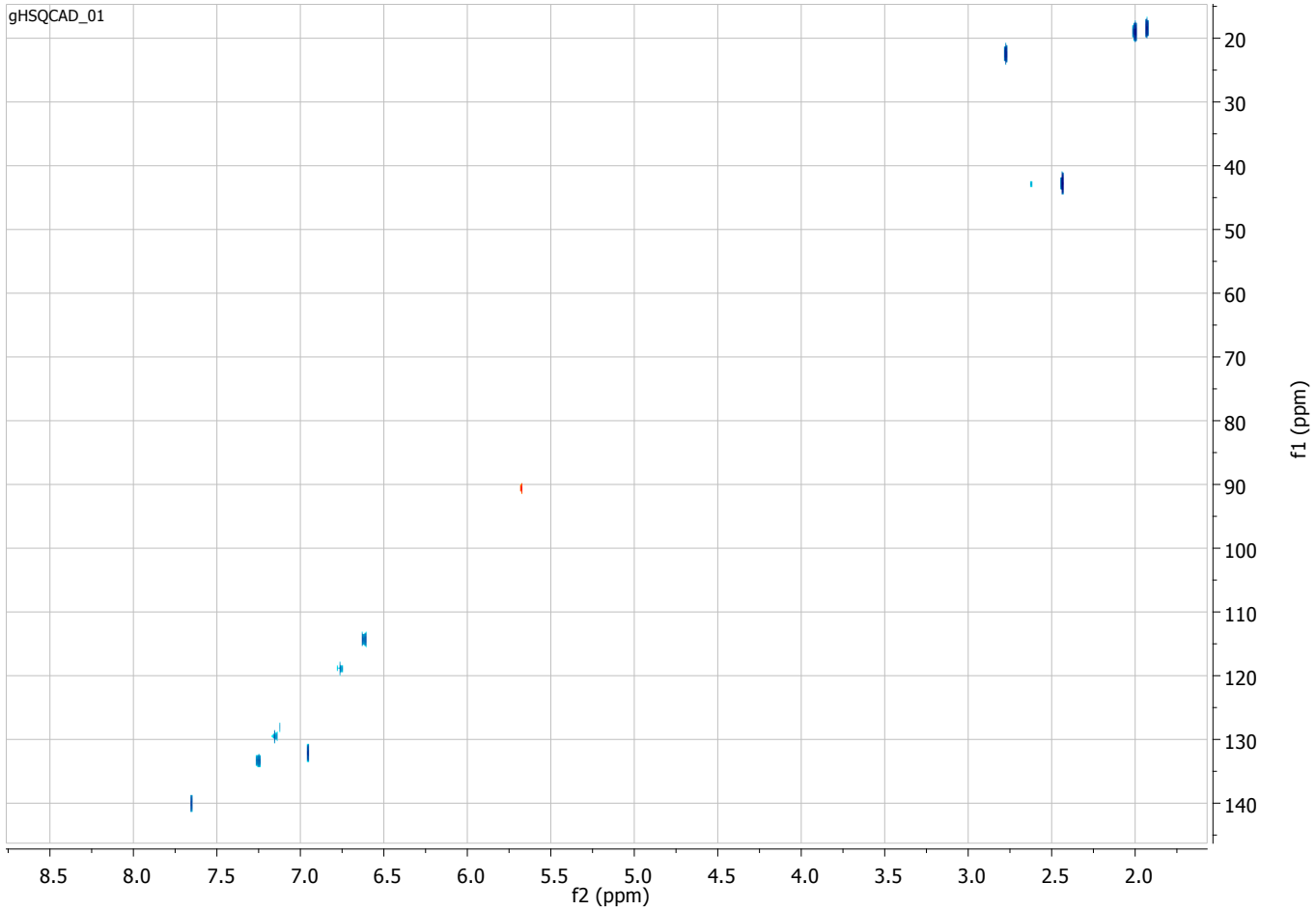


Figure S6-2: HSQC NMR spectra of the crystals of **4** in benzene-d6. *n*-hexane was found to co-crystallize with the product, explaining the presence of small amounts of n-hexane in the product

S7: Additional computational details and figures

Computational details:

All the calculations were performed on the full structures of the reported compounds. Calculations were performed with the GAUSSIAN 03 and GAUSSIAN 09 suite of programs.[7,8] The ωB97XD functional[9] was qualified as promising by Grimme[10] and was used to accurately describe the mechanism of FLP mediated hydrogenation of alkynes[11] and was thus used in combination with the 6-31G** basis set for all atoms[12] The transition states were located and confirmed by frequency calculations (single imaginary frequency). The stationary points were characterized as minima by full vibration frequencies calculations (no imaginary frequency). All geometry optimizations were carried out without any symmetry constraints. The energies were then refined by single point calculations to include solvent effects using the SMD solvation model[13] with the experimental solvent (benzene) at the ωB97XD /6-31++G** level of theory.[14] All structures with their associated free enthalpy and Gibbs free energies as well as their cartesian coordinates are fully detailed in section S8

Figure S7-1: Protodeborylation for 1

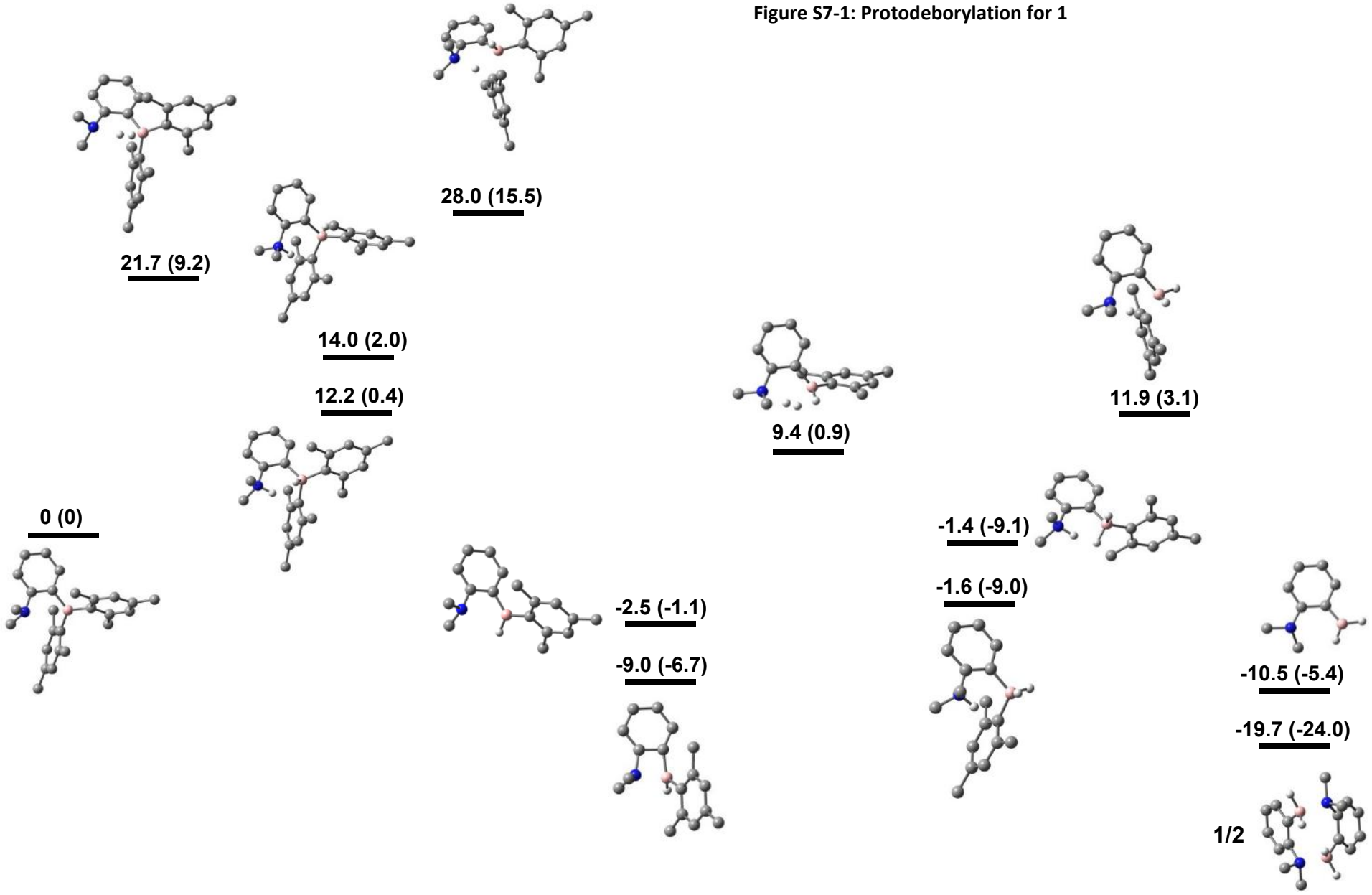
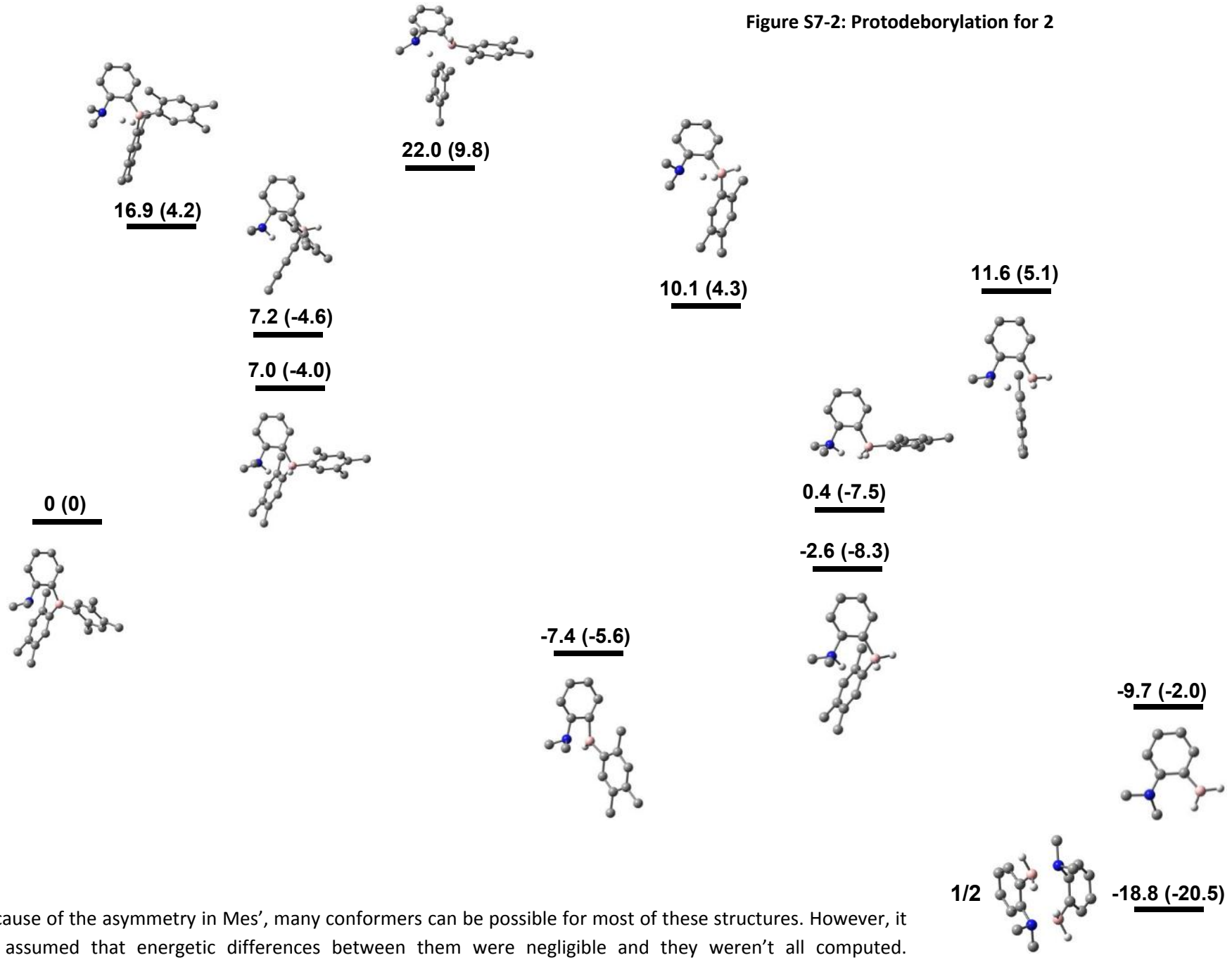


Figure S7-2: Protodeborylation for 2



*Because of the asymmetry in Mes', many conformers can be possible for most of these structures. However, it was assumed that energetic differences between them were negligible and they weren't all computed. Nevertheless, uncertainty on the values reported might be slightly higher than for NMe_2BMes_2, but still we are confident that the conclusions based on those calculations should not be altered significantly

Figure S7-3: Identification of the resting state of 4

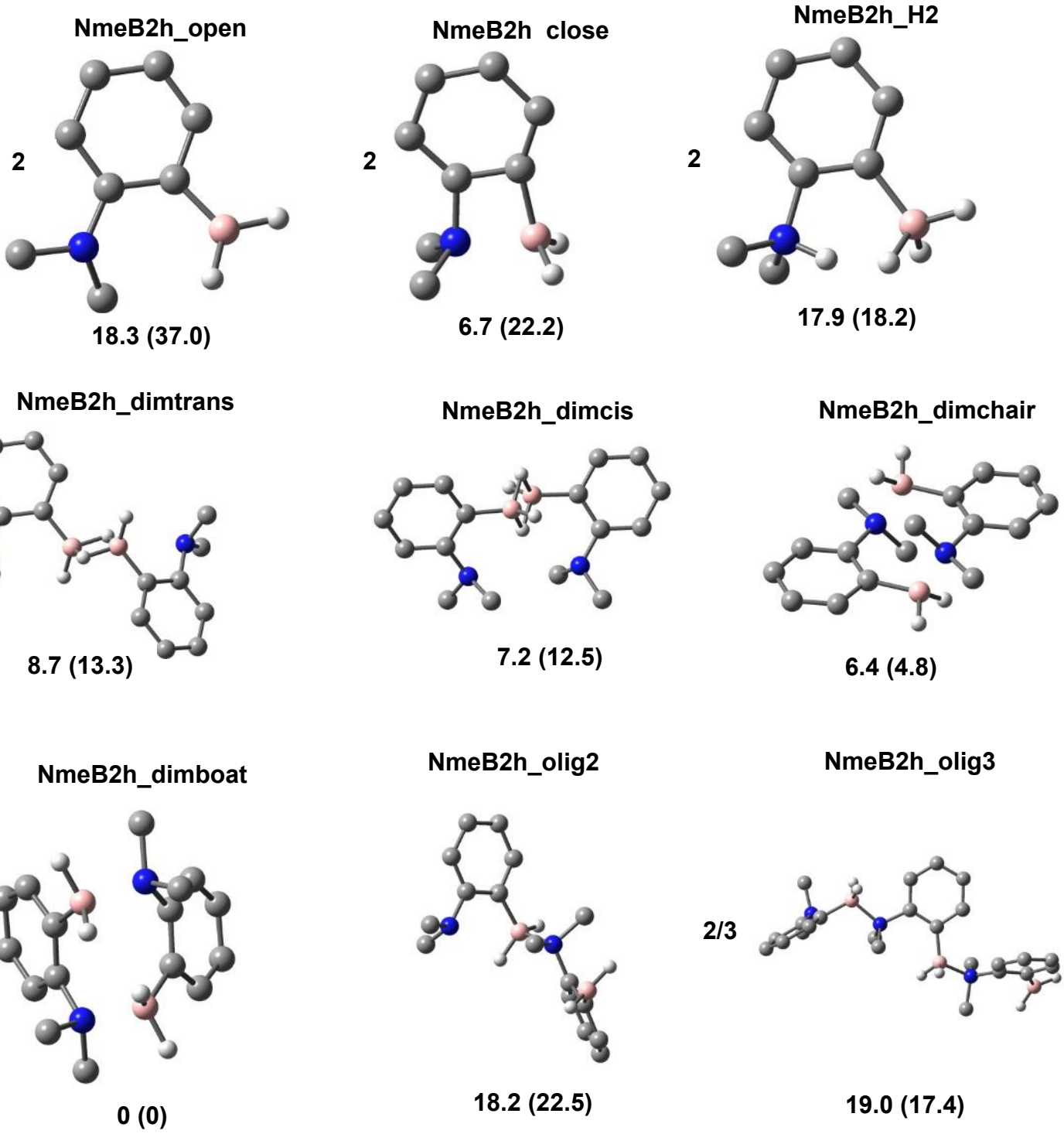
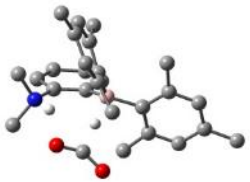
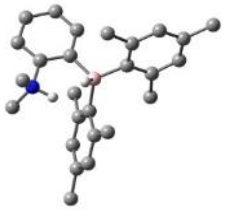


