SUPPORTING INFORMATION FOR

Metal-free Disproportionation of Formic Acid Mediated by Organoboranes

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1. Experimental details

a) General considerations

All reactions and manipulations were performed at 20 ºC in a recirculating mBraun LabMaster DP inert atmosphere (Ar) drybox and vacuum Schlenk lines. Glassware was dried overnight at 120 ºC or flame-dried in vacuum before use. ^{1}H, ^{13}C, ^{31}P and ^{11}B NMR spectra were obtained using a Bruker DPX 200 MHz spectrometer. Chemical shifts for ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced to solvent impurities. ^{11}B NMR spectra were externally referenced using neat $BF_3 \bullet Et_2O$. ^{31}P spectra were externally referenced using H_3PO_4 (85 %). Mass spectrometer data were collected on a Shimadzu GCMS-QP2010 Ultra gas chromatograph mass spectrometer equipped with a Supelco SLBTM-ms fused silica capillary column (30 m × 0.25 mm × 0.25 μm).
Tetrahydrofuran (THF), d_8-tetrahydrofuran (d_8-THF), toluene, pentane and d_6-benzene were dried over a sodium(0)/benzophenone mixture and vacuum-distilled before use. CD_3CN and CD_2Cl_2 were dried over CaH_2 and vacuum-distilled before use. Boranes (*B*-I-9-BBN, *B*-OMe-9-BBN, 9-BBN dimer) and $H^{13}CO_2H$ were obtained from Aldrich and used as received. HCO_2H (> 99 % grade) was obtained from Acros and degassed prior to use. $H^{13}CO2H$ and HCO_2D were obtained from Aldrich and degassed prior to use. Sodium formate (HCO_2Na) was purchased from Aldrich and dried at 120°C under high-vacuum for 2 hours prior to use. Triethylamine and *N*,*N*-diisopropylethylamine (DIPEA) were purchased respectively from Carlo Erba and Aldrich and degassed prior to use. 2,2,6,6-tetramethylpiperidine (TMP) was purchased from Alfa Aesar and degassed prior to use. 1,2,2,6,6-pentamethylpiperidine (PMP) was purchased from Aldrich and degassed prior to use. Cyclohexene was purchased from Aldrich, passed through a column of alumina, dried over CaH_2 and vacuum-distilled before use. Tricyclohexylphosphine (Cy_3P) solution (20 wt. % in toluene) was purchased from Aldrich and used as received. [Et_3NH^+, $\mathbf{1}^-$] and [Et_3NH^+, $\mathbf{2}^-$] were prepared by a previously reported procedure.[1] Crown ethers Dibenzo-18-crown-6 (DB18C6) and 15-Crown-5 (15C5) were purchased from Aldrich and used a received. Benzaldehyde, 4-chlorobenzaldehyde and cinnamaldehyde were purchased from Aldrich and degassed prior to use.

b) Crystallography

The data were collected at 150(2) K on a Nonius Kappa-CCD area detector diffractometer[2] using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The crystals were introduced into glass capillaries with a protective coating of Paratone-N oil (Hampton Research). The unit cell parameters were determined from ten frames, then refined on all data. The data (combinations of φ- and ω-scans with a minimum redundancy of 4 for 90% of the reflections) were processed with HKL2000.[3] Absorption effects in [Cy_3PH^+, $\mathbf{1}^-$] and **4** were corrected empirically with the program SCALEPACK.[3] The structures were solved by intrinsic phasing with SHELXT,[4] expanded by subsequent difference Fourier synthesis and refined by full-matrix least-squares on F^2 with SHELXL-2014.[5] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms bound to N1 in

[$TMPH^+$, **1**$^-$] and [Et_3NH^+, **2**$^-$], and to P1 in [Cy_3PH^+, **1**$^-$] were found on a difference Fourier map; the carbon-bound hydrogen atoms were introduced at calculated positions in all compounds. All hydrogen atoms were treated as riding atoms with an isotropic displacement parameter equal to 1.2 times that of the parent atom (1.5 for CH_3, with optimized geometry). The structure of complex **4** was refined as a two-component inversion twin, with a Flack parameter of 0.48(10). In compound **SI1**, restraints on some bond lengths and displacement parameters had to be applied for atoms C3–C6 which may be affected by unresolved disorder. Crystal data and structure refinement parameters are given in Table S1. The molecular plots were drawn with ORTEP-3.[6] CCDC-1450409, -1450410, -1454182, -1450411, -1450412 and -1450413 contain the supplementary crystallographic data for compounds [$TMPH^+$, **1**$^-$], [Cy_3PH^+, **1**$^-$], [Et_3NH^+, **2**$^-$], **3**, **4** and **SI1**, respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement details

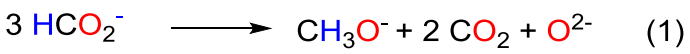
	[$TMPH^+$, **1**$^-$]	[Cy_3PH^+, **1**$^-$]	[Et_3NH^+,**2**$^-$]	**3**	**4**	**SI1**
chemical formula	$C_{19}H_{36}BNO_4$	$C_{28}H_{50}BO_4P$	$C_{20}H_{40}BNO_4$	$C_{25}H_{47}B_2NO_5$	$C_{28}H_{50}BO_3P$	$C_{32}H_{60}B_3NO_4$
M (g mol^{-1})	353.30	492.46	369.34	463.25	476.46	555.24
crystal system	monoclinic	triclinic	triclinic	monoclinic	monoclinic	triclinic
space group	$P2_1/c$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	Cc	$P\bar{1}$
a (Å)	11.0485(6)	11.1604(7)	10.8630(6)	10.6867(2)	19.1313(10)	10.5845(9)
b (Å)	22.2891(12)	11.4336(7)	11.2446(7)	14.3031(2)	21.5741(15)	11.0144(7)
c (Å)	8.1947(3)	12.9009(9)	11.3017(4)	17.0535(3)	16.3900(11)	13.8285(13)
α (°)	90	64.743(3)	72.947(5)	90	90	90.335(5)
β (°)	95.694(3)	68.006(3)	65.299(4)	91.9943(6)	124.724(3)	90.142(4)
γ (°)	90	77.056(4)	62.655(4)	90	90	90.788(5)
V (Å^3)	2008.08(17)	1376.43(16)	1105.23(11)	2605.10(8)	5560.0(6)	1612.0(2)
Z	4	2	2	4	8	2
D_{calcd} (g cm^{-3})	1.169	1.188	1.110	1.181	1.138	1.144
μ(Mo Kα) (mm^{-1})	0.079	0.131	0.074	0.079	0.125	0.071
F(000)	776	540	408	1016	2096	612
reflections collected	73000	70576	51755	87423	80213	78638
independent reflections	3789	5204	4192	4906	10370	6116
"observed" reflections [$I > 2\sigma(I)$]	3037	4441	3115	4413	9104	4369
R_{int}	0.023	0.036	0.026	0.016	0.039	0.046
parameters refined	238	307	238	301	596	364
R1[a]	0.037	0.047	0.039	0.036	0.048	0.074
wR2[b]	0.101	0.131	0.112	0.095	0.099	0.203
S	1.047	1.083	1.061	1.041	1.066	1.107
$\Delta\rho_{min}$ (e Å^{-3})	–0.17	–0.27	–0.18	–0.16	–0.25	–0.39
$\Delta\rho_{max}$ (e Å^{-3})	0.25	0.35	0.14	0.27	0.37	0.84

[a] R1 = $\Sigma||F_o| - |F_c||/|F_o|$ ("observed" reflections); [b] wR2 = $[\Sigma w(|F_o^2| - |F_c^2|)^2/\Sigma w|F_o^2|^2]^{1/2}$ (all reflections).

2. Determination of methanol yields

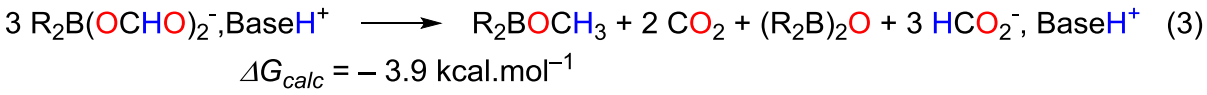
Chemical equations for the formation of methoxyboranes by thermolysis of bis(formyloxy)borates.

- Formal disproportionation of the formate anion:

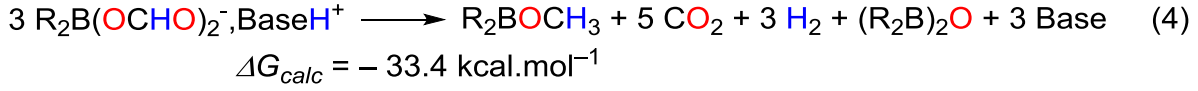


- Formal disproportionation of mono(formyloxy)boranes:

- Disproportionation of bis(formyloxy)borates[1]:



- Disproportionation of bis(formyloxy)borates with concomitant dehydrogenation[1]:



According to equations (1) or (2), 3 moles of formate anion are required to formally obtain one mole of methoxide anion. The yield of methoxyborane was therefore calculated as follows:

$$\rho(MeO[B]) = \frac{3 \times n(MeO[B])}{n_0(HCOOH)}$$

- $\rho(MeO[B])$ is the yield of methoxyborane
- $n(MeO[B])$ is the number of moles of methoxyborane at time *t* as determined by NMR spectroscopy *vs* an internal standard
- $n_0(HCOOH)$ is the initial number of moles of formic acid/formate anion

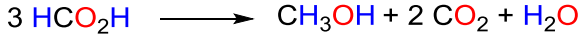
Yields of free methanol were calculated using the same formula after hydrolysis of the methoxyboranes with H_2O.

Experimental yield determination: From ^{1}H NMR experiments, yields of methoxyborane were determined by integration of the CH_3O protons ($\underline{H_3}CO[B]$, δ =3.71 ppm for [B] = BBN and δ = 3.65 ppm for [B] = BCy_2 in CD_3CN) *vs* mesitylene as an internal standard (C_{Ar}-$\underline{H}$, δ = 6.79 ppm in CD_3CN). Yields of free methanol were determined with the same method. Qualitatively, H_2 (δ = 4.57 ppm in CD_3CN, δ = 4.55 ppm in d_8-THF) and $^{13}CO_2$ (δ = 125.8 ppm in CD_3CN, δ = 125.69 ppm in d_8-THF) are detected by ^{1}H and ^{13}C NMR spectroscopy.

[1] ΔG_{calc} were determined by calculations at the M062X/PCM=MeCN/6-311+G(d,p) level of theory.

State of the art in the disproportionation of formic acid to methanol

Table S2: State of the art for the disproportionation of formic acid to MeOH



Entry		Metal	Best MeOH Selectivity (conversion) [%]	Best MeOH Yield (conversion) [%]	Ref.
1	**Goldberg *et al.***	Ir	12 (3)	2.6[a] (50)	[7]
2	**Parkin *et al.***	Mo	21[a] (100)	21[a] (100)	[8]
3	**Cantat *et al.***	Ru	50.2 (100)	50.2 (100)	[9]

[a] these yields of methanol also include the yield of methyl formate

3. Preparation and characterization of new bis(formoxy)borates

a) X-ray diffraction of [Et_3NH^+, 2^-]

Crystals suitable for X-ray diffraction were obtained from the oily solid upon standing.

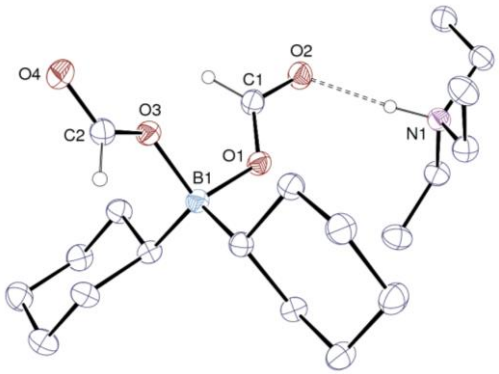


Figure S1. ORTEP view of [Et_3NH^+, **2**$^-$]. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms of the ethyl and cyclohexyl groups have been omitted for clarity. The hydrogen bond is shown as a dashed line.

b) Synthesis of [*i*-Pr_2EtNH^+, **1**$^-$]

A 100-mL, flame dried round-bottomed flask equipped with a stirring bar and a J-Young valve was charged with 9-BBN dimer (356 mg, 1.46 mmol, 0.5 equiv.) and 10 mL of toluene. The resulting suspension was stirred vigorously at RT to ensure complete dissolution of the hydroborane reagent. The flask was then sequentially charged with formic acid (221 µL, 5.85 mmol, 2 equiv.) added *via* syringe, and *N*,*N*-diisopropylethylamine (498 µL, 2.93 mmol, 1 equiv.), added as a single portion. While H_2 release is quite slow when only formic acid is added, the addition of the base considerably increases the rate of H_2 evolution. The reaction mixture was stirred at RT for 15 h to ensure full conversion of the starting hydroborane (evolution of H_2 ends after *ca.* 30 min) The volatiles were removed *in vacuo* to afford a colorless crude oil, which upon trituration in pentane gives a white solid. The solid was further washed with pentane (3 × 2 mL) and Et_2O (3 × 2 mL), filtered and dried under high-vacuum to afford [*i*-Pr_2EtNH^+, **1**$^-$] as a white powder, in 76 % yield (766 mg).

^{1}H NMR (200 MHz, CD_3CN) δ 8.44 (s, 2H), 7.87 (bs, 1H), 3.68 (h, 2H), 3.15 (q, *J* = 7.2 Hz, 2H), 1.88 – 1.15 (m, 27H), 0.74 (s, 2H).
^{13}C NMR (50 MHz, CD_3CN) δ 167.75, 55.47, 43.61, 32.08, 25.60, 18.57, 17.26, 12.85.
^{11}B NMR (64 MHz, CD_3CN) δ 9.03.
Elem. Anal. : calc (%) for $C_{18}H_{36}BNO_4$ (341.29 g.mol^{-1}): C 63.35, H 10.63, N 4.10; found: C 62.80, H 10.67, N 3.99.

c) Synthesis of [Cy_3PH^+, 1^-]

The procedure detailed for the synthesis of [*i*-Pr_2EtNH^+, $\mathbf{1}^-$] was employed for the synthesis of [Cy_3PH^+, $\mathbf{1}^-$], by replacing *i*-Pr_2EtN with Cy_3P (20 wt % in toluene). [Cy_3PH^+, $\mathbf{1}^-$] was obtained as a white powder, in 73 % yield. Crystals suitable for X-Ray analysis were obtained by diffusion of pentane through a saturated solution of [Cy_3PH^+, $\mathbf{1}^-$] in THF, at room temperature.

^{1}H NMR (200 MHz, CD_3CN) δ 8.44 (s, 2H), 2.51 (q, *J* = 11.7 Hz, 3H), 1.87 – 1.22 (m, 43H), 0.72 (s, 2H).
^{13}C NMR (50 MHz, CD_3CN) δ 166.85, 32.22, 28.88, 28.46, 28.12, 26.92, 26.66, 25.79.
^{11}B NMR (64 MHz, CD_3CN) δ 8.46
^{31}P NMR (81 MHz, CD_3CN) δ 31.5 (s).
Elem. Anal. : calc (%) for $C_{28}H_{50}BO_4P$ (492.49 g.mol^{-1}): C 68.29, H 10.23 found: C 68.56, H 10.33

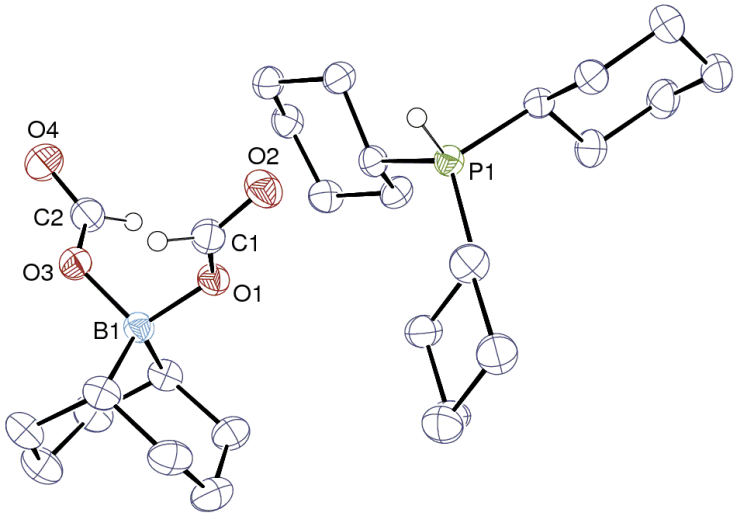


Figure S2. ORTEP view of [Cy_3PH^+, $\mathbf{1}^-$]. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms of the BBN and cyclohexyl groups have been omitted for clarity.

d) Synthesis of [$TMPH^+$, 1^-]

The procedure detailed for the synthesis of [*i*-Pr_2EtNH^+, $\mathbf{1}^-$] was employed for the synthesis of [$TMPH^+$, $\mathbf{1}^-$], by replacing *i*-Pr_2EtN with TMP. [$TMPH^+$, $\mathbf{1}^-$] was obtained as a white powder in 89 % yield and was recrystallized from acetonitrile. Crystals suitable for X-Ray diffraction were obtained from the recrystallization crop.

^{1}H NMR (200 MHz, CD_3CN) δ 8.44 (s, 2H), 7.87 (bs, 1H), 3.68 (h, 2H), 3.15 (q, *J* = 7.2 Hz, 2H), 1.88 – 1.15 (m, 27H), 0.74 (s, 2H).

^{13}C NMR (50 MHz, CD_3CN) δ 169.13, 60.45, 37.22, 33.97, 29.24, 27.52, 18.51.
^{11}B NMR (64 MHz, CD_3CN) δ 8.30.
Elem. Anal. : calc (%) for $C_{19}H_{36}BNO_4$ (353.31 g.mol^{-1}): C 64.59, H 10.27, N 3.96; found: C 64.15, H 10.31, N 4.02.

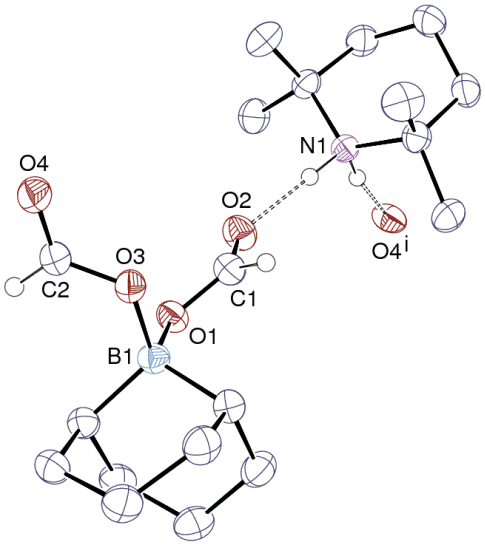


Figure S3. ORTEP view of [TMPH$^+$, **1**$^-$]. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms of the BBN and 1,1,3,3-tetramethylpiperidine groups have been omitted for clarity. Hydrogen bonds are shown as dashed lines. Symmetry code: i = *x*, 3/2 – *y*, *z* + 1/2.

e) Synthesis of [Na$^+$, 1$^-$]

A 50-mL, flame dried round-bottomed flask equipped with a stirring bar and a J-Young valve was charged with 9-BBN dimer (512 mg, 2.10 mmol, 0.50 equiv.) and 10 mL of THF. The resulting suspension was stirred vigorously at RT to ensure complete dissolution of the hydroborane reagent. The flask was then sequentially charged with formic acid (159 µL, 4.20 mmol, 1 equiv.) added *via* syringe, and anhydrous sodium formate (286 mg, 4.20 mmol, 1 equiv.), poured in one portion. While H_2 release is quite slow when only formic acid is added, the addition of sodium formate considerably increases the rate of H_2 evolution. In THF, H_2 evolution ceases after *ca.* 15 min affording a colorless homogeneous solution. The reaction mixture was further stirred at RT for 15 h to ensure full conversion of the starting hydroborane. Pentane (3 mL) was then added to precipitate a white solid that was filtered and washed with pentane (3 × 2 mL) and Et_2O (3 × 2 mL). The resulting white powder was dried under high-vacuum to afford [Na$^+$, **1**$^-$] in 83 % yield (830 mg).

^{1}H NMR (200 MHz, DMSO-d_6) δ 8.34 (s, 2H), 2.05 – 1.11 (m, 12H), 0.68 (s, 2H).
^{13}C NMR (50 MHz, DMSO-d_6) δ 165.45, 31.02, 24.65.
^{11}B NMR (64 MHz, DMSO-d_6) δ 8.77 (bs).

4. Procedures for the disproportionation of formate anions

Caution: *Release of CO_2 and H_2 generates pressure in sealed tubes!*

a) Procedure and spectra for the *in-situ* preparation and thermolysis of [Et_3NH^+, 1^-]

In a glovebox, an oven-dried J-Young NMR tube was sequentially charged with formic acid (0.2 mmol, 7.4 µL, 2 equiv.), triethylamine (0.2 mmol, 27.8 µL, 2 equiv) and d_3-MeCN (0.25 mL). The tube was then shaken vigourously for 1 min to ensure complete protonation of the base and BBNI (100 µL, 0.1 mmol, 0.1 M in hexanes, 1 equiv.) was added in one portion using a syringe. The tube was brought out of the glovebox and immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reactions were periodically cooled down to room temperature and monitored by NMR spectroscopy. Representative NMR spectra acquired before heating and after 18 h at 130°C are given in Figure S4.

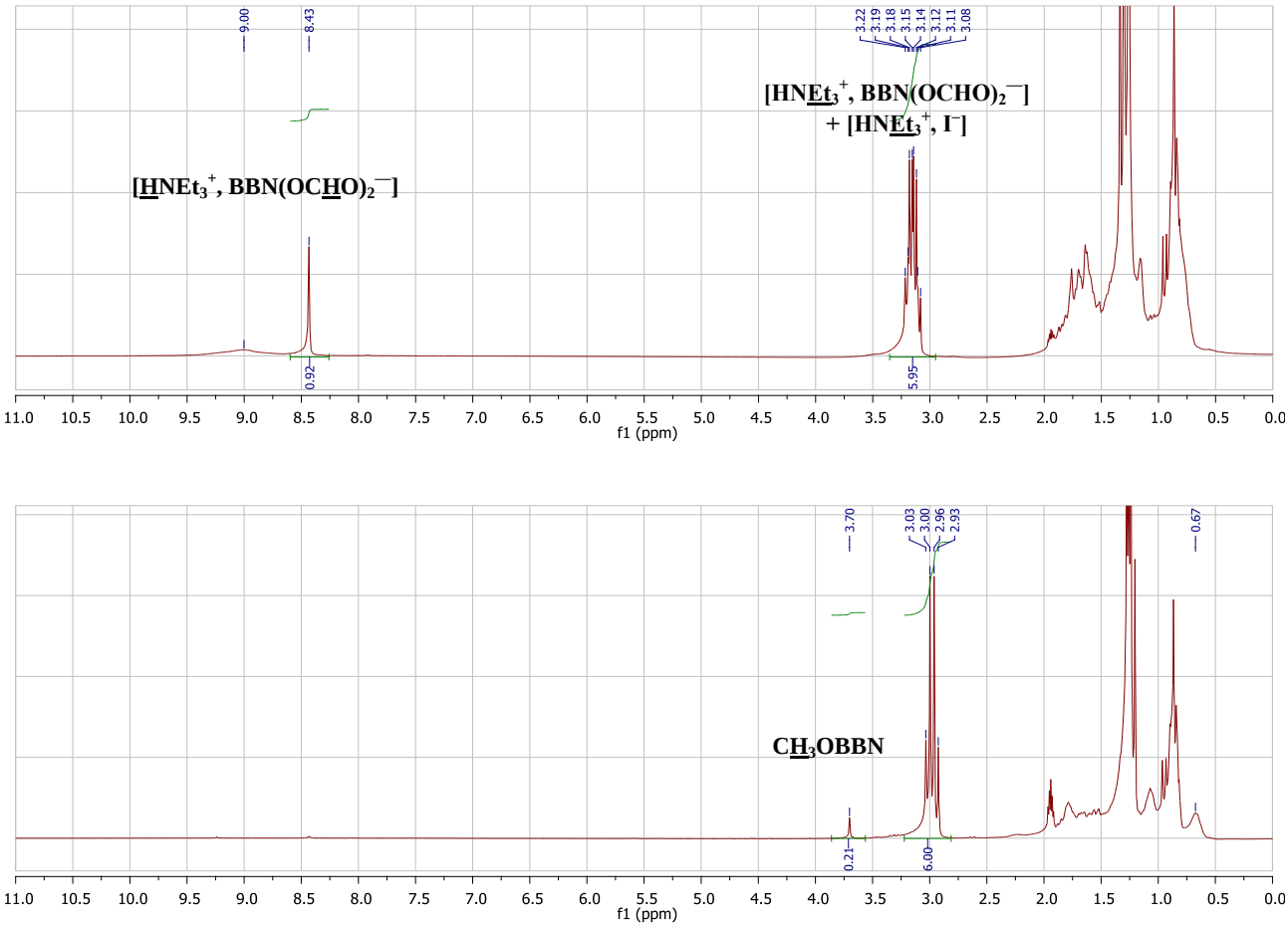


Figure S4. Representative ^{1}H NMR spectra obtained in CD_3CN for the thermolysis of *in-situ* formed [Et_3NH^+, **1**$^-$]. a) crude reaction mixture before heating; t = 0. b) crude reaction mixture after 18 h at 130°C.

