# Supporting Information

***for***

# Taming the parent oxoborane

Gargi Kundu,[a,b] P. R. Amrutha,[a] K. Vipin Raj,[b,c] Srinu Tothadi,[b,d] Kumar Vanka,[b,c] and Sakya S. Sen*[a,b]

[a]*Inorganic Chemistry and Catalysis Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune 411008, India;* [b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India;*[c] *Physical and Materials Chemistry Division CSIR-National Chemical Laboratory Dr. Homi Bhabha Road, Pashan, Pune 411008, India;* [d]*Analytical and Environmental Science Division, CSIR-Central Salt & Marine Chemicals Research Institute, Gijubhai Badheka Marg, Bhavnagar-364002, India.*

Author to whom correspondence should be addressed: E-mail: ss.sen@ncl.res.in

**Table of Contents**

## S1. General procedures and instrumentation

All manipulations were carried out in an inert atmosphere of argon using standard Schlenk techniques and in argon filled glove box. The solvents, especially toluene, tetrahydrofuran, dichloromethane and *n*-hexane were purified by MBRAUN solvent purification system MB SPS-800. Other chemicals were purchased from Sigma Aldrich and TCI Chemicals and were used without further purification. The starting material, 6-SIDipp was synthesized by using literature procedure.[1] The $^{1}H$, $^{13}C$, and $^{11}B$ NMR spectra were recorded in $CDCl_3$, using a Bruker Avance DPX 400, and a Bruker Avance DPX 500 spectrometer. Chemical shifts (δ) are given in ppm. NMR spectra were referenced to external $SiMe_4$ ($^{1}H$ and $^{13}C$), $BF_3{\cdot}OEt_2$ ($^{11}B$). High resolution mass spectra (HRMS) were obtained using a Q Exactive Thermo Scientific, and IR spectra were recorded on Perkinelmer spectrum two FTIR Spectrometer at the CSIR National Chemical Laboratory, Pune. Elemental analyses were performed at the CSIR National Chemical Laboratory, Pune, India.

## S2. Synthetic procedure and spectroscopic characterization of 1-3

**1**: 1.2 equivalent of gallium chloride (0.11 g, 0.58 mmol) and 6-SIDipp-$BH_3$ (0.20 g, 0.48 mmol) were taken in a Schlenk flask and 10 ml of toluene was added to the reaction mixture. The reaction was run for 6 hours at room temperature which afforded white precipitation. The toluene solution was concentrated to 2 ml and the precipitate was filtered through cannula. The precipitate was further dissolved in 5 ml dichloromethane solution and colorless crystals of **1** was isolated after keeping the solution at 4 °C for a day with 80 % yield (0.23 g).

$^{1}H$ NMR (400 MHz, 298 K, $CDCl_3$): $\delta$ = 1.30 (d, $J$ = 6.8 Hz, 12 H, $CH(CH_3)_2$), 1.38 (d, $J$ = 6.8 Hz, 12 H, $CH(CH_3)_2$), 2.40 (quint, $J$ = 5.1 Hz, 2 H, $NCH_2CH_2CH_2N$), 2.93 (sept, $J$ = 6.8 Hz, 4 H,

C*H*($CH_3$)$_2$), 3.64 (t, *J* = 5.5 Hz, 4 H, NC*H*$_2$C$H_2$C*H*$_2$N), 7.25 (m, 4 H, Ar-*H*), 7.41 (t, *J* = 7.6 Hz, 2 H, Ar-*H*) ppm.

$^{13}$C{$^1$H} NMR (125 MHz, 298 K, $CDCl_3$): $\delta$ = 18.8 ($CH_2CH_2CH_2$), 22.5 ($CH(CH_3)_2$), 26.5 ($CH(CH_3)_2$), 29.1 ($CH(CH_3)_2$), 48.4 ($NCH_2$), 124.9 (Ar-*C*), 128.2 (Ar-*C*), 129.0 (Ar-*C*), 130.9 (Ar-*C*), 131.54 (Ar-*C*), 135.7 (Ar-*C*), 136.5 (Ar-*C*), 145.8 (Ar-*C*), 146.2 (Ar-*C*) ppm, N*C*N signal not observed.

$^{11}$B{$^1$H} NMR (128 MHz, 298 K, $CDCl_3$): $\delta$ = -27.4 (quartet, 1 B, $BH_2$Ga) ppm.

ESI-MS ($CH_3CN$): m/z Calcd. for $C_{28}H_{43}N_2BGaCl_3$ $[M+2H]^+$ 600.1903, found 600.1685.