Figure S7-4: Hydrogenation of CO2 by 1

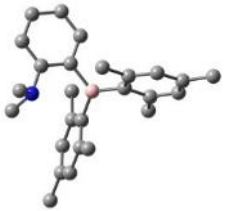


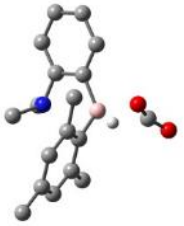
34.7 (9.4)



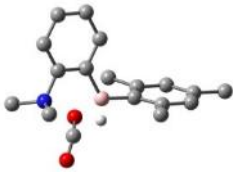
12.2 (0.4)

0 (0)



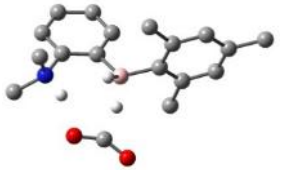


31.7 (19.9)

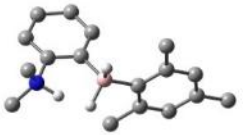


29.3 (16.3)

24.4 (1.9)



7.6 (-2.4)



0 (0)

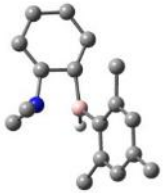


Figure S7-6: Hydrogenation of CO2 by 2

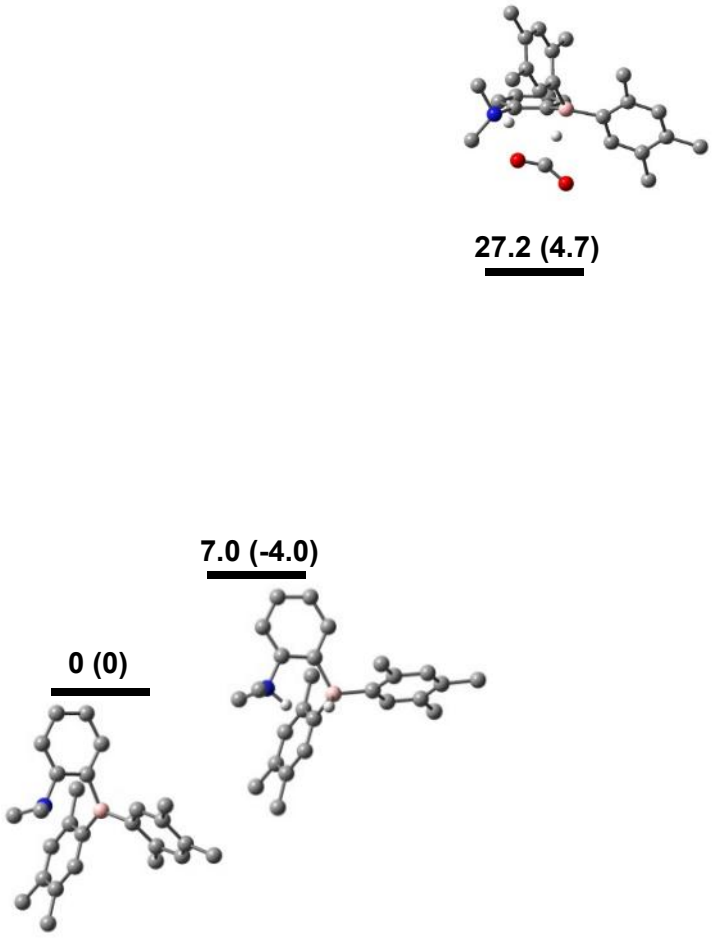
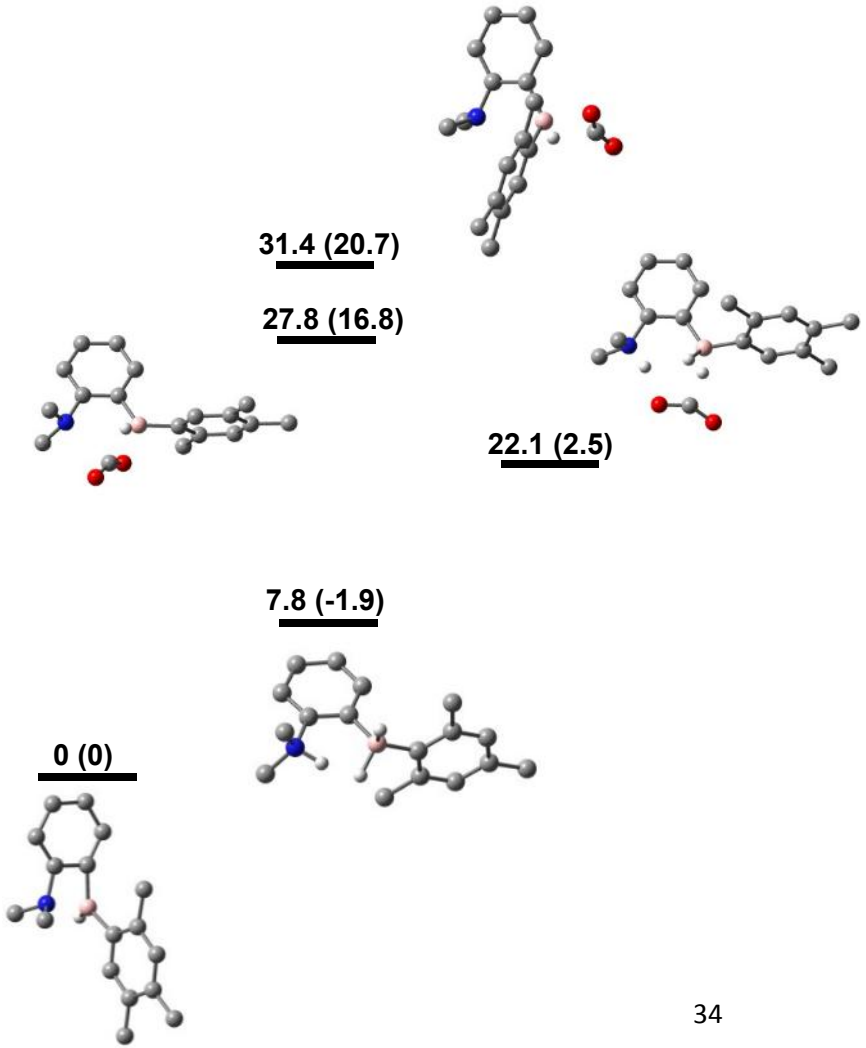


Figure S7-7: Hydrogenation of CO2 by 2



S8: **Optimized geometries with cartesian coordinates and electronic energies.**

H_2

Sum of electronic and thermal Enthalpies=-1.161392

Sum of electronic and thermal Free Energies= -1.176183

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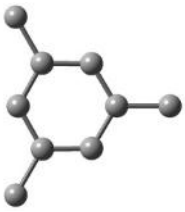
H	2.04240800	0.63636400	0.00000000

Mes



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Sum of electronic and thermal Free Energies= -349.967313

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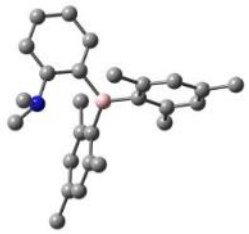
C	-1.48221700	-0.08192100	-0.00213000	H	1.13993700	0.28171800	0.56575300
C	-0.77204800	1.12051100	0.00843000	C	-3.63109500	3.63991300	0.00702100
C	-1.48528200	2.31700900	0.00729300	H	-3.52648900	4.13880600	0.97649900
C	-2.88182400	2.33115700	-0.00853200	H	-3.24854600	4.32636200	-0.75459300
C	-3.56059700	1.11496700	-0.02312500	H	-4.69797200	3.49111400	-0.17732000
H	-0.93588600	-1.02303800	-0.00023100	C	-3.62983100	-1.40706600	0.00798000
H	-0.94408300	3.26109800	0.01636100	H	-3.82062400	-1.72746500	1.03830500
H	-4.64855900	1.11191500	-0.03854700	H	-4.59815100	-1.31622000	-0.49166400
C	0.73603700	1.11858700	-0.01094100	H	-3.06647600	-2.20430300	-0.48461600
H	1.11445000	1.02242300	-1.03473800				

NMeBMes



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Sum of electronic and thermal Free Energies= -1088.970774

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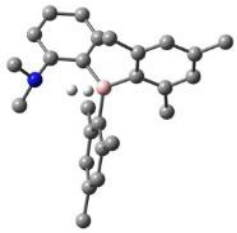
C	1.26535500	0.18579900	0.05282800	C	6.10535100	-0.66778800	0.81403100
C	2.00604400	1.35554400	-0.08470900	H	5.98539300	-1.76351900	0.74433400
C	1.91789100	-1.04332500	0.05796000	H	7.17927700	-0.45283900	0.81908400
C	3.39716600	1.32541000	-0.24793000	H	5.68213200	-0.33874700	1.76618300
H	1.49847900	2.31722300	-0.06287200	N	5.48229800	0.06016500	-0.28125900
C	3.30353100	-1.09377000	-0.06755700	C	7.69451300	3.01228400	-5.24467100
H	1.35266800	-1.96310600	0.17469200	H	7.71675800	2.05543400	-5.77706000
C	4.04291200	0.08000600	-0.21620100	H	7.33830500	3.76848600	-5.95189700
H	3.81376400	-2.05258600	-0.03880900	H	8.72174000	3.26603000	-4.97015000
B	4.18649400	2.66771600	-0.49544600	C	7.09318100	3.22662700	-0.25242100
C	3.95188300	3.87846900	0.48626300	H	8.16142600	3.44836300	-0.32054400
C	3.66373300	5.17758900	0.00317400	H	6.61146200	4.02818000	0.31505000
C	4.01944800	3.68866000	1.88700200	H	6.97291500	2.29775400	0.31729400
C	3.41642900	6.21550500	0.90111100	C	3.14904900	2.19542100	-3.29849300
C	3.79743000	4.75887200	2.75191900	H	2.96381500	1.14744200	-3.03926700
C	3.47785800	6.02865600	2.27931000	H	2.46122100	2.79205600	-2.69201500
H	3.18226400	7.20416800	0.51161000	H	2.87600300	2.33721400	-4.34749300
H	3.87797600	4.59678200	3.82476000	C	3.60567800	5.50090300	-1.47345700
C	5.10812400	2.78231700	-1.76892300	H	4.58592800	5.38945000	-1.94416600
C	4.59826700	2.56155700	-3.06549400	H	2.91756200	4.84594300	-2.01514600
C	6.47984700	3.06462900	-1.62239100	H	3.26835400	6.52916300	-1.62722500
C	5.44245700	2.65794100	-4.17005300	C	3.19253500	7.16509000	3.22671500
C	7.30242700	3.12780800	-2.74796100	H	3.56014400	8.11522100	2.82836900
C	6.80164600	2.93638900	-4.03228200	H	2.11454500	7.27407200	3.39053500
H	5.03063200	2.50289200	-5.16571800	H	3.65946700	6.99978200	4.20136200
H	8.36301000	3.33208300	-2.61545500	C	4.38475000	2.35307000	2.49577400
C	5.99251700	-0.38569000	-1.57138600	H	3.57125900	1.62915100	2.39350400
H	5.52170600	0.18334200	-2.37447000	H	5.26498800	1.91908700	2.01231800
H	7.06996200	-0.19659700	-1.61618800	H	4.60806300	2.46467000	3.56001500

NMeBMes_H2_TSsplit



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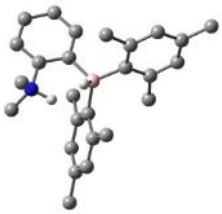
Sum of electronic and thermal Free Energies= -1090.112362

H	0.30760000	0.52535900	0.41501900	C	6.12042700	-0.86949900	1.17498500
C	1.38033700	0.38636800	0.32406000	H	5.91276000	-1.94959100	1.10537600
C	2.21114400	1.48362900	0.13356500	H	7.20705800	-0.73966900	1.19147500
C	1.93146500	-0.88816400	0.41051600	H	5.71241600	-0.49791300	2.11794900
C	3.59981500	1.35153900	-0.00334600	N	5.57006700	-0.09777600	0.06915600
H	1.77615500	2.47880800	0.08760600	H	5.83909400	2.46308300	0.69734800
C	3.30903600	-1.04667400	0.31877100	H	5.86094100	1.72178800	0.46169100
H	1.29444500	-1.75426500	0.56057000	C	3.44567700	5.23396900	-1.65136900
C	4.13797100	0.05781900	0.11428400	H	4.43494400	5.31584200	-2.10906300
H	3.74483400	-2.03796300	0.40495200	H	2.95970500	4.36703200	-2.10499600
B	4.46221800	2.66656800	-0.30397700	H	2.86920600	6.11933000	-1.93203400
C	4.00589300	3.96779900	0.52359300	C	4.46563200	2.81439600	2.77936000
C	3.52847200	5.12263500	-0.14380200	H	4.09843900	1.85842500	2.40066000
C	3.99144800	3.98156700	1.94084400	H	5.56048500	2.75791600	2.80857900
C	3.08831500	6.22664300	0.58775000	H	4.12113300	2.92298600	3.81064600
C	3.55765300	5.11217900	2.63382100	C	2.60031900	7.44631300	2.74309600
C	3.10209800	6.24924400	1.97763900	H	3.08112800	7.52367200	3.72211700
H	2.72138000	7.09877900	0.05036600	H	2.78779200	8.37502800	2.19695400
H	3.57013500	5.09892900	3.72181400	H	1.51973300	7.37735900	2.91180700
C	5.24124900	2.79933600	-1.70502400	C	3.35911200	1.59904100	-3.00067700
C	4.71032500	2.27771000	-2.91051700	H	3.35959300	0.60942200	-2.53439900
C	6.48020200	3.47856300	-1.78289500	H	2.57085700	2.17242900	-2.50652600
C	5.41997500	2.40222400	-4.10516600	H	3.07078500	1.47445100	-4.04757100
C	7.16427100	3.57325700	-2.99629900	C	7.42302500	3.11615300	-5.46678900
C	6.65886700	3.03138500	-4.17102800	H	8.04137400	2.22359700	-5.61495600
H	4.98434700	2.00143500	-5.01823200	H	6.74754500	3.19162000	-6.32356300
H	8.11674100	4.09897300	-3.02293000	H	8.08929800	3.98302300	-5.48078400
C	6.07486800	-0.55528300	-1.22120600	C	7.13138000	4.13613000	-0.58589300
H	5.69931700	0.08885100	-2.01624900	H	7.85746400	4.88494700	-0.91208500
H	7.16725800	-0.49168100	-1.22246800	H	6.40425000	4.63318300	0.06014700
H	5.78546400	-1.59785400	-1.43424200	H	7.67423200	3.40741200	0.02797700

NMeBMes_H2_HH



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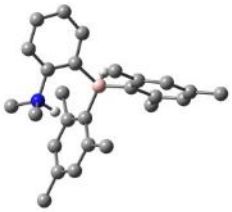
C	1.52892800	0.25017000	0.53941400	H	6.18182500	-1.38968200	1.06878300
C	2.27882400	1.41554600	0.42372100	H	7.48603000	-0.24255200	0.63028800
C	2.12154100	-0.99836700	0.34974800	H	6.13625000	0.29559500	1.67420500
C	3.64462400	1.39774500	0.10576100	N	5.64129300	0.08251000	-0.34444800
H	1.80571800	2.38151100	0.58066100	H	5.56958400	2.42378700	0.68619600
C	3.47755600	-1.06941300	0.05326100	H	5.86405900	1.08582300	-0.49863600
H	1.53797200	-1.90850600	0.43892100	C	3.58510100	5.30357200	-1.60116500
C	4.18402300	0.12152400	-0.05866500	H	4.62091200	5.29354200	-1.95056400
H	3.95850100	-2.03460800	-0.08266700	H	3.07539400	4.48211500	-2.10963100
B	4.61187400	2.71512300	-0.04401600	H	3.12473800	6.23628100	-1.94006900
C	3.95795900	4.05552500	0.61639300	C	4.31720100	2.97376800	2.91244500
C	3.49546600	5.18653000	-0.09480500	H	3.84356100	2.01979800	2.66011100
C	3.82948200	4.10204800	2.02946800	H	5.39814600	2.83170700	2.80397800
C	2.93091000	6.27556400	0.57871100	H	4.10650200	3.18419700	3.96498600
C	3.25608000	5.20089100	2.67004600	C	2.20714600	7.49972500	2.66869600
C	2.79734400	6.30629800	1.96087900	H	2.99159900	8.18315300	3.01458500
H	2.58118800	7.12769700	-0.00218100	H	1.54624800	8.06901200	2.00853200
H	3.16673700	5.19444200	3.75555400	H	1.62950500	7.19695000	3.54767800
C	5.29187600	2.78843100	-1.55012800	C	3.26205600	1.83474000	-2.81712100
C	4.69943200	2.31160900	-2.74590500	H	3.14708100	0.78095400	-2.53715700
C	6.61042200	3.30149800	-1.65996700	H	2.61295200	2.40208800	-2.14862900
C	5.41786800	2.29616100	-3.94622000	H	2.87848200	1.94700000	-3.83547700
C	7.30048200	3.27431200	-2.87359300	C	7.47435100	2.76571100	-5.34182400
C	6.72667200	2.75967000	-4.03246700	H	7.36987500	3.73247000	-5.84721900
H	4.92992300	1.92597200	-4.84706700	H	8.54405800	2.59147200	-5.19148700
H	8.31010500	3.68019800	-2.91803900	H	7.09662500	1.99805900	-6.02353000
C	6.01260000	-0.64047100	-1.58596000	C	7.30112600	3.92983100	-0.47004200
H	5.44445900	-0.21136700	-2.41010000	H	8.19386400	4.47814200	-0.78419300
H	7.07827300	-0.49213500	-1.76604800	H	6.63244100	4.61884900	0.05307900
H	5.79477300	-1.70236700	-1.47177500	H	7.60719700	3.18077400	0.26941300