CH_3OBBN yield: **19 %** (average of three runs).

b) Procedure for the thermolysis of isolated [Et_3NH^+, 1^-]

In a glovebox, a flame-dried NMR tube equipped with a J-Young valve was charged with [Et_3NH^+, **1**$^-$] (0.125 mmol in typical experiments), mesitylene (as an internal standard) and acetonitrile-d_3.

The tube was immersed in a pre-heated silicon-oil bath at the indicated temperature (oil-bath temperature). The reactions were periodically cooled down to room temperature and monitored by NMR spectroscopy. Products yields were determined after complete decomposition of the formate ligands (> 95% conversion).

Representative NMR spectra are given in Figures S5 (^{1}H) and S6 (^{11}B).

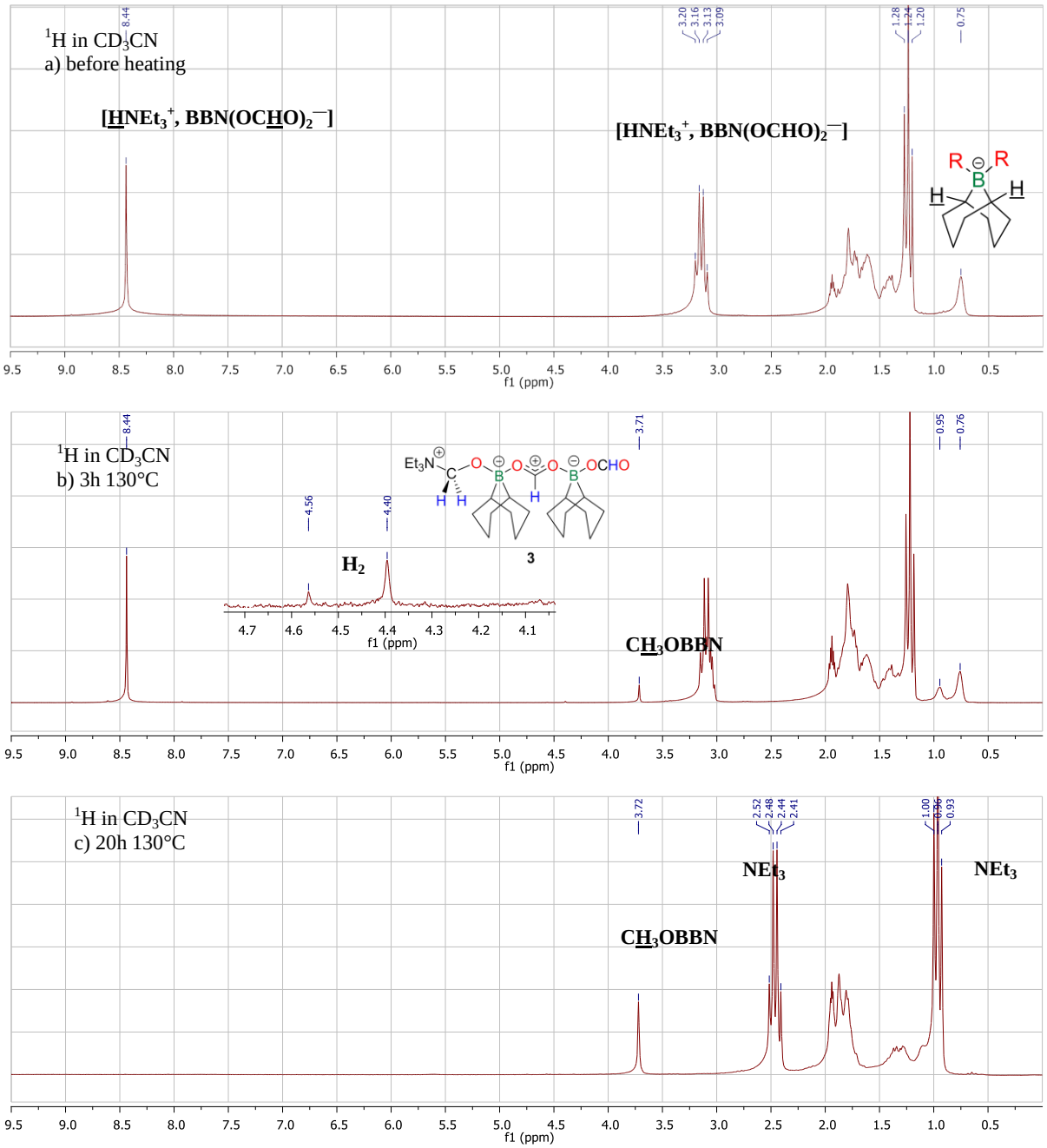


Figure S5. Representative ^{1}H NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$]. a) crude reaction mixture before heating; t = 0. b) crude reaction mixture after 3

h at 130°C, H_2 gas (δ = 4.56 ppm) and intermediate **3** (δ = 4.40 ppm) are observed. c) crude reaction mixture after 20 h at 130°C.

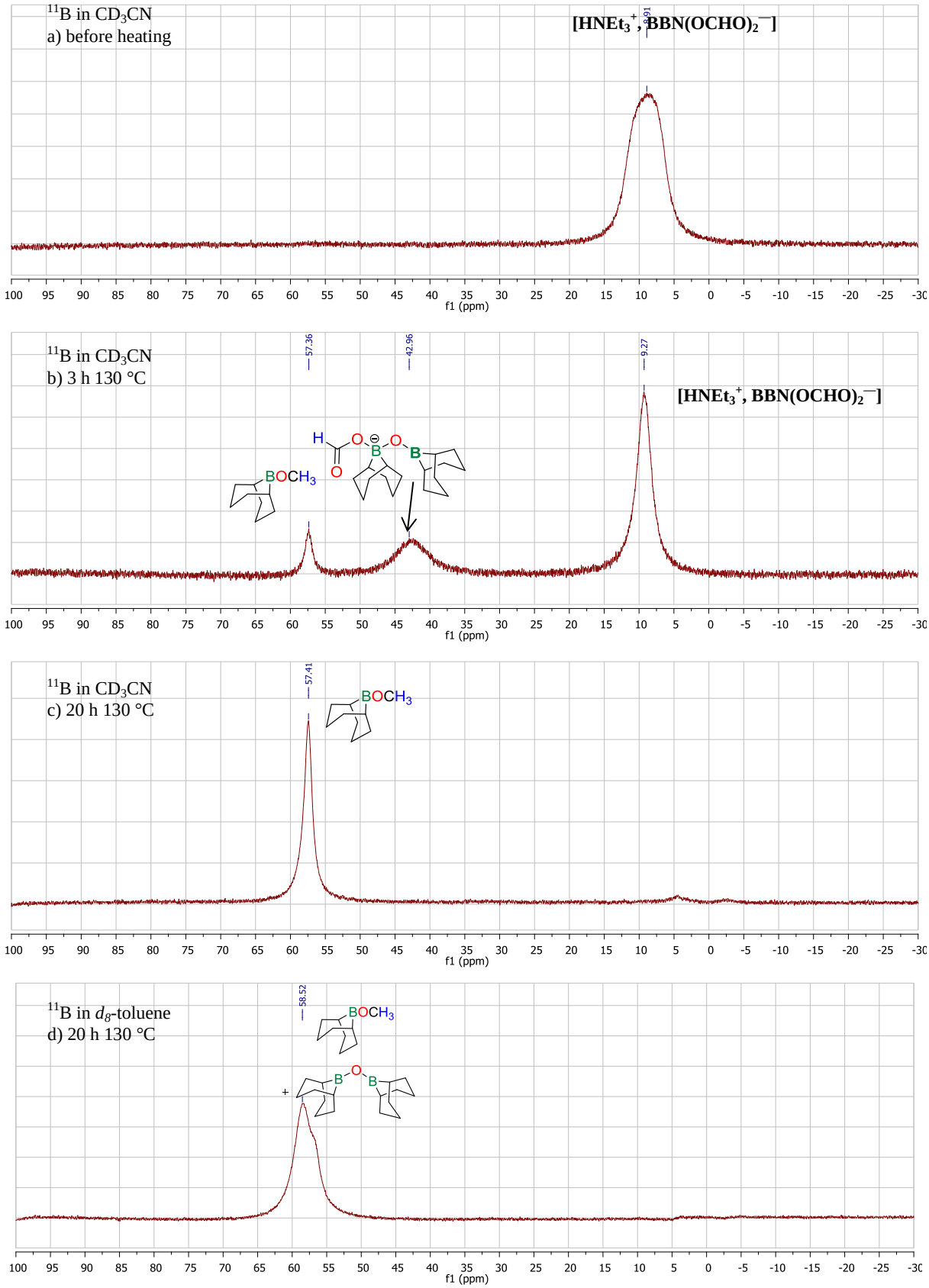


Figure S6. Representative ^{11}B NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$]. a) crude reaction mixture before heating; t = 0. b) crude reaction mixture after 3 h at 130°C. The broad signal (δ_{11B} = 42.96 ppm) was attributed to the tricoordinate boroxane. See figure S17 c) crude reaction mixture after 20 h at 130°C. d) crude reaction mixture taken-up in d_8-toluene after evaporation of volatiles (comprising NEt_3 and traces of $BBNOCH_3$). The spectrum shows the overlap between the signals of $BBNOCH_3$ and $(BBN)_2O$. On the contrary, due to the insolubility of $(BBN)_2O$ in CH_3CN at room temperature, no overlap is observed in the latter solvent.

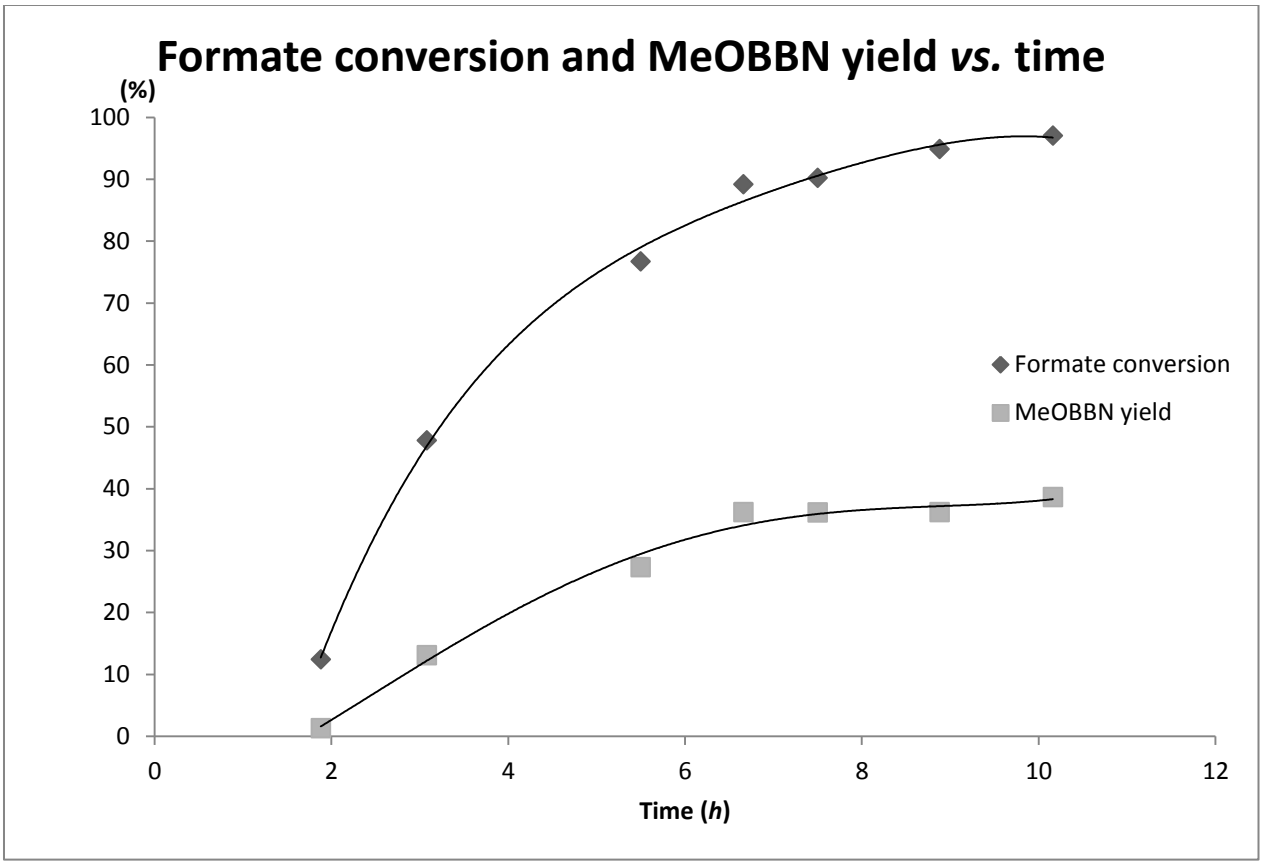


Figure S7. Plot of the conversion of [Et_3NH^+, **1**$^-$] and corresponding yield of CH_3OBBN (as defined p. S5) over time. 10.5 h are required to reach > 95 % conversion (39 % yield of CH_3OBBN).

As depicted in Figure S7, the formation of CH_3OBBN is observed after an initiation period of ca. 2 h during which 12 % of the formate ligands are decomposed. After this period, CH_3OBBN production follows the decomposition of formates and the yield difference is attributed to the competitive evolution of H_2 (observed by ^1H NMR).

c) Hydrolysis of CH_3OBBN within the crude reaction mixture

When full conversion of the formate anions was reached, H_2O (*ca.* 10 equiv.) was added to the reaction mixture *via* syringe and the resulting solution was stirred at RT for 1 h. The reaction mixture was then distilled under reduced pressure to afford a MeCN solution of methanol. The formation of methanol was determined by ^1H NMR in d_3-MeCN (δ = 3.28 ppm) using mesitylene as an internal standard.

Alternatively, to obtain a solution consisting only in MeOH, triethylamine may be removed *in vacuo* prior to carrying out the hydrolysis.

d) Procedure for the thermolysis of $[Et_3NH^+,BBN(O^{13}CHO)_2^-]$

The same procedure given for the thermolysis of $[Et_3NH^+, \mathbf{1}^-]$ was carried out by replacing $H^{12}CO_2H$ with $H^{13}CO_2H$. $^{13}CO_2$ and $^{13}CH_3OBBN$ were the sole ^{13}C-enriched products detected by NMR. Representative spectra are provided in Figure S8 (^{13}C) and S9 (^1H).

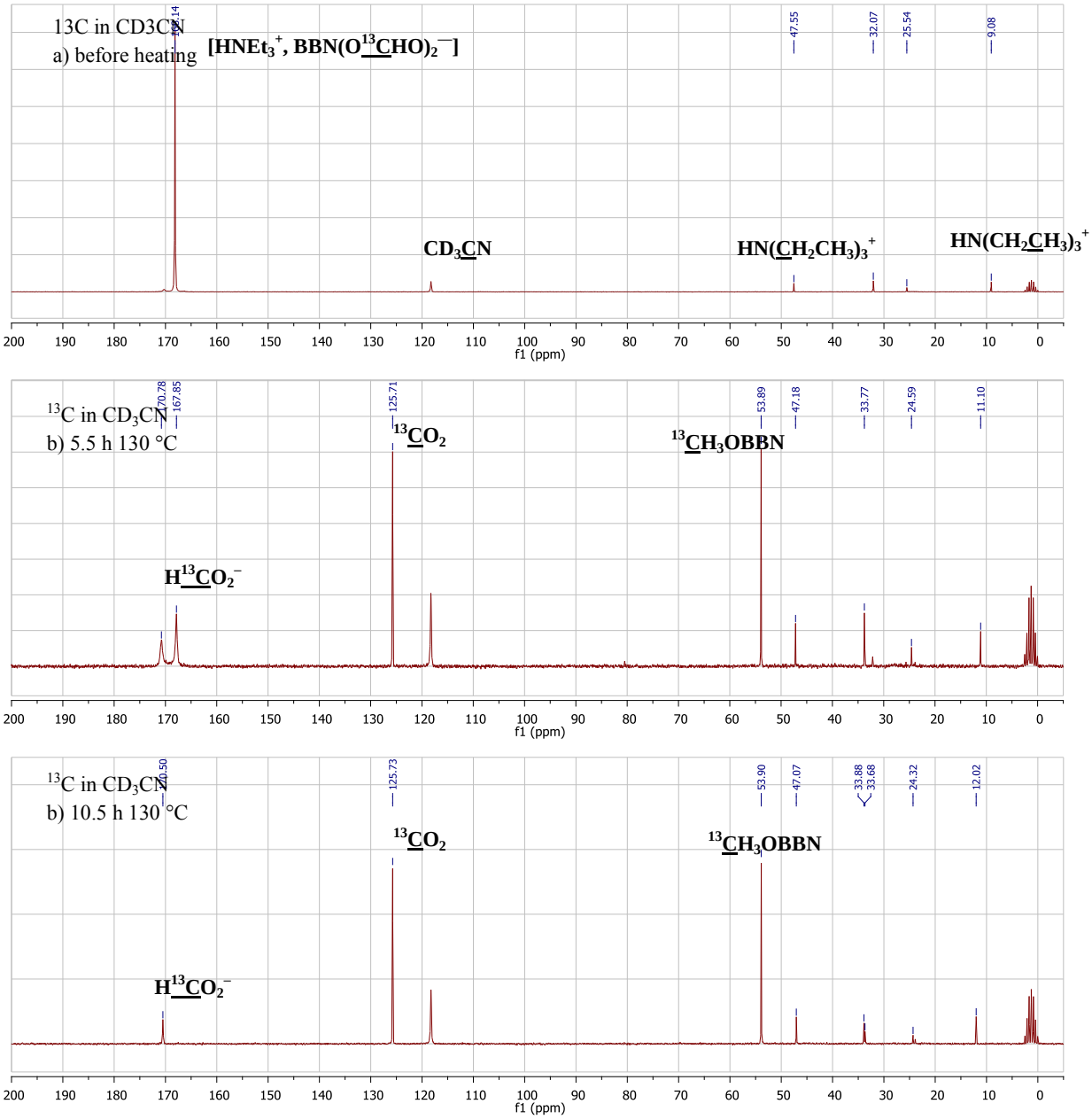


Figure S8. ^{13}C NMR spectra obtained in CD_3CN for the thermolysis of $[Et_3NH^+,BBN(O^{13}CHO)_2^-]$ a) crude reaction mixture before heating consisting of pure $[Et_3NH^+,BBN(O^{13}CHO)_2^-]$. b) crude reaction mixture after 5.5 h at 130°C. c) crude reaction mixture after 10.5 h at 130°C.

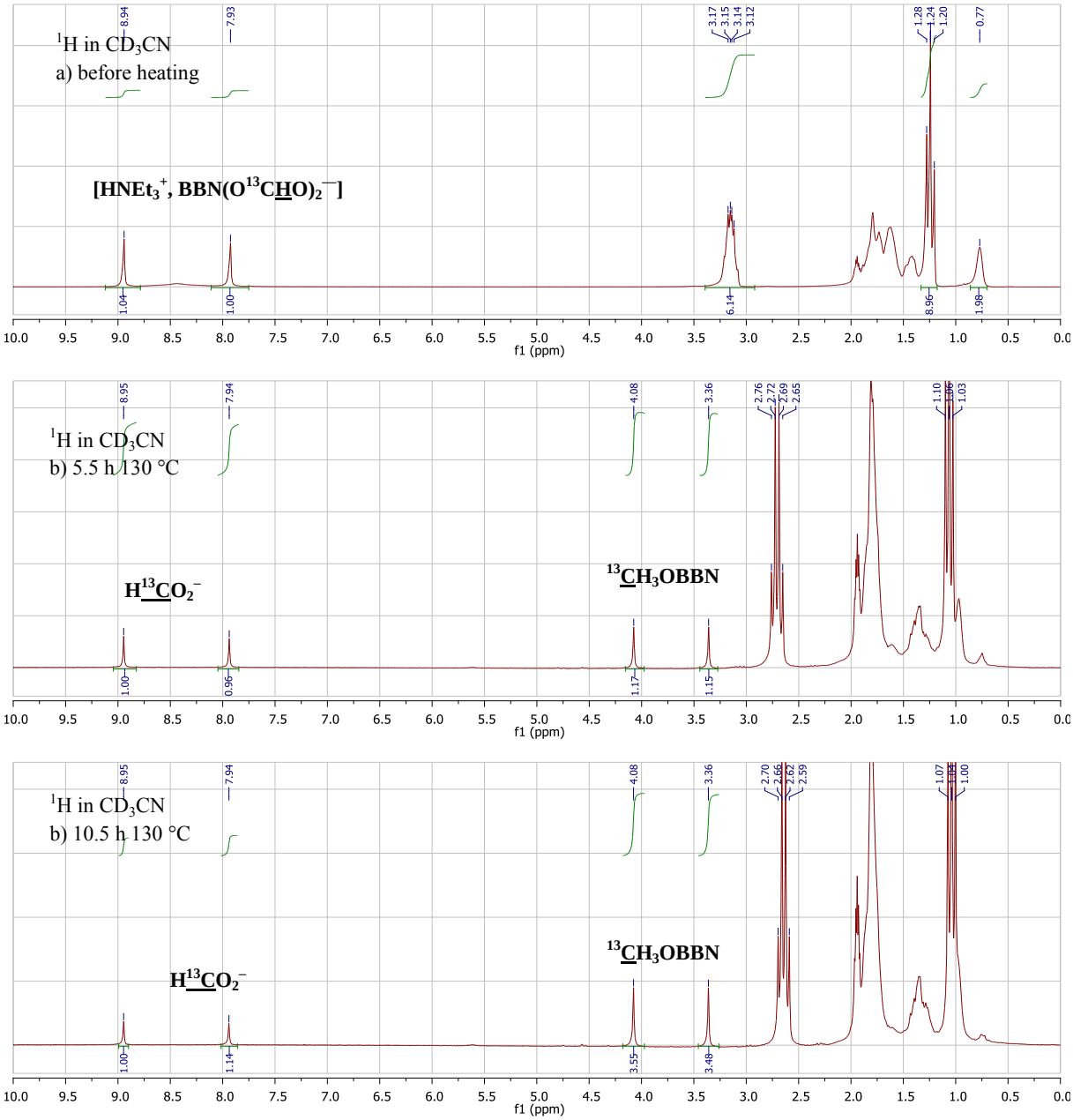


Figure S9. ^{1}H NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+,$BBN(O^{13}CHO)_2^-$]. a) Crude reaction mixture before heating consisting of pure [Et_3NH^+,$BBN(O^{13}CHO)_2^-$] ($^1J_{C\text{-}H}$ = 203.3 Hz). b) Crude reaction mixture after 5.5 h at 130°C ($^1J_{C\text{-}H}$($^{13}CH_3OBBN$) = 143.1 Hz). c) Crude reaction mixture after 10.5 h at 130°C.

e) Procedure for the thermolysis of [Na^+, 1^-]

In a glovebox, a flame-dried NMR tube equipped with a J-Young valve was charged with [Na^+, $\mathbf{1}^-$] (0.125 mmol in typical experiments), mesitylene (as an internal standard) and acetonitrile-d_3. Crown ethers (DB18C6 or 15C5, 1 equiv) were used as additives in order to obtain a homogeneous solution at room temperature.

The tube was immersed in a pre-heated silicon-oil bath at the indicated temperature (oil-bath temperature). The reactions were periodically cooled down to room temperature and monitored by NMR spectroscopy. Products yields were determined when the formate conversion reached a plateau (typically within 20-25h).