Anal. Calcd for $C_{28}H_{43}BCl_3GaN_2$: C, 56.57; H, 7.29; N, 4.71. Found: C, 56.88; H, 7.40; N, 4.62.

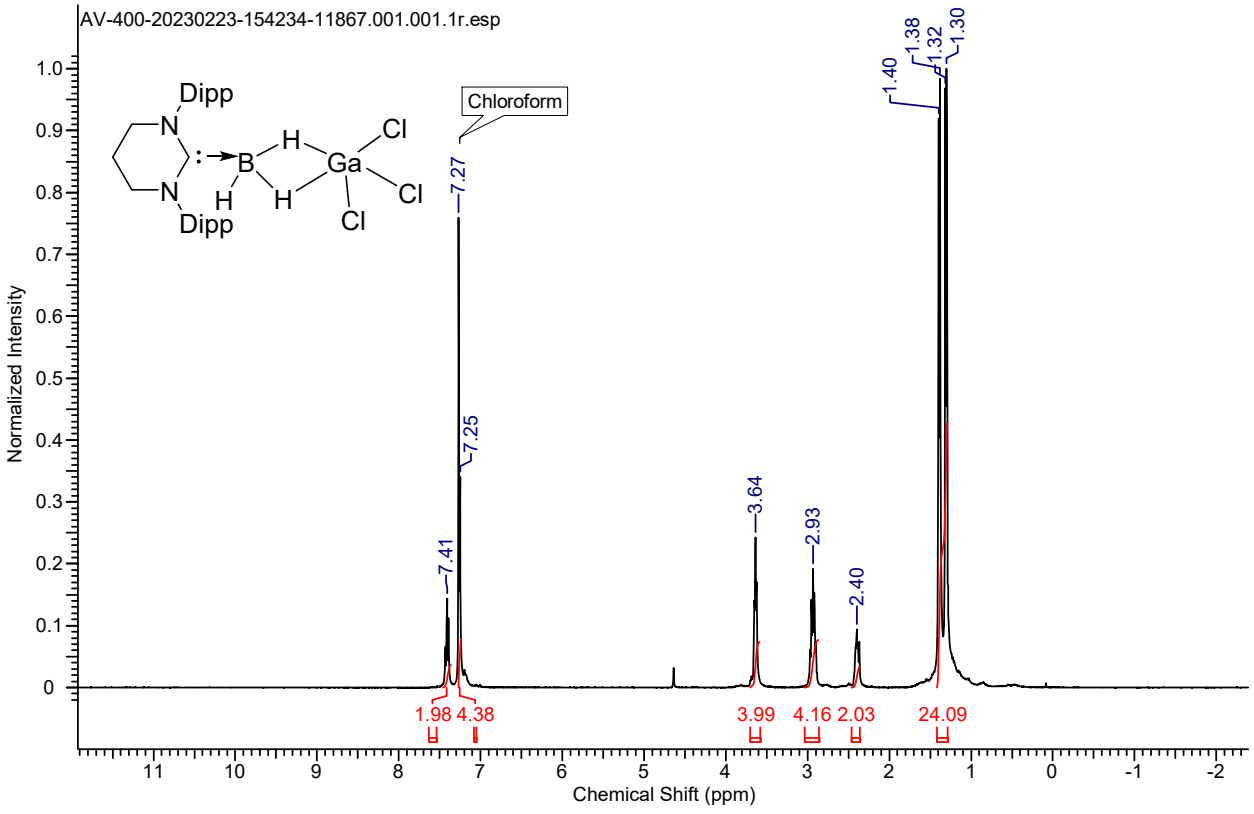



Figure S1. $^1$H NMR spectrum of **1**.