NMeBMes_H2_HMes

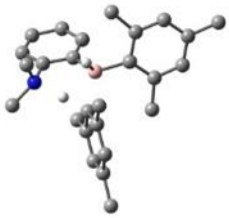


Sum of electronic and thermal Enthalpies= -1090.038800

Sum of electronic and thermal Free Energies= -1090.124613

C	0.53661800	-0.73585200	0.71747800	H	1.51515600	-0.40439800	0.38091600
C	0.05829400	-0.20414300	1.93364900	H	-1.02078900	0.40559400	3.96594700
C	-1.19605600	-0.69335900	2.29967500	H	2.09565400	0.21416500	2.72953800
C	-1.95482200	-1.59667900	1.55444100	H	0.47849600	4.48458300	-0.46102100
C	-1.44440700	-2.06843200	0.35787900	H	-0.93927400	3.03634200	6.62673900
C	-0.18336800	-1.63129600	-0.05603500	H	3.91419800	4.56698900	2.06386100
B	1.05049600	0.84095300	2.74025000	H	0.99580600	-0.71100000	7.28497400
C	1.40441700	2.23095500	1.94625700	C	-0.66120800	2.30235200	0.40704900
C	0.65633400	2.84705600	0.91844800	H	-1.22256200	3.08435600	-0.11285200
C	1.08821200	4.03765300	0.32317300	H	-0.52524600	1.47025700	-0.29065300
C	2.25847300	4.67647700	0.70760300	H	-1.29221500	1.92090900	1.21329600
C	2.99716000	4.08507400	1.72810800	C	3.48631600	2.35127800	3.43091600
C	2.59811400	2.89472500	2.33460700	H	4.32888200	3.02342500	3.61732500
N	-1.77374900	-0.20628200	3.57595800	H	2.94177700	2.22262500	4.37116100
C	-2.98253600	0.63825100	3.41460900	H	3.88467900	1.36686600	3.16501600
H	-3.20684800	1.10640700	4.37451800	C	2.72137500	5.94796000	0.04296100
C	0.65808500	1.03215300	4.34323400	H	3.13814100	6.65030000	0.77176300
C	1.02609100	0.00895000	5.26205400	H	3.50327900	5.74627700	-0.69828400
C	0.69532000	0.09292800	6.61502200	H	1.89827900	6.44852400	-0.47545200
C	-0.01189500	1.17447500	7.13433600	C	1.77869500	-1.21970000	4.80615500
C	-0.38453600	2.17904700	6.24898600	H	1.30608200	-1.69424900	3.94045100
C	-0.05752100	2.13208200	4.88797800	H	2.79099200	-0.95640300	4.48572500
C	-1.96808900	-1.27631900	4.58847500	H	1.85066800	-1.95587200	5.61240500
H	-2.19749600	-0.80717100	5.54622600	C	-0.51562600	3.29597500	4.03782300
H	-2.77989000	-1.93319800	4.27456900	H	-0.98802800	2.97187400	3.10816400
H	-1.03870900	-1.83689600	4.66987500	H	-1.22761500	3.91878900	4.58748600
H	-2.77340800	1.40380200	2.66941300	H	0.32958800	3.92069300	3.73704300
H	-3.81892000	0.02031500	3.08597800	C	-0.33595400	1.26533000	8.60348800
H	-2.93035000	-1.92920400	1.90051600	H	-0.44979400	0.27396500	9.05172800
H	-2.01553800	-2.76884200	-0.24184800	H	0.46496800	1.77889500	9.14678500
H	0.23577400	-2.00032200	-0.98728400	H	-1.25925200	1.82582600	8.77631300

NMeBMes_H2_TSprot



Sum of electronic and thermal Enthalpies= -1090.017364

Sum of electronic and thermal Free Energies= -1090.017364

C	0.00864700	-0.04409500	0.14815900	H	0.85357300	0.38026300	-0.38889100
C	-0.00334100	0.04435900	1.54407700	H	0.37088600	-0.31356700	3.76870200
C	-1.11880700	-0.50794300	2.19273000	H	0.61747000	1.58360700	3.10250200
C	-2.15313300	-1.14321900	1.51390300	H	3.11628200	-3.51593900	4.05987300
C	-2.09862100	-1.22472100	0.12469800	H	5.57490700	1.41430000	0.46389400
C	-1.01920300	-0.66744800	-0.55583200	H	3.65175100	-0.03283300	6.48027500
B	1.15593500	0.72613900	2.44270100	H	2.59890700	4.41586800	-0.10233100
C	1.63209700	-0.44220700	3.73921400	C	1.40520600	-2.56881800	2.29203400
C	1.96666100	-1.80696900	3.46892700	H	1.87085400	-3.55482700	2.22085400
C	2.86959500	-2.48022600	4.28206600	H	0.32410100	-2.71032700	2.35434100
C	3.48701500	-1.85847800	5.36804300	H	1.57801600	-2.03410200	1.35508100
C	3.17422900	-0.52852000	5.63839900	C	1.96647700	1.60418400	5.24209100
C	2.25389700	0.17405600	4.86477200	H	2.42693700	1.85025400	6.20235300
N	-1.09514600	-0.40591200	3.64264000	H	2.35855200	2.28442500	4.47969400
C	-1.77105700	0.80432400	4.13004200	H	0.89255300	1.79524600	5.31007700
H	-1.53057100	0.95390500	5.18681300	C	4.44720800	-2.62443700	6.23759800
C	2.35568900	1.45700300	1.62051400	H	5.06641900	-1.95555700	6.84002700
C	2.00021100	2.71643600	1.06248200	H	3.90020000	-3.28180000	6.92260600
C	2.91185700	3.45836700	0.31099000	H	5.10544300	-3.25657500	5.63502400
C	4.20880300	3.01393400	0.07899300	C	0.62645000	3.32529900	1.25167000
C	4.56581900	1.78943300	0.62684900	H	-0.17106200	2.64151800	0.94702900
C	3.67399200	1.01356200	1.37571400	H	0.44474100	3.57799400	2.30192800
C	-1.53187000	-1.58998100	4.38095300	H	0.52811600	4.24193200	0.66338000
H	-1.27814000	-1.45393100	5.43574700	C	4.21292500	-0.29951000	1.89436700
H	-2.61384700	-1.75472900	4.30241700	H	3.61507500	-1.14750400	1.55337200
H	-1.00879500	-2.47145200	4.00895600	H	5.23419000	-0.46007900	1.53738300
H	-1.42173100	1.66358800	3.55906900	H	4.23786700	-0.33172100	2.98666500
H	-2.85960700	0.70883300	4.02011200	C	5.17113600	3.81720300	-0.75854700
H	-2.99586600	-1.56924800	2.05096000	H	5.01631800	3.62874600	-1.82732200
H	-2.89987000	-1.71418400	-0.42017800	H	5.03874700	4.89118700	-0.59564900
H	-0.97514600	-0.72746500	-1.63944200	H	6.21028100	3.56505800	-0.52787900

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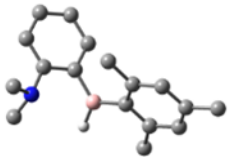

Sum of electronic and thermal Enthalpies= -740.117667

Sum of electronic and thermal Free Energies= -740.183701

H	0.16051300	-0.17475800	0.27026800	H	6.93696800	0.35762200	-1.70187500
C	1.23774400	-0.11159500	0.15105200	H	5.79208100	-0.98014100	-1.98318300
C	1.84772400	1.12323000	-0.06198700	C	6.22098300	-0.56916200	0.66988500
C	2.01732400	-1.26030500	0.23646300	H	6.25437200	-1.64424400	0.41998900
C	3.23362100	1.22611300	-0.21177000	H	7.25057700	-0.19747300	0.66514300
H	1.23922100	2.02406100	-0.08972500	H	5.82069100	-0.46374300	1.68143100
C	3.40166100	-1.17703800	0.09596500	N	5.42833200	0.22426100	-0.25474200
H	1.55058000	-2.22384300	0.41719100	C	3.83512000	5.37452300	-1.49394400
C	4.00454300	0.05813800	-0.13119200	H	4.75657200	4.98461300	-1.93641500
H	4.00668800	-2.07574200	0.17216900	H	3.00152300	4.89424100	-2.01530900
B	3.95791100	2.59837500	-0.44722200	H	3.78358600	6.44594400	-1.70337400
C	3.86192300	3.80637200	0.52790200	C	3.44615900	7.25002500	3.13761200
C	3.79079000	5.11808100	-0.00405200	H	3.87176100	8.15322000	2.69185100
C	3.83048300	3.65061700	1.93583900	H	2.38386300	7.44405800	3.32431200
C	3.65430300	6.21181200	0.84810000	H	3.92548100	7.08690500	4.10668200
C	3.72162000	4.77116800	2.75663700	C	3.96247900	2.29609400	2.59479200
C	3.61578200	6.05790100	2.23207000	H	3.05734000	1.69722600	2.46039300
H	3.58388200	7.21099300	0.42352900	H	4.79162400	1.72532800	2.16808000
H	3.71868600	4.63825000	3.83650900	H	4.14109300	2.40740900	3.66747000
C	5.88567200	0.06150900	-1.62961000	H	4.52400000	2.75213400	-1.49485300
H	5.30127300	0.70401400	-2.29156200				

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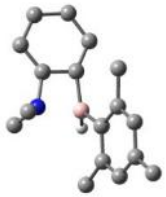

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Sum of electronic and thermal Free Energies= -740.194023

H	0.25836100	-0.69165900	-1.75014000	H	6.88729100	0.87788100	-0.11521800
C	1.21072500	-0.43339100	-1.29605800	H	6.20269400	-0.76236000	0.02728100
C	1.70392300	0.86685600	-1.42547300	C	4.96652600	0.94674000	1.72870400
C	1.91331300	-1.41951900	-0.59479700	H	5.16827700	-0.03253000	2.17708900
C	2.92304800	1.17801500	-0.82982700	H	5.78748700	1.63251200	1.95044500
H	1.13193800	1.60951400	-1.97494000	H	4.05043400	1.36225600	2.14784400
C	3.14687400	-1.13473600	-0.00629600	N	4.82075500	0.82997000	0.26985200
H	1.49463700	-2.41743100	-0.51065900	C	1.61201100	3.07559600	1.15564300
C	3.58899000	0.16831200	-0.16058500	H	1.13875300	3.11954200	0.17082400
H	3.70826800	-1.89237100	0.53261500	H	1.76540000	2.01626200	1.37874100
B	4.09862900	2.25219900	-0.57860700	H	0.90044000	3.47203800	1.88528200
C	4.02764700	3.51779800	0.40480300	C	4.09702600	6.96281600	3.08038500
C	2.90242700	3.86529200	1.18821800	H	3.11586700	7.44198800	3.14515800
C	5.17585000	4.33631200	0.52734400	H	4.37699300	6.65455200	4.09442300
C	2.94022000	4.97896800	2.03053800	H	4.82163400	7.71390400	2.75377400
C	5.18265700	5.44014800	1.38114700	C	6.44110300	4.05612400	-0.25350000
C	4.07063400	5.78179600	2.14381800	H	6.84893100	3.06501200	-0.03082200
H	2.05630700	5.22764900	2.61534600	H	6.26265400	4.08550900	-1.33195500
H	6.08012500	6.05241100	1.44959700	H	7.21506900	4.79029500	-0.01416500
C	6.02386400	0.25153300	-0.34872300	H	4.80519500	2.40792000	-1.54717300
H	5.88362600	0.22244800	-1.42937700				

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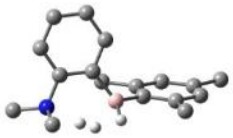

Sum of electronic and thermal Enthalpies= -741.271820

Sum of electronic and thermal Free Energies= -741.336716

H	1.00727300	0.20444100	2.18245000	C	3.23037600	4.18323700	-0.13717700
C	1.90219400	0.23233600	1.56886900	C	3.33187000	5.31654200	0.69986000
C	2.47493700	1.45256600	1.22440100	C	2.20748600	4.16398700	-1.11093500
C	2.46906300	-0.94767100	1.10173300	C	2.43652700	6.37558200	0.55787600
C	3.62864400	1.53239900	0.43471300	C	1.33816800	5.24782300	-1.23526900
H	2.00448200	2.37534500	1.55377600	C	1.43231800	6.36191900	-0.40677500
C	3.61227500	-0.90129000	0.31050100	H	2.52517500	7.23665500	1.21732700
H	2.02498800	-1.90653600	1.35082800	H	0.56258200	5.21903300	-1.99796800
C	4.19802100	0.32380400	-0.01051300	H	4.73342500	2.96572000	-1.49909500
H	4.05054800	-1.82590900	-0.05151500	C	4.38812800	5.40976600	1.77832100
B	4.22123100	2.96620100	0.09523400	H	4.33018600	4.56914500	2.47661300
C	5.48311300	-0.60526000	-1.87660000	H	5.39588300	5.40032600	1.35179900
H	4.53507400	-0.69224900	-2.41157400	H	4.27400100	6.33104700	2.35532200
H	6.25629600	-0.29505300	-2.58604400	C	2.04379000	3.00526000	-2.06720900
H	5.76358200	-1.59991300	-1.49280500	H	2.85234000	2.98157200	-2.80772300
C	6.60425400	0.53031100	-0.06786500	H	2.05564500	2.04478900	-1.54657600
H	6.86454800	-0.40955600	0.44514000	H	1.10257700	3.08429700	-2.61676000
H	7.42491100	0.80010500	-0.73995500	C	0.45721500	7.50498000	-0.52593600
H	6.49638900	1.31719600	0.67954400	H	-0.39266400	7.36501200	0.15157800
N	5.36829400	0.40417000	-0.83653800	H	0.92748400	8.45809000	-0.26810600
H	5.31567300	3.21907600	0.52280300	H	0.05837500	7.58518500	-1.54082700
H	4.95976200	2.22640400	-1.38849300				

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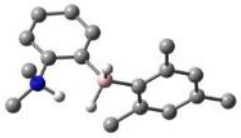
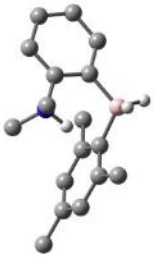


Sum of electronic and thermal Enthalpies= -741.291712

Sum of electronic and thermal Free Energies= -741.358015

H	1.01720800	0.08502600	2.21778400	C	3.34280000	3.96357100	-0.13189100
C	1.92506800	0.08979500	1.62183200	C	3.19858200	4.94264700	0.87401900
C	2.48101700	1.29937200	1.22156200	C	2.48179900	4.05005900	-1.24464600
C	2.51590000	-1.12221600	1.26137400	C	2.25558600	5.96319400	0.74520600
C	3.65324900	1.35959100	0.45218200	C	1.54760700	5.08252600	-1.35175900
H	1.99923800	2.23432900	1.49465200	C	1.42055700	6.05525100	-0.36599000
C	3.66943200	-1.11424400	0.48762800	H	2.16817300	6.70787200	1.53531200
H	2.07907900	-2.06415000	1.57543800	H	0.89816200	5.12477300	-2.22497400
C	4.18881500	0.11856700	0.11194100	H	4.94608500	2.57238600	-1.11559800
H	4.14076200	-2.04814000	0.19320400	C	4.05069400	4.90617600	2.12257000
B	4.38866300	2.74342600	0.00237300	H	3.97312300	3.93892200	2.62924100
C	5.38249800	-0.59864900	-1.95088200	H	5.10973100	5.05096800	1.88778300
H	4.45643300	-0.37367500	-2.47905600	H	3.74756900	5.68507500	2.82855200
H	6.24127000	-0.33061000	-2.56835200	C	2.54085500	3.01792700	-2.34731500
H	5.42271400	-1.66134200	-1.70888100	H	3.50927600	3.03745500	-2.85928500
C	6.64826000	0.01024900	0.08930300	H	2.41102600	2.00656000	-1.94547700
H	6.66872100	-1.01020500	0.47525400	H	1.75888700	3.18797200	-3.09317400
H	7.51907400	0.19523100	-0.54232400	C	0.40390100	7.16385200	-0.47810200
H	6.62467200	0.72629700	0.91035300	H	-0.36787300	7.07602200	0.29486800
N	5.41443300	0.20605500	-0.70999900	H	0.87216400	8.14627700	-0.35602800
H	5.30968600	2.94348000	0.78293300	H	-0.09616700	7.14914500	-1.45040700
H	5.37443700	1.23672100	-0.97940700				