Representative NMR spectra are given in Figures S10 (^{1}H)

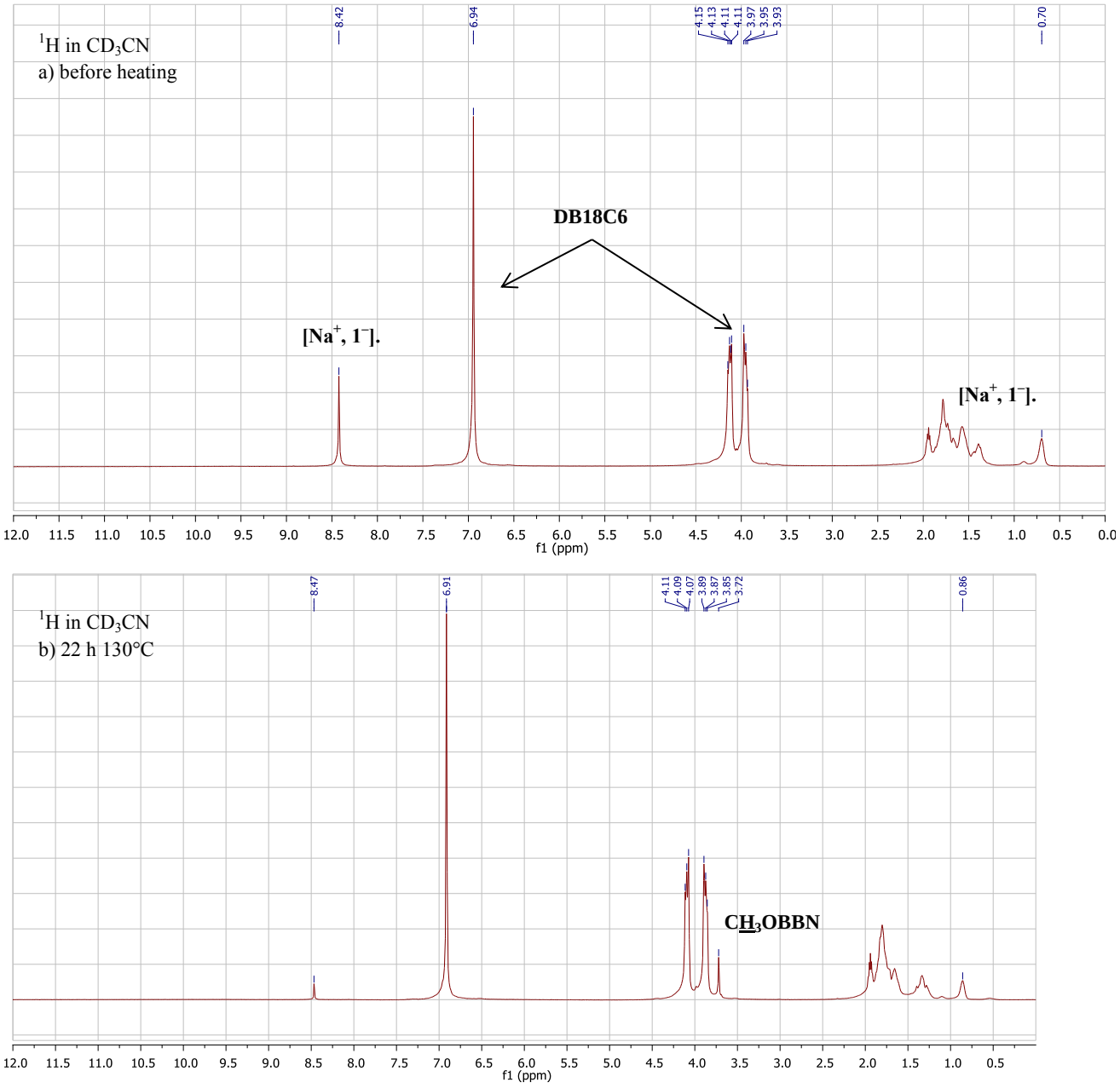


Figure S10. ^{1}H NMR spectra obtained in CD_3CN for the thermolysis of [Na^+, $\mathbf{1}^-$]. a) Crude reaction mixture before heating b) Crude reaction mixture after 22 h at 130°C

f) Thermolysis of [Cy_3PH^+, 1^-]:

In a glovebox, a flame-dried J-Young NMR tube was charged with **[**Cy_3PH^+, **1**$^-$**]** (0.125 mmol) and acetonitrile-d_3 (0.4 mL), sealed and brought out of the glovebox.
The tube was immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reaction was periodically cooled down to room temperature and monitored by NMR spectroscopy.
Representative NMR spectra obtained during the thermolysis of ^{13}C-enriched [Cy_3PH^+, **1**$^-$] are given in figures S11 (^{13}C) and S12 (^{31}P).

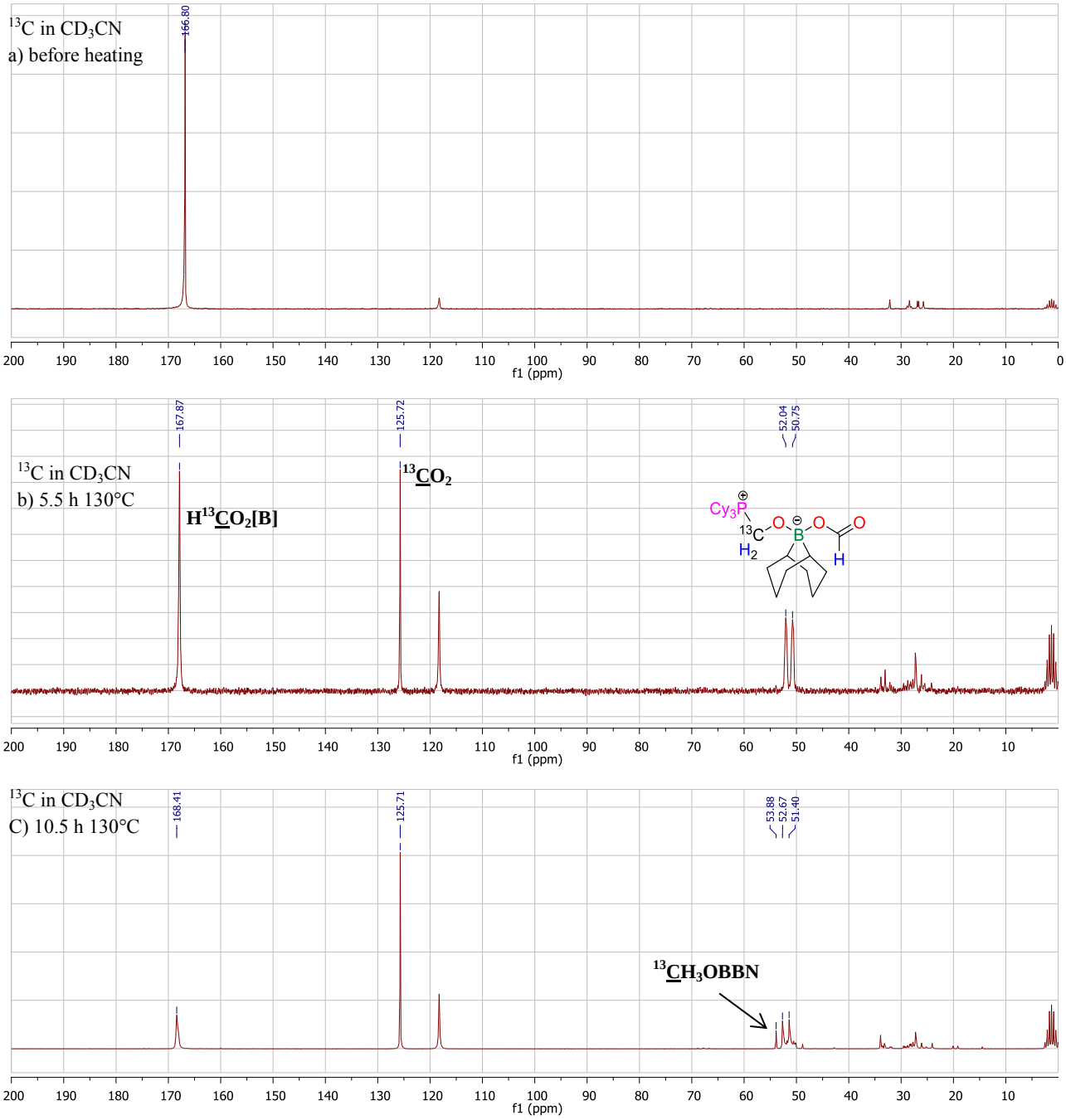


Figure S11. ^{13}C NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$] under $^{13}CO_2$ atmosphere a) Crude reaction mixture before heating. b) Crude reaction mixture after 5.5 h at 130°C ($^1J_{C\text{-}H}$ = 145 Hz). c) Crude reaction mixture after 10.5 h at 130°C.

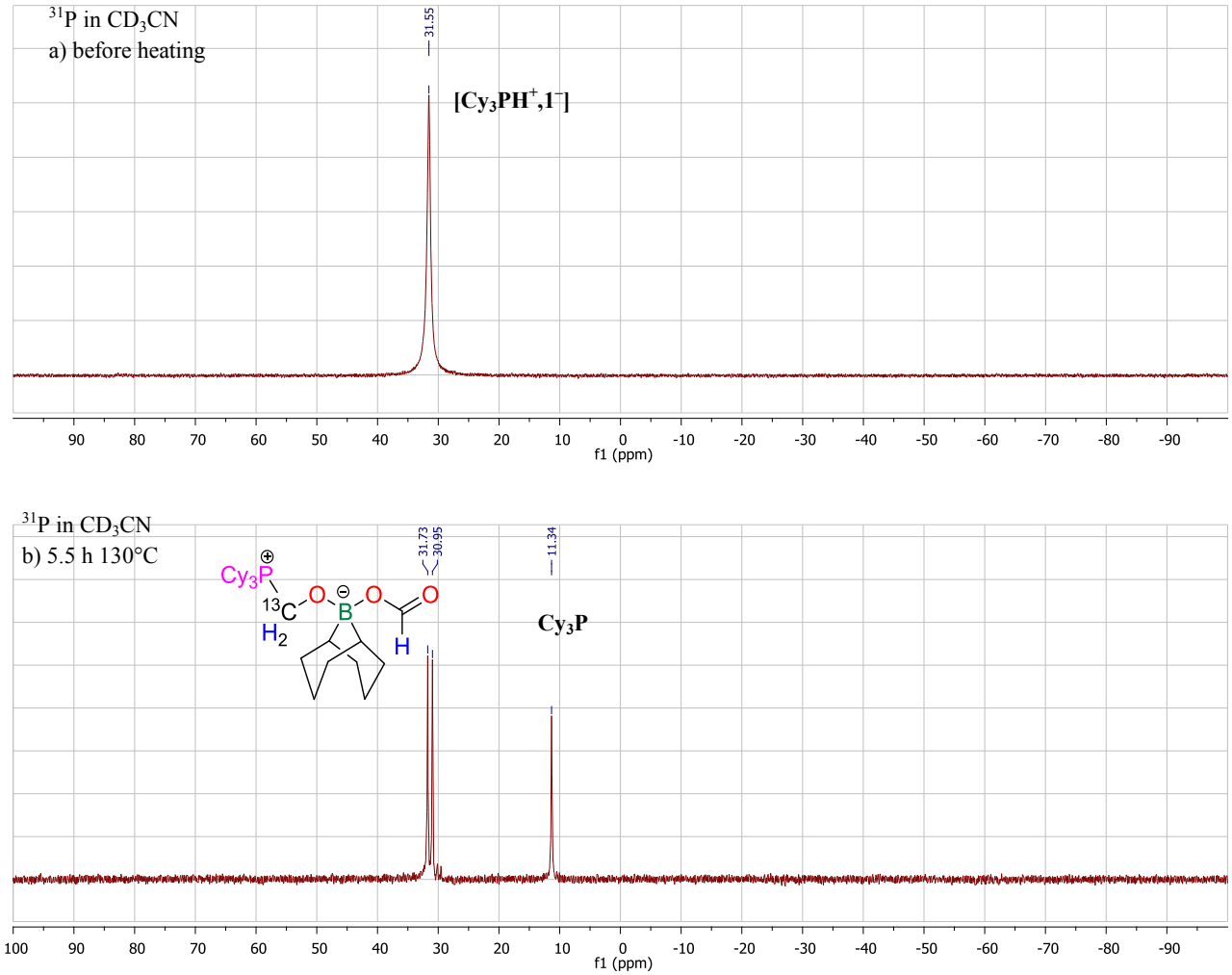


Figure S12. ^{31}P NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$] under $^{13}CO_2$ atmosphere a) Crude reaction mixture before heating. b) Crude reaction mixture after 5.5 h at 130°C ($^1J_{C\text{-}P}$ = 64 Hz).

Crystals of **4** suitable for X-ray diffraction were obtained by slow cooling of the crude reaction mixture, which had been taken up in THF (after removal of the volatiles).

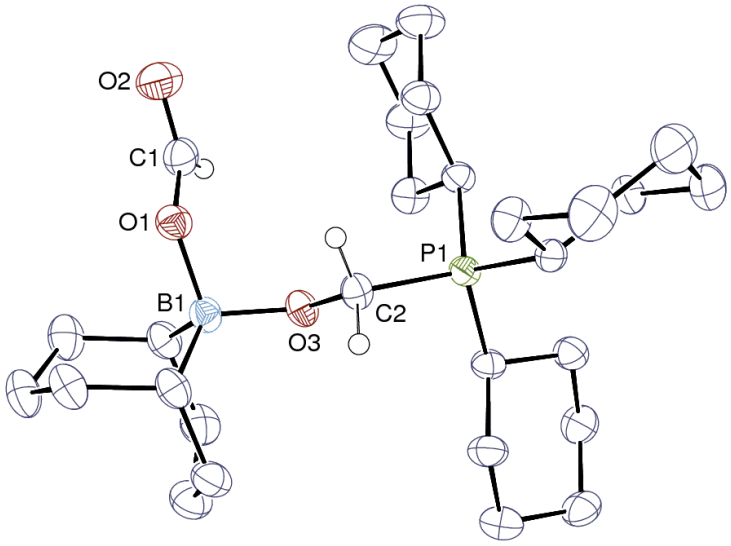


Figure S13. ORTEP view of **4**. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms of the BBN and cyclohexyl groups have been omitted for clarity.

g) Methylation of TMP *via* the thermolysis of [$TMPH^+$, 1^-]

In a glovebox, a flame-dried J-Young NMR tube was charged with **[**$TMPH^+$,**1**$^-$**]** (35.3 mg, 0.1 mmol), diphenylmethane as internal standard (10 µL) and acetonitrile-d_3 (0.4 mL), sealed and brought out of the glovebox.
The tube was immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reaction was periodically cooled down to room temperature and monitored by NMR spectroscopy. After 18 h, full conversion was reached and vacuum-transfer of the volatiles reveals the clean formation of PMP (1,2,2,6,6-pentamethylpiperidine) and free TMP as judged by NMR and GC/MS analysis. Comparison with a commercial sample ultimately confirmed the formation of PMP.
Yield of PMP: **23 %** (calculated *vs.* initial amount of $TMPH^+$ in [$TMPH^+$, **1**$^-$])

h) Transfer hydroboration of aldehydes

General procedure for the reduction of aldehydes with [Et_3NH^+, 1^-]:
In a glovebox, a flame-dried J-Young NMR tube was charged with **[**Et_3NH^+, **1**$^-$**]** (31.4 mg, 0.1 mmol, 2 equiv.), mesitylene as internal standard (10 µL) and acetonitrile-d_3 (0.4 mL). To the resulting homogeneous colorless solution was added the aldehyde (0.05 mmol, 1 equiv) and the tube was sealed and brought out of the glovebox.
The tube was immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reaction was periodically cooled down to room temperature and monitored by NMR spectroscopy. Yields were determined *vs*. mesitylene by ^{1}H NMR for borylethers **10a** (δ_{CH2} = 5.07 ppm, s), **10b** (δ_{CH2} = 5.06 ppm, s), and **10c** (δ_{CH2} = 4.69 ppm, d, J = 4.8 Hz).
Borylethers **10a**, **10b** and **10c** may be hydrolyzed with H_2O (10 equiv.) following the same procedure as with the methoxyborane CH_3OBBN (see p. S13), to afford the known benzyl[10], 4-chlorobenzyl[11] and cinnamyl[12] alcohols respectively.

5. Experimental mechanistic investigations

a) Thermolysis of [Et_3NH^+, 1^-] under $^{13}CO_2$ atmosphere.

In a glovebox, a flame-dried medium-walled Wilmad NMR tube was charged with the [Et_3NH^+, **1**$^-$] (0.125 mmol) and acetonitrile-d_3 (0.3 mL; 0.4 mol.L^{-1}), sealed and brought out of the glovebox. $^{13}CO_2$ (1 atm) was then introduced by three freeze-pump-thaw cycles.
The tube was immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reaction was periodically cooled down to room temperature and monitored by NMR spectroscopy.
NMR spectra showing the involvement of an equilibrium between H$^{12}CO_2$[B] and H$^{13}CO_2$[B] are provided in Figures S14 (^{1}H) and S15 (^{13}C).

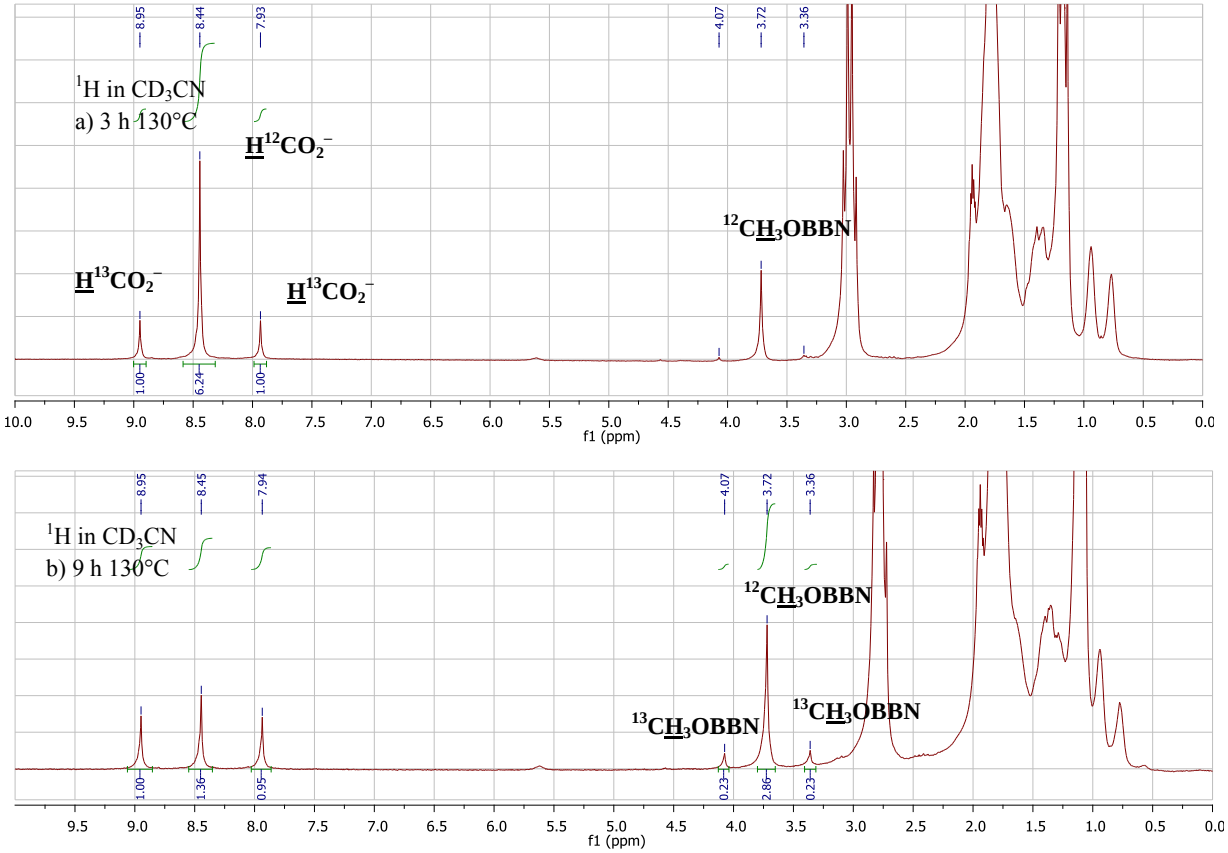


Figure S14. ^{1}H NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$] under $^{13}CO_2$ atmosphere a) Crude reaction mixture after 3 h at 130°C; appearance of signals for $H^{13}CO_2^-$ ($^1J_{C\text{-}H}$ = 202.7 Hz) demonstrates the borane-mediated interconversion of CO_2 and formate anions. b) Crude reaction mixture after 9 h at 130°C ($^1J_{C\text{-}H}$($^{13}CH_3OBBN$) = 143.0 Hz).

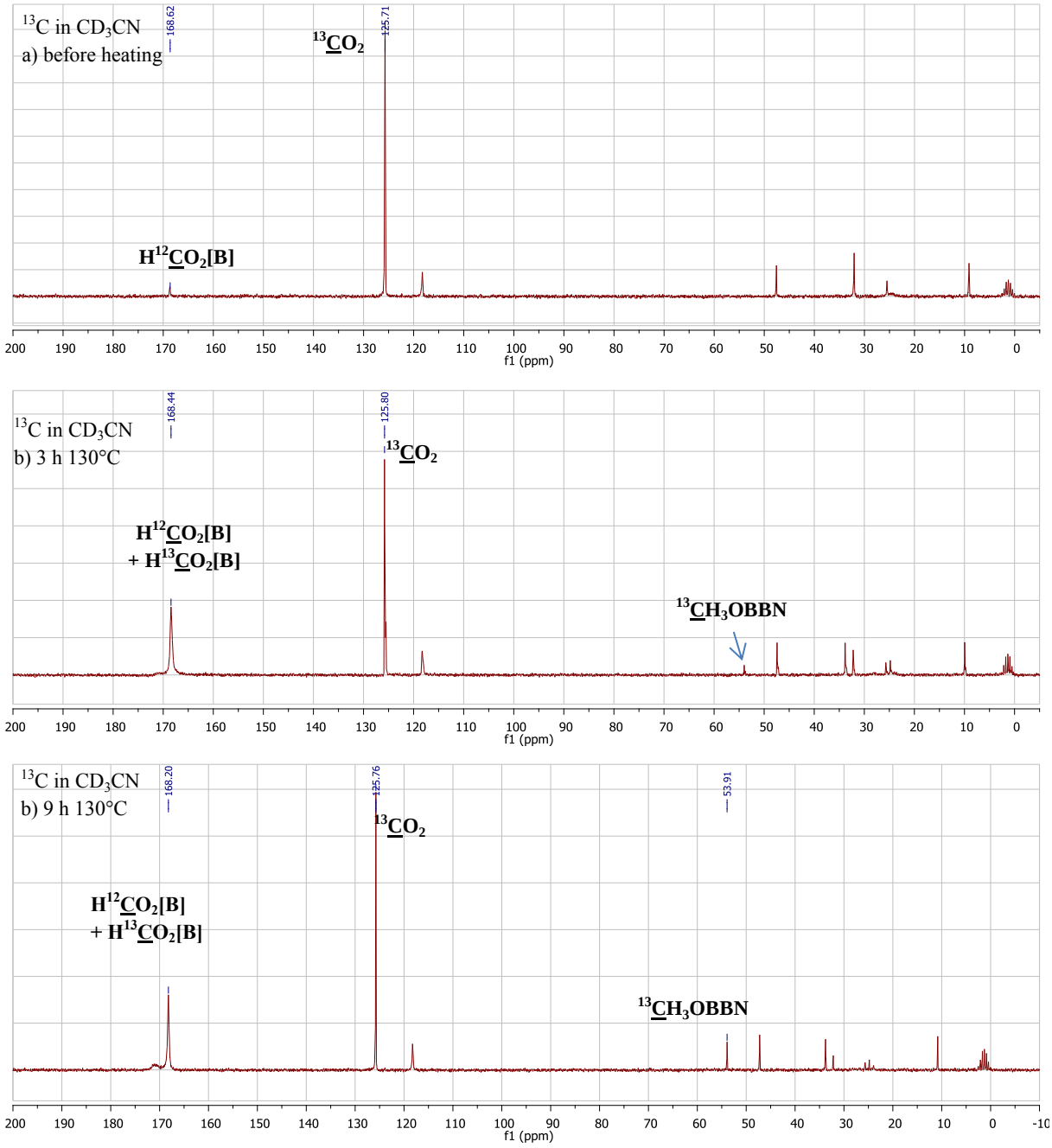


Figure S15. ^{13}C NMR spectra obtained in CD_3CN for the thermolysis of [Et_3NH^+, **1**$^-$] under $^{13}CO_2$ atmosphere a) Crude reaction mixture before heating. b) Crude reaction mixture after 3 h at 130°C. c) Crude reaction mixture after 9 h at 130°C.

b) Thermolysis of [Et_3ND^+, 1^-]

In a glovebox, a flame-dried J-Young NMR tube was charged with the [Et_3ND^+, **1**$^-$] (0.125 mmol) and acetonitrile-d_3 (0.3 mL; 0.4 mol.L^{-1}), sealed and brought out of the glovebox.