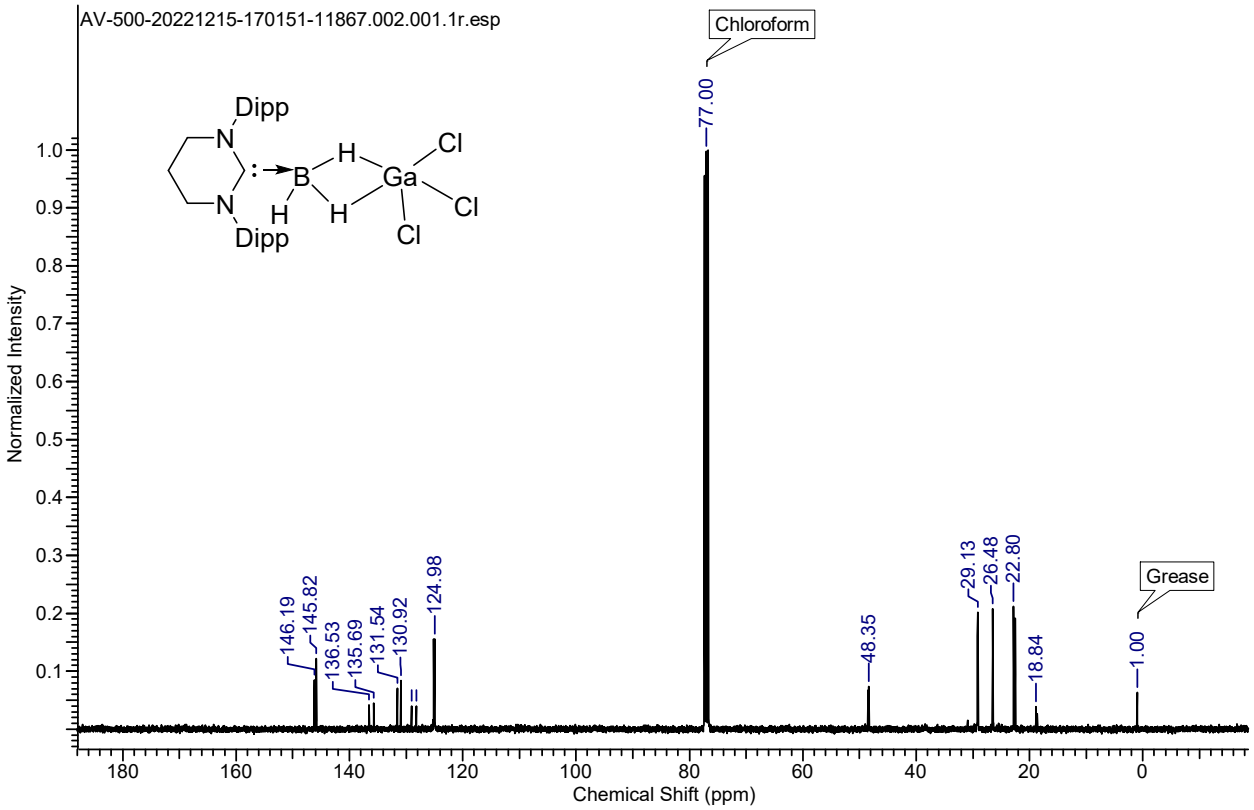



Figure S2. $^{13}$C NMR spectrum of **1**.