NMeB1H1Mes_H2_HMes



Sum of electronic and thermal Enthalpies= -741.291551

Sum of electronic and thermal Free Energies= -741.358385

H	0.55624500	-0.00122500	0.91479800	H	5.94400100	-1.61659600	-1.48745400
C	1.60497700	0.02844000	0.63339800	C	6.54776000	-0.06434000	0.72097300
C	2.23228200	1.25206100	0.42999100	H	6.41915800	-1.10195700	1.03211500
C	2.30810800	-1.16640000	0.47301900	H	7.58481200	0.12285800	0.43649700
C	3.58378300	1.35807500	0.05991100	H	6.24843000	0.61094400	1.52248900
H	1.66830300	2.17245700	0.55155100	N	5.66750200	0.20793300	-0.44164500
C	3.64739300	-1.11838500	0.10962200	H	5.09373500	2.91186400	0.82912200
H	1.82033500	-2.12285100	0.62851100	H	5.78583100	1.20990900	-0.70403100
C	4.23010800	0.12932300	-0.08457300	C	3.12465400	2.27264100	-2.86688200
H	4.21349000	-2.03815700	-0.01449900	H	2.85694400	1.26713500	-2.52395300
B	4.35701900	2.78676500	-0.14428200	H	2.58224900	2.97327100	-2.22659400
C	5.23110200	2.81828200	-1.54053200	H	2.76602500	2.38348300	-3.89436900
C	4.61339300	2.51705800	-2.78444800	C	7.51536300	2.59451100	-5.26466400
C	6.62041900	3.09047600	-1.57622700	H	7.18094500	3.35519100	-5.97813200
C	5.35635400	2.45176400	-3.96233400	H	8.58444400	2.74649800	-5.09293300
C	7.34402800	3.00428800	-2.77363500	H	7.38639000	1.62052000	-5.74923700
C	6.73350500	2.67667900	-3.97783200	C	7.37673500	3.49813600	-0.32854600
H	4.84750400	2.22639300	-4.89884900	H	8.42236000	3.72054600	-0.56105100
H	8.41242000	3.21487400	-2.76245200	H	6.92488600	4.38273300	0.12701400
C	6.04592300	-0.54567300	-1.66288700	H	7.35929900	2.72505100	0.44721200
H	5.38853100	-0.22047800	-2.46890700	H	3.53213400	3.68584500	-0.13438200
H	7.07787400	-0.29610300	-1.91437500				

NMeB1H1Mes_H2_TSprot

Sum of electronic and thermal Enthalpies= -741.272373

Sum of electronic and thermal Free Energies= -741.336838

H	0.85607500	1.73944200	-2.07959300
C	1.76406500	1.28281900	-1.69622000
C	2.73321100	2.07197300	-1.08351500
C	1.95969500	-0.08989100	-1.83719800
C	3.92095300	1.52784300	-0.57857600
H	2.57735900	3.14449400	-1.00218700
C	3.12585700	-0.66836000	-1.34737500
H	1.21004700	-0.70613100	-2.32362000
C	4.07016700	0.14329000	-0.72509500
H	3.29023800	-1.73778500	-1.44885200
B	5.07177900	2.41617300	0.11860900
C	6.72730900	1.91808600	-0.36737300
C	7.76418000	1.99004900	0.59862300
C	7.07567400	2.13602400	-1.73226600
C	9.07012300	2.28526700	0.21146600
C	8.38757600	2.43162000	-2.08048500
C	9.40011500	2.50969100	-1.12196500
H	9.84991200	2.34057300	0.96776800
H	8.63306900	2.61161200	-3.12500800
C	6.03248000	-1.32487900	-1.04481400
H	6.13601400	-0.88943100	-2.03983000
H	7.03075400	-1.48002600	-0.62615400
H	5.52950800	-2.29645200	-1.12679800
C	5.13536500	-0.90845600	1.17828900
H	4.50379600	-1.80665900	1.18168100
H	6.11357400	-1.15763800	1.59950200
H	4.66449700	-0.13659200	1.78902500
N	5.30685500	-0.39253500	-0.18407900
C	7.49288600	1.77829700	2.06563800
H	6.77043400	0.97981900	2.24016200
H	8.41537600	1.54212700	2.60308200
H	7.06125500	2.68418900	2.50292100
C	10.81920100	2.80015500	-1.53383900
H	11.28714400	1.90639900	-1.96167500
H	10.85592900	3.58294700	-2.29679500
H	11.42672900	3.11974100	-0.68349900
C	6.03364400	2.11350500	-2.82009500
H	5.46846600	1.17835000	-2.84050000
H	5.29833600	2.90721100	-2.65167300
H	6.49072400	2.26219900	-3.80162200
H	6.03317400	0.86014300	-0.18127300
H	5.03099000	2.30812100	1.32600200
H	5.03806000	3.57309900	-0.24351600

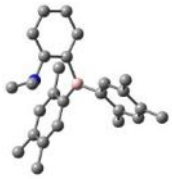
Mes’

Sum of electronic and thermal Enthalpies= -349.925550

Sum of electronic and thermal Free Energies= -349.968804

C	-0.22106100	-1.95839200	-0.01662500	H	-0.78620000	-3.83476400	0.89932500
C	1.18459700	-1.95084500	0.02016100	H	-2.06239100	-3.08188100	-0.06650600
C	1.85805300	-0.73074700	0.01522200	C	1.94958400	1.79308100	0.00606500
C	1.18636900	0.49285100	-0.02380700	H	2.13965600	2.11207000	1.03715200
C	-0.20599700	0.47127600	-0.06437100	H	2.91914100	1.69745600	-0.49096200
C	-0.89344300	-0.73842400	-0.05953700	H	1.39294000	2.59428300	-0.48808100
H	2.94630900	-0.73320600	0.04128400	C	1.95644800	-3.24509300	0.05692200
H	-0.75926000	1.40619700	-0.10146900	H	1.68540600	-3.84886300	0.93055700
H	-1.98018400	-0.73434400	-0.09397900	H	1.75123400	-3.85751200	-0.82862600
C	-0.98529600	-3.25736400	-0.01096100	H	3.03313200	-3.06329300	0.09660400
H	-0.70539800	-3.89363900	-0.85836400				

NmeBMes’

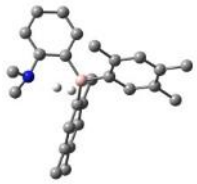


Sum of electronic and thermal Enthalpies= -1088.884902

Sum of electronic and thermal Free Energies= -1088.975124

H	0.09420700	-0.14288300	-0.23092500	H	5.96983800	-0.79144900	1.55692200
C	1.17343500	-0.02795300	-0.19630600	H	6.95612800	0.66387900	1.29332500
C	1.75235900	1.20525300	-0.48292300	H	5.35843300	0.81040400	2.04400900
C	1.97733800	-1.11402000	0.14525400	N	5.34916400	0.52158600	-0.02666400
C	3.14079900	1.36782500	-0.45720300	C	7.63259100	2.83040400	-5.35642200
H	1.11499400	2.04919100	-0.73569400	H	8.47322200	2.15241300	-5.16795200
C	3.35964100	-0.96304900	0.20317900	H	7.14771200	2.51344200	-6.28284800
H	1.52567900	-2.07459100	0.37377400	H	8.06019500	3.82568700	-5.52236200
C	3.93160900	0.27368100	-0.09446800	C	3.00561800	1.91305900	-3.63866500
H	3.99189100	-1.80097200	0.48509000	H	2.81438500	0.94171600	-3.17207700
B	3.93141600	2.70364600	-0.76644100	H	2.25440600	2.60686600	-3.24784100
C	3.87266800	3.86072300	0.28853100	H	2.83739900	1.81113200	-4.71414700
C	4.01189200	5.23768700	0.00416500	C	4.13425900	5.79120800	-1.39797000
C	3.70431200	3.49037900	1.63474300	H	5.17469400	5.79208600	-1.73764000
C	4.00731200	6.14537800	1.06429300	H	3.56991600	5.20379000	-2.12449700
C	3.72565100	4.39228300	2.69239500	H	3.76887200	6.82164200	-1.43257100
C	3.88569200	5.75528700	2.39685500	C	3.90336500	6.78345400	3.49708700
H	4.10298400	7.20694500	0.84340000	H	4.05867100	7.78871800	3.09843600
C	4.80596600	2.80447800	-2.06849300	H	2.96030900	6.78364400	4.05573600
C	4.41021900	2.38929900	-3.35244900	H	4.70011500	6.57853400	4.22092100
C	6.13040900	3.23400100	-1.89754400	H	3.55047200	2.43760000	1.86112200
C	5.34250500	2.42619100	-4.39100500	H	6.44311800	3.55735800	-0.90621900
C	7.06931300	3.24244500	-2.92388700	C	8.48501200	3.69126000	-2.66775200
C	6.66246900	2.83189800	-4.20385400	H	9.20855300	2.90880400	-2.92400000
H	5.02929000	2.11960600	-5.38749100	H	8.74436900	4.57100100	-3.26845200
C	6.09766800	-0.11384700	-1.10027200	H	8.63058300	3.94943600	-1.61595300
H	5.63616100	0.13107100	-2.05960300	C	3.56704400	3.91923700	4.11426800
H	7.11800300	0.28321200	-1.10953800	H	4.44272400	4.17419300	4.72268300
H	6.14973200	-1.21215800	-0.99889900	H	2.69848400	4.38056900	4.59813900
C	5.93180700	0.27745500	1.28114300	H	3.43513200	2.83516900	4.15505100

NmeBMes'_H2_TSsplit

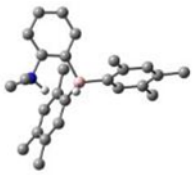


Sum of electronic and thermal Enthalpies= -1090.039560

Sum of electronic and thermal Free Energies= -1090.124378

H	0.58543400	-0.06568700	0.50541200	H	7.62445100	-0.34361400	1.25442500
C	1.66844800	-0.06306300	0.42984600	H	6.13859000	-0.30522000	2.22954200
C	2.34626700	1.12882800	0.19937000	N	5.87384400	0.03590200	0.18191300
C	2.38035800	-1.25094100	0.57695900	H	5.74106300	2.50301200	0.67837900
C	3.74109200	1.17458700	0.09391400	H	5.84660400	1.71478600	0.44810400
H	1.78538600	2.05603900	0.11611300	C	3.85817000	2.71848500	2.87245600
C	3.76739500	-1.23540100	0.49392300	H	3.12011400	1.92805200	2.70643100
H	1.85824500	-2.18472700	0.76043200	H	4.84382600	2.26403800	2.72439900
C	4.43246600	-0.03449000	0.25141400	H	3.79166500	3.02874400	3.91871400
H	4.32954900	-2.15705600	0.61449300	C	2.24987500	7.43392700	2.34475000
B	4.53261000	2.55253000	-0.16760500	H	2.91664400	8.29770900	2.24204800
C	3.95634700	3.85148000	0.57776800	H	1.30189300	7.70760800	1.86759800
C	3.72858500	5.01105000	-0.17349400	H	2.05780400	7.28327600	3.40986700
C	3.63158200	3.89343400	1.94956100	C	2.90911600	2.55733100	-2.76646900
C	3.17345500	6.17489700	0.35414100	H	2.64629100	1.52510700	-2.51539600
C	3.09199000	5.06391700	2.48368500	H	2.44054300	3.19980000	-2.01405200
C	2.84556600	6.20086700	1.71661200	H	2.46020300	2.79351500	-3.73502200
H	2.85181900	5.09228700	3.54518200	C	7.02491100	3.32570000	-5.52860000
C	5.18209400	2.76597500	-1.62753500	H	7.52325500	4.29838500	-5.61148300
C	4.40566800	2.75495700	-2.80221700	H	7.78507000	2.56229900	-5.73056700
C	6.55649300	2.98945800	-1.77753600	H	6.27326000	3.26660000	-6.31950100
C	5.03063600	2.93931700	-4.03742300	H	7.18447900	3.01847300	-0.88769600
C	7.18494100	3.17133800	-3.00696300	H	4.00212100	5.00626400	-1.22642200
C	6.40211100	3.13900900	-4.16942300	C	8.67277900	3.39867000	-3.08256400
H	4.41826200	2.92788200	-4.93743100	H	9.16903800	2.62540100	-3.68055900
C	6.39971500	-0.35858300	-1.12657200	H	8.90950500	4.36091100	-3.55084100
H	5.85781400	0.17215600	-1.90979000	H	9.12396100	3.39328500	-2.08711500
H	7.45591400	-0.08158000	-1.19190100	C	2.94271000	7.37952000	-0.52147100
H	6.30304200	-1.44296100	-1.28887900	H	1.88426900	7.66398300	-0.54445700
C	6.56849000	-0.62856200	1.27879800	H	3.49777700	8.25295500	-0.16003300
H	6.51194000	-1.72584000	1.22287500	H	3.25911300	7.18382700	-1.54881100

NmeBMes'_H2_HH



Sum of electronic and thermal Enthalpies= -1090.052631

Sum of electronic and thermal Free Energies= -1090.140111

H	0.66804900	0.10817200	0.88051000
C	1.72445200	0.08595700	0.62951500
C	2.45015600	1.27136700	0.59171000
C	2.33867700	-1.13323600	0.34156900
C	3.81488800	1.30556000	0.26726600
H	1.95646800	2.21404100	0.81412400
C	3.69102400	-1.15336800	0.02419500
H	1.77330200	-2.05882000	0.36671900
C	4.37410900	0.05671700	0.00062300
H	4.18878400	-2.09414300	-0.19726500
B	4.73972400	2.66305600	0.16433300
C	4.00214200	3.97616100	0.75513200
C	3.63664200	5.04265000	-0.07480300
C	3.69270500	4.10938000	2.12576300
C	2.97692800	6.18841200	0.37150600
C	3.03418400	5.25295000	2.58053800
C	2.66192200	6.29481000	1.73242300
H	2.80664000	5.34146600	3.64235800
C	5.31646200	2.81908200	-1.36863400
C	4.54150100	2.70339500	-2.54444100
C	6.69574800	3.01012200	-1.55237500
C	5.16580100	2.76034100	-3.79415100
C	7.32676000	3.06592500	-2.79641300
C	6.54131800	2.92855300	-3.94922200
H	4.55171100	2.67233900	-4.68968400
C	6.13831400	-0.37898400	-1.69916400
H	5.54386400	0.22252600	-2.38693700
H	7.19839900	-0.20587700	-1.88883800
H	5.89877800	-1.43803000	-1.79964500
C	6.64008900	-0.60697100	0.72278500
H	6.39868700	-1.66992700	0.74427700
H	7.69709900	-0.46620500	0.49107400
H	6.40104600	-0.14751500	1.68163500
N	5.82402800	0.06692300	-0.31674800
H	5.74185500	2.42025700	0.86844200
H	6.05567100	1.07784900	-0.26404200
C	4.08132600	3.04525600	3.12433500
H	3.55973300	2.10050700	2.93581900
H	5.15356600	2.82994400	3.06328600
H	3.85136600	3.35727500	4.14746500
C	1.94879500	7.50818600	2.27244500
H	2.51815800	8.42721500	2.08908300
H	0.96957600	7.64499900	1.79788800
H	1.78803300	7.42387900	3.35055100
C	3.04401800	2.50086900	-2.49902700
H	2.78614800	1.45359200	-2.30439000
H	2.58672300	3.09357700	-1.70332200
H	2.58267700	2.78630600	-3.44910200
C	7.16107200	2.98402100	-5.32211700
H	7.65669500	3.94587100	-5.49765200
H	7.92412800	2.20761300	-5.45450300
H	6.40733000	2.84996100	-6.10224100
H	7.31298600	3.12650900	-0.66070800
H	3.89182300	4.98616900	-1.13183000
C	8.81610300	3.27777600	-2.89656500
H	9.31012300	2.45610700	-3.42962200
H	9.05364400	4.19613700	-3.44586400
H	9.27064300	3.35902800	-1.90569900
C	2.61615100	7.29025600	-0.59234400
H	1.53435100	7.46962500	-0.61588000
H	3.08764900	8.24065300	-0.31465500
H	2.93591500	7.04358300	-1.60818800

NmeBMes'_H2_HMes'