The tube was immersed in a pre-heated silicon-oil bath at 130°C (oil-bath temperature). The reaction was periodically cooled down to room temperature and monitored by NMR spectroscopy.

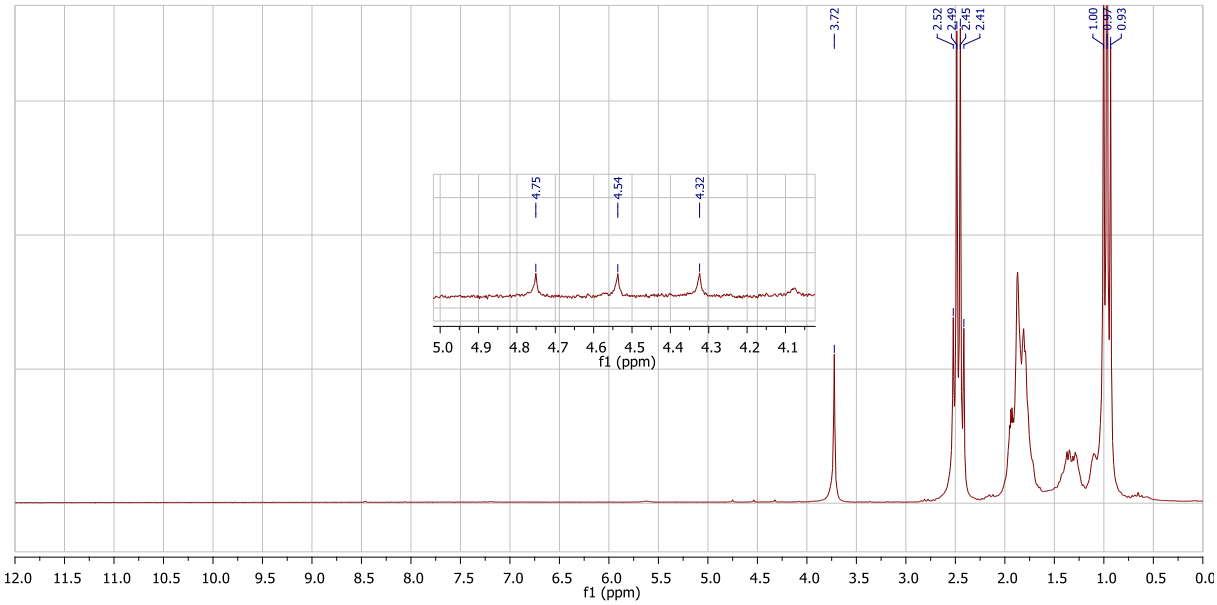


Figure S16. ^{1}H NMR spectrum obtained in CD_3CN for the thermolysis of [Et_3ND^+, **1**$^-$]. Crude reaction mixture after 15 h at 130°C; HD (δ_H = 4.54 ppm, t, $^1J_{HD}$ = 43 Hz).

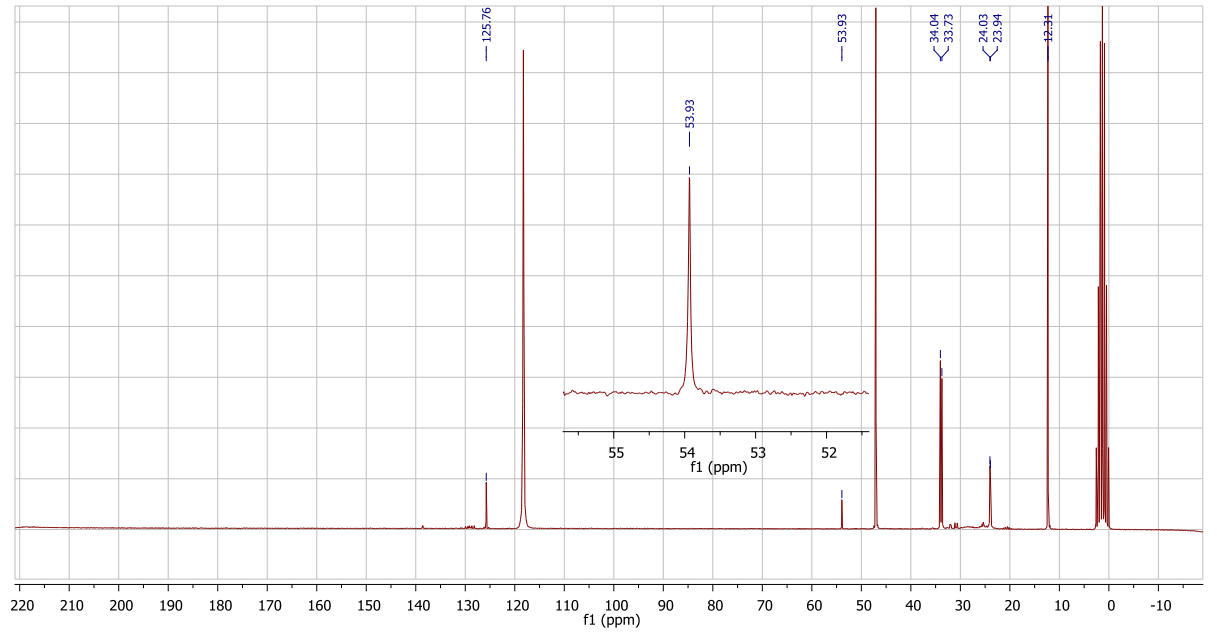


Figure S17. ^{13}C NMR spectrum obtained in CD_3CN for the thermolysis of [Et_3ND^+, **1**$^-$]. Crude reaction mixture after 15 h at 130°C.

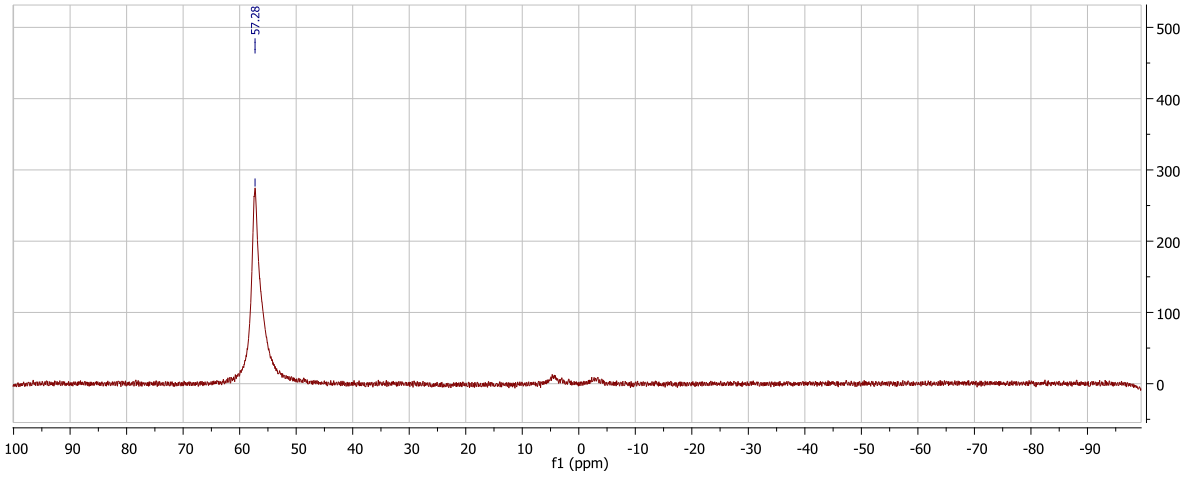
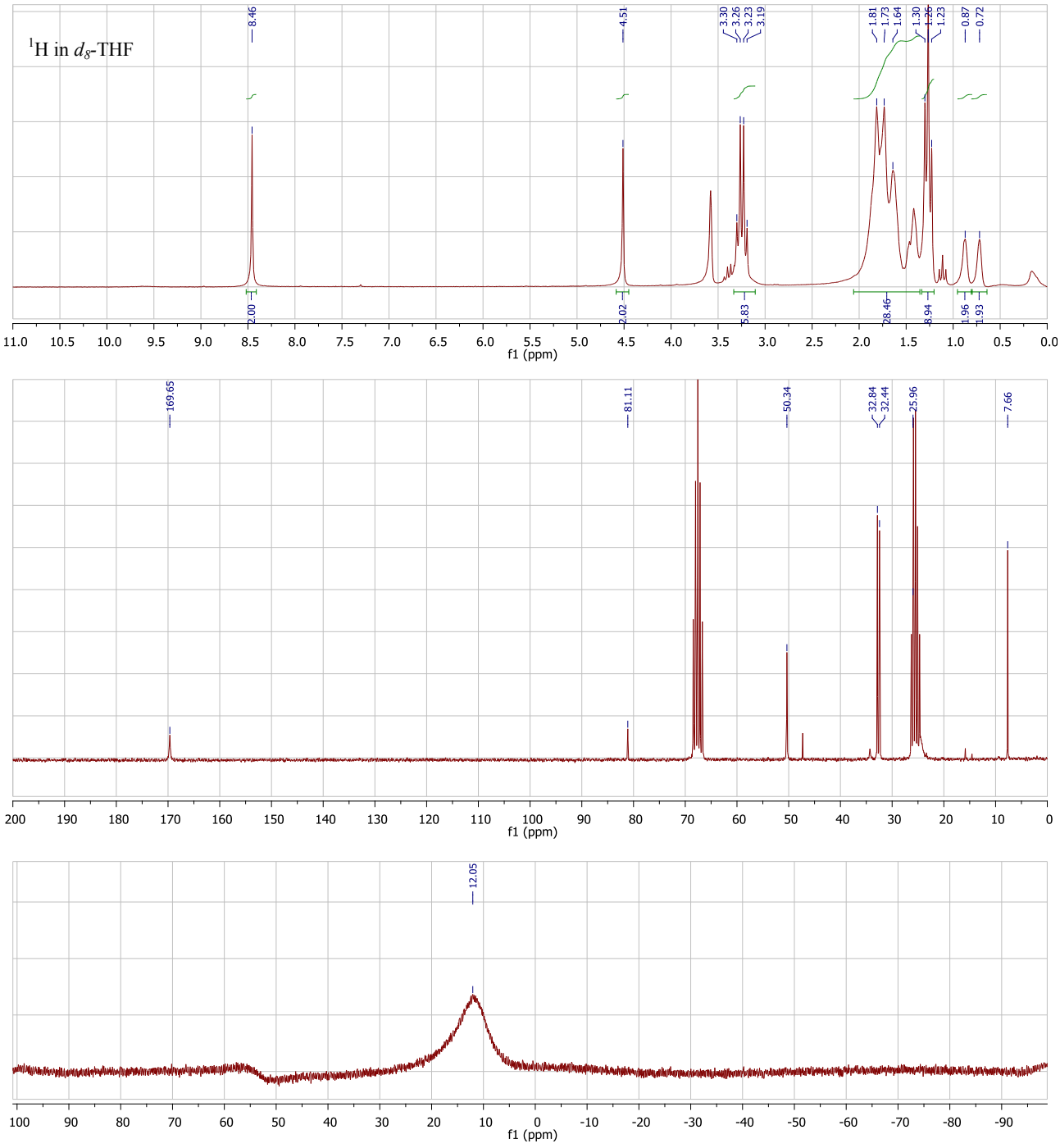


Figure S18. ^{11}B NMR spectrum obtained in CD_3CN for the thermolysis of [Et_3ND^+, **1**$^-$]. Crude reaction mixture after 15 h at 130°C.

c) *In-situ* characterization of 3.

In a glovebox, a flame-dried J-Young NMR tube was charged with [Et_3NH^+**, 1**$^-$] (62.7 mg, 0.2 mmol) and THF (0.35 mL). The tube was shaken vigorously until the resulting solution was homogeneous and 9-BBN dimer (24.4 mg, 0.1 mmol, 0.5 equiv) was then added in one portion. After *ca.* 1 min, copious H_2 evolution was noted with concomitant borane dissolution, which lasted over a period of 5 min to yield a colorless, homogeneous solution. Volatiles were removed under high-vacuum to afford a crude white solid that was taken-up in a minimum amount of THF (*ca.*0.05 mL) and layered with pentane to obtain colorless crystals suitable for X-Ray diffraction. The crystals were then isolated by filtration and washed with cold pentane and Et_2O to afford **3** (11 mg, < 92 % pure as judged by ^{1}H NMR analysis). Dissolution of the crystals in d_8-THF allowed further characterization:

^{1}H NMR (200 MHz, d_8-THF) δ 8.46 (s, 2H), 4.51 (s, 2H), 3.25 (q, J = 7.2 Hz, 6H), 2.01 – 1.34 (m, 24H), 1.26 (t, J = 7.2 Hz, 9H), 0.87 (bs, 2H), 0.72 (bs, 2H).
^{13}C NMR (50 MHz, d_8-THF) δ 169.65, 81.11, 50.34, 32.84, 32.44, 25.96, 7.66.
^{11}B NMR (64 MHz, d_8-THF) δ 12.05 (bs).



In the solid state and in solution at room temperature, **3** is a zwitterionic adduct of formaldehyde in which the carbon atom is bound to NEt_3 and the oxygen atom coordinates a mono(formoxy)borane, namely BBNOCHO. The latter formate ligand coordinates a second equivalent of the Lewis acid BBNOCHO (Fig. S16). Additionally, we have also found that the formate ligand can also combine within the crude reaction medium with the somewhat higher Lewis-acid diboroxane BBN_2O formed during the reduction of formate anions. The crystal structure of such adduct is presented in Fig. S17. For the latter compound, crystals suitable for X-ray diffraction were obtained from an upscaled experiment (same procedure as above on 0.8 mmol scale) by allowing the crude reaction mixture to stand overnight.

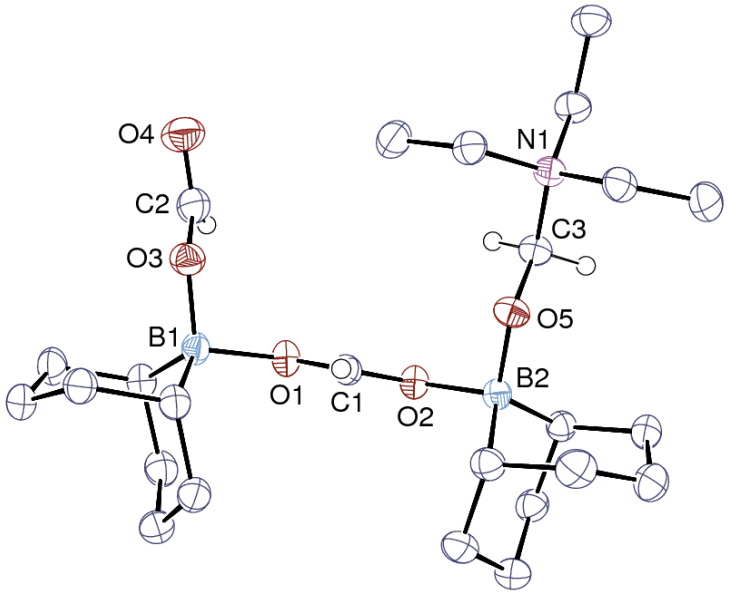


Figure S19. ORTEP view of **3**. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms of the BBN and ethyl groups have been omitted for clarity.

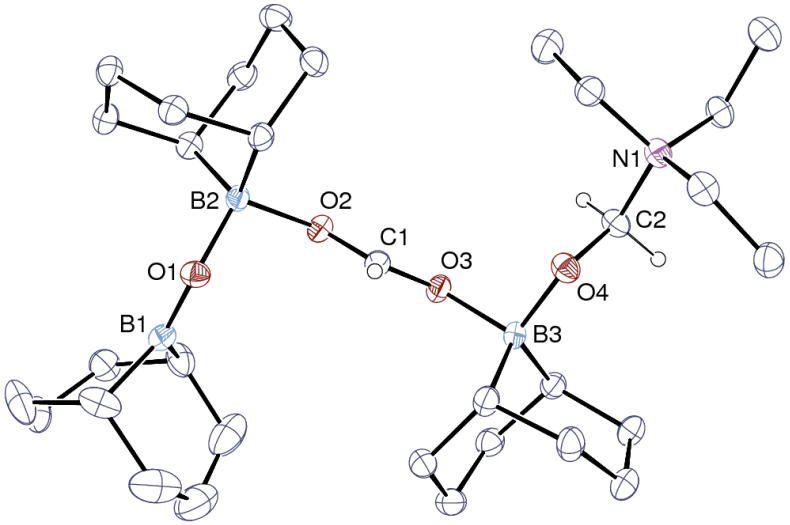


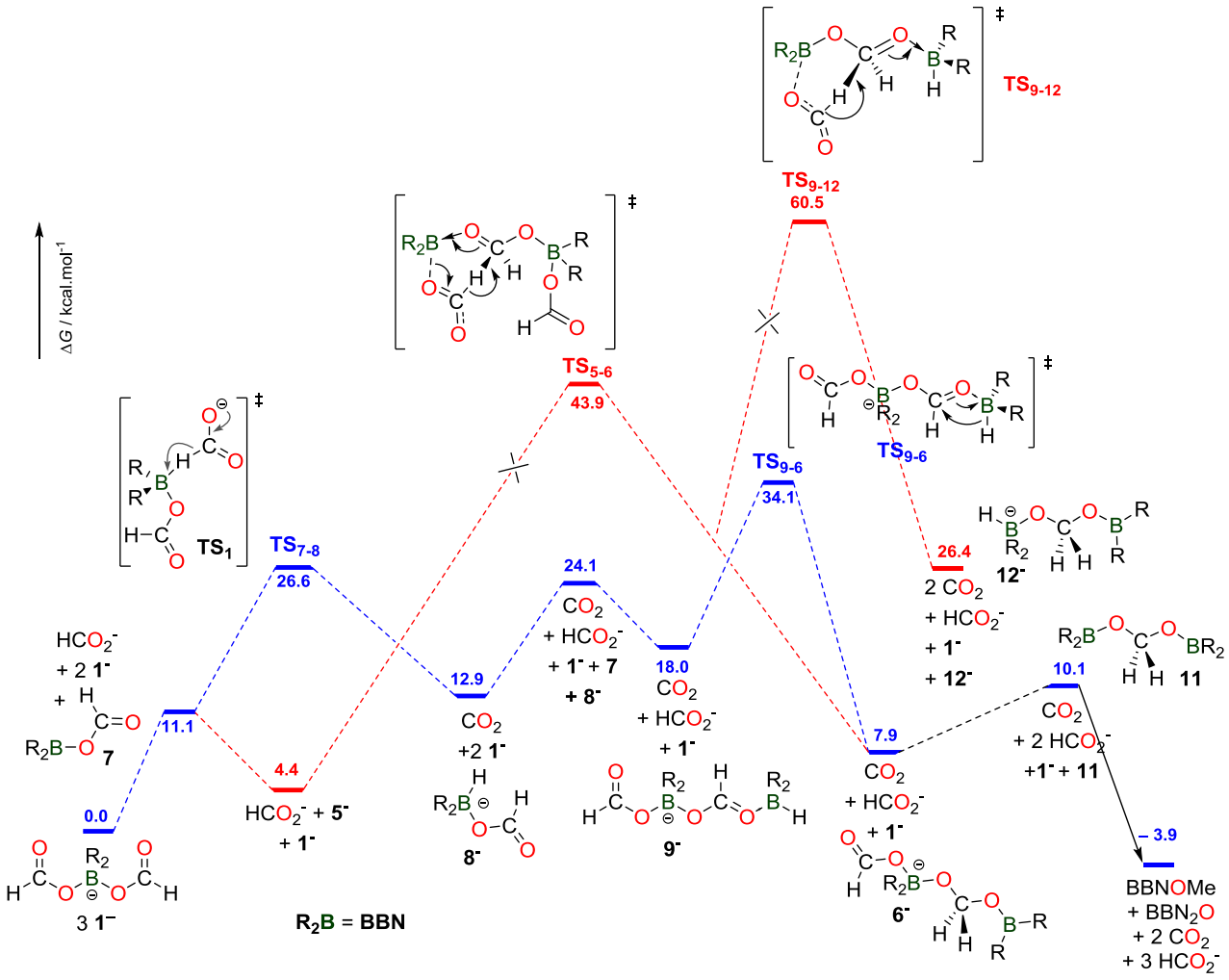
Figure S20. ORTEP view of **SI1**. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms of the BBN and ethyl groups have been omitted for clarity

6. Computational details and structures

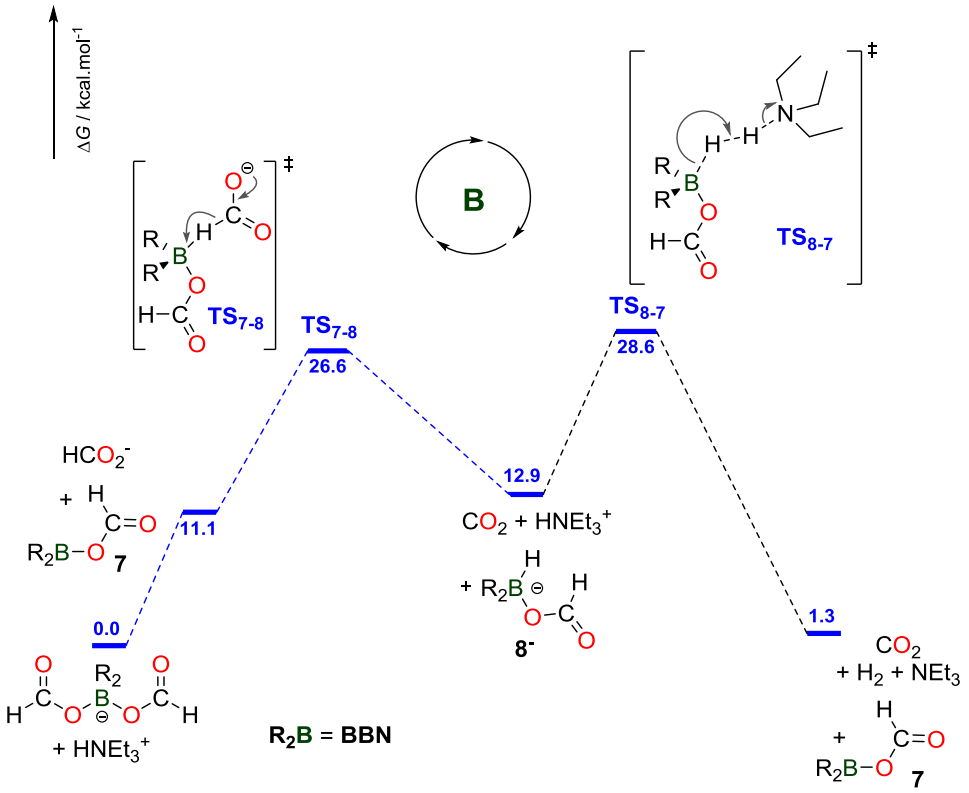
Density functional theory[13a] was applied to determine the structural and energetic features of the intermediates and transition states described herein. Calculations were performed using Gaussian09 version D.01 code.[7b] The 6-311+G(d,p) basis set[13c,d] was used for atoms C, H, B and O. The hybrid exchange correlation functional M06-2X was used.[13e] All structures were calculated without geometrical constraint; stationary points were characterized by frequency calculations (one negative frequency for a transition state, no negative frequency for minima). Solvent effects (acetonitrile) were included in structure-optimization and frequency calculations using the PCM model implemented in the Gaussian code.[13f,g] All relative energies (corrected for ZPE contributions) and Gibbs free energies (T = 298 K, P = 1 atm) are reported in kcal.mol^{-1}. NBO analysis was performed using program NBO 3.1 implemented in Gaussian version B.01 code[14].

Hydride donor abilities were calculated according to the method established by Heiden *et al.* at the M06-2X/6-311++G(d,p) level of theory in acetonitrile (PCM).[15]

a) Computed surface for the disproportionation of the formate anions



Scheme S1. Computed pathways for the disproportionation of formate anions mediated by formoxyborane derivatives in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory).