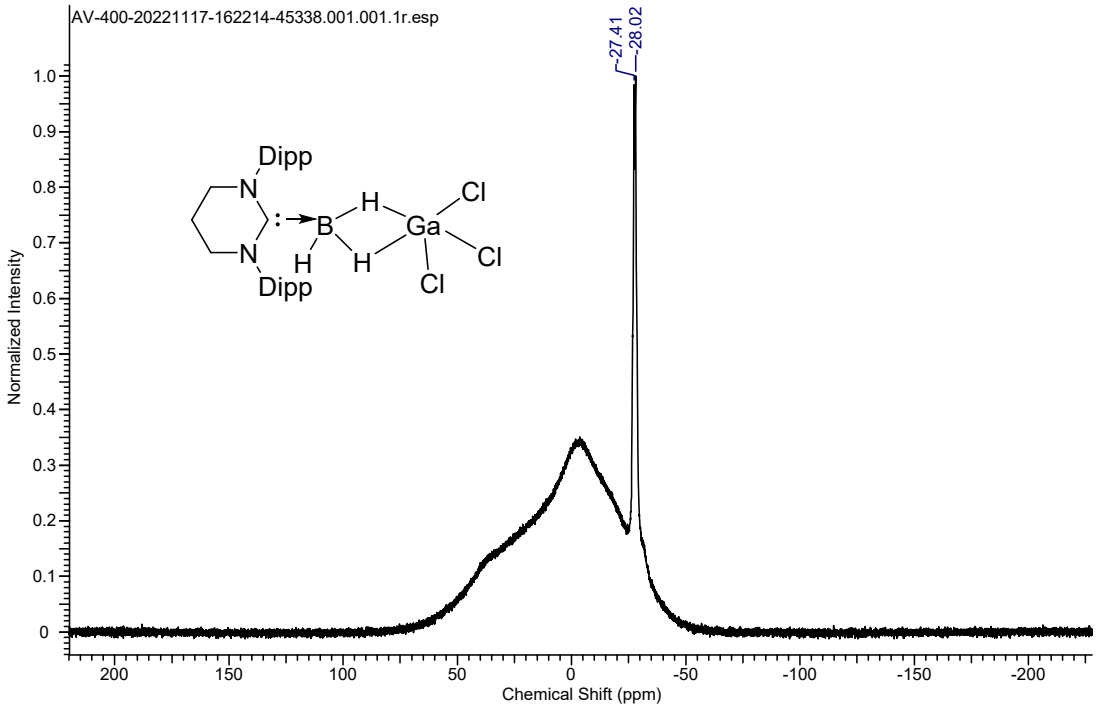



Figure S3. $^{11}$B NMR spectrum of **1**.

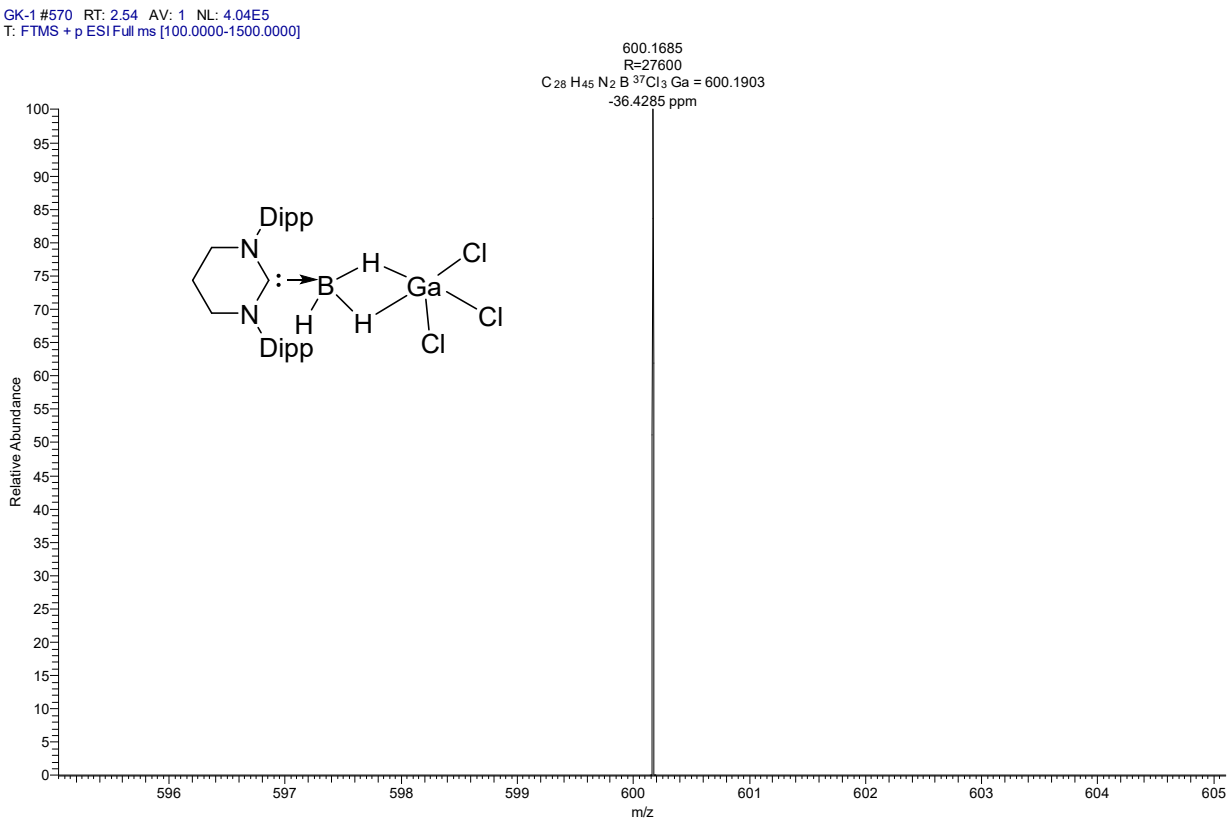



Figure S4. ESI Mass spectrum of **1**.

**2**: 1.1 equivalent of degassed water (6.6 µL, 0.37 mmol) was added to a 10 ml toluene a solution of **1** (0.20 g, 0.34 mmol) at -30 °C in a Schlenk flask. Stirring the resultant mixture for further 6 hours at room temperature accessed a colorless solution. The toluene solution was dried completely and washed with hexane. 5 ml of toluene was added to dissolve the white precipitate and the toluene solution was filtered through the cannula filtration. Colorless crystals of **2**·$GaCl_3$ were isolated after keeping the solution at room temperature for 2-3 days with 58 % yield (0.12 g).