Sum of electronic and thermal Enthalpies= -1090.053643

Sum of electronic and thermal Free Energies= -1090.139829

C	0.92975900	-1.16608600	1.00237300
C	0.41044900	-0.34886100	2.02235300
C	-0.97526300	-0.44144800	2.17030600
C	-1.81044200	-1.24647700	1.39948900
C	-1.24548800	-2.02809600	0.40347700
C	0.13514800	-1.98342100	0.20983000
B	1.41299600	0.65995900	2.85684200
C	1.47531500	2.11540300	2.12092200
C	0.62006500	2.46620600	1.06793500
C	0.60993000	3.71272300	0.43819500
C	1.51872000	4.68587600	0.86893800
C	2.40418400	4.35010900	1.89223900
C	2.40749500	3.10151900	2.51526900
N	-1.59776500	0.39099200	3.22916400
C	-2.40670300	1.52232900	2.70941500
H	-2.74023800	2.12580200	3.55551900
C	0.96222600	0.77381500	4.43874100
C	1.00465400	-0.34432700	5.30612000
C	0.52514300	-0.23062600	6.61141100
C	-0.01484500	0.95191700	7.12080600
C	-0.05980900	2.07551400	6.28553400
C	0.42986000	1.95718500	4.98090300
C	-2.31169200	-0.39846000	4.26547100
H	-2.56002300	0.26800600	5.09283100
H	-3.21548200	-0.83516100	3.84028400
H	-1.63701100	-1.17741100	4.61686800
H	-1.77133000	2.11970100	2.05574400
H	-3.26411300	1.13168300	2.16040000
H	-2.88464900	-1.26621100	1.56499800
H	-1.87302000	-2.66320200	-0.21253300
H	0.58971500	-2.59225500	-0.56590700
H	2.00271900	-1.13929300	0.83721900
H	-0.78488700	0.80877800	3.73047900
H	2.51961200	0.13739300	2.81665300
H	3.13057800	5.09564400	2.21337200
H	0.57128000	-1.10112800	7.26458800
C	3.42467400	2.83109500	3.59673400
H	4.18360000	3.61797800	3.63155900
H	2.95575500	2.76814200	4.58429800
H	3.92286500	1.87176600	3.42891200
C	1.55704600	6.05164000	0.23241400
H	2.32579300	6.67961600	0.68989700
H	1.77099800	5.99006300	-0.84116600
H	0.59667500	6.57129000	0.33339000
C	1.55844900	-1.66540900	4.83389400
H	0.95334900	-2.08775200	4.02395600
H	2.56279900	-1.53446700	4.42118200
H	1.60151500	-2.39560800	5.64691900
C	-0.51933000	1.01821900	8.53945000
H	-1.57320000	1.31755300	8.58296500
H	-0.42509900	0.05051000	9.03827000
H	0.04109800	1.75292600	9.12865500
H	0.40138600	2.83976700	4.34121500
H	-0.06633300	1.71240300	0.68256100
C	-0.35490300	3.99576500	-0.68560100
H	-1.02691000	4.82869700	-0.44488000
H	0.16826300	4.27130600	-1.60872300
H	-0.97129700	3.11912600	-0.90469600
C	-0.60690400	3.38979100	6.78183300
H	-1.64237300	3.29563000	7.13067400
H	-0.02499400	3.76946800	7.62934600
H	-0.58168200	4.14800000	5.9954540

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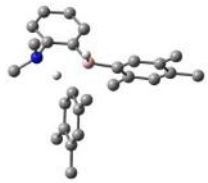

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Sum of electronic and thermal Free Energies= -1090.116214

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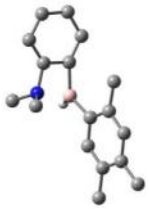
C	-0.10204100	-0.15483200	1.48013100
C	-1.13478400	-0.80641800	2.17077500
C	-2.07232700	-1.62234100	1.54396900
C	-2.00414600	-1.79267600	0.16488000
C	-1.00786000	-1.14197200	-0.55933500
B	0.92012700	0.78216800	2.30277000
C	1.49399500	-0.14845600	3.75959400
C	1.92343600	-1.47712900	3.57209800
C	2.93199000	-2.07472300	4.31437300
C	3.55255000	-1.30941300	5.31770500
C	3.12166300	-0.00114800	5.54326700
C	2.10377300	0.59136700	4.80050800
N	-1.16532200	-0.56257600	3.60358600
C	-2.05626600	0.54246200	3.97670100
H	-1.88111100	0.80546400	5.02404500
C	2.20564000	1.38785000	1.53864400
C	2.30685400	2.78919400	1.51982500
C	3.32832500	3.49768200	0.89054100
C	4.32732300	2.77585000	0.22370600
C	4.24463900	1.38611200	0.22172900
C	3.22044300	0.68028800	0.85938700
C	-1.36774300	-1.74436800	4.43945500
H	-1.16382000	-1.47787700	5.48018700
H	-2.39086100	-2.13401400	4.37090800
H	-0.66594500	-2.52256500	4.13517300
H	-1.83071700	1.40458400	3.34950800
H	-3.10936500	0.26058500	3.84711600
H	-2.85463000	-2.11352000	2.11599700
H	-2.72904000	-2.42311000	-0.34056600
H	-0.95459500	-1.26695600	-1.63689300
H	0.70014900	0.16015100	-0.48209600
H	0.21817700	-0.16494700	3.73560400
H	0.28724000	1.70486200	2.78226100
H	5.01579600	0.82317700	-0.30291400
H	3.60149500	0.57425500	6.33228500
C	1.70587300	2.01215000	5.09047300
H	2.10350600	2.34643100	6.05239100
H	2.09192500	2.67267200	4.30655400
H	0.61935500	2.13362300	5.09529800
C	4.66428100	-1.89502100	6.14615000
H	5.03148700	-1.17825100	6.88394400
H	4.33265500	-2.79308500	6.67937000
H	5.50865400	-2.19469300	5.51530000
C	3.27874100	-0.82803300	0.80148800
H	2.28843600	-1.27705000	0.70202400
H	3.88458500	-1.15995300	-0.04723800
H	3.73218700	-1.23729100	1.71066300
C	5.45677300	3.48157100	-0.48148300
H	5.08485500	4.15886400	-1.25933000
H	6.04563100	4.09268800	0.21279600
H	6.13522900	2.76756700	-0.95564500
H	1.52566400	3.36042300	2.01879200
C	3.35059600	5.00472900	0.92013900
H	4.26692100	5.38731900	1.38521400
H	3.30776600	5.42979100	-0.08981700
H	2.50029100	5.39890200	1.48265900
C	3.36061700	-3.49198600	4.03661200
H	2.76320800	-3.92997800	3.23341500
H	4.41243100	-3.53885300	3.73173100
H	3.25693700	-4.12939300	4.92211500
H	1.43520100	-2.06017700	2.79303400

NmeB1H1Mes'_close



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Sum of electronic and thermal Free Energies= -740.194267

H	0.31188700	-0.67917000	-1.89504600	H	6.25739400	-0.67544100	0.20208400
C	1.24759700	-0.42279400	-1.40645600	C	4.84873800	0.96518600	1.78719600
C	1.75859500	0.87130100	-1.53428500	H	5.04721800	-0.01030100	2.24518700
C	1.91004600	-1.40434400	-0.66152400	H	5.64349800	1.66754700	2.04760700
C	2.95468300	1.17820000	-0.89280200	H	3.90548700	1.36159700	2.16177100
H	1.21758300	1.61177700	-2.11696800	N	4.78013400	0.84517800	0.32318300
C	3.11800100	-1.12155900	-0.02006100	C	1.59793300	3.04260200	1.20937300
H	1.47861600	-2.39718400	-0.58162400	H	1.10696500	3.09181600	0.23306100
C	3.57915500	0.17441900	-0.17416400	H	1.76045300	1.98058100	1.41689000
H	3.64530400	-1.87463800	0.55815300	H	0.89793500	3.42734900	1.95650900
B	4.11338400	2.25263300	-0.57814800	C	4.14713900	6.91876200	3.09726400
C	3.98178700	3.51366300	0.39392900	H	3.20445500	7.02103900	3.64068800
C	2.88465200	3.83694800	1.21884900	H	4.95141500	6.81675800	3.83538000
C	5.11008000	4.34235800	0.48351500	H	4.32768300	7.85748800	2.56097100
C	2.97369300	4.93877300	2.07263300	H	4.90586400	2.42815100	-1.47813700
C	5.20752200	5.43804700	1.33926800	H	5.95943200	4.11852800	-0.16088900
C	4.10887700	5.74320600	2.15517800	C	6.45842600	6.27820700	1.37851100
H	2.12001200	5.18321700	2.70287500	H	6.24850500	7.32650600	1.13650400
C	6.03327700	0.30751800	-0.22804000	H	6.91933300	6.27044500	2.37340900
H	5.93333000	0.22088100	-1.30994500	H	7.19981000	5.91335500	0.66306700
H	6.84545100	1.00066600	0.00274900				

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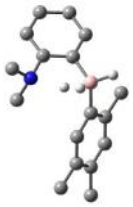
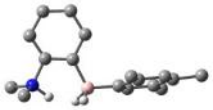


Sum of electronic and thermal Enthalpies= -741.275307

Sum of electronic and thermal Free Energies=-741.342636

H	0.66358700	-0.51420300	0.81796100	H	3.60227700	3.49506100	0.18517200
C	1.71301800	-0.36066700	0.58602000	C	4.37519200	2.92688800	-2.00922500
C	2.17218700	0.90948200	0.25161500	C	5.67645300	3.07893100	-2.50187700
C	2.60011700	-1.43242500	0.63408700	C	3.32151400	3.08807200	-2.92687100
C	3.51526200	1.14616300	-0.06053500	C	5.97214100	3.35601700	-3.83518900
H	1.47225700	1.74013600	0.23933300	C	3.61005400	3.36999400	-4.26211200
C	3.94520800	-1.22446300	0.35104500	C	4.91188900	3.50136000	-4.74033900
H	2.24744700	-2.42507600	0.89598000	H	2.78459500	3.49208700	-4.96141400
C	4.38827000	0.05061600	0.00671700	C	1.88344100	2.95427400	-2.49133400
H	4.64585300	-2.05372900	0.39409000	H	1.62682000	1.90826500	-2.29220200
B	4.07736000	2.59399800	-0.46742400	H	1.69619600	3.51215500	-1.56729700
C	6.16631400	-0.08922500	-1.62910800	H	1.19836300	3.32843200	-3.25677900
H	5.45464300	0.31449500	-2.34982500	C	5.17003000	3.79901300	-6.19476800
H	7.15731100	0.31159700	-1.86186600	H	4.23427800	3.86620900	-6.75498700
H	6.19490800	-1.18553700	-1.72328900	H	5.70516700	4.74709600	-6.32208100
C	6.71038100	-0.16056100	0.73211300	H	5.78587700	3.02178400	-6.66170200
H	6.80735500	-1.25656500	0.73620300	H	6.51676600	2.96884800	-1.81598600
H	7.69976500	0.26503800	0.53977300	C	7.40170000	3.49144400	-4.29274100
H	6.37478200	0.16241700	1.72011500	H	7.65437600	2.74081600	-5.05080300
N	5.77882900	0.32659600	-0.27978800	H	7.58901300	4.47203000	-4.74483900
H	5.31114200	2.80893500	0.17649200	H	8.09817500	3.37064700	-3.45886800
H	5.48551500	2.02964500	-0.07765400				

NmeB1H1Mes'_H2_HH



Sum of electronic and thermal Enthalpies= -741.294148

Sum of electronic and thermal Free Energies= -741.357986

H	1.30812600	0.09349800	2.50899800	C	3.19198000	3.93108900	-0.32340700
C	2.17096500	0.10427600	1.84958700	C	3.05717500	4.75092800	0.81445600
C	2.54952400	1.28969000	1.22790600	C	2.33957400	4.20279900	-1.39941800
C	2.88575400	-1.07438600	1.63597100	C	2.10247100	5.76911700	0.82651500
C	3.65869300	1.35766300	0.37266800	C	1.38538900	5.22009100	-1.39830000
H	1.97606800	2.19723900	1.39690200	C	1.26135400	6.02212200	-0.25533700
C	3.98385100	-1.06105400	0.78387200	H	2.00928600	6.39310300	1.71465700
H	2.58983600	-1.99669700	2.12429700	H	4.43810700	2.38752200	-1.57228600
C	4.32194100	0.14587000	0.18651300	C	3.93614500	4.54997000	2.02633700
H	4.54842800	-1.97177100	0.60254500	H	3.85272600	3.53150300	2.42126400
B	4.21820800	2.69631200	-0.37414900	H	4.99115900	4.70277000	1.77657800
C	5.47445600	-0.75951700	-1.82596700	H	3.67070500	5.24518300	2.82840100
H	4.50570400	-0.71523100	-2.32213500	C	0.24235800	7.13129000	-0.19226300
H	6.27043400	-0.51724400	-2.53158000	H	-0.77689800	6.75017200	-0.32774500
H	5.63665100	-1.75642400	-1.41562700	H	0.28040000	7.64721000	0.77069400
C	6.77336700	0.30381100	-0.00695400	H	0.40680200	7.87789700	-0.97840700
H	6.94088300	-0.64669200	0.50156200	C	0.50534200	5.44987700	-2.60091000
H	7.57574800	0.50068200	-0.72008600	H	-0.55773700	5.34737800	-2.35202900
H	6.70561400	1.11732800	0.71409100	H	0.63750200	6.45704400	-3.01411800
N	5.48032800	0.23983000	-0.73323000	H	0.73202200	4.73245300	-3.39396300
H	5.31600900	2.96092500	0.11915100	H	2.42628700	3.58422500	-2.29206200
H	5.30493800	1.18709300	-1.16389300				

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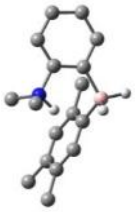

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Sum of electronic and thermal Free Energies= -741.362798

H	0.58612500	-0.04578600	0.96981300	C	6.58650200	0.02053700	0.71419700
C	1.63215100	-0.00429100	0.67998200	H	6.48702200	-1.00322300	1.07734600
C	2.23705800	1.22533300	0.44452000	H	7.61322000	0.21689600	0.39975900
C	2.35540500	-1.18969400	0.54328600	H	6.28850100	0.72901500	1.48690400
C	3.58378400	1.34542500	0.06303700	N	5.67985000	0.22055700	-0.44236900
H	1.65888800	2.13871900	0.55099400	H	5.14209400	2.93142200	0.73232800
C	3.69084700	-1.12747200	0.16690100	H	5.78112100	1.21411200	-0.73993600
H	1.88546100	-2.15041600	0.72523700	C	3.07342100	2.27565900	-2.95457000
C	4.24982200	0.12488100	-0.06234800	H	2.79728800	1.29301900	-2.55590200
H	4.27191100	-2.03991400	0.05938400	H	2.52302700	3.01292600	-2.36287100
B	4.33073900	2.78085700	-0.18534000	H	2.73090100	2.32940500	-3.99217900
C	5.15806100	2.80215100	-1.60107300	C	7.52344300	2.62869200	-5.26754500
C	4.55905800	2.51993100	-2.85177900	H	8.02064500	3.58321500	-5.47512800
C	6.54400300	3.03652100	-1.61799700	H	8.31121100	1.86753200	-5.21555600
C	5.34307300	2.47366200	-4.00509300	H	6.88617600	2.39115000	-6.12321100
C	7.33777300	2.98775700	-2.76882900	H	3.49548600	3.66884900	-0.14902200
C	6.72264200	2.69178900	-3.99179600	H	7.02618900	3.27467900	-0.66913300
H	4.86130900	2.26350900	-4.95940500	C	8.81862500	3.26178900	-2.69315200
C	6.05653500	-0.56631800	-1.64210200	H	9.41040300	2.42193100	-3.07702800
H	5.37935200	-0.28329900	-2.44780000	H	9.09426300	4.13834400	-3.29113600
H	7.07881400	-0.30310400	-1.91816600	H	9.13082600	3.45247100	-1.66306800
H	5.98190300	-1.63305500	-1.43107200				

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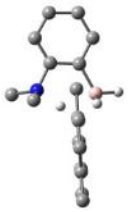

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Sum of electronic and thermal Free Energies= -741.340265