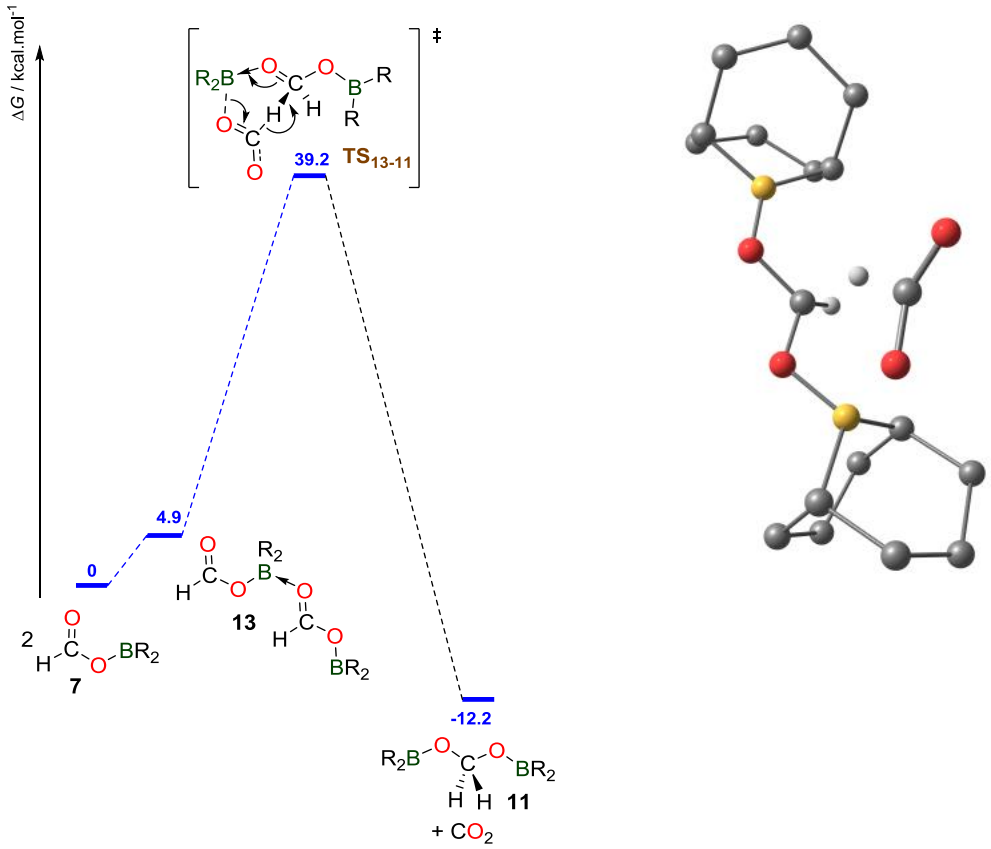


Scheme S2. Computed pathway for the dehydrogenation of formic acid catalyzed by formoxyborane derivatives in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory).

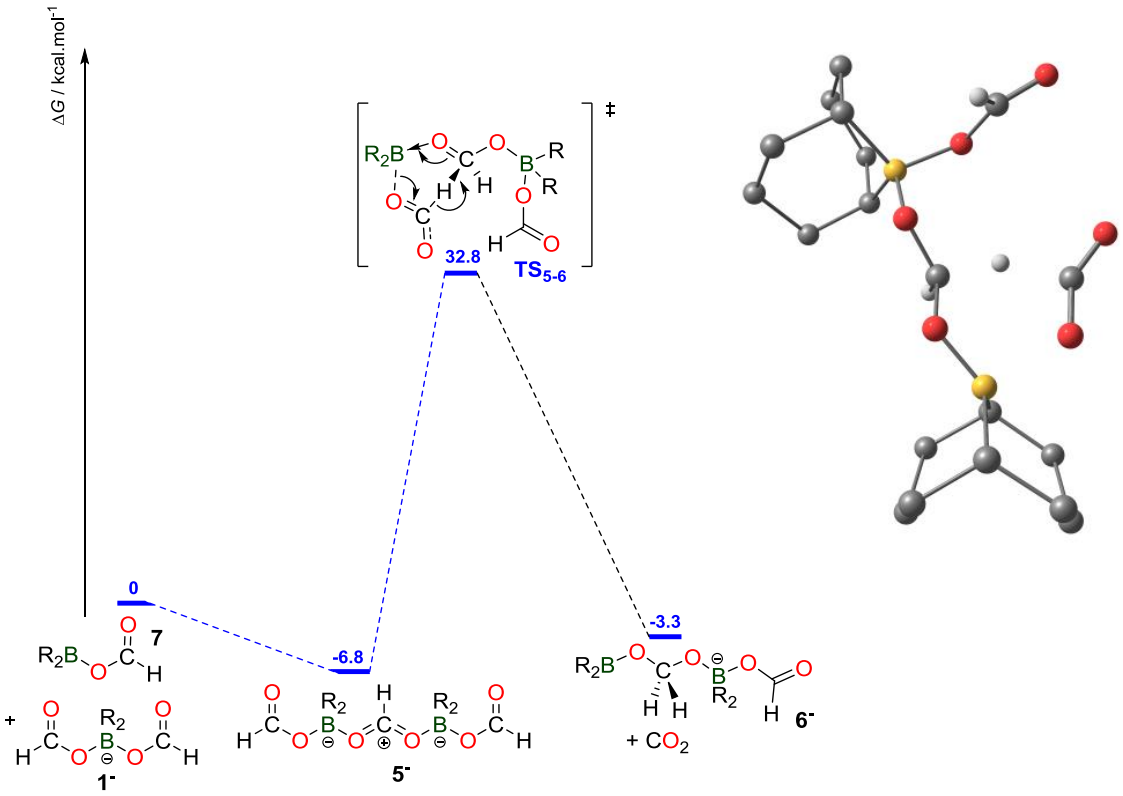
Scheme S2 shows that the dehydrogenation pathway is competing with the disproportionation of formate anions (overall barriers are 28.6 *vs.* 34.1 kcal.mol^{-1} respectively) as observed experimentally. In addition, the dehydrogenation path produces the Lewis acidic mono(formoxy)borane BBNOCHO, that in turn allows the disproportionation to occur directly *via* **9**$^{-}$ and **TS$_{9\text{-}6}$** (Scheme S1). The thermodynamics of the overall thermolysis is also influenced by the dehydrogenation since the coupling of both dehydrogenation and disproportionation of formates induces a change in free energy as high as 29.5 kcal.mol^{-1} (see thermodynamics p. S5 eq. 3 and 4). Free NEt_3 is also produced during the dehydrogenation thus shifting the disproportionation to the right by stabilization of the acetal **11** (see Scheme S10).

b) Computed elementary steps

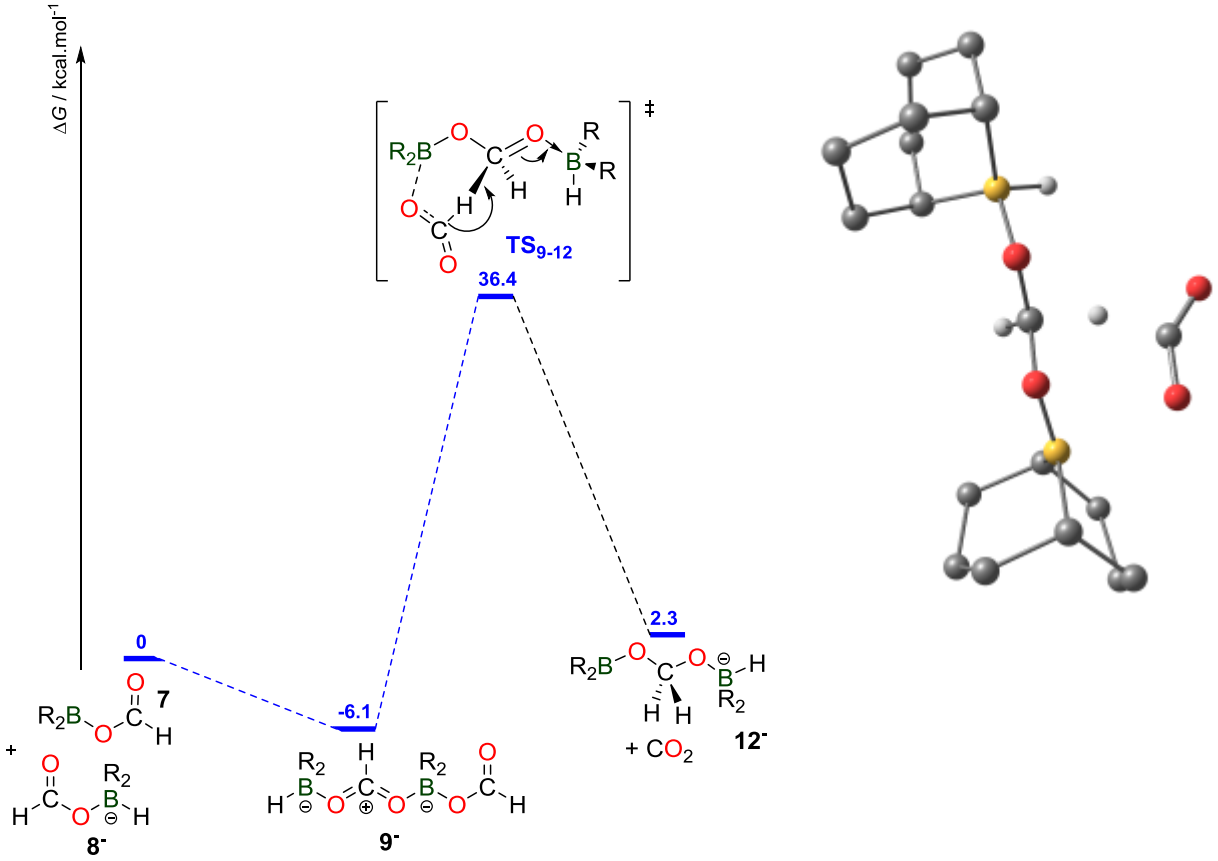
Computed elementary steps and additional alternative pathways are depicted in Schemes S3-S10.



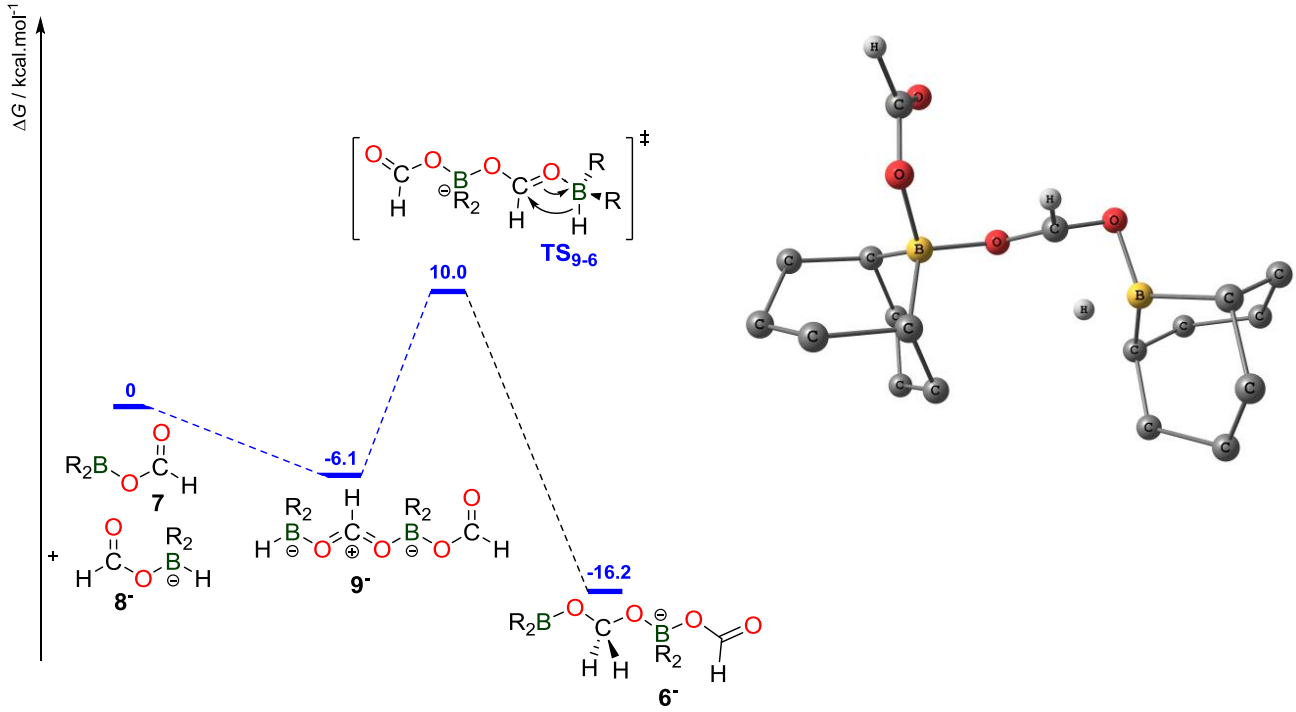
Scheme S3. Computed elementary steps for the MPV-type reduction of μ^2(O,O')-$HCOO^-$ *via* **TS$_{13\text{-}11}$** in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



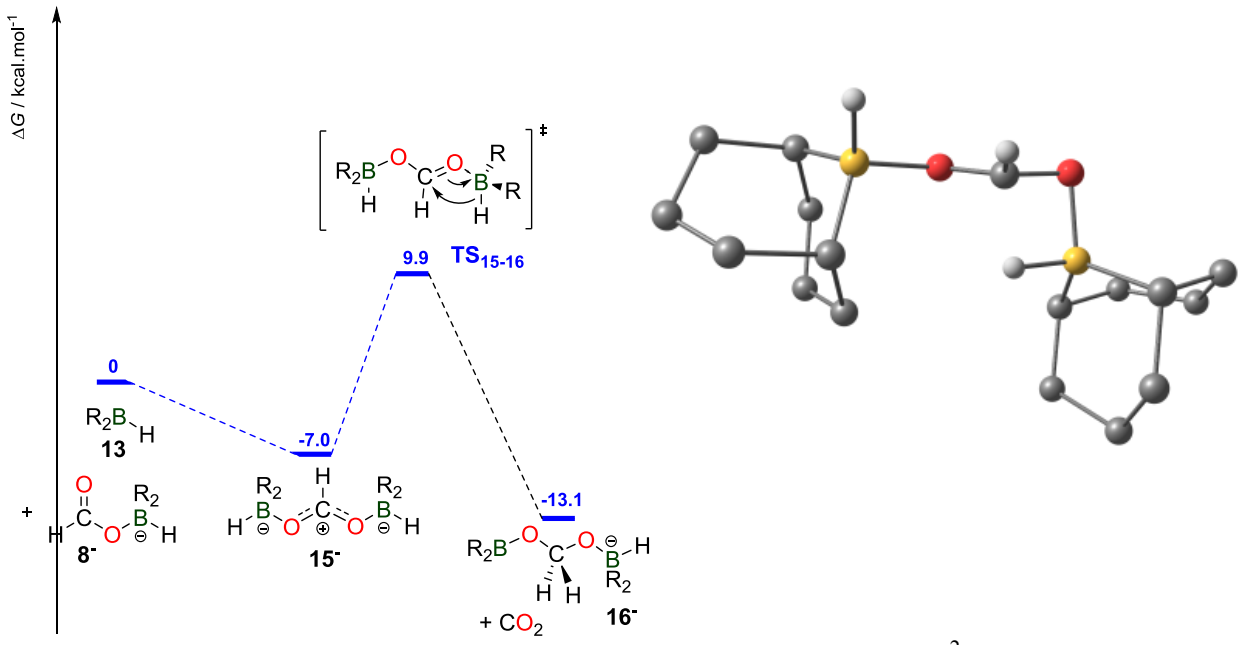
Scheme S4. Computed elementary steps for the MPV-type reduction of μ^2(O,O')-$HCOO^-$ *via* **$TS_{5\text{-}6}$** in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



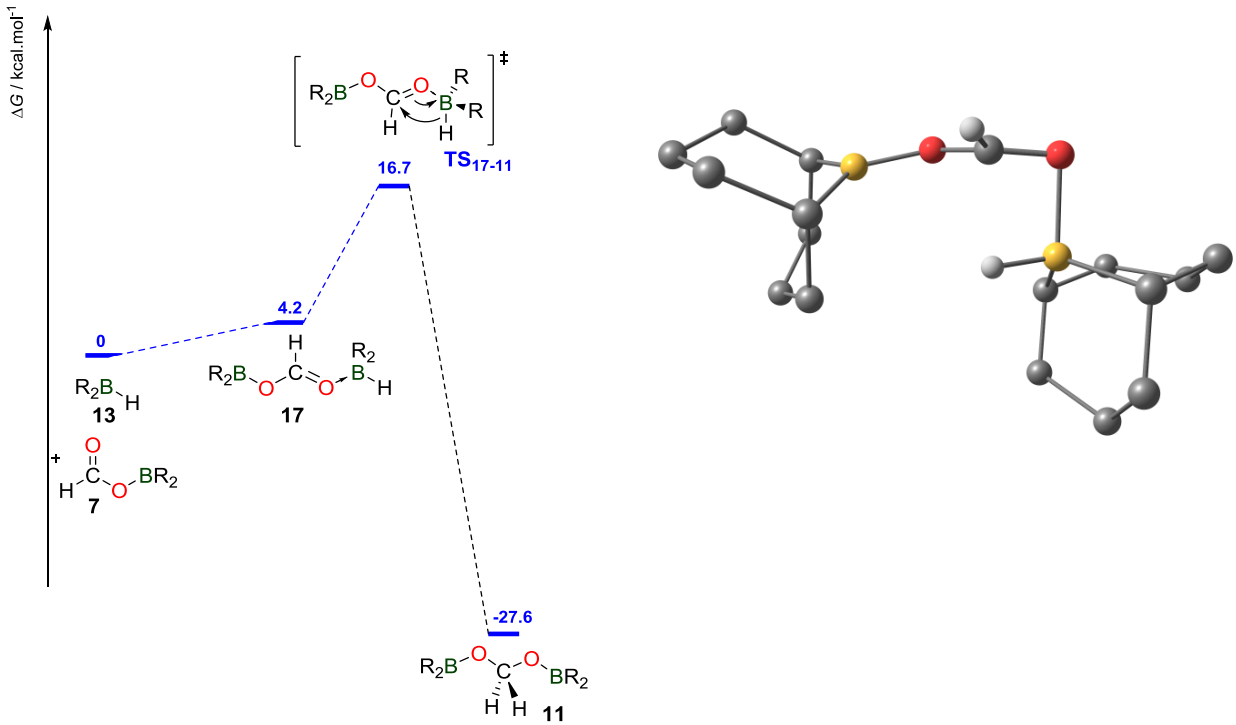
Scheme S5. Computed elementary steps for the MPV-type reduction of μ^2(O,O')-$HCOO^-$ *via* **$TS_{9\text{-}11}$** in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



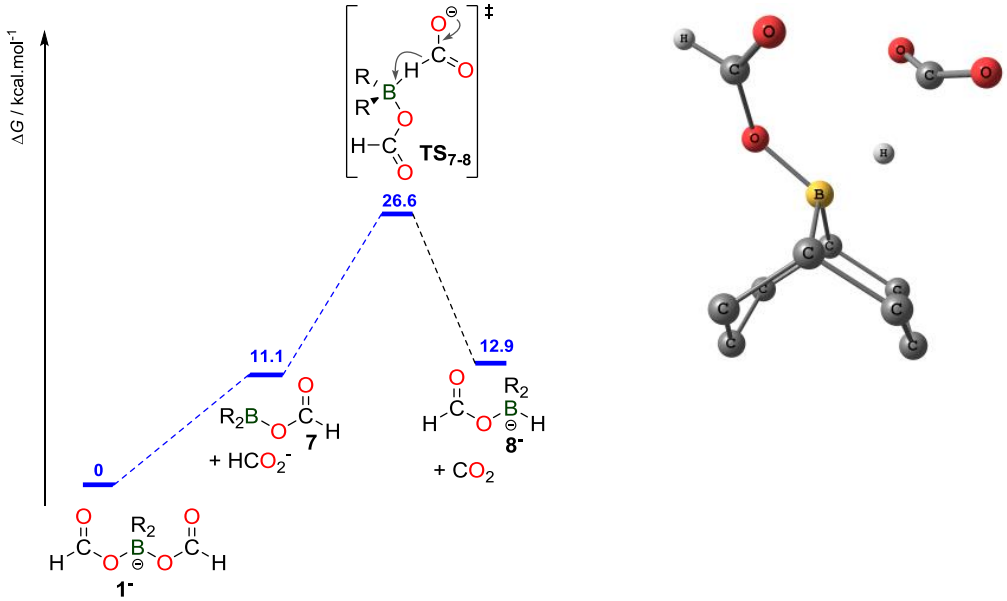
Scheme S6. Computed elementary steps for the hydridic reduction of μ^2(O,O')-HCOO$^-$ *via* **TS$_{9\text{-}6}$** in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



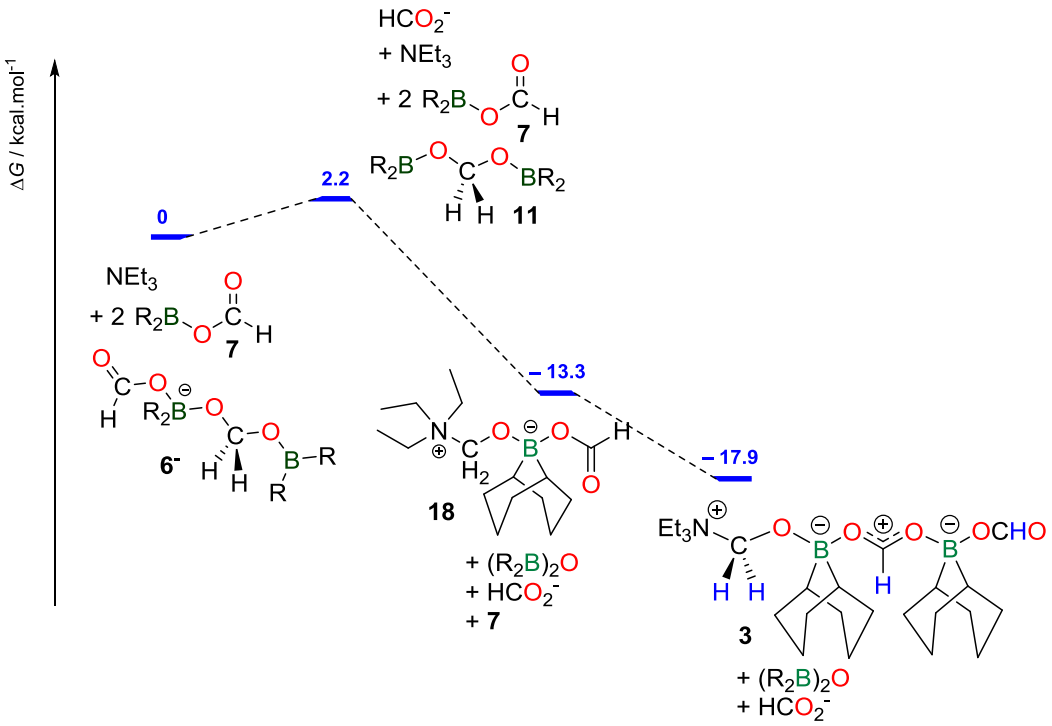
Scheme S7. Computed elementary steps for the hydridic reduction of μ^2(O,O')-HCOO$^-$ *via* **TS$_{14\text{-}15}$** in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



Scheme S8. Computed elementary steps for the hydridic reduction of μ^2(O,O')-$HCOO^-$ *via* $\mathbf{TS_{16\text{-}10}}$ in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



Scheme S9. Computed elementary steps for the generation of the borohydride $\mathbf{8}^-$ *via* $\mathbf{TS_{7\text{-}8}}$ in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).



Scheme S10. Computed elementary steps for the thermodynamic stabilization of the bis(boryl)acetal **11** by formation of adducts **18** and **3** with NEt_3 in acetonitrile (at the M06-2X/6-311+G(d,p) level of theory; R_2B = BBN).