$^1$H NMR (400 MHz, 298 K, $CDCl_3$): $\delta$ = 1.27 (d, $J$ = 6.9 Hz, 12 H, $CH(CH_3)_2$), 1.39 (d, $J$ = 6.8 Hz, 12 H, $CH(CH_3)_2$, 2.48 (quint, $J$ = 5.8 Hz, 2 H, $NCH_2CH_2CH_2N$), 3.01 (sept, $J$ = 6.8 Hz, 4 H,

C*H*($CH_3$)$_2$), 3.71 (t, *J* = 5.8 Hz, 4 H, NC*H*$_2$C$H_2$C*H*$_2$N), 4.64 (s, 1 H, B*H*OGa), 7.23 (d, *J* = 7.8 Hz, 4 H, Ar-*H*), 7.43 (t, *J* = 7.8 Hz, 2 H, Ar-*H*) ppm.

$^{13}$C{$^1$H} NMR (101 MHz, 298 K, $CDCl_3$): $\delta$ = 22.5 ($CH_2CH_2CH_2$), 26.5 ($CH(CH_3)_2$), 29.3 ($CH(CH_3)_2$), 48.4 ($NCH_2$), 125.2 (Ar-*C*), 129.0 (Ar-*C*), 131.7 (Ar-*C*), 135.6 (Ar-*C*), 146.1(Ar-*C*) ppm, N*C*N signal not observed.

$^{11}$B{$^1$H} NMR (128 MHz, 298 K, $CDCl_3$): $\delta$ = 21.6 (s, 1 B, *B*HOGa) ppm.

HRMS ($CH_3CN$): m/z Calcd. for $C_{28}H_{41}BCl_3GaO_2N_2$ $[M+H]^+$ 607.1706, found 607.1782.

IR (ATR, cm$^{-1}$): 1665 ($\upsilon_{B=O}$).

Anal. Calcd for $C_{28}H_{41}BCl_3GaN_2O$: C, 55.27; H, 6.79; N, 4.60. Found: C, 53.92; H, 5.20; N, 3.31.