H	0.79311500	1.76938500	-1.95201700
C	1.70950900	1.30073600	-1.60503400
C	2.71005500	2.07564900	-1.02430800
C	1.88543300	-0.07264700	-1.76010900
C	3.90821800	1.51451200	-0.56647300
H	2.56908700	3.14924500	-0.93091100
C	3.06318600	-0.66766900	-1.31902900
H	1.11118600	-0.67777200	-2.22149300
C	4.03960900	0.12794000	-0.72654500
H	3.21339300	-1.73741700	-1.43608900
B	5.08941300	2.38425600	0.09847000
C	6.73830800	1.88843300	-0.45812800
C	7.74945000	1.93472700	0.51978700
C	7.10569500	2.14546300	-1.80000900
C	9.07202900	2.24859700	0.23731400
C	8.43041500	2.46370800	-2.08621400
C	9.41602900	2.52126800	-1.09936000
H	8.71062000	2.67847500	-3.11544100
C	5.94257500	-1.39725500	-1.12156000
H	5.91697900	-1.04451800	-2.15397500
H	6.98675200	-1.50414700	-0.81328000
H	5.45952000	-2.38176700	-1.06745500
C	5.26939600	-0.83010900	1.14654700
H	4.68947600	-1.75356400	1.27535000
H	6.29447700	-0.99852100	1.49123200
H	4.82213900	-0.03315000	1.74154600
N	5.29787800	-0.41380300	-0.25806800
C	10.83415000	2.87071800	-1.46354000
H	11.52925900	2.08004200	-1.15974300
H	10.94476400	3.02483900	-2.53914900
H	11.15645400	3.78680800	-0.95581600
C	6.08158300	2.12849300	-2.90195900
H	5.53877500	1.17981100	-2.94269700
H	5.32714200	2.90237700	-2.72399500
H	6.54353000	2.30439200	-3.87674500
H	6.03077600	0.86394500	-0.30455700
H	5.14533900	2.24152800	1.30514200
H	5.05561900	3.54764600	-0.23605300
H	7.46671700	1.72650300	1.54954800
C	10.10840800	2.29631500	1.33013100
H	10.90920700	1.56722300	1.15988300
H	10.58252000	3.28211300	1.39306500
H	9.65980900	2.08098200	2.30276300

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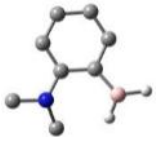

Sum of electronic and thermal Enthalpies= -391.359816

Sum of electronic and thermal Free Energies= -391.405317

H	0.15271400	0.35510100	0.19720300	C	6.10648900	0.21210600	-1.43105200
C	1.23037200	0.25683900	0.12528400	H	5.42412200	0.72249500	-2.11063400
C	2.00561400	1.27317800	-0.40744300	H	6.94220300	0.88536900	-1.21229600
C	1.87425000	-0.89240900	0.58242000	H	6.49976200	-0.67377700	-1.95067300
C	3.41244700	1.19897600	-0.49035800	C	6.06794300	-1.27275300	0.48142500
H	1.52770700	2.18999500	-0.74247800	H	5.92180100	-2.25357900	-0.00067600
C	3.24972700	-1.03737400	0.47735300	H	7.14213200	-1.06982300	0.50963800
H	1.29315100	-1.70659300	1.00680500	H	5.71431800	-1.33216400	1.51316800
C	4.04184400	-0.01719900	-0.08367100	N	5.41071100	-0.19124400	-0.21951800
H	3.70126100	-1.96810000	0.79966900	H	3.52152600	3.45436400	-1.17216300
B	4.14721300	2.51509300	-0.76346500	H	5.30981400	2.66745900	-0.52231200

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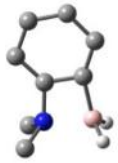
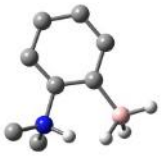


Sum of electronic and thermal Enthalpies= -391.371616

Sum of electronic and thermal Free Energies= -391.414550

C	-1.26622800	-2.39098400	0.64957700	C	-2.34637500	-0.98487000	-1.06212500
C	0.08192100	-2.12438300	0.80935500	H	-2.51670500	0.06438300	-1.31218800
C	0.91117300	-3.18362200	1.16443300	H	-1.62699000	-1.40672000	-1.76368300
C	0.33764100	-4.44670100	1.33813500	H	-3.29162500	-1.53496200	-1.12536100
C	-1.03264100	-4.66532700	1.16398200	C	-2.70825800	-0.50522100	1.29764200
C	-1.88469400	-3.61733200	0.80791200	H	-2.87465000	0.55099400	1.07597000
H	1.97918600	-3.04959000	1.30885500	H	-3.66512000	-1.03844500	1.28503200
H	0.96874900	-5.28584500	1.61682500	H	-2.25016600	-0.59536900	2.28228200
H	-1.43915000	-5.66118500	1.30884000	B	-0.13012400	-0.56576100	0.45255800
H	-2.95067600	-3.77133200	0.66958100	H	0.24445500	-0.16728000	-0.62610000
N	-1.78618300	-1.06593600	0.29634800	H	-0.06547200	0.24512700	1.34722200

NmeB2h_H2



Sum of electronic and thermal Enthalpies= -392.536223

Sum of electronic and thermal Free Energies= -392.581801

H	0.45094500	0.33390000	0.65686200	H	5.44531400	0.40625900	-2.18719300
C	1.52245400	0.25855300	0.49530800	H	7.07539800	-0.13872000	-1.69862000
C	2.26867200	1.41068600	0.26939900	H	5.71621700	-1.30698000	-1.73258100
C	2.13394700	-0.99595100	0.51924400	C	6.45065200	-0.69366500	0.85451200
C	3.65540800	1.37174900	0.05432400	H	6.25055600	-1.75994200	0.74166600
H	1.77381100	2.37734100	0.25768400	H	7.51273100	-0.50273100	0.69219100
C	3.50611400	-1.08824100	0.31868000	H	6.15825600	-0.36497900	1.85132600
H	1.54987500	-1.89334800	0.69445500	N	5.66838800	0.07422400	-0.13794200
C	4.20805800	0.09055900	0.09961600	H	5.69881000	2.51923100	0.33138200
H	3.99947700	-2.05653900	0.33299900	H	5.88075800	1.11029400	-0.00938300
B	4.59878300	2.64942300	-0.26917200	H	4.10947300	3.69302500	0.10363800
C	6.00324700	-0.27151500	-1.54180300	H	4.84948200	2.67068100	-1.47092000

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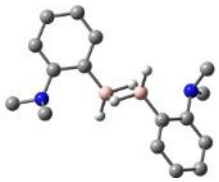

Sum of electronic and thermal Enthalpies= -782.757436

Sum of electronic and thermal Free Energies= -782.825897

C	0.28937700	-1.83795900	0.66463600	H	-2.52042800	-1.93311600	3.57575100
C	1.26909800	-0.86628400	0.85372800	B	-2.90967800	-2.85113400	-0.73464900
C	0.94378100	0.31599200	1.50727600	H	-2.44431600	-2.16741200	-1.59468500
C	-0.34980900	0.51720000	1.98171200	C	-4.11914600	-3.81466100	-1.02137700
C	-1.32614100	-0.46208500	1.79808700	C	-4.29500800	-4.40990200	-2.29235600
C	-1.01670500	-1.65511200	1.12274300	C	-5.11799300	-4.00788400	-0.06004200
H	0.54418700	-2.74982600	0.12964400	C	-5.46490100	-5.12881000	-2.56297100
H	2.27496900	-1.02602100	0.47854300	C	-6.27687900	-4.72832500	-0.32862900
H	1.69638200	1.08501100	1.65239500	H	-4.99740200	-3.55172000	0.91925300
H	-0.59520500	1.44201600	2.49434800	C	-6.44928200	-5.27906000	-1.59190400
N	-2.67299500	-0.30309800	2.25975900	H	-5.60941100	-5.58863400	-3.53418200
B	-2.16980500	-2.70407400	0.87237100	H	-7.04043700	-4.84403100	0.43356100
H	-2.59943500	-3.41313400	1.73729400	H	-7.34984300	-5.83880400	-1.82664500
H	-3.18949900	-2.08944200	0.31193800	N	-3.28770500	-4.24512700	-3.27510600
H	-1.87648400	-3.47138100	-0.14431900	C	-3.68164500	-4.42047000	-4.65762500
C	-3.20320900	1.04695200	2.19963700	H	-2.89469600	-4.01651500	-5.30173500
H	-4.28873600	1.00624800	2.33391000	H	-3.83491500	-5.47649300	-4.94333800
H	-2.80008300	1.71948600	2.97720600	H	-4.60251000	-3.86841600	-4.85789600
H	-2.99344100	1.48399200	1.22089100	C	-2.02090200	-4.90419800	-2.99866900
C	-2.90289500	-0.91084800	3.56474000	H	-2.06570200	-5.98904400	-3.19751800
H	-2.41327300	-0.35060200	4.38016400	H	-1.23552500	-4.47014200	-3.62520600
H	-3.97834100	-0.94470000	3.76660300	H	-1.73173000	-4.77046900	-1.95609500

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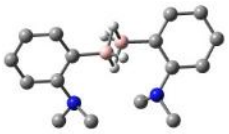
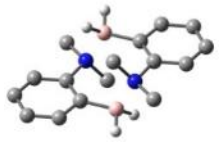


Sum of electronic and thermal Enthalpies= -782.758807

Sum of electronic and thermal Free Energies= -782.828329

C	-1.22497000	-1.51746100	2.78332900	H	-4.03577800	-0.12341100	0.31184900
C	-0.22575700	-0.67326400	3.26064100	B	-2.47932500	-3.43219800	-0.31211100
C	0.16951400	0.41309600	2.49032600	H	-1.34822700	-3.39252700	-0.70320300
C	-0.44241500	0.66018900	1.26479600	C	-3.56673000	-4.38478900	-0.94426700
C	-1.44502700	-0.18730800	0.78506900	C	-4.54414800	-3.87827900	-1.82652200
C	-1.83639100	-1.30987000	1.54456700	C	-3.60894500	-5.74169600	-0.61629700
H	-1.52066200	-2.37613700	3.38222800	C	-5.54016000	-4.72604800	-2.31959400
H	0.24314700	-0.86708200	4.22007900	C	-4.60118400	-6.58605700	-1.10760900
H	0.94797300	1.08215300	2.84463100	H	-2.86032700	-6.14565900	0.06166200
H	-0.13590800	1.52483000	0.68563600	C	-5.57267500	-6.06923300	-1.95544000
N	-2.08398300	0.04029000	-0.46967500	H	-6.29516200	-4.34325700	-2.99827600
B	-2.90234300	-2.33396000	0.99210600	H	-4.61892900	-7.63377100	-0.82478100
H	-4.02171400	-2.39214200	1.41351300	H	-6.35582200	-6.71193100	-2.34640600
H	-2.95774400	-2.20997300	-0.31323100	N	-4.49131800	-2.49592700	-2.17580400
H	-2.42602300	-3.57328600	1.00495600	C	-5.74108400	-1.88653800	-2.58428500
C	-1.33184200	0.79950600	-1.44799200	H	-5.62283800	-0.79804900	-2.57386400
H	-1.81190600	0.68875600	-2.42572800	H	-6.06568400	-2.17357500	-3.60014900
H	-1.27622700	1.88036900	-1.22830500	H	-6.53117100	-2.15122300	-1.87797100
H	-0.31535000	0.40591900	-1.52142500	C	-3.40414100	-2.14887900	-3.08190200
C	-3.45929900	0.50945100	-0.36617700	H	-3.56801400	-2.54045200	-4.10021800
H	-3.52165000	1.54932400	-0.00266600	H	-3.31494800	-1.05923900	-3.13913200
H	-3.93400700	0.45635800	-1.35131600	H	-2.45329400	-2.53977600	-2.71436200

NmeB2h_dimchair



Sum of electronic and thermal Enthalpies= -782.771074

Sum of electronic and thermal Free Energies= -782.829692

B	0.14348100	14.31204200	5.03590800	B	-1.46627500	11.33682200	4.01550700
H	0.94919500	15.21328200	5.11019600	H	-2.27199700	10.43551600	3.94128400
C	0.93838300	12.94125000	5.41861300	H	-0.48701100	11.03986000	3.37482900
C	2.33018000	13.13433600	5.50595900	C	-2.26112500	12.70757800	3.63284400
H	2.70560000	14.13400200	5.31336200	C	-3.65293300	12.51462300	3.54539900
C	3.24596400	12.14001900	5.82375000	C	-1.82251200	14.02136700	3.35354300
H	4.30694200	12.36443200	5.87023600	C	-4.56852900	13.50892400	3.22705700
C	2.77709500	10.86414100	6.07827600	H	-4.02845700	11.51506100	3.73832600
H	3.45559100	10.05461300	6.32763000	C	-2.73391700	15.03107900	3.03519800
C	1.41157900	10.61757400	6.01529000	C	-4.09944400	14.78462800	2.97202400
H	1.08722200	9.60669500	6.21124100	H	-5.62953000	13.28464800	3.18044800
C	0.49999300	11.62731100	5.69755100	H	-2.40942400	16.04184900	2.83890500
N	-0.94333600	11.25846200	5.61300100	H	-4.77780800	15.59411400	2.72217600
C	-1.19568000	9.84865200	6.01817600	N	-0.37916600	14.39007000	3.43836100
H	-2.27139800	9.68917400	5.99867500	C	0.44478600	13.55915000	2.51576600
H	-0.73756800	9.16645400	5.30355900	H	0.16036700	13.77726000	1.48253500
H	-0.81787300	9.66634300	7.02775100	H	1.49450200	13.80696900	2.67916500
H	-0.83591700	14.60895200	5.67644300	H	0.29199400	12.50697300	2.72528500
C	-1.76725000	12.08925600	6.53568600	C	-0.12663500	15.79989500	3.03310000
H	-2.81693200	11.84117100	6.37253200	H	0.94907900	15.95930000	3.05299500
H	-1.48255400	11.87135300	7.56889300	H	-0.50407500	15.98209300	2.02337800
H	-1.61470500	13.14144400	6.32604200	H	-0.58502300	16.48213600	3.74749700

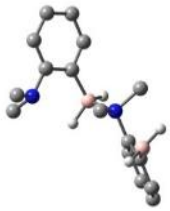
NmeB2h_dimboat

Sum of electronic and thermal Enthalpies= -782.778655

Sum of electronic and thermal Free Energies= -782.839826

B	1.32958400	14.05787600	5.24130000	C	1.06173400	14.25898900	9.04244500
H	2.33113500	14.56613800	4.78384800	H	1.95335000	14.84784100	9.20278100
H	0.40000000	14.25972500	4.51172600	C	0.45711200	14.16761600	7.78881800
C	1.63780500	12.52895200	5.66206200	N	-0.71562000	11.65843400	5.49992500
C	2.98059400	12.23505900	5.94101400	N	1.01785900	14.96126600	6.65466100
H	3.71198600	13.02010500	5.76910000	C	2.30176800	15.62052700	7.00859000
C	3.41895700	11.00651600	6.42135500	H	3.04535300	14.86234200	7.25421600
H	4.47164600	10.83878900	6.62654000	H	2.64111700	16.17551200	6.13734500
C	2.48776800	10.00479600	6.63446400	H	2.17112500	16.31133400	7.84555100
H	2.78810600	9.03554000	7.01953000	C	0.05996800	16.05513300	6.31979500
C	1.14794900	10.23767600	6.34120800	H	-0.04478000	16.72436500	7.17897600
H	0.45425700	9.42803800	6.51635900	H	0.45254000	16.60002300	5.45994900
C	0.72379500	11.47310500	5.85170000	H	-0.90140200	15.62096100	6.06208800
B	-1.44848000	13.02702500	6.20853100	C	-0.83414700	11.76593800	4.01653700
H	-1.46127000	13.87152100	5.35718600	H	-1.88310300	11.93831600	3.77079300
H	-2.58044500	12.66202300	6.44491000	H	-0.24049000	12.60683700	3.67045500
C	-0.68557200	13.36564900	7.59218900	H	-0.48186700	10.83897600	3.55436300
C	-1.19017200	12.72747800	8.73486300	C	-1.54671300	10.49492400	5.90490900
H	-2.09329100	12.13430300	8.61972700	H	-2.57404600	10.70181200	5.61519700
C	-0.60391300	12.81724900	9.99194100	H	-1.21032200	9.58109500	5.40841400
H	-1.03691900	12.29651900	10.84034900	H	-1.50392900	10.37625200	6.98770700
C	0.54113000	13.58061100	10.13992200				
H	1.03377600	13.66839000	11.10291700				

NmeB2h_olig2



Sum of electronic and thermal Enthalpies= -782.742766

Sum of electronic and thermal Free Energies= -782.810765

C	-0.43063900	0.39700200	0.23141800	N	2.63350900	-1.23907000	1.11653400
C	0.88984400	0.32492500	-0.27427500	C	3.31482700	-2.55631200	1.17823100
C	1.45320000	1.52704400	-0.72339800	C	3.70698200	-3.18227700	0.00042700
C	0.79826700	2.75421700	-0.64227900	C	3.57237700	-3.14084700	2.42560800
C	-0.48113300	2.80130600	-0.10778300	C	4.36512200	-4.40620400	0.05048500
C	-1.09433900	1.62496300	0.31403600	H	3.48645000	-2.71977100	-0.95117700
H	2.45481900	1.49421000	-1.14670600	C	4.20204600	-4.39325700	2.44365800
H	1.28408000	3.66043300	-0.99133600	C	4.61092000	-5.01886200	1.27247400
H	-1.01409300	3.74451700	-0.03138600	H	4.66603600	-4.88606300	-0.87479400
H	-2.10596400	1.66949400	0.70423900	H	4.38122800	-4.88440300	3.39679100
N	-1.07046000	-0.80521000	0.67429600	H	5.10505800	-5.98394500	1.31514400
C	-1.58219400	-1.62307500	-0.41736800	C	1.65639000	-1.11297300	2.21996100
H	-1.84623100	-2.61610300	-0.03811200	H	1.17507000	-0.13864300	2.14971000
H	-2.48066800	-1.17841400	-0.88053000	H	0.90133100	-1.89012500	2.12848700
H	-0.81720200	-1.74304200	-1.18346100	H	2.14695700	-1.13511500	3.20947600
C	-2.05854100	-0.65598700	1.72359300	C	3.66405300	-0.17129600	1.24819600
H	-2.28496100	-1.64406400	2.13849900	H	4.36533400	-0.26923000	0.42067200
H	-1.66175900	-0.02837900	2.52659500	H	3.16798900	0.79827400	1.18828500
H	-3.01504600	-0.21807900	1.38523800	H	4.19376100	-0.26779900	2.19944600
B	1.78205200	-1.02019900	-0.34810600	B	3.27265700	-2.49475700	3.81652200
H	2.65959500	-0.88321900	-1.17656600	H	3.91978500	-1.56581800	4.21343200
H	1.18200600	-2.06045900	-0.47148400	H	2.51203200	-3.02045200	4.57615200