$HCOO^-$

Element	X	Y	Z
C	0.00000000	0.33119401	0.00000000
H	-0.00024200	1.44935596	0.00000000
O	1.12426603	-0.21451300	0.00000000
O	-1.12423503	-0.21505199	0.00000000

Frequencies -- 758.0618 1088.4566 1393.9831

Sum of electronic and zero-point Energies= -189.274828
Sum of electronic and thermal Energies= -189.271860
Sum of electronic and thermal Enthalpies= -189.270916
Sum of electronic and thermal Free Energies= -189.298627

CO_2

Element	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15488803
O	0.00000000	0.00000000	-1.15488803

Frequencies -- 682.4198 682.4198 1419.6703

Sum of electronic and zero-point Energies= -188.565905
Sum of electronic and thermal Energies= -188.563298
Sum of electronic and thermal Enthalpies= -188.562354
Sum of electronic and thermal Free Energies= -188.586584

H_2

Element	X	Y	Z
H	0.00000000	0.00000000	0.37033200
H	0.00000000	0.00000000	-0.37033200

Frequencies -- 4463.4965

Sum of electronic and zero-point Energies= -1.158289
Sum of electronic and thermal Energies= -1.155928
Sum of electronic and thermal Enthalpies= -1.154984
Sum of electronic and thermal Free Energies= -1.169771

NEt_3

Element	X	Y	Z
N	-0.31493300	-0.42759100	-0.27341899
C	-0.17995200	0.42884901	0.90786099
C	-1.09007299	0.03299100	2.06584597
H	-0.43471599	1.44655204	0.61080903
H	0.87213498	0.44648099	1.24954402
H	-1.10894299	0.83657497	2.80442595
H	-2.11044002	-0.12692399	1.70838106
H	-0.75557297	-0.87192100	2.57409906
C	0.00604200	-1.81843603	0.05859900

C	-0.17274500	-2.79101992	-1.10213494
H	-0.65929902	-2.12913394	0.86473000
H	1.03900504	-1.88954401	0.44850999
H	-0.13733201	-3.81526709	-0.72623003
H	-1.14266098	-2.63636398	-1.58167899
H	0.60674900	-2.69276404	-1.85850406
C	0.54077101	0.05291000	-1.36168396
C	0.23454300	1.47843504	-1.80885196
H	0.39274701	-0.60834098	-2.21589804
H	1.60622597	-0.02597300	-1.07402503
H	0.73359001	1.67570698	-2.75951004
H	-0.84080398	1.60938799	-1.95412004
H	0.58122599	2.22713995	-1.09565103

Frequencies -- 57.0473 101.0586 108.8369

Sum of electronic and zero-point Energies= -292.135907
Sum of electronic and thermal Energies= -292.126568
Sum of electronic and thermal Enthalpies= -292.125623
Sum of electronic and thermal Free Energies= -292.169841

$HNEt_3^+$

Element	X	Y	Z
N	-0.94654000	0.00397000	-0.21478701
C	-0.95918202	1.17894101	0.73045999
C	-1.36490500	0.81303197	2.14651489
H	-1.66239405	1.89593601	0.31368199
H	0.04314100	1.60909700	0.68952900
H	-1.54104602	1.74047697	2.69167590
H	-2.29377198	0.23825100	2.15994310
H	-0.59109002	0.25794700	2.67448592
C	-0.12455000	-1.13827300	0.32804000
C	-0.07340700	-2.33829308	-0.59948301
H	-0.57727998	-1.41737700	1.27632499
H	0.86779600	-0.72658402	0.52127600
H	0.38291201	-3.16341805	-0.05235700
H	-1.07593799	-2.65139389	-0.89949501
H	0.52775699	-2.15596604	-1.48872995
C	-0.48874900	0.40555701	-1.59425998
C	-1.25316203	1.58562398	-2.16536188
H	-0.62490499	-0.46841800	-2.22708511
H	0.57995802	0.61065698	-1.50731695
H	-0.98715901	1.67593002	-3.21871591
H	-2.33221412	1.42544901	-2.10702395
H	-1.00233996	2.52571297	-1.67650902
H	-1.91380203	-0.32675099	-0.29971001

Frequencies -- 76.6578 88.2070 128.2755

Sum of electronic and zero-point Energies= -292.578334
Sum of electronic and thermal Energies= -292.569130
Sum of electronic and thermal Enthalpies= -292.568186
Sum of electronic and thermal Free Energies= -292.611920

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Element	X	Y	Z
C	1.05915797	-1.13929605	1.51527095
C	0.17455401	0.05529400	1.10582805
C	1.06853902	-0.11813400	-1.32162905
C	1.99688995	-1.27571595	-0.90108800

H	1.41012895	-1.01790094	2.54933310
H	2.95557809	-1.21723402	-1.43536305
H	1.52181196	-2.20815992	-1.22533000
C	0.88542300	1.41816795	1.24937606
H	0.12398600	2.19475508	1.12268400
H	1.27686095	1.53565204	2.26979303
C	1.70283306	1.27748895	-1.19280505
H	2.61691689	1.34977806	-1.79787505
H	-0.68936503	0.07203300	1.77720797
H	0.82186902	-0.26999599	-2.38300109
C	2.28219604	-1.38667595	0.61132097
H	3.08136606	-0.69780099	0.88864398
H	2.67992592	-2.38677001	0.81876898
C	2.02628207	1.69439697	0.25131199
H	2.94165111	1.19879305	0.57722801
H	2.25517011	2.76627803	0.26856700
H	0.99584299	2.00410795	-1.61248696
H	0.43380800	-2.04037809	1.51001406
B	-0.27313799	-0.16377901	-0.42885199
O	-1.27216399	0.82843000	-1.03006101
C	-2.13951898	1.59739101	-0.44293901
H	-2.81393790	2.05804992	-1.18515098
O	-2.25415111	1.85490894	0.73690099
O	-0.91018099	-1.54380000	-0.67280602
C	-2.05190897	-1.90903997	-0.17966500
H	-2.29956603	-2.94704604	-0.45775300
O	-2.81013393	-1.24685502	0.50210202

Frequencies -- 68.7113 95.4055 117.8045

Sum of electronic and zero-point Energies= -716.350288
Sum of electronic and thermal Energies= -716.336383
Sum of electronic and thermal Enthalpies= -716.335438
Sum of electronic and thermal Free Energies= -716.390012

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Element	X	Y	Z
C	0.93404901	-0.87517202	1.63186502
C	-0.18572199	0.05613200	1.10169804
C	0.66825300	-0.39439800	-1.32716405
C	1.83040500	-1.24398398	-0.76275402
H	1.25296295	-0.53028703	2.62178898
H	2.73100305	-1.08489799	-1.36713505
H	1.55824995	-2.29815507	-0.88960999
C	0.23455700	1.54554999	0.96534503
H	-0.67422402	2.12171793	0.75680703
H	0.61591202	1.90429103	1.92805898
C	0.99421299	1.12043297	-1.46721399
H	1.85303199	1.24563003	-2.13587189
H	-1.02344501	0.01137900	1.80133104
H	0.41015401	-0.77374399	-2.32050109
C	2.16520905	-1.00619197	0.72164297
H	2.79751992	-0.12561800	0.82907599
H	2.77184606	-1.84498799	1.07646203
C	1.26612496	1.84549296	-0.13880600
H	2.27097201	1.61022401	0.20881200
H	1.26575994	2.92351389	-0.32611600
H	0.14491101	1.60629499	-1.96396899
H	0.49995500	-1.87159503	1.77976596
B	-0.54080802	-0.42176300	-0.34294999
O	-1.79841399	-0.81575203	-0.80321598
C	-2.96447492	-0.51381600	-0.20772400
H	-3.72433805	-1.27281904	-0.42264199
O	-3.16432595	0.47620100	0.43286100

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Frequencies -- 26.7083 56.6508 78.2604

Sum of electronic and zero-point Energies= -527.035464
Sum of electronic and thermal Energies= -527.024174
Sum of electronic and thermal Enthalpies= -527.023230
Sum of electronic and thermal Free Energies= -527.073633

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Element	X	Y	Z
C	1.15919900	-1.75665700	0.48103899
C	-0.09712400	-0.89239597	0.70318598
C	0.69215000	0.71299100	-1.17517197
C	1.93684304	-0.16447100	-1.40518999
H	1.51600301	-2.18307710	1.43010795
H	2.80397201	0.44587100	-1.69641399
H	1.72445500	-0.82230002	-2.25808001
C	0.09295400	0.22815600	1.74185300
H	-0.89059502	0.68053401	1.92467797
H	0.42441699	-0.18090700	2.70758200
C	0.89551502	1.82725298	-0.12940700
H	1.75516903	2.46141195	-0.39175501
H	-0.87743598	-1.55901003	1.09250796
H	0.47458899	1.21299899	-2.13107896
C	2.33934903	-1.04665697	-0.20894299
H	2.88564205	-0.44663599	0.52036500
H	3.05450702	-1.80340099	-0.55263501
C	1.06545699	1.34829605	1.32528901
H	2.09343505	1.01964402	1.48797095
H	0.92749900	2.20447397	1.99635601
H	0.01193600	2.47519112	-0.17052200
H	0.86510301	-2.60979605	-0.14425300
B	-0.53255701	-0.25199199	-0.72525501
O	-1.78861904	0.66210502	-0.58107799
C	-2.94939089	0.20645000	-0.25536501
H	-3.70391893	1.01013994	-0.19422799
O	-3.26404500	-0.95118499	-0.03011900
H	-0.79038799	-1.11032295	-1.56848800

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Frequencies -- 48.3704 105.0733 117.3057

Sum of electronic and zero-point Energies= -527.746017
Sum of electronic and thermal Energies= -527.734894
Sum of electronic and thermal Enthalpies= -527.733949
Sum of electronic and thermal Free Energies= -527.782793

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Element	X	Y	Z
C	-4.04731989	1.04585600	1.35139894
C	-2.66993594	0.40134200	1.07590199
C	-3.65990710	-0.77207798	-1.02105999
C	-5.04242420	-0.15534900	-0.72278202
H	-4.21033907	1.13866699	2.43269706
H	-5.84338093	-0.85878599	-0.98553902
H	-5.16341209	0.71006298	-1.38348806
C	-2.49522996	-0.97748500	1.74991000
H	-1.44405901	-1.28293705	1.66255999
H	-2.68763208	-0.89395100	2.82722497
C	-3.42002892	-2.14207697	-0.36098501
H	-4.18814802	-2.86111903	-0.67353803

H	-1.92323899	1.07813001	1.51169503
H	-3.59317994	-0.91393399	-2.10904193
C	-5.25281191	0.31436601	0.73087102
H	-5.52510691	-0.53516901	1.35802102
H	-6.11935616	0.98378998	0.75997198
C	-3.36337590	-2.11268711	1.17577100
H	-4.37405777	-2.04456711	1.57838500
H	-2.96956801	-3.06946111	1.53507197
H	-2.46516299	-2.53190804	-0.73508197
H	-4.02043819	2.06840992	0.95710999
B	-2.53920197	0.25701699	-0.52439898
O	-1.14788198	-0.27215499	-1.01860797
C	-0.08849400	-0.12369200	-0.35554200
H	-0.13850600	0.26296300	0.66220999
O	1.02013195	-0.43337300	-0.85499001
O	-2.71080995	1.56172800	-1.27988696
C	-1.87092495	2.54856205	-1.17246997
H	-2.18166304	3.41882396	-1.76899600
O	-0.84618503	2.56067991	-0.51732802
B	2.36514592	-0.50342298	-0.03912200
C	2.37811899	0.35099801	1.32551897
C	3.53724790	0.05465700	-0.97909701
C	3.71899891	0.03336900	2.02590394
C	2.18201590	1.85491097	1.04533005
H	1.58705401	0.03576900	2.02293611
C	4.88369179	-0.21392000	-0.27756399
C	3.26094007	1.54229903	-1.28005099
H	3.55832005	-0.47112501	-1.93936896
H	3.80035996	0.60896999	2.95699310
C	4.97901106	0.28829300	1.17671394
H	3.70307589	-1.02293801	2.31408405
H	1.14520895	2.02836204	0.73771501
H	2.32004499	2.42857909	1.97156096
C	3.09740901	2.44394803	-0.04507000
H	5.71252298	0.21556000	-0.85555702
H	5.04458618	-1.29951894	-0.27738500
H	4.05307293	1.95618498	-1.91743302
H	2.33646703	1.59415698	-1.86915803
H	5.21506310	1.35279500	1.18434203
H	5.83090115	-0.20011500	1.66236901
H	4.07808495	2.67488003	0.37227401
H	2.68324304	3.40646791	-0.36558601
O	2.46265411	-1.96812797	0.33803099
C	2.62020802	-2.94667292	-0.50978702
H	2.72382903	-3.91068101	0.01258200
O	2.65241003	-2.87902403	-1.71965599

Frequencies -- 22.7976 35.8450 50.9784

Sum of electronic and zero-point Energies= -1243.420004
Sum of electronic and thermal Energies= -1243.394537
Sum of electronic and thermal Enthalpies= -1243.393593
Sum of electronic and thermal Free Energies= -1243.474451

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Element	X	Y	Z
C	4.29601097	0.11694300	1.85662305
C	3.06171703	0.50262702	1.01596904
C	3.74847007	-1.24753904	-0.77441400
C	4.98572111	-1.62087595	0.06611100
H	4.69382286	0.99209398	2.38824511
H	5.83404779	-1.88165200	-0.58137900
H	4.73969316	-2.52958012	0.63045901
C	3.31657696	1.63793397	0.00599000
H	2.34673309	1.93661404	-0.41245201

H	3.71320200	2.52833509	0.51308000
C	3.99093390	-0.10759100	-1.78387296
H	4.82558584	-0.35447201	-2.45458698
H	2.30123496	0.86914998	1.72266805
H	3.47827601	-2.13905907	-1.35793996
C	5.44321680	-0.54449302	1.06870699
H	6.01795387	0.22243300	0.54795098
H	6.14222479	-0.99833202	1.78024495
C	4.25213194	1.27799106	-1.16388905
H	5.29088497	1.34499800	-0.83730203
H	4.14514017	2.03882504	-1.94530201
H	3.09900188	-0.03620100	-2.41763806
H	3.96154499	-0.58715397	2.62935591
B	2.57802606	-0.83443302	0.25021800
O	1.27969801	-0.49326000	-0.63913602
C	0.19487301	-0.27356100	-0.06206200
H	0.15590000	-0.30628899	1.03284895
O	-0.85878199	-0.01596800	-0.70611298
B	-2.19308901	0.28115499	0.06777400
C	-2.55479503	-0.89983302	1.09983504
C	-3.37938595	0.37738901	-1.00579095
C	-3.85226202	-0.50129902	1.83533001
C	-2.64805388	-2.23524690	0.33768699
H	-1.78479099	-1.02045000	1.87624097
C	-4.66947794	0.77513200	-0.26126000
C	-3.47192502	-0.96553200	-1.76117694
H	-3.18023491	1.15350604	-1.75298703
H	-4.16484213	-1.30274296	2.51735091
C	-5.04004717	-0.13168600	0.92723602
H	-3.61813998	0.36569300	2.46337104
H	-1.64192295	-2.50060010	-0.01205400
H	-2.95309305	-3.04337096	1.01490796
C	-3.59245300	-2.22183704	-0.87830102
H	-5.51866722	0.81372201	-0.95576000
H	-4.53695011	1.79806602	0.11413200
H	-4.31400824	-0.94826603	-2.46542096
H	-2.56551194	-1.06099796	-2.37048507
H	-5.52112484	-1.03899097	0.55994499
H	-5.79940987	0.37423399	1.53339696
H	-4.62296391	-2.34049511	-0.54256397
H	-3.38404012	-3.10397410	-1.49352396
O	-1.92134094	1.54045999	0.86771798
C	-1.66693604	2.70464706	0.33401999
H	-1.57754004	3.48559189	1.10489297
O	-1.52375805	2.95717096	-0.84264499
H	2.22087407	-1.73048604	1.00130999

Frequencies -- 25.9929 28.9890 46.8648

Sum of electronic and zero-point Energies= -1054.813774
Sum of electronic and thermal Energies= -1054.790809
Sum of electronic and thermal Enthalpies= -1054.789865
Sum of electronic and thermal Free Energies= -1054.866076

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Element	X	Y	Z
C	-3.95950389	0.39880699	1.48687994
C	-2.53801394	-0.05141400	1.09556997
C	-3.37481809	-0.53347200	-1.31320202
C	-4.79065609	-0.07306600	-0.92063898
H	-4.18037510	0.11840400	2.52665806
H	-5.55488300	-0.65705401	-1.45287204
H	-4.90420294	0.96330601	-1.25757003
C	-2.28457499	-1.56061900	1.29360700
H	-1.21670699	-1.74562204	1.11735296

H	-2.47665405	-1.85118604	2.33644891
C	-3.12516189	-2.03916788	-1.10325301
H	-3.87533092	-2.63911605	-1.63794601
H	-1.85223603	0.47930399	1.76559901
H	-3.25300694	-0.33187100	-2.38852310
C	-5.09663486	-0.12358000	0.58796197
H	-5.35107183	-1.14433599	0.87713701
H	-6.00011015	0.46506900	0.78591299
C	-3.08929992	-2.49138308	0.36820501
H	-4.10688496	-2.59353209	0.74856299
H	-2.65839911	-3.49814391	0.41902700
H	-2.15619302	-2.27629495	-1.55660200
H	-3.97793198	1.49597704	1.46219301
B	-2.27320600	0.29579100	-0.46905100
O	-0.92705101	-0.03090200	-0.98709500
O	1.26631796	-0.48896301	-0.76594698
O	-2.55318093	1.81251001	-0.78782600
C	-2.08225489	2.81369901	-0.12291900
H	-2.47984290	3.77428198	-0.49401999
O	-1.29275501	2.79316211	0.80659801
B	2.52674603	-0.33996400	-0.29149100
C	3.01136708	0.68459201	0.80577201
C	3.72392297	-1.13967800	-0.92565298
C	3.78998208	-0.08461900	1.90003896
C	3.86321998	1.72971702	0.03600800
H	2.19655490	1.22593200	1.29759300
C	4.48298979	-1.89072096	0.19079500
C	4.57508278	-0.07842300	-1.67384803
H	3.38186502	-1.87328303	-1.66351104
H	4.22036409	0.62628800	2.61568999
C	4.89814901	-1.02265096	1.39064097
H	3.06425190	-0.68406898	2.46351004
H	3.18562293	2.30026197	-0.61196202
H	4.28987789	2.45102811	0.74317300
C	4.99009609	1.14404595	-0.83397502
H	5.37224197	-2.38151407	-0.22300901
H	3.83060002	-2.69394302	0.55512100
H	5.47289181	-0.54799598	-2.09359598
H	3.98551297	0.27460799	-2.52907395
H	5.78778505	-0.44575199	1.13970697
H	5.19869089	-1.68132603	2.21165991
H	5.84556198	0.89126599	-0.20881300
H	5.34571791	1.92595899	-1.51245904
C	0.19163901	0.32729000	-0.28073201
H	0.46352801	1.37840796	-0.44225299
H	0.07523700	0.15319499	0.79617500

Frequencies -- 17.9828 39.1045 44.2910

Sum of electronic and zero-point Energies= -1054.829692
Sum of electronic and thermal Energies= -1054.806802
Sum of electronic and thermal Enthalpies= -1054.805858
Sum of electronic and thermal Free Energies= -1054.882252

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Element	X	Y	Z
C	3.76171803	-1.30282497	1.34810805
C	2.76782894	-0.14071900	1.09615397
C	3.62829089	0.01101800	-1.36746001
C	4.59219980	-1.16743696	-1.09506202
H	4.13211203	-1.25011802	2.37856603
H	5.51119614	-1.04034996	-1.67924905
H	4.11590385	-2.08243489	-1.46804798
C	3.35479307	1.27116299	1.36770797
H	2.53769398	1.99801099	1.27523994

H	3.70134807	1.33011496	2.40587592
C	4.22837496	1.40839601	-1.06241095
H	5.15717411	1.54429400	-1.62877095
H	1.92243195	-0.27925000	1.77794003
H	3.35098100	-0.01129500	-2.42654800
C	4.95825481	-1.37767100	0.38377500
H	5.72252512	-0.66104603	0.68228698
H	5.42491007	-2.36189389	0.49087301
C	4.49475813	1.69832003	0.42624000
H	5.42645311	1.22717702	0.73713303
H	4.65715694	2.77396202	0.54629499
H	3.52512002	2.16054702	-1.44023800
H	3.19879198	-2.24119401	1.27312601
B	2.38233900	-0.14579099	-0.42880499
O	1.12169397	-0.20112801	-0.94699198
O	-1.12170005	-0.20119800	-0.94699103
B	-2.38234401	-0.14583001	-0.42880201
C	-2.76783109	-0.14070401	1.09615695
C	-3.62829399	0.01097100	-1.36746097
C	-3.35476303	1.27119601	1.36767495
C	-3.76174688	-1.30278206	1.34814298
H	-1.92243695	-0.27924201	1.77794600
C	-4.22834110	1.40837598	-1.06245399
C	-4.59223318	-1.16745102	-1.09502399
H	-3.35098600	-0.01138100	-2.42654800
H	-3.70132494	1.33018506	2.40583801
C	-4.49471521	1.69835603	0.42618901
H	-2.53764796	1.99802399	1.27519298
H	-3.19884300	-2.24116492	1.27317798
H	-4.13213205	-1.25004303	2.37860203
C	-4.95829105	-1.37762403	0.38382000
H	-5.15713692	1.54428101	-1.62881696
H	-3.52506495	2.16049504	-1.44030404
H	-5.51122379	-1.04036200	-1.67921805
H	-4.11595821	-2.08247304	-1.46797800
H	-5.42642307	1.22724903	0.73709702
H	-4.65708303	2.77400589	0.54620701
H	-5.72253609	-0.66096401	0.68230897
H	-5.42497587	-2.36182904	0.49095300
C	0.00000100	-0.27834901	-0.10257400
H	0.00003000	-1.22841203	0.43975401
H	-0.00002500	0.55842203	0.60205603

Frequencies -- 15.6248 16.1346 33.1012

Sum of electronic and zero-point Energies= -865.528408
Sum of electronic and thermal Energies= -865.508305
Sum of electronic and thermal Enthalpies= -865.507361
Sum of electronic and thermal Free Energies= -865.580161

BBNOMe

Element	X	Y	Z
C	1.07649601	1.32024801	-1.15411794
C	0.35317901	-0.03247800	-1.38178504
C	-0.37908500	-0.05034600	1.12660897
C	0.30330700	1.33052003	1.31487203
H	1.98932803	1.36020100	-1.76046503
H	0.69743800	1.41198897	2.33455706
H	-0.47180501	2.10232401	1.22291303
C	1.23690403	-1.27525997	-1.12172198
H	0.66589499	-2.16234899	-1.42321897
H	2.12329006	-1.24723101	-1.76650405
C	0.55497199	-1.26252604	1.37040401
H	0.99277800	-1.19320500	2.37338305
H	0.01931000	-0.06355900	-2.42440701

H	-1.19718206	-0.11342200	1.85096204
C	1.42622399	1.64561105	0.31071299
H	2.33685088	1.12445700	0.60361099
H	1.66492105	2.71148705	0.38123199
C	1.68113804	-1.45584202	0.33922100
H	2.50895596	-0.78269601	0.55899203
H	2.08796906	-2.46501994	0.45823401
H	-0.06951900	-2.16427803	1.37045002
H	0.42057300	2.11295891	-1.53402495
B	-0.85101998	-0.08089100	-0.37462899
O	-2.13272905	-0.08842400	-0.82547498
C	-3.23248911	-0.09303900	0.08166300
H	-4.14560795	-0.08852200	-0.51145798
H	-3.21604204	-0.98636103	0.70893902
H	-3.21409607	0.79374403	0.71860200

Frequencies -- 39.5813 78.3552 177.4019

Sum of electronic and zero-point Energies= -452.981819
Sum of electronic and thermal Energies= -452.971094
Sum of electronic and thermal Enthalpies= -452.970150
Sum of electronic and thermal Free Energies= -453.018108

BBN_2O

Element	X	Y	Z
C	3.37853098	0.59624600	-1.57587504
C	2.47801495	-0.62791300	-1.26281595
C	1.66606903	0.54267102	0.92476702
C	2.57757092	1.75630498	0.59060597
H	4.29343987	0.26310501	-2.07981110
H	2.96305990	2.19097209	1.52018201
H	1.94777799	2.52728796	0.12957500
C	3.16387510	-1.71975303	-0.40773600
H	2.49295902	-2.58697605	-0.37464300
H	4.07954121	-2.06052089	-0.90527600
C	2.36072707	-0.56179398	1.75786304
H	2.74515104	-0.13510001	2.69176602
H	2.17984295	-1.07626402	-2.21623302
H	0.81221902	0.91968799	1.49881697
C	3.75302196	1.45870495	-0.35765600
H	4.56634521	0.98918301	0.19375899
H	4.15525913	2.41089392	-0.71739900
C	3.49624205	-1.30987501	1.03784502
H	4.40491819	-0.70894599	1.05478799
H	3.73329592	-2.21285200	1.60899603
H	1.59497797	-1.29220498	2.04755902
H	2.84369206	1.22747099	-2.29625010
B	1.25211704	-0.06338500	-0.46457899
O	-0.00001300	0.00172400	-1.01867104
B	-1.25224197	0.06490400	-0.46463600
C	-1.66559505	-0.54308498	0.92402202
C	-2.47865009	0.62922603	-1.26225996
C	-2.36105299	0.56000203	1.75835598
C	-2.57618403	-1.75703204	0.58871001
H	-0.81147802	-0.92003000	1.49771202
C	-3.16479301	1.71993899	-0.40595600
C	-3.37862897	-0.59509403	-1.57624495
H	-2.18084598	1.07862604	-2.21529508
H	-2.74528408	0.13194101	2.69171095
C	-3.49697304	1.30823898	1.03914297
H	-1.59578001	1.29053700	2.04898405
H	-1.94592798	-2.52697897	0.12657200
H	-2.96109700	-2.19311094	1.51786005
C	-3.75211406	-1.45919502	-0.35884601
H	-4.08058405	2.06103897	-0.90303600

H	-2.49410892	2.58731198	-0.37188500
H	-4.29397106	-0.26194799	-2.07939196
H	-2.84373999	-1.22517598	-2.29757810
H	-4.40527391	0.70672798	1.05528998
H	-3.73463011	2.21041107	1.61131895
H	-4.56553698	-0.99079198	0.19336100
H	-4.15384722	-2.41123700	-0.71953398

Frequencies -- 40.6902 40.8429 50.9573

Sum of electronic and zero-point Energies= -751.043388
Sum of electronic and thermal Energies= -751.025776
Sum of electronic and thermal Enthalpies= -751.024831
Sum of electronic and thermal Free Energies= -751.089165

$\mathbf{12}^{-}$

Element	X	Y	Z
C	-3.97896791	1.46970201	1.15969098
C	-2.73716903	0.58336401	0.95210999
C	-3.68395591	-0.18821900	-1.33704805
C	-4.91963387	0.70613402	-1.13055301
H	-4.26674509	1.51027405	2.22106504
H	-5.82038593	0.24623400	-1.56367803
H	-4.75202894	1.63627005	-1.68873894
C	-2.88666201	-0.84921098	1.49683702
H	-1.90750599	-1.33876801	1.41053200
H	-3.13528204	-0.84560400	2.56887197
C	-3.84928608	-1.61538398	-0.77808100
H	-4.73902607	-2.10557103	-1.20152700
H	-1.92297196	1.05660105	1.52397501
H	-3.54132390	-0.28991401	-2.42402506
C	-5.21945381	1.07640195	0.33457100
H	-5.73829603	0.24970900	0.82256198
H	-5.93088579	1.91086304	0.34992301
C	-3.91761899	-1.72088802	0.75713098
H	-4.92249489	-1.47182298	1.10235500
H	-3.76624990	-2.76835799	1.04504299
H	-2.98466492	-2.19852090	-1.11600494
H	-3.69836402	2.49371696	0.88079602
B	-2.39613008	0.52256399	-0.64788997
O	-1.14960897	-0.29049700	-0.95162201
O	1.11822200	-0.40767899	-0.93974698
B	2.35535598	-0.15353100	-0.44833699
C	2.69905496	0.69614297	0.83671802
C	3.64855504	-0.74326199	-1.12571704
C	3.36033511	-0.27527899	1.84756505
C	3.60684896	1.86858296	0.39199799
H	1.82327700	1.13122702	1.32776403
C	4.28431177	-1.71024001	-0.09502900
C	4.56120300	0.43917301	-1.53442502
H	3.41413999	-1.31877697	-2.02769995
H	3.69462109	0.28200200	2.73102903
C	4.53512096	-1.10454202	1.29736996
H	2.58386111	-0.96714699	2.19798589
H	2.99727011	2.54688406	-0.21850400
H	3.92304397	2.44595695	1.26906002
C	4.84693909	1.46581197	-0.42373300
H	5.22622824	-2.11125302	-0.48849201
H	3.60888600	-2.56756806	0.01729000
H	5.51216888	0.05864800	-1.92666900
H	4.07327318	0.96090502	-2.36702704
H	5.44003296	-0.49833900	1.27892804
H	4.74280787	-1.91837299	1.99936402
H	5.62169313	1.08849394	0.24318101

H	5.26897907	2.36565709	-0.88241303
C	-0.04154400	0.14037000	-0.28894499
H	0.04324700	1.23970699	-0.30788699
H	-0.02517400	-0.19351900	0.76047403
H	-2.21562099	1.67867506	-1.08820605

Frequencies -- 22.7843 32.8928 49.5387

Sum of electronic and zero-point Energies= -866.217283
Sum of electronic and thermal Energies= -866.197505
Sum of electronic and thermal Enthalpies= -866.196561
Sum of electronic and thermal Free Energies= -866.266111

TS_{7-8}

Element	X	Y	Z
C	1.40316200	1.67659903	-1.01899397
C	0.92658597	0.24789301	-1.34025800
C	0.61450100	-0.21692701	1.20459998
C	1.07904005	1.22107601	1.50846505
H	2.17445993	1.99995399	-1.73109496
H	1.63353896	1.25782394	2.45598602
H	0.17700399	1.82915294	1.65409994
C	2.05805898	-0.80201399	-1.38579500
H	1.62452197	-1.73648405	-1.76147497
H	2.83017397	-0.50695699	-2.10947490
C	1.75311506	-1.25845206	1.14464700
H	2.32447696	-1.26250505	2.08285308
H	0.46690100	0.27168700	-2.33811498
H	-0.05916900	-0.51846802	2.01541495
C	1.93235397	1.88543499	0.41234601
H	2.96184301	1.53178000	0.48129100
H	1.98354995	2.96145797	0.61299098
C	2.73335600	-1.09390700	-0.03247800
H	3.45530295	-0.30916899	0.19621401
H	3.32414508	-2.01206398	-0.12657700
H	1.28797102	-2.24953890	1.06595004
H	0.54843402	2.34964800	-1.16716099
C	-2.51930904	1.11041796	-0.23108800
H	-1.06517506	0.67488998	-0.17518300
O	-2.64319205	1.77937305	0.74013603
O	-2.95121002	0.64795500	-1.23317504
B	-0.12647900	-0.21334700	-0.22080299
O	-0.77553201	-1.51462400	-0.62121201
C	-1.79580998	-2.01093698	0.01437100
H	-2.10319209	-2.98058009	-0.40640900
O	-2.38540602	-1.51133001	0.95172697

Frequencies -- –380.2809 32.7153 48.9445

Sum of electronic and zero-point Energies= -716.305526
Sum of electronic and thermal Energies= -716.291144
Sum of electronic and thermal Enthalpies= -716.290199
Sum of electronic and thermal Free Energies= -716.347562

TS_{5-6}

Element	X	Y	Z
C	-4.08174419	0.48189500	1.58305895
C	-2.81132293	-0.27700999	1.14675701
C	-3.70200300	-0.29732400	-1.30561602
C	-4.94083786	0.50041199	-0.85816401

H	-4.38539696	0.15638800	2.58556104
H	-5.81421614	0.21007800	-1.45480001
H	-4.75406790	1.55767703	-1.07721102
C	-2.93951392	-1.81958401	1.19965303
H	-1.95108402	-2.24738407	0.98654300
H	-3.20156002	-2.14173388	2.21428704
C	-3.86797309	-1.83611405	-1.22138596
H	-4.75206280	-2.15058303	-1.78921902
H	-2.01381803	0.00743200	1.84607196
H	-3.49341202	-0.04746600	-2.35313892
C	-5.28991604	0.36727500	0.63472301
H	-5.81123209	-0.57430899	0.80800402
H	-6.00990391	1.14955294	0.89658701
C	-3.95444608	-2.41469789	0.20523299
H	-4.96347904	-2.29014301	0.59775400
H	-3.79450107	-3.49632597	0.15086800
H	-3.00335002	-2.28795195	-1.72170699
H	-3.81782198	1.54172599	1.67328405
B	-2.47360206	0.03530200	-0.37539700
O	-1.18360198	-0.28749201	-0.91485500
C	-0.10593700	0.05129500	-0.17927000
O	-2.27715707	1.87725699	-0.41434601
C	-1.25170302	2.36206698	0.00886700
H	-0.33601901	1.25686598	0.16217600
O	-0.67501998	3.33500600	0.33775100
H	-0.07719400	-0.38718399	0.82636201
B	2.34131193	0.12654901	-0.10488300
C	2.47369909	-0.87272900	1.15444899
C	3.52760196	-0.23823901	-1.13324201
C	2.26031590	-2.31656909	0.65967202
C	3.83978009	-0.62912899	1.83000398
H	1.71743703	-0.67724901	1.92872095
C	3.31966710	-1.68696296	-1.61959898
C	4.88542223	0.00787300	-0.44937301
H	3.49444008	0.40049201	-2.02848697
H	2.38581395	-3.03118300	1.48372900
C	3.17147112	-2.74212909	-0.50745201
H	1.21668506	-2.41366005	0.33138701
H	3.80850506	0.37288299	2.27229691
H	3.98388290	-1.33076000	2.66245604
C	5.06712484	-0.70634001	0.90322000
H	4.13920784	-1.99104798	-2.28455305
H	2.40764499	-1.69997299	-2.22692800
H	5.71104479	-0.27879801	-1.11408901
H	4.99034309	1.08760500	-0.28322700
H	4.15506220	-3.01280689	-0.12186300
H	2.77069497	-3.66179895	-0.94786501
H	5.33881903	-1.74914598	0.73413002
H	5.92489004	-0.26399499	1.42188895
O	1.02365601	0.02677400	-0.85744601
O	2.42566800	1.57144403	0.42505601
C	2.47481799	2.56330609	-0.41346201
H	2.29585505	2.29042912	-1.46651495
O	2.69310808	3.71567798	-0.09360000

Frequencies -- -1000.3312 26.1292 33.5619

Sum of electronic and zero-point Energies= -1243.356236
Sum of electronic and thermal Energies= -1243.330789
Sum of electronic and thermal Enthalpies= -1243.329844
Sum of electronic and thermal Free Energies= -1243.411373

$TS_{9\text{-}6}$

Element	X	Y	Z
C	-3.69053411	-0.54281700	-1.85385394

C	-3.29084992	0.76065302	-1.13677299
C	-2.43483901	-0.64412099	0.90241700
C	-2.85598111	-1.93259299	0.16845299
H	-4.58888388	-0.38979900	-2.46641588
H	-3.21275902	-2.68574405	0.88363397
H	-1.95750403	-2.35555005	-0.29848999
C	-4.39203596	1.36269498	-0.23345099
H	-4.03652811	2.34470606	0.10216700
H	-5.30659485	1.54833102	-0.81200403
C	-3.53860497	-0.02357400	1.78495705
H	-3.89428592	-0.74747300	2.52997088
H	-3.05567288	1.50799203	-1.90591502
H	-1.58784997	-0.89281398	1.55636895
C	-3.92273092	-1.75175095	-0.92806298
H	-4.91170692	-1.68025994	-0.47474900
H	-3.94966888	-2.65977192	-1.54037905
C	-4.75221920	0.53196400	1.01435697
H	-5.41655684	-0.28622499	0.73496503
H	-5.33803177	1.16200805	1.69259501
H	-3.08222294	0.80096298	2.34559298
H	-2.88130903	-0.79570901	-2.55115509
B	-2.04674411	0.46482399	-0.18091300
O	-1.39048898	1.72201097	0.41839701
C	-0.28810099	1.30192196	-0.17031799
H	-0.04077400	1.71112096	-1.15407205
O	0.67337799	0.85365498	0.55378002
B	2.00049806	0.42495501	-0.09995700
C	1.79759204	-0.86526400	-1.04166603
C	3.04527593	0.02666900	1.05413795
C	3.15059090	-1.21170604	-1.69501805
C	1.18899405	-1.99856997	-0.19280601
H	1.09215295	-0.65610301	-1.86051297
C	4.39545584	-0.31563100	0.39376101
C	2.44273400	-1.12327695	1.88799298
H	3.21975708	0.86463100	1.73935401
H	3.06534290	-2.12191701	-2.30407000
C	4.32871580	-1.38210106	-0.71635002
H	3.39650011	-0.39858001	-2.38737607
H	0.18269999	-1.68147099	0.10742400
H	1.05985498	-2.90947294	-0.79349399
C	1.97658896	-2.34946895	1.08198094
H	5.12326193	-0.63999403	1.14960301
H	4.79914999	0.60853398	-0.03963000
H	3.15443110	-1.45493805	2.65619302
H	1.57578695	-0.71934402	2.42360806
H	4.29232216	-2.37484097	-0.26648399
H	5.26421213	-1.35665298	-1.28630197
H	2.83376002	-2.97422290	0.82703298
H	1.34389699	-2.97254896	1.72454703
O	2.45977902	1.58162200	-0.98896700
C	2.77614903	2.76330090	-0.54302400
H	3.16358995	3.40582800	-1.34999800
O	2.67292404	3.17566705	0.59370500
H	-1.01706803	0.04880500	-0.85338598

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Frequencies -- -456.5921 24.1152 50.0385

Sum of electronic and zero-point Energies= -1054.790322
Sum of electronic and thermal Energies= -1054.768336
Sum of electronic and thermal Enthalpies= -1054.767392
Sum of electronic and thermal Free Energies= -1054.840513

$TS_{9\text{-}12}$

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Element	X	Y	Z
C	-3.88722396	0.60769498	1.44916201
C	-2.57692003	-0.15124901	1.14683104
C	-3.38897491	-0.51066101	-1.31156194
C	-4.64765692	0.32484600	-1.00734305
H	-4.21755600	0.37343401	2.46823812
H	-5.49311495	-0.04254900	-1.60119402
H	-4.45371294	1.35002697	-1.34003794
C	-2.66604590	-1.68705404	1.38458395
H	-1.66546202	-2.11530399	1.23949099
H	-2.93442011	-1.88124704	2.42903399
C	-3.54400897	-2.03310299	-1.02840102
H	-4.41434908	-2.42230010	-1.56956804
H	-1.81049895	0.23990400	1.82480502
H	-3.14044309	-0.39624900	-2.37186694
C	-5.05385399	0.35881299	0.47475901
H	-5.57007313	-0.56543899	0.73397702
H	-5.79419279	1.15281296	0.61522698
C	-3.65458012	-2.42145991	0.46003601
H	-4.67166615	-2.26027489	0.81486899
H	-3.47939897	-3.49796510	0.55034602
H	-2.66699004	-2.53762102	-1.45127404
H	-3.65253496	1.67641401	1.43558705
B	-2.21247292	-0.07315600	-0.37940401
O	-0.91361701	-0.09780400	-0.89455599
C	0.13372999	0.32562399	-0.14999200
O	-2.07559395	2.28903294	-0.53422701
C	-1.03467000	2.67277288	-0.05823100
H	-0.23634300	1.60258603	0.14019200
O	-0.43849301	3.64968395	0.30168700
H	0.14056601	-0.01121200	0.89300197
B	2.54537392	0.62464601	0.07786800
C	2.84035397	-0.62949401	1.06762397
C	3.78769994	0.70012498	-0.95151299
C	2.91776800	-1.93251002	0.25031599
C	4.12119818	-0.30528200	1.86298394
H	2.04624391	-0.77217603	1.81662905
C	3.86831999	-0.60813302	-1.76388705
C	5.06101179	1.02215600	-0.14893800
H	3.65143895	1.51560998	-1.67675805
H	3.16658807	-2.78739810	0.89500099
C	3.90610790	-1.90409100	-0.93102401
H	1.91475499	-2.13425207	-0.14820200
H	3.89472795	0.54910398	2.51385903
H	4.38713884	-1.13773501	2.52952504
C	5.35483789	0.05627200	1.01402998
H	4.73916721	-0.59883201	-2.43490195
H	2.98351693	-0.64499903	-2.41023207
H	5.94235086	1.05983806	-0.80457401
H	4.94336510	2.03094101	0.26749399
H	4.91859198	-2.07513690	-0.56238502
H	3.69124889	-2.75273991	-1.59067094
H	5.81493998	-0.85423797	0.62720102
H	6.11043406	0.50734001	1.66758096
O	1.25487494	0.36988300	-0.77806699
H	2.35124612	1.67424095	0.69198197

Frequencies -- -1013.7341 23.1162 28.1831

Sum of electronic and zero-point Energies= -1054.745567
Sum of electronic and thermal Energies= -1054.722798
Sum of electronic and thermal Enthalpies= -1054.721854
Sum of electronic and thermal Free Energies= -1054.798477

$TS_{8\text{-}7}$

Element	X	Y	Z
N	-2.41894603	0.34940699	0.02393600
C	-2.72192693	1.34859598	1.06231296
C	-2.10639811	2.71921492	0.80409497
H	-2.32616591	0.96344799	2.00526190
H	-3.81282210	1.44167197	1.18349302
H	-2.16643310	3.31585598	1.71583402
H	-1.05196095	2.63098502	0.52846903
H	-2.62389207	3.26533103	0.01484600
C	-2.73808098	0.85029000	-1.32225394
C	-2.38040709	-0.13158800	-2.43110895
H	-2.17573404	1.77056098	-1.47795701
H	-3.80770493	1.11377501	-1.37327099
H	-2.37217402	0.39146301	-3.38902593
H	-1.38990104	-0.55598700	-2.25234509
H	-3.09414697	-0.95279998	-2.50776505
C	-3.13594890	-0.91055202	0.28710499
C	-2.85504508	-1.50612903	1.66240704
H	-2.81686211	-1.62701595	-0.46688399
H	-4.21894693	-0.74460101	0.16377001
H	-3.24020290	-2.52695704	1.69208002
H	-1.78149903	-1.54825699	1.86234999
H	-3.33400393	-0.94818902	2.46809602
H	-0.78021002	0.03631900	0.42366800
H	0.34703100	-3.83429790	0.62541902
C	0.18055899	-2.81694794	0.24753200
O	0.95731002	-1.94724202	0.86456001
O	-0.63371700	-2.56063700	-0.60430700
B	1.10329497	-0.55846000	0.44131500
C	1.34729302	-0.19935100	-1.08303499
C	2.06399012	0.29339901	1.37941098
H	-0.15594099	0.05792500	0.96237898
C	1.08984399	1.30440795	-1.29889596
C	2.79739094	-0.65004200	-1.38995600
H	0.69265699	-0.75210398	-1.76087606
C	1.83933699	1.80021405	1.14549696
C	3.49645400	-0.19150500	1.04697394
H	1.88833404	0.08576300	2.44157195
H	1.34514594	1.58719897	-2.32745790
C	1.82221401	2.25253201	-0.32939300
H	0.00927500	1.46723104	-1.20168400
H	2.82302094	-1.74607098	-1.33800900
H	3.05603790	-0.38639399	-2.42244601
C	3.87348199	-0.09638800	-0.43989199
H	2.59819388	2.38122702	1.68316805
H	0.87867600	2.06341290	1.60487902
H	4.22694492	0.36907300	1.64233994
H	3.57714510	-1.23888898	1.36158597
H	2.84414697	2.40532994	-0.67761701
H	1.34889901	3.23912311	-0.38446501
H	4.10034513	0.93847501	-0.69663501
H	4.80361414	-0.65003401	-0.60371798

Frequencies -- -347.1370 27.9725 40.7695

Sum of electronic and zero-point Energies= -820.319828
Sum of electronic and thermal Energies= -820.298042
Sum of electronic and thermal Enthalpies= -820.297098
Sum of electronic and thermal Free Energies= -820.369742

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Element	X	Y	Z
C	-3.71142411	0.49900901	1.67527401
C	-2.43621993	-0.15761600	1.09508801

C	-3.53070688	-0.13901900	-1.26603794
C	-4.81271315	0.48589900	-0.67301798
H	-3.88728189	0.13324900	2.69405007
H	-5.69977379	0.09599400	-1.18742096
H	-4.78154087	1.56044900	-0.88489002
C	-2.48228502	-1.70107901	1.09099698
H	-1.48644400	-2.08212590	0.82846999
H	-2.68055201	-2.07160592	2.10413790
C	-3.51885700	-1.67966604	-1.27445900
H	-4.38013983	-2.06546807	-1.83344996
H	-1.61249697	0.14926200	1.75314999
H	-3.45146394	0.20154700	-2.30714393
C	-4.99408007	0.29796600	0.84599102
H	-5.41096878	-0.68804598	1.05123997
H	-5.74832678	1.00931501	1.19833004
C	-3.49782801	-2.32977509	0.11918500
H	-4.49603510	-2.29763389	0.55557799
H	-3.26191306	-3.39323902	0.00900800
H	-2.62671399	-2.00658202	-1.82302296
H	-3.52017307	1.57480597	1.76473498
B	-2.30294704	0.39096701	-0.40538400
O	-0.93924397	-0.12559800	-1.14358497
O	1.22136104	-0.42970401	-1.11769402
O	-2.17377400	1.88021696	-0.53284502
C	-1.16988504	2.56147504	-0.05603900
H	-1.31354105	3.64341497	-0.17673300
O	-0.16471000	2.10262799	0.45348999
B	2.47150612	-0.37676099	-0.44774601
C	2.69970202	0.10065500	1.01650202
C	3.76974511	-0.64668798	-1.25171196
C	3.55372500	-0.96294397	1.75052702
C	3.39854288	1.48661494	0.85194200
H	1.79636800	0.27940100	1.60566401
C	4.61606789	-1.69657004	-0.49010500
C	4.44852400	0.74783099	-1.38537800
H	3.57195091	-1.02266705	-2.25956011
H	3.82896996	-0.58248198	2.73991394
C	4.82280588	-1.41535902	1.00870895
H	2.91769600	-1.83883297	1.92305005
H	2.65433788	2.18418598	0.45113099
H	3.66899300	1.85974395	1.84534895
C	4.63703394	1.50275397	-0.05924600
H	5.59153605	-1.79979396	-0.97756898
H	4.11568403	-2.66588402	-0.59622401
H	5.41636086	0.62840700	-1.88373995
H	3.82992792	1.36013198	-2.05214906
H	5.61324120	-0.67905301	1.14538598
H	5.19092894	-2.32994890	1.48270702
H	5.50104809	1.10943496	0.47379500
H	4.88077688	2.54471898	-0.28665099
C	0.09142000	-0.28113699	-0.49156800
H	0.08627200	-0.33616799	0.59366298

Frequencies -- 23.2591 27.9550 37.1256

Sum of electronic and zero-point Energies= -1054.086937
Sum of electronic and thermal Energies= -1054.064221
Sum of electronic and thermal Enthalpies= -1054.063277
Sum of electronic and thermal Free Energies= -1054.139535

$TS_{13\text{-}11}$

Element	X	Y	Z
C	-3.71044707	0.68268299	1.60870194
C	-2.54914093	-0.20989600	1.12136102
C	-3.53142905	-0.12471300	-1.29142594

C	-4.67805099	0.77438003	-0.78874499
H	-3.99422407	0.40029499	2.62951112
H	-5.59898996	0.55789298	-1.34313297
H	-4.41490221	1.81256795	-1.02251601
C	-2.84010291	-1.72676098	1.18479896
H	-1.90925503	-2.26098990	0.95484799
H	-3.11371589	-2.01569605	2.20630407
C	-3.82411289	-1.64188695	-1.21188104
H	-4.74332190	-1.87750304	-1.76121998
H	-1.70107305	-0.01011600	1.79266906
H	-3.34606695	0.12020900	-2.34482789
C	-4.96760511	0.67654699	0.72009200
H	-5.56143618	-0.21374001	0.92694002
H	-5.59993410	1.52196395	1.00984502
C	-3.93155193	-2.21692896	0.21397500
H	-4.91526508	-1.99763298	0.62818700
H	-3.87735605	-3.30858898	0.15345600
H	-3.01221800	-2.16292810	-1.73304200
H	-3.33712006	1.71174705	1.67061400
B	-2.24556994	0.11971500	-0.40865901
O	-1.01036894	-0.46692199	-0.99954802
C	0.08621300	-0.26661900	-0.32196400
O	-1.82828796	1.74231005	-0.49730200
C	-0.72407800	2.12957001	-0.12428100
H	0.05149500	1.01325595	0.00723400
O	-0.09380800	3.08744502	0.14064001
H	0.13606200	-0.65673101	0.69991601
O	1.21332204	-0.41683301	-1.05491805
B	2.47004008	-0.26028100	-0.47921300
C	2.74809694	0.18116599	0.99609101
C	3.75846791	-0.59306997	-1.28838098
C	3.41347194	-1.04056096	1.68921697
C	3.64150691	1.44641304	0.93437099
H	1.86030698	0.44404501	1.58071601
C	4.36688519	-1.83496296	-0.57996601
C	4.67878723	0.65282500	-1.29373801
H	3.54263496	-0.86782098	-2.32524204
H	3.73637295	-0.75064200	2.69502497
C	4.59748077	-1.67128098	0.93213201
H	2.64157200	-1.80802798	1.82373905
H	3.03353095	2.26573896	0.53217798
H	3.91930008	1.74017298	1.95244098
C	4.91080904	1.30938697	0.07929900
H	5.31106806	-2.10364699	-1.06605506
H	3.68652201	-2.68012094	-0.74090302
H	5.64528894	0.39138401	-1.73904204
H	4.22516203	1.39586794	-1.95984495
H	5.50469589	-1.09533405	1.10861099
H	4.79006815	-2.65890002	1.36168396
H	5.67229223	0.76242501	0.63372397
H	5.32809687	2.30792499	-0.08138100