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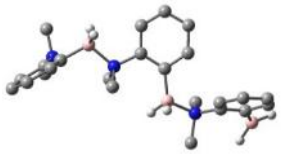


Sum of electronic and thermal Enthalpies= -1174.126497

Sum of electronic and thermal Free Energies= -1174.214267

C	-0.45333900	0.44440600	-0.45319600
C	0.95014900	0.30602200	-0.56100000
C	1.65498900	1.44863500	-0.96803200
C	1.04869100	2.68029500	-1.20045200
C	-0.32549000	2.79776500	-1.04205000
C	-1.07019000	1.67890500	-0.68424200
H	2.73244300	1.36359500	-1.09087300
H	1.64470700	3.53785200	-1.49890800
H	-0.82378200	3.74768800	-1.21338700
H	-2.14833400	1.76910300	-0.59462300
N	-1.24649500	-0.70029900	-0.11151900
C	-1.51396800	-1.56872700	-1.24741500
H	-1.92726800	-2.51968800	-0.89282100
H	-2.23555300	-1.12059800	-1.95457200
H	-0.58644000	-1.77709600	-1.78037600
C	-2.45011500	-0.44089600	0.64936800
H	-2.81901600	-1.38640000	1.06270500
H	-2.22880900	0.23431300	1.48074800
H	-3.27556300	-0.00045800	0.05978400
B	1.77780300	-1.06062500	-0.28615700
H	2.85027500	-1.03172200	-0.85852500
H	1.13958900	-2.05435900	-0.54151600
N	2.19574700	-1.21158800	1.35483800
C	3.01556500	-2.42623200	1.67244800
C	3.15379100	-3.36307300	0.64905300
C	3.61564100	-2.63842800	2.94424400
C	3.86741800	-4.54029300	0.82770000
H	2.69311300	-3.16794300	-0.30579800
C	4.33304200	-3.84259000	3.06339900
C	4.46318600	-4.78485200	2.05118800
H	3.95156200	-5.24698400	0.00855500
H	4.83295500	-4.06873000	3.99708300
H	5.03284000	-5.69277100	2.22555600
C	0.91589100	-1.27823200	2.11696400
H	0.38369500	-0.33825400	1.97500900
H	0.31259500	-2.07859800	1.69310800
H	1.10498500	-1.44359600	3.17512700
C	2.95670300	0.01937800	1.70542700
H	3.88838500	0.00978500	1.13909900
H	2.36602300	0.88400900	1.40795300
H	3.16820300	0.07229300	2.76876300
B	3.58641900	-1.61905000	4.21625600
H	4.45656700	-0.77691000	4.18243400
H	2.52440100	-1.07119400	4.38880900
N	3.74297200	-2.36538400	5.73225700
C	5.07384800	-2.92995800	6.08795800
C	6.18150700	-2.47784200	5.38508800
C	5.21891500	-3.89819700	7.10833000
C	7.45086900	-2.98264000	5.65882700
H	6.05134900	-1.75203600	4.59477000
C	6.50688500	-4.43103500	7.30755100
C	7.62049300	-3.97141700	6.61477300
H	8.29868400	-2.61351500	5.09141700
H	6.63130700	-5.21548200	8.04818300
H	8.60059600	-4.39299400	6.80934700
C	2.65418600	-3.38559700	5.80236500
H	1.76145600	-2.94136700	5.36264800
H	2.93726100	-4.25857900	5.21816100
H	2.43776000	-3.66622200	6.83313600
C	3.45899400	-1.27693500	6.71908800
H	4.16695100	-0.46713000	6.54573300
H	2.44724700	-0.90953700	6.55256100
H	3.56145300	-1.65528200	7.73662100
B	4.21949000	-4.35330900	8.20319300
H	4.35383000	-5.44134100	8.68080300
H	3.38894500	-3.63582800	8.67751600

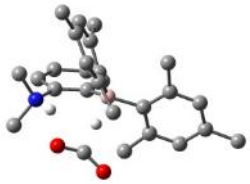
CO2

Sum of electronic and thermal Enthalpies= -188.512018

Sum of electronic and thermal Free Energies= -188.536311

C	0.00000000	0.00000000	0.00000000	O	-1.16509200	0.00000000	0.00000000
O	1.16509200	0.00000000	0.00000000				

NMeBMes_H2CO2TS



Sum of electronic and thermal Enthalpies= -1278.539112

Sum of electronic and thermal Free Energies= -1278.627963

C	-0.09945200	0.11928800	-0.83603800	H	-1.21389400	-1.53438900	-2.53161300
C	1.28930700	0.22827500	-0.94176200	H	-1.93827200	-2.67490600	-1.37490400
C	1.74490200	1.50448000	-1.31922800	H	-2.57880100	-1.00575800	-1.50531200
C	0.89743400	2.58337100	-1.52414600	C	-1.30625900	-1.26600500	0.84893700
C	-0.47694300	2.43179500	-1.35759100	H	-0.53469900	-1.01675700	1.57619100
C	-0.97960400	1.18462200	-1.01815400	H	-2.13745300	-0.56285100	0.90975700
H	2.81645400	1.64271700	-1.42999400	H	-1.65812800	-2.28478000	1.01611100
H	1.30866900	3.54844900	-1.80308300	N	-0.71161200	-1.19682100	-0.51579900
H	-1.15268600	3.26837600	-1.49987800	C	1.73228600	1.00714300	1.87731400
H	-2.05093400	1.05360700	-0.89786600	H	2.54389100	1.36081700	1.23823100
B	2.38265800	-0.92028500	-0.52535600	H	0.79780800	1.36351900	1.43059900
H	1.96421500	-1.99953800	-1.22835600	H	1.83874400	1.49589300	2.84983200
H	0.02413400	-1.92829700	-0.55746000	C	3.08939600	-3.75007900	0.54051800
C	3.84746300	-0.71129900	-1.18037500	H	3.81885700	-4.30178400	1.14175700
C	5.04949000	-0.65076600	-0.42667400	H	2.39110500	-4.48917900	0.13450600
C	3.97654000	-0.61375400	-2.59021100	H	3.63069000	-3.29032200	-0.28693600
C	6.28455000	-0.53138100	-1.06564500	C	1.11250300	-2.80712100	5.02647400
C	5.23257000	-0.50566000	-3.19189500	H	1.32243300	-3.87262600	5.15100700
C	6.40457400	-0.47009000	-2.45007500	H	1.64704600	-2.26418100	5.81293700
H	7.18668400	-0.48287700	-0.45838100	H	0.04150400	-2.65499400	5.20046900
H	5.29021500	-0.44100900	-4.27729900	C	5.09332600	-0.68643000	1.08669600
C	2.18412400	-1.39343500	1.02761500	H	4.40174000	0.02615900	1.53981800
C	2.38822900	-2.73601100	1.41752000	H	4.83466400	-1.67067300	1.48554300
C	1.77176300	-0.49838100	2.05435400	H	6.09981100	-0.44175900	1.43764700
C	2.02396800	-3.18056300	2.69434300	C	2.80395600	-0.55447900	-3.54921700
C	1.44324200	-0.96996700	3.32559400	H	1.88466300	-0.97408600	-3.14841300
C	1.51655800	-2.32226100	3.65772400	H	2.58818500	0.48620700	-3.81894300
H	2.17447600	-4.23010500	2.94193000	H	3.03986500	-1.09631000	-4.46881000
H	1.13663600	-0.25517900	4.08789600	C	7.75495200	-0.38056100	-3.11325100
C	1.54466700	-3.21031700	-1.87923500	H	8.45256700	0.21336700	-2.51516700
O	2.37484300	-3.51184300	-2.67276300	H	8.19707500	-1.37543100	-3.23990700
O	0.47537400	-3.48402000	-1.36768500	H	7.68229600	0.07563800	-4.10466500
C	-1.68813800	-1.63096000	-1.55671600				

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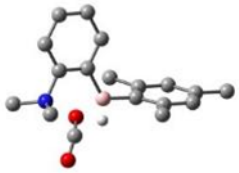

Sum of electronic and thermal Enthalpies= -928.612565

Sum of electronic and thermal Free Energies= -928.683661

H	0.32571600	0.37901300	0.78950700	H	5.30057700	-1.49812600	-2.41703800
C	1.34985100	0.28918100	0.44073800	C	6.18274000	-0.76037900	0.06742600
C	2.22029800	1.37079400	0.54696400	H	5.94313000	-1.83531500	0.08357600
C	1.79689800	-0.90606200	-0.11394700	H	7.23469900	-0.63605400	-0.20601000
C	3.54247700	1.28753500	0.09940800	H	6.03840900	-0.35893100	1.07432900
H	1.87158700	2.30429800	0.98137700	N	5.35340700	-0.01243600	-0.86864100
C	3.11322900	-1.01829000	-0.55391000	C	2.92638200	4.62245500	-1.21511800
H	1.12357000	-1.75350900	-0.20032900	H	2.14989300	5.33457300	-1.50597100
C	3.97578000	0.07060900	-0.44745100	H	3.77277100	4.75123100	-1.89660500
H	3.46768600	-1.95409100	-0.97728800	H	2.53562800	3.61279200	-1.37645300
B	4.53488300	2.51552300	0.22296600	C	2.84695500	7.52580200	2.88530300
C	4.10900400	3.87488300	0.91125800	H	3.63007800	8.28748500	2.79810800
C	3.33928100	4.83366500	0.22306900	H	1.93771400	7.93780400	2.43871400
C	4.42089200	4.10701900	2.26576300	H	2.66183400	7.36775500	3.95158900
C	2.93727600	6.00038100	0.87445900	C	5.19344700	3.08730500	3.07169800
C	3.99892500	5.28012600	2.88908900	H	4.73298300	2.09549600	3.00739800
C	3.26412300	6.24680600	2.20532300	H	6.22521000	2.98998300	2.71502100
H	2.34276000	6.73112000	0.32942800	H	5.23386900	3.36818500	4.12719300
H	4.24162300	5.44209300	3.93747600	H	5.65104500	2.10351000	0.67590800
C	5.53990400	-0.43626000	-2.24925500	O	5.22035100	2.79078800	-1.29324100
H	4.90782700	0.17236400	-2.89983300	C	6.22719400	2.26768400	-0.81733500
H	6.58665200	-0.27578400	-2.52709700	O	7.37901900	2.05077600	-0.81650800

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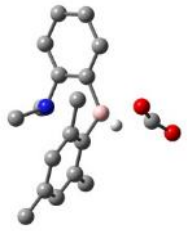
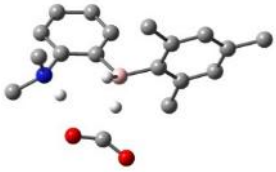


Sum of electronic and thermal Enthalpies= -928.606820

Sum of electronic and thermal Free Energies= -928.679788

H	2.21384500	-0.45446300	-2.54129000
C	2.30461500	-0.08438800	-1.52484600
C	3.23794700	0.90280500	-1.22342200
C	1.49325500	-0.60007300	-0.51931800
C	3.37887700	1.39420100	0.07728200
H	3.87408400	1.29341000	-2.01259600
C	1.61754000	-0.12408800	0.78186200
H	0.76321500	-1.37049800	-0.74721400
C	2.55543500	0.86415800	1.08035300
H	0.98214000	-0.52177800	1.56779700
B	4.41736000	2.50723200	0.51420400
C	4.06706100	3.97174200	0.98748700
C	3.29939200	4.81657400	0.15923100
C	4.44262700	4.43767000	2.26495500
C	2.92732800	6.08250100	0.60938800
C	4.04726700	5.70717400	2.68456400
C	3.29077300	6.54644600	1.87076600
H	2.33337100	6.72173000	-0.04050600
H	4.33516100	6.05053800	3.67608500
C	2.84036600	0.36596300	3.44250700
H	3.58553500	-0.37460900	3.14333100
H	3.17665800	0.83916300	4.37103800
H	1.89443400	-0.15895700	3.66147500
C	1.71712200	2.38534200	2.75264500
H	0.71494900	1.94544800	2.89648300
H	2.01214100	2.89115100	3.67785300
H	1.66274400	3.13751400	1.96378500
N	2.72051200	1.38380700	2.41118400
C	2.85063700	4.37597300	-1.21426400
H	2.38946300	5.20493100	-1.75679800
H	3.68692700	4.00672300	-1.81461900
H	2.11749900	3.56568500	-1.15176500
C	2.90061300	7.92771700	2.33010800
H	3.67284200	8.65846300	2.06528700
H	1.96728500	8.25389300	1.86324900
H	2.77108500	7.96638600	3.41520100
C	5.24249000	3.58039700	3.21829000
H	4.74470300	2.61878000	3.37650700
H	6.24723400	3.37278800	2.83411300
H	5.35932100	4.07655400	4.18487200
H	5.33725000	1.97883300	1.20691400
O	5.58767000	2.64616600	-0.82407200
C	6.36555000	2.21010300	0.00459200
O	7.41545400	1.87396600	0.39599600

NMeB1H1Mes_H2CO2TS

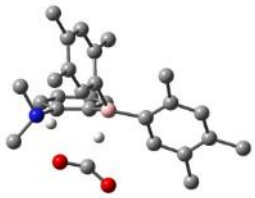


Sum of electronic and thermal Enthalpies= -929.796987

Sum of electronic and thermal Free Energies= -929.867679C -0.08715300 0.13223100 -0.87545400

C	1.22128600	0.11014800	-1.36779200
C	1.66954900	1.32771900	-1.90458700
C	0.87573500	2.46925800	-1.93730300
C	-0.41406800	2.44107800	-1.41589900
C	-0.90234100	1.25870000	-0.87254200
H	2.68245600	1.36930300	-2.29452400
H	1.26781500	3.38685500	-2.36481600
H	-1.03803900	3.32853900	-1.42845900
H	-1.90553200	1.23191800	-0.45896100
B	2.21103000	-1.17524400	-1.27440900
H	1.74094000	-2.00266200	-2.18829200
H	-0.08692600	-1.91071600	-0.72393700
C	3.74532200	-0.88142800	-1.61436300
C	4.63902600	-0.57328900	-0.56706600
C	4.24293800	-0.84573300	-2.93300000
C	5.97517400	-0.27768500	-0.83709300
C	5.58533600	-0.54694000	-3.17407900
C	6.47260100	-0.26939900	-2.13803400
H	6.64512700	-0.04036500	-0.01216700
H	5.94768900	-0.52747800	-4.20065200
C	1.16339400	-3.32547800	-2.27861200
O	1.91247500	-3.97655300	-2.92854600
O	0.10352900	-3.28886100	-1.68372700
C	-2.02652600	-1.42466600	-0.58774100
H	-2.17915600	-1.28944300	-1.65708900
H	-2.21397800	-2.46466700	-0.32054700
H	-2.68803800	-0.76968800	-0.02123600
C	-0.34015400	-1.16958000	1.19062000
H	0.72957200	-1.03342600	1.34233600
H	-0.89871100	-0.36710500	1.67468800
H	-0.65300300	-2.14142800	1.57578100
N	-0.60641100	-1.12049100	-0.27237700
C	4.16531300	-0.52660500	0.86819400
H	3.33655400	0.18103300	0.98865200
H	3.80375600	-1.50506600	1.20159200
H	4.96989100	-0.21415000	1.53980700
C	3.34359500	-1.12897400	-4.11441400
H	3.06079700	-2.18548100	-4.14687600
H	2.41784800	-0.54524300	-4.06524000
H	3.84365600	-0.88457700	-5.05581500
C	7.92777000	0.01453600	-2.41306300
H	8.06640300	0.46991000	-3.39808300
H	8.35084700	0.69066800	-1.66407100
H	8.51823500	-0.90878500	-2.39267100
H	2.04476500	-1.80008100	-0.24423000