Frequencies -- -1012.5733 -9.6975 21.9622

Sum of electronic and zero-point Energies= -1054.034610
Sum of electronic and thermal Energies= -1054.013485
Sum of electronic and thermal Enthalpies= -1054.012541
Sum of electronic and thermal Free Energies= -1054.084763

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Element	X	Y	Z
C	1.28324401	1.28705597	-0.18703000
C	0.00551800	1.30078602	0.71087199
C	0.00265000	-1.30066705	0.71095800
C	1.27948403	-1.29026496	-0.18811400

H	1.25309396	2.15040898	-0.86133200
H	1.24593902	-2.15280795	-0.86330998
H	2.15123606	-1.44378698	0.46006700
C	-1.32131100	1.29034102	-0.07789400
H	-2.13345098	1.44726706	0.64201200
H	-1.35205901	2.14625096	-0.76246500
C	-1.32488894	-1.28715801	-0.07659400
H	-1.35880101	-2.14374495	-0.76016301
H	0.04490400	2.21980596	1.30260003
H	0.04029300	-2.21963310	1.30289102
C	1.49835896	-0.00154200	-0.99949402
H	0.85912102	-0.00017000	-1.88134301
H	2.52386999	-0.00288900	-1.38165498
C	-1.61229002	0.00156600	-0.86361802
H	-1.05122101	0.00024200	-1.79735804
H	-2.66679192	0.00289700	-1.15703404
H	-2.13694000	-1.44071805	0.64414501
H	2.15497994	1.43703306	0.46203199
B	0.18900099	-0.00007600	1.55997896
H	0.61623001	-0.00047800	2.67649794

Frequencies -- 41.8686 182.4140 207.3760

Sum of electronic and zero-point Energies= -338.429544
Sum of electronic and thermal Energies= -338.421224
Sum of electronic and thermal Enthalpies= -338.420280
Sum of electronic and thermal Free Energies= -338.462437

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Element	X	Y	Z
C	-4.24445200	1.76915002	0.50993299
C	-3.00183511	0.92195499	0.85122699
C	-3.47434711	-0.59153098	-1.20322001
C	-4.72028208	0.25388700	-1.53840899
H	-4.73151779	2.13446999	1.42464304
H	-5.51718283	-0.37476000	-1.95913696
H	-4.43674088	0.96002698	-2.32916808
C	-3.28999496	-0.26545101	1.79042196
H	-2.32547808	-0.69992900	2.08265591
H	-3.76300597	0.07915700	2.72066808
C	-3.75591898	-1.77447498	-0.25492701
H	-4.53505898	-2.42948294	-0.66935998
H	-2.29963398	1.58565795	1.37910402
H	-3.11378694	-1.01811802	-2.15017605
C	-5.30076885	1.06111205	-0.36125201
H	-5.91421986	0.41011000	0.26306200
H	-5.99091101	1.81450796	-0.75766599
C	-4.15288305	-1.38468599	1.18059099
H	-5.20423079	-1.09448397	1.20606101
H	-4.08234787	-2.27249789	1.81949997
H	-2.84268594	-2.37977195	-0.20482400
H	-3.89924097	2.66011596	-0.03018300
B	-2.38658094	0.39837101	-0.54727298
O	-1.06816602	-0.45917100	-0.25629100
C	-0.00007400	0.14687000	-0.00022400
H	-0.00014000	1.24410498	-0.00026600
O	1.06809402	-0.45901400	0.25589299
B	2.38643289	0.39868101	0.54673702
C	3.00204206	0.92145598	-0.85191000
C	3.47403908	-0.59084398	1.20353699
C	4.24462080	1.76880705	-0.51084697
C	3.29037905	-0.26652700	-1.79032195
H	2.29998493	1.58485198	-1.38036096
C	4.71981478	0.25484499	1.53862000
C	3.75594807	-1.77431095	0.25601599

H	3.11322498	-1.01690602	2.15063190
H	4.73197794	2.13344002	-1.42567503
C	5.30066586	1.06133497	0.36114901
H	3.89930105	2.66018105	0.02852100
H	2.32591605	-0.70121902	-2.08242393
H	3.76353693	0.07749600	-2.72070909
C	4.15321779	-1.38533294	-1.17963898
H	5.51660681	-0.37347901	1.96004295
H	4.43595982	0.96148998	2.32881904
H	4.53504610	-2.42900109	0.67103302
H	2.84278202	-2.37971807	0.20604099
H	5.91435194	0.40996400	-0.26255101
H	5.99065208	1.81500399	0.75731301
H	5.20453978	-1.09503400	-1.20503497
H	4.08292103	-2.27353597	-1.81803095
H	-2.02680993	1.30465698	-1.28786194
H	2.02646995	1.30536795	1.28674102

Frequencies -- 31.8289 33.1368 46.4692

Sum of electronic and zero-point Energies= -866.207893
Sum of electronic and thermal Energies= -866.188015
Sum of electronic and thermal Enthalpies= -866.187071
Sum of electronic and thermal Free Energies= -866.256311

$TS_{15\text{-}16}$

Element	X	Y	Z
C	3.21758389	1.38244605	-1.40668499
C	3.03040409	-0.14513800	-1.33686900
C	2.03360200	0.10495300	1.07060206
C	2.24354410	1.62980497	0.98290801
H	4.11288309	1.63882804	-1.98842204
H	2.50798798	2.04116011	1.96627903
H	1.28024900	2.07978797	0.71162897
C	4.23068380	-0.91471601	-0.74033099
H	4.02854919	-1.98511696	-0.87044698
H	5.14616203	-0.70258600	-1.30825806
C	3.24041200	-0.67076498	1.64145398
H	3.50474906	-0.29624501	2.63924599
H	2.88450599	-0.51244599	-2.36127806
H	1.17878199	-0.07944900	1.73531997
C	3.29243588	2.09736300	-0.04466500
H	4.29405594	1.99027300	0.37303701
H	3.16242599	3.17276907	-0.20863099
C	4.50103378	-0.65687197	0.75509799
H	5.02722502	0.29018399	0.87797898
H	5.19360399	-1.42298400	1.12066698
H	2.92656398	-1.71314096	1.77566504
H	2.36347890	1.79239595	-1.96167195
B	1.78308702	-0.47502899	-0.39641100
O	1.29926598	-1.92277598	-0.43838799
C	0.15047300	-1.40563595	-0.86323899
H	-0.02523500	-1.38660502	-1.94467294
O	-0.87654603	-1.44207001	-0.09764300
B	-2.24164605	-0.91990501	-0.66880703
C	-2.17296910	0.68566197	-0.88769102
C	-3.37433910	-1.18308604	0.45376101
C	-3.53117800	1.15302205	-1.44327605
C	-1.75935698	1.35994804	0.43468800
H	-1.41529202	0.96477997	-1.63658702
C	-4.72868681	-0.70896298	-0.10742000

C	-2.97097802	-0.49513000	1.77366400
H	-3.47776389	-2.25610089	0.67296398
H	-3.54545212	2.24334598	-1.58270001
C	-4.75596380	0.74912101	-0.60196900
H	-3.64727497	0.71530199	-2.44353008
H	-0.72987300	1.04760695	0.64924002
H	-1.73301196	2.45461512	0.32988200
C	-2.62467909	1.00158703	1.65766096
H	-5.52864885	-0.84308100	0.63448000
H	-4.98318577	-1.35945499	-0.95435500
H	-3.75618196	-0.61543399	2.53401589
H	-2.08773994	-1.01838505	2.15878010
H	-4.85644913	1.42521703	0.24818100
H	-5.66147804	0.90188199	-1.20083702
H	-3.54071593	1.59451604	1.64996505
H	-2.09141302	1.30936396	2.56510711
H	0.68595302	0.05492300	-0.87470597
H	-2.43855810	-1.53409195	-1.71816504

Frequencies -- -475.5413 28.7683 37.2611

Sum of electronic and zero-point Energies= -866.182512
Sum of electronic and thermal Energies= -866.163481
Sum of electronic and thermal Enthalpies= -866.162537
Sum of electronic and thermal Free Energies= -866.229450

16^{-}

Element	X	Y	Z
C	-3.97896791	1.46970201	1.15969098
C	-2.73716903	0.58336401	0.95210999
C	-3.68395591	-0.18821900	-1.33704805
C	-4.91963387	0.70613402	-1.13055301
H	-4.26674509	1.51027405	2.22106504
H	-5.82038593	0.24623400	-1.56367803
H	-4.75202894	1.63627005	-1.68873894
C	-2.88666201	-0.84921098	1.49683702
H	-1.90750599	-1.33876801	1.41053200
H	-3.13528204	-0.84560400	2.56887197
C	-3.84928608	-1.61538398	-0.77808100
H	-4.73902607	-2.10557103	-1.20152700
H	-1.92297196	1.05660105	1.52397501
H	-3.54132390	-0.28991401	-2.42402506
C	-5.21945381	1.07640195	0.33457100
H	-5.73829603	0.24970900	0.82256198
H	-5.93088579	1.91086304	0.34992301
C	-3.91761899	-1.72088802	0.75713098
H	-4.92249489	-1.47182298	1.10235500
H	-3.76624990	-2.76835799	1.04504299
H	-2.98466492	-2.19852090	-1.11600494
H	-3.69836402	2.49371696	0.88079602
B	-2.39613008	0.52256399	-0.64788997
O	-1.14960897	-0.29049700	-0.95162201
O	1.11822200	-0.40767899	-0.93974698
B	2.35535598	-0.15353100	-0.44833699
C	2.69905496	0.69614297	0.83671802
C	3.64855504	-0.74326199	-1.12571704
C	3.36033511	-0.27527899	1.84756505
C	3.60684896	1.86858296	0.39199799
H	1.82327700	1.13122702	1.32776403
C	4.28431177	-1.71024001	-0.09502900
C	4.56120300	0.43917301	-1.53442502
H	3.41413999	-1.31877697	-2.02769995
H	3.69462109	0.28200200	2.73102903
C	4.53512096	-1.10454202	1.29736996
H	2.58386111	-0.96714699	2.19798589

H	2.99727011	2.54688406	-0.21850400
H	3.92304397	2.44595695	1.26906002
C	4.84693909	1.46581197	-0.42373300
H	5.22622824	-2.11125302	-0.48849201
H	3.60888600	-2.56756806	0.01729000
H	5.51216888	0.05864800	-1.92666900
H	4.07327318	0.96090502	-2.36702704
H	5.44003296	-0.49833900	1.27892804
H	4.74280787	-1.91837299	1.99936402
H	5.62169313	1.08849394	0.24318101
H	5.26897907	2.36565709	-0.88241303
C	-0.04154400	0.14037000	-0.28894499
H	0.04324700	1.23970699	-0.30788699
H	-0.02517400	-0.19351900	0.76047403
H	-2.21562099	1.67867506	-1.08820605

Frequencies -- 22.7843 32.8928 49.5387

Sum of electronic and zero-point Energies= -866.217283
Sum of electronic and thermal Energies= -866.197505
Sum of electronic and thermal Enthalpies= -866.196561
Sum of electronic and thermal Free Energies= -866.266111

17

Element	X	Y	Z
C	-4.00965786	1.48663604	-1.10397303
C	-2.65937304	1.01596296	-0.51719499
C	-3.70365596	-1.32112801	-0.06170600
C	-5.05673599	-0.82583898	-0.61668497
H	-4.16323805	2.55296206	-0.89468199
H	-5.89003611	-1.28476095	-0.06867900
H	-5.13754177	-1.18028402	-1.65199006
C	-2.52865696	1.25449204	1.00129104
H	-1.48547304	1.07362700	1.29662704
H	-2.71634293	2.30980897	1.23810506
C	-3.52256489	-1.09603095	1.45268703
H	-4.33332205	-1.57939100	2.01359606
H	-1.89151001	1.62888896	-1.01073301
H	-3.66351199	-2.40463090	-0.23607300
C	-5.24248314	0.70309401	-0.61951202
H	-5.52657890	1.04510403	0.37608099
H	-6.09142685	0.95310700	-1.26499796
C	-3.43251610	0.37710601	1.88935602
H	-4.43316793	0.80763698	1.93266797
H	-3.05639291	0.41729799	2.91729307
H	-2.59888506	-1.60427904	1.75581598
H	-3.94756889	1.39158702	-2.19523907
B	-2.55991602	-0.55047899	-0.87701899
O	-1.11935103	-1.16742396	-0.29550600
O	1.02321196	-1.05484402	0.10255900
B	2.27932811	-0.40263799	0.07793100
C	2.61466193	0.98055899	-0.55814999
C	3.50828004	-1.16259098	0.64511299
C	3.28197598	1.84178305	0.54811001
C	3.54495096	0.65976000	-1.76722205
H	1.76761603	1.55102003	-0.94751102
C	4.21399498	-0.27289000	1.69814706
C	4.37842894	-1.48842204	-0.60217297
H	3.23101711	-2.10857010	1.11874795
H	3.60438704	2.79302597	0.11182900
C	4.46912813	1.18166494	1.26577103
H	2.51307893	2.08723307	1.29014301
H	2.92726398	0.19707599	-2.54566789
H	3.91336894	1.60221601	-2.18602490
C	4.73426008	-0.27122101	-1.47044301

H	5.16156483	-0.73793399	1.99107802
H	3.58567691	-0.26193601	2.59596610
H	5.29636812	-1.99045801	-0.27860799
H	3.83105898	-2.21258497	-1.21753597
H	5.35650110	1.23766506	0.63692302
H	4.70424318	1.77091897	2.15692592
H	5.54433584	0.28927001	-1.00693202
H	5.13275480	-0.62977999	-2.42396688
C	-0.07983900	-0.53374898	-0.36569500
H	-0.03774900	0.46258101	-0.80997097
H	-2.48562002	-0.80780399	-2.06048298

Frequencies -- 18.6456 27.2533 33.0277

Sum of electronic and zero-point Energies= -865.479162
Sum of electronic and thermal Energies= -865.459107
Sum of electronic and thermal Enthalpies= -865.458163
Sum of electronic and thermal Free Energies= -865.529260

$TS_{17\text{-}11}$

Element	X	Y	Z
C	-3.39908409	1.07078600	1.58848095
C	-3.06540990	-0.40489501	1.27261698
C	-1.92959905	0.35625800	-0.96758902
C	-2.26776695	1.82413304	-0.61998600
H	-4.35919905	1.13899505	2.11521411
H	-2.48465800	2.39155698	-1.53362894
H	-1.36906099	2.27694201	-0.18201700
C	-4.14302683	-1.14259303	0.45243099
H	-3.85673189	-2.19994307	0.41087100
H	-5.10892010	-1.10429299	0.97207701
C	-3.02775788	-0.37623700	-1.76352000
H	-3.26478195	0.17259599	-2.68395400
H	-2.95596409	-0.92938399	2.22934890
H	-1.02006805	0.36809701	-1.58286500
C	-3.43290210	2.01334405	0.37010801
H	-4.38255405	1.90401399	-0.15355200
H	-3.41816211	3.04736996	0.73053199
C	-4.33581877	-0.63599300	-0.99045998
H	-4.94778919	0.26650500	-0.98524702
H	-4.92227316	-1.37865603	-1.54201198
H	-2.61600590	-1.34238195	-2.07656503
H	-2.63714504	1.43910599	2.28673291
B	-1.71980405	-0.38703901	0.42467901
O	-1.26380897	-1.99034798	0.11554500
C	-0.11571700	-1.69447505	0.51398402
H	0.19499999	-1.82528806	1.55225301
O	0.83447301	-1.46463895	-0.36935899
B	2.02716994	-0.77590901	-0.07796900
C	2.26294494	0.10993200	1.18002999
C	3.09926295	-0.62338001	-1.19033003
C	3.69221592	-0.09748400	1.73048103
C	1.99111104	1.53805804	0.60282999
H	1.55326605	-0.04001300	1.99847102
C	4.50377989	-0.87438703	-0.59754997
C	2.87401891	0.82737702	-1.71623003
H	2.94042397	-1.30862403	-2.02786994
H	3.89989710	0.65917999	2.49492908
C	4.81967211	-0.08491700	0.68306202
H	3.70763898	-1.06544399	2.24394107
H	0.92815500	1.59460199	0.33422101
H	2.14851308	2.27437091	1.39781296
C	2.82939005	1.91695797	-0.62952298
H	5.26581001	-0.65636802	-1.35380399
H	4.58691406	-1.94517398	-0.37797701

H	3.65102005	1.06798899	-2.44982505
H	1.92104399	0.83954602	-2.25857806
H	5.08498383	0.94096297	0.43075800
H	5.71671677	-0.51284599	1.14019704
H	3.83875108	2.18721199	-0.32395500
H	2.40228295	2.82388806	-1.06757700
H	-0.73113197	0.03520000	1.04600894

Frequencies -- -221.0491 25.2654 31.4282

Sum of electronic and zero-point Energies= -865.461318
Sum of electronic and thermal Energies= -865.442004
Sum of electronic and thermal Enthalpies= -865.441060
Sum of electronic and thermal Free Energies= -865.509462

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Element	X	Y	Z
O	0.29026499	3.68301392	-0.48983800
O	0.85688502	1.68930197	0.31072801
O	-0.19025800	-0.39619499	-0.38393199
N	-2.51235294	-0.27212900	-0.02138300
B	1.13944900	0.19244100	0.00051500
C	0.57523203	2.51084995	-0.65215802
H	0.60496902	2.07328606	-1.66396999
C	-1.12801600	-0.43940800	0.60046798
H	-1.03237903	0.36469200	1.33566594
H	-1.16204095	-1.39859998	1.12997198
C	1.77763999	-0.45068800	1.33503401
H	1.11327803	-0.31666100	2.20304203
C	1.93999004	-1.96732497	1.11673498
H	2.39326406	-2.44221711	1.99704301
H	0.93760902	-2.40474200	1.01629806
C	2.75331807	-2.35441995	-0.13088401
H	2.60397291	-3.42100406	-0.33276799
H	3.81831408	-2.24621701	0.07769200
C	2.38293195	-1.55746901	-1.39464998
H	1.43644702	-1.95252895	-1.78191102
H	3.13898396	-1.75056005	-2.16776395
C	2.19866991	-0.03807300	-1.19352198
H	1.83524704	0.35398600	-2.15435505
C	3.50182009	0.71194202	-0.85916299
H	4.26027203	0.53352100	-1.63298798
H	3.29147601	1.78894496	-0.88623297
C	4.11179590	0.37590799	0.51623398
H	4.67275476	-0.55706298	0.44832799
H	4.85475683	1.14136696	0.76646900
C	3.08941698	0.28809801	1.66687799
H	2.82080698	1.30881703	1.96138704
H	3.58096099	-0.16632800	2.53780293
C	-2.62886095	1.10851598	-0.63068902
H	-1.76768994	1.19115806	-1.29347801
H	-3.52702403	1.09670997	-1.24797201
C	-2.66889000	2.25808191	0.35960099
H	-3.56196404	2.24236107	0.98495001
H	-2.68693590	3.18104196	-0.22155400
H	-1.78079998	2.29721904	0.99148297
C	-3.51941299	-0.49298799	1.07635200
H	-3.33016491	-1.48747694	1.47773194
H	-3.27399206	0.22323599	1.86041903
C	-4.96814108	-0.35477200	0.64516503
H	-5.18239594	0.62210500	0.20979300
H	-5.58883190	-0.46283200	1.53532100
H	-5.26546001	-1.13208199	-0.05900700
C	-2.67436695	-1.26048303	-1.15539896
H	-3.67741990	-1.10894799	-1.55111504

H	-1.95636404	-0.94776702	-1.91085899
C	-2.44017601	-2.70992494	-0.77500898
H	-1.40832400	-2.88291693	-0.46669900
H	-2.62620902	-3.31302094	-1.66481602
H	-3.11872911	-3.06082106	0.00358400

Frequencies -- 19.6416 44.7154 51.0698

Sum of electronic and zero-point Energies= -933.704566
Sum of electronic and thermal Energies= -933.682130
Sum of electronic and thermal Enthalpies= -933.681185
Sum of electronic and thermal Free Energies= -933.755547

3

Element	X	Y	Z
O	-1.70198298	-0.15572000	-1.04684603
O	0.38130301	-0.84035099	-1.16310596
O	-2.78208899	1.88685000	-0.29190901
O	-2.82954311	3.70525599	-1.55992401
O	2.13671088	0.01515000	0.31662101
N	2.69196010	2.28490901	0.26456800
B	-2.92568302	0.38829100	-0.19577099
B	1.70432603	-1.24721599	-0.31711900
C	-0.58775800	-0.38471699	-0.51116002
H	-0.45601499	-0.18217200	0.55602700
C	-2.95126390	2.50605702	-1.42908394
H	-3.20942593	1.85956395	-2.28180003
C	2.69612598	0.96669400	-0.48847100
H	2.14196610	1.13941205	-1.41647005
H	3.74292588	0.76455998	-0.73926699
C	-4.25397110	-0.23236400	-0.84697998
H	-4.34078789	-0.00173000	-1.91747999
C	-5.47380781	0.39846399	-0.14481300
H	-5.50858498	1.45991802	-0.42176300
H	-6.40420818	-0.04395100	-0.52222800
C	-5.46172190	0.30332899	1.39263797
H	-5.80417585	-0.68374002	1.70434403
H	-6.20031214	1.00581396	1.79316604
C	-4.09732389	0.60845202	2.03582907
H	-4.13287115	0.32147899	3.09421992
H	-3.93947291	1.69227505	2.01308393
C	-2.87929702	-0.04935600	1.34927404
H	-1.99539602	0.34282100	1.87346494
C	-2.85142803	-1.58563805	1.47230697
H	-1.87507904	-1.95139098	1.12599301
H	-2.91503000	-1.88262105	2.52671099
C	-3.94452691	-2.32465005	0.67742699
H	-3.66534901	-3.38075209	0.59808201
H	-4.87866211	-2.31320000	1.23930597
C	-4.18231297	-1.77050495	-0.73904699
H	-5.09694719	-2.22116804	-1.14440000
H	-3.36250997	-2.10864806	-1.38434005
C	2.71873403	-1.92400503	-1.35630000
H	3.00120592	-1.23876202	-2.16922688
C	4.00715113	-2.27111197	-0.57902700
H	4.72425413	-2.78340507	-1.23279405
H	4.48800993	-1.32921505	-0.28428400
C	3.79787207	-3.11766291	0.69123697
H	4.71338797	-3.07928991	1.29138899
H	3.67716503	-4.16555023	0.41582301
C	2.61531305	-2.66973901	1.56959701
H	2.91616392	-1.76875603	2.11736608
H	2.42382407	-3.44298410	2.32452202
C	1.32042205	-2.33123207	0.80097699
H	0.61433297	-1.92291796	1.54108703

C	0.64186901	-3.54376793	0.13594100
H	0.43601701	-4.32400417	0.87987202
H	-0.33748901	-3.22386003	-0.24450199
C	1.42745197	-4.16497517	-1.03461504
H	2.21369600	-4.81207514	-0.64539498
H	0.75765997	-4.82656717	-1.59419405
C	2.03211093	-3.13922596	-2.01306605
H	1.22749400	-2.75844789	-2.65195894
H	2.73311901	-3.65958595	-2.67831302
C	1.26486599	2.71640110	0.53792799
H	0.81429601	1.87961698	1.06999302
H	1.33029497	3.55454397	1.23101902
C	0.44844800	3.09064293	-0.68500900
H	0.84801602	3.96086597	-1.20694494
H	-0.55582500	3.34256911	-0.34153301
H	0.34700799	2.26861596	-1.39658904
C	3.42866993	3.28270507	-0.59485900
H	4.42683506	2.87692404	-0.75197202
H	2.92295790	3.28180003	-1.56022894
C	3.50049591	4.68594599	-0.02162700
H	2.51414108	5.11957216	0.14663200
H	4.01505899	5.31115007	-0.75200897
H	4.07199287	4.72666979	0.90562397
C	3.34870911	2.09895897	1.61799097
H	3.33623791	3.07755709	2.09512091
H	2.68288994	1.43946803	2.17113400
C	4.74794197	1.51615095	1.57830799
H	4.74580812	0.49162599	1.20497203
H	5.11673117	1.49162400	2.60466003
H	5.44590378	2.11802912	0.99549103

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Frequencies -- 11.4675 17.2052 26.6867

Sum of electronic and zero-point Energies= -1460.770333
Sum of electronic and thermal Energies= -1460.736096
Sum of electronic and thermal Enthalpies= -1460.735152
Sum of electronic and thermal Free Energies= -1460.836616

7. References

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