NMeBMes'_H2CO2TS

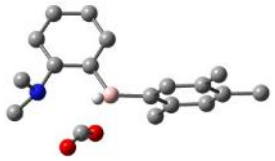


Sum of electronic and thermal Enthalpies= -1278.550825

Sum of electronic and thermal Free Energies= -1278.64432

C	-0.09826700	-0.27474300	-0.95132000	H	-2.49824200	-1.69111500	-1.33189300
C	1.27642200	-0.04534600	-1.08659100	C	-1.09616300	-1.50904100	0.95832300
C	1.60149000	1.21710300	-1.61404000	H	-0.34794600	-1.02435300	1.58332700
C	0.64865500	2.17071700	-1.94735200	H	-2.02420100	-0.93618200	0.95166600
C	-0.70359000	1.90278100	-1.75871700	H	-1.27538100	-2.52308200	1.31710100
C	-1.07950400	0.66503800	-1.25714800	N	-0.57601800	-1.58781200	-0.43773800
H	2.65200400	1.45263600	-1.74781400	C	2.23673900	1.10599500	1.66452200
H	0.96275000	3.13036100	-2.34593600	H	3.03594800	1.24378300	0.93065800
H	-1.45873700	2.64214500	-2.00289900	H	1.32929800	1.54061400	1.23008200
H	-2.13280800	0.44636800	-1.10940300	H	2.49016400	1.68631400	2.55648600
B	2.45438600	-1.04040400	-0.51750000	C	1.20037100	-2.31091000	5.18517000
H	2.21769100	-2.20301400	-1.14207000	H	1.95495600	-2.96016200	5.64345400
H	0.22606900	-2.24346900	-0.43948000	H	1.13950100	-1.39635600	5.78040700
C	3.93288100	-0.74293700	-1.07491800	H	0.24022200	-2.83302500	5.27231900
C	5.13479900	-0.69517100	-0.33677200	C	5.21626900	-0.91607700	1.15751800
C	4.04593200	-0.58395800	-2.46765100	H	4.71327700	-0.12675500	1.72332800
C	6.33663000	-0.45057300	-1.00970600	H	4.75083900	-1.85880000	1.45381100
C	5.24066600	-0.35286200	-3.14011800	H	6.26101300	-0.93782300	1.48057100
C	6.42040600	-0.27214200	-2.38680200	C	7.74895800	-0.01792500	-3.05016300
H	7.25643700	-0.40716500	-0.42858700	H	8.55903300	0.00258100	-2.31678200
C	2.18114800	-1.37368500	1.04372600	H	7.98310700	-0.79324000	-3.78876600
C	2.00212400	-2.69050000	1.48932000	H	7.75449200	0.93980800	-3.58390200
C	2.04586000	-0.35303800	2.01000800	H	3.14100300	-0.66072300	-3.06796000
C	1.68184300	-3.03039100	2.80526200	H	2.10432500	-3.50216500	0.77431600
C	1.73443300	-0.68895800	3.32885200	C	5.26624100	-0.20557500	-4.63966300
C	1.53829800	-2.00463900	3.74887000	H	5.68211500	0.76216500	-4.94462700
H	1.64567700	0.10909700	4.06464000	H	5.88700500	-0.97902500	-5.10676800
C	1.88977400	-3.35790600	-1.87339000	H	4.26118900	-0.28910500	-5.06064100
O	2.72406000	-3.51402000	-2.70522800	C	1.50176600	-4.47426200	3.19890500
O	0.85545300	-3.76932600	-1.37802400	H	2.24208400	-4.77957100	3.94733300
C	-1.55950600	-2.24311800	-1.34769800	H	0.51492000	-4.65325000	3.64222300
H	-1.13963500	-2.26046800	-2.35078000	H	1.60830600	-5.13494100	2.33518700
H	-1.71173200	-3.26467100	-1.00201500				

NMeB1H1Mes'_CO2TS_inside



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H	0.29156100	0.34640400	0.65616100	C	6.16350600	-0.84527600	0.06634700
C	1.32803600	0.26524000	0.34419900	H	5.91485500	-1.91453500	-0.02149300
C	2.18399700	1.35417300	0.47882900	H	7.22466600	-0.71007700	-0.16222300
C	1.80464200	-0.92842900	-0.18896200	H	5.98957200	-0.53386700	1.09951100
C	3.52188300	1.28261800	0.07781100	N	5.37507800	-0.00591200	-0.82592200
H	1.81200600	2.28371100	0.90200000	C	2.77801600	4.55642100	-1.17818100
C	3.13602800	-1.02933300	-0.58078500	H	1.98706900	5.25614700	-1.46019100
H	1.14289000	-1.78231600	-0.29626300	H	3.60652400	4.68346300	-1.88246400
C	3.98354000	0.06828200	-0.44833200	H	2.39531800	3.54042400	-1.31549500
H	3.51496300	-1.96258500	-0.98839200	C	2.78504100	7.50791600	2.88912900
B	4.50813000	2.51074400	0.24481800	H	3.63529500	8.13521300	3.17983200
C	4.07335500	3.87826500	0.90394900	H	2.14230900	8.09821100	2.23176600
C	3.23448400	4.79322900	0.24146700	H	2.22260600	7.29220200	3.80464300
C	4.47297900	4.17892700	2.20989300	H	5.59422300	2.08874400	0.78543100
C	2.84056300	5.95185100	0.91000200	O	5.29539900	2.77527000	-1.20289800
C	4.07781300	5.33411000	2.88116900	C	6.25804400	2.24388600	-0.64025000
C	3.24225600	6.24144600	2.21311900	O	7.40900900	2.02818700	-0.56988600
H	2.19312500	6.65929000	0.39517400	C	4.54013100	5.60144500	4.29013500
C	5.58953900	-0.32151400	-2.23201400	H	3.69388500	5.69534800	4.98027100
H	5.00380400	0.36561500	-2.84657400	H	5.18019900	4.79432300	4.65455500
H	6.64988700	-0.18512300	-2.46712200	H	5.10912900	6.53581000	4.35642100
H	5.30841400	-1.35393700	-2.49231800	H	5.12241600	3.47870100	2.73312800

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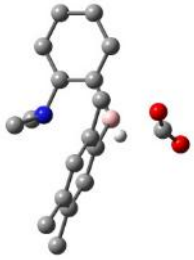

Sum of electronic and thermal Enthalpies= -928.608791

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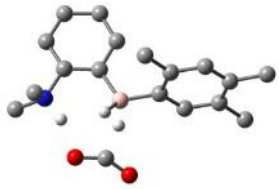
H	2.20306800	-0.49626500	-2.51842700	C	1.72999800	2.37930100	2.75124700
C	2.30433200	-0.11735300	-1.50626600	H	0.73895900	1.91832700	2.90818300
C	3.22115500	0.89254500	-1.22892600	H	2.02190100	2.90015800	3.66878300
C	1.52520300	-0.64504400	-0.48142100	H	1.64944800	3.12410200	1.95694200
C	3.37385100	1.39393900	0.06636600	N	2.75361100	1.40096700	2.40678000
H	3.83521700	1.29129100	-2.03161300	C	2.80205300	4.43580900	-1.26922700
C	1.65988200	-0.15623600	0.81434100	H	2.27371500	5.24860600	-1.77387000
H	0.81117100	-1.43580200	-0.69013100	H	3.65194800	4.14783700	-1.89618200
C	2.57790100	0.85750400	1.08811000	H	2.13122300	3.57198700	-1.22354800
H	1.04906100	-0.56398400	1.61458600	C	2.85934000	7.91037900	2.36132100
B	4.39383700	2.52937300	0.48081100	H	3.72969800	8.52907200	2.60726400
C	4.02134400	3.99592700	0.91806600	H	2.27358600	8.44005600	1.60644300
C	3.25172600	4.85155200	0.10987700	H	2.25210100	7.84155600	3.27099800
C	4.40010300	4.44900500	2.18589600	H	5.29995900	2.05278300	1.23922800
C	2.90049800	6.10722600	0.60457500	O	5.58301600	2.63708800	-0.81560000
C	4.04274400	5.69860300	2.68554400	C	6.34807900	2.22706600	0.04061400
C	3.27466400	6.54689100	1.87358400	O	7.39185400	1.89554600	0.44987800
H	2.30795400	6.77047800	-0.02259200	C	4.47096900	6.12584800	4.06562000
C	2.92944600	0.40600000	3.45054300	H	3.60821000	6.35178100	4.70270700
H	3.69489400	-0.31276600	3.14847000	H	5.05320400	5.34243200	4.55673200
H	3.26676800	0.90555900	4.36439500	H	5.08764500	7.03126900	4.03414500
H	2.00810800	-0.15056600	3.69731700	H	4.98047200	3.78510200	2.82396000

NMeB1H1Mes'_H2CO2TS



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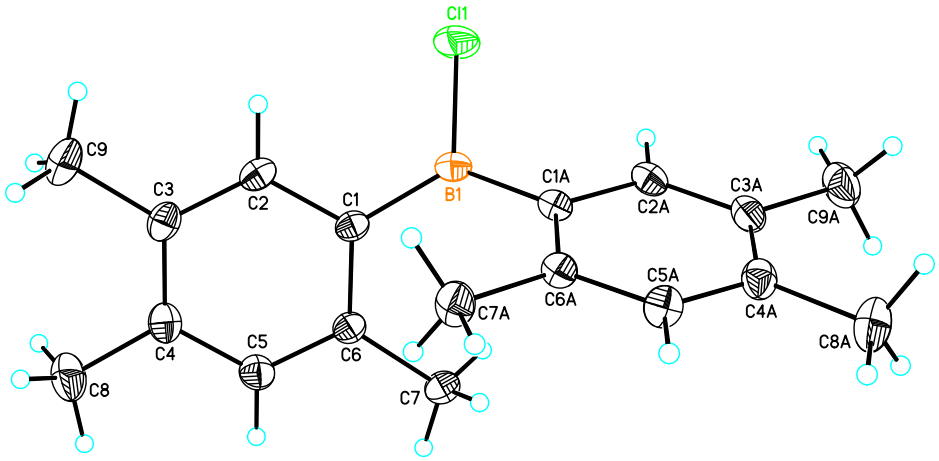
Sum of electronic and thermal Free Energies= -929.87156

C	-0.07839600	0.11017100	-0.76596800
C	1.24395700	0.14606200	-1.21700700
C	1.69804000	1.41089900	-1.62119100
C	0.89884500	2.54669500	-1.55839300
C	-0.40413400	2.46004200	-1.07820400
C	-0.90100800	1.22692900	-0.67394000
H	2.71871700	1.49051500	-1.98354500
H	1.29424600	3.50467200	-1.88101600
H	-1.03366500	3.34140700	-1.01915100
H	-1.91707300	1.15507600	-0.29990200
B	2.23335900	-1.13881600	-1.23818000
H	1.78351500	-1.84200700	-2.26568200
H	-0.07382200	-1.93462900	-0.84858000
C	3.76403100	-0.83724600	-1.56486000
C	4.61780600	-0.28565600	-0.59106600
C	4.30382800	-1.08456900	-2.83099200
C	5.94455800	-0.00902500	-0.91780200
C	5.63183400	-0.81420800	-3.16195400
C	6.47071200	-0.26153200	-2.18405100
H	6.59691000	0.41792700	-0.15734200
C	1.13934600	-3.02315300	-2.69645100
O	1.81604800	-3.48649800	-3.55567500
O	0.11175300	-3.13027000	-2.05201300
C	-2.01678000	-1.47227900	-0.70913800
H	-2.12907700	-1.24872500	-1.76840800
H	-2.21667500	-2.52963100	-0.53658000
H	-2.69630500	-0.86319900	-0.11379700
C	-0.38339800	-1.41393000	1.13528700
H	0.67888300	-1.28237100	1.33429800
H	-0.96884400	-0.67850500	1.68878300
H	-0.69174500	-2.42670100	1.39887600
N	-0.60787800	-1.20375600	-0.32007000
C	4.10740800	0.01273200	0.79804000
H	3.30058400	0.75482900	0.77586300
H	3.69949300	-0.88978100	1.26744700
H	4.90111000	0.40049400	1.44265100
C	7.91334400	0.05053300	-2.48942600
H	8.00496600	0.76316600	-3.31740300
H	8.41757300	0.48095200	-1.62038600
H	8.46517400	-0.84934900	-2.78498300
H	2.05117500	-1.88888900	-0.29515300
H	3.66408700	-1.52583600	-3.59292100
C	6.15140800	-1.11421300	-4.54476400
H	6.52530900	-0.21077800	-5.04111500
H	6.98386000	-1.82694600	-4.51599200
H	5.36747800	-1.54300200	-5.17352500

S9: Crystallographic information

S9-1: Crystal structure of chlorobis(2,4,5-trimethylphenyl)borane



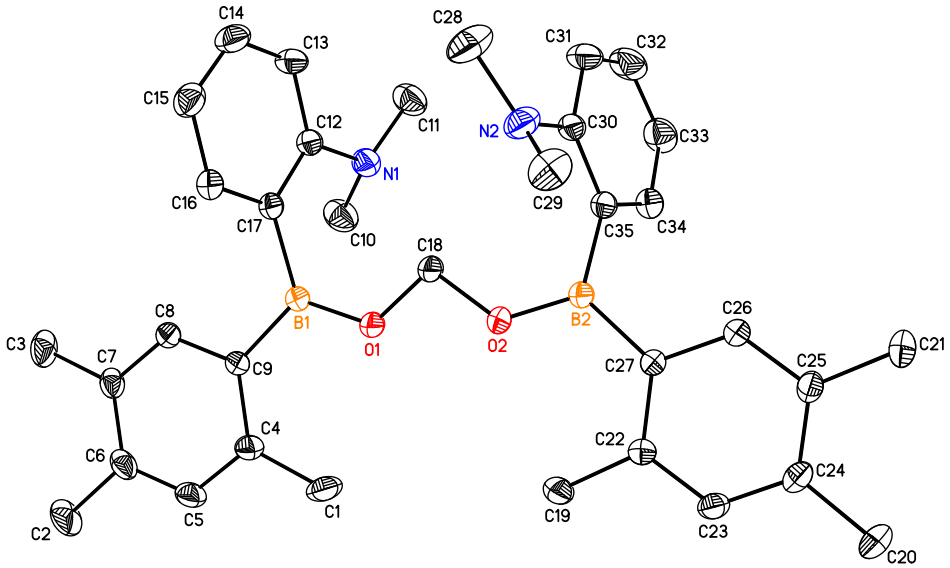
The ORTEP of chlorobis(2,4,5-trimethylphenyl)borane with thermal ellipsoids set at the 50% probability level. H atoms are shown as spheres with arbitrary radii. [Symmetry codes: (A) -x+1, y, -z+1/2]

Table S9-1. Crystal data and structure refinement for chlorobis(2,4,5-trimethylphenyl)borane .

Identification code	chlorobis(2,4,5-trimethylphenyl)borane	
Empirical formula	C18 H22 B Cl	
Formula weight	284.61	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 14.1030(9) Å	α= 90°.
	b = 7.4414(5) Å	β= 110.7640(8)°.
	c = 16.5975(10) Å	γ = 90°.
Volume	1628.71(18) $Å^3$	
Z	4	
Density (calculated)	1.161 Mg/m^3	
Absorption coefficient	0.222 mm^{-1}	
F(000)	608	
Crystal size	0.520 x 0.360 x 0.300 mm^3	
Theta range for data collection	2.625 to 30.498°.	
Index ranges	-20<=h<=20, -10<=k<=10, -23<=l<=23	
Reflections collected	10052	
Independent reflections	2489 [R(int) = 0.0180]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.936 and 0.909	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	2489 / 0 / 95
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.1149
R indices (all data)	R1 = 0.0410, wR2 = 0.1186
Extinction coefficient	n/a
Largest diff. peak and hole	0.396 and -0.281 e.$Å^{-3}$

S9-2: Crystal structure of **4**



The ORTEP of **4** with thermal ellipsoids set at the 50% probability level. H atoms are shown as spheres with arbitrary radii. [Symmetry codes: (A) -x+1, y, -z+1/2]

Table S9-7. Crystal data and structure refinement for **4**

Identification code	4	
Empirical formula	C35 H44 B2 N2 O2	
Formula weight	546.34	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.8272(10) Å	α= 90°.
	b = 21.1220(16) Å	β= 93.3920(10)°.
	c = 14.0969(11) Å	γ = 90°.
Volume	3812.7(5) $Å^3$	
Z	4	
Density (calculated)	0.952 Mg/m^3	
Absorption coefficient	0.057 mm^{-1}	
F(000)	1176	
Crystal size	0.520 x 0.460 x 0.320 mm^3	
Theta range for data collection	1.590 to 28.308°.	
Index ranges	-17<=h<=17, -28<=k<=28, -18<=l<=18	
Reflections collected	40253	
Independent reflections	9480 [R(int) = 0.0307]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.979 and 0.969	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9480 / 0 / 380
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0570, wR2 = 0.1663
R indices (all data)	R1 = 0.0720, wR2 = 0.1751
Extinction coefficient	n/a
Largest diff. peak and hole	0.581 and -0.192 e.$Å^{-3}$

S10: References

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