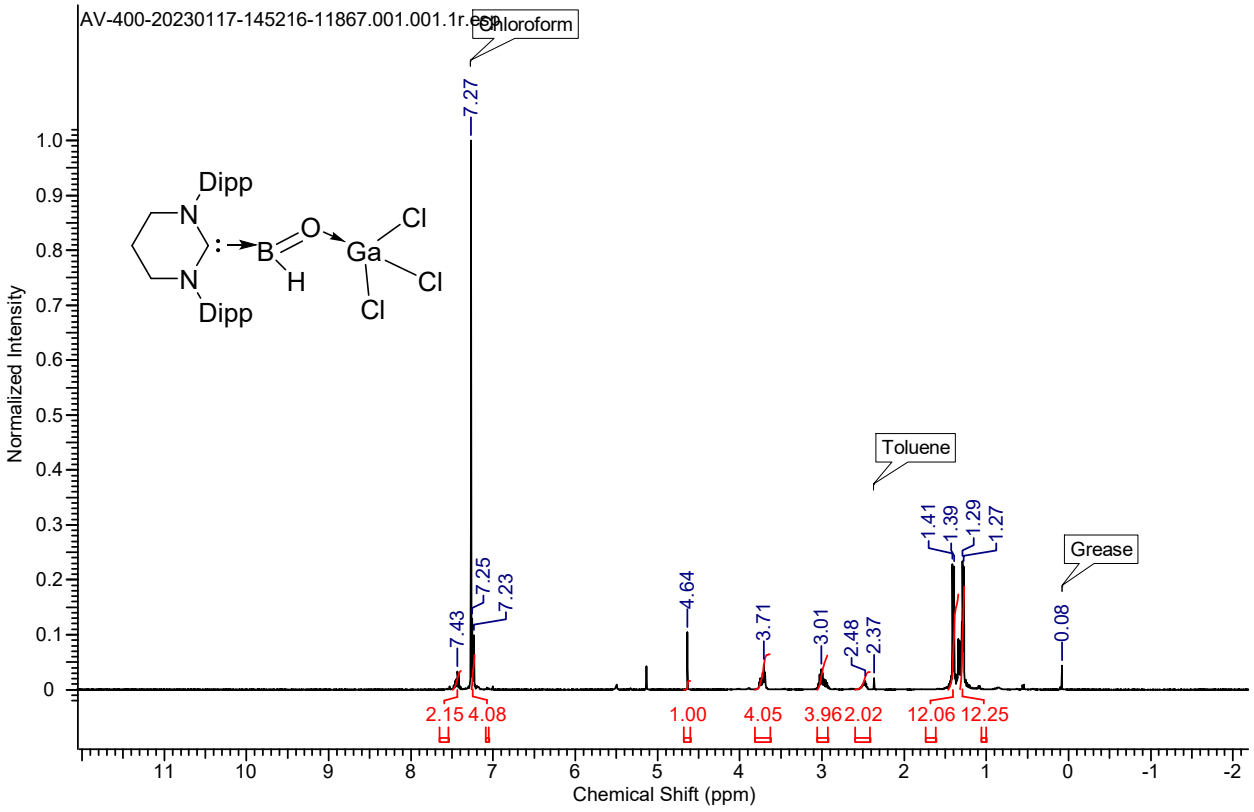



Figure S5. $^1$H NMR spectrum of **2**.

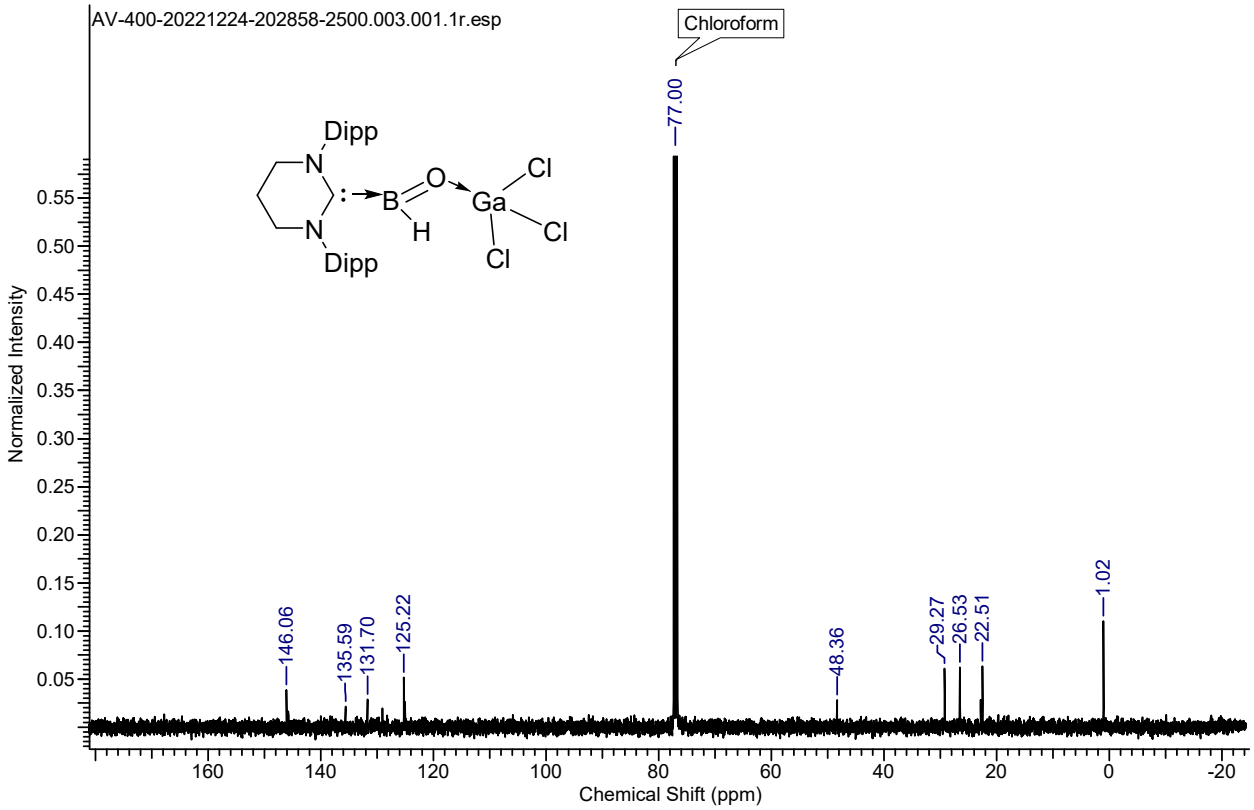



Figure S6. $^{13}C$ NMR spectrum of **2**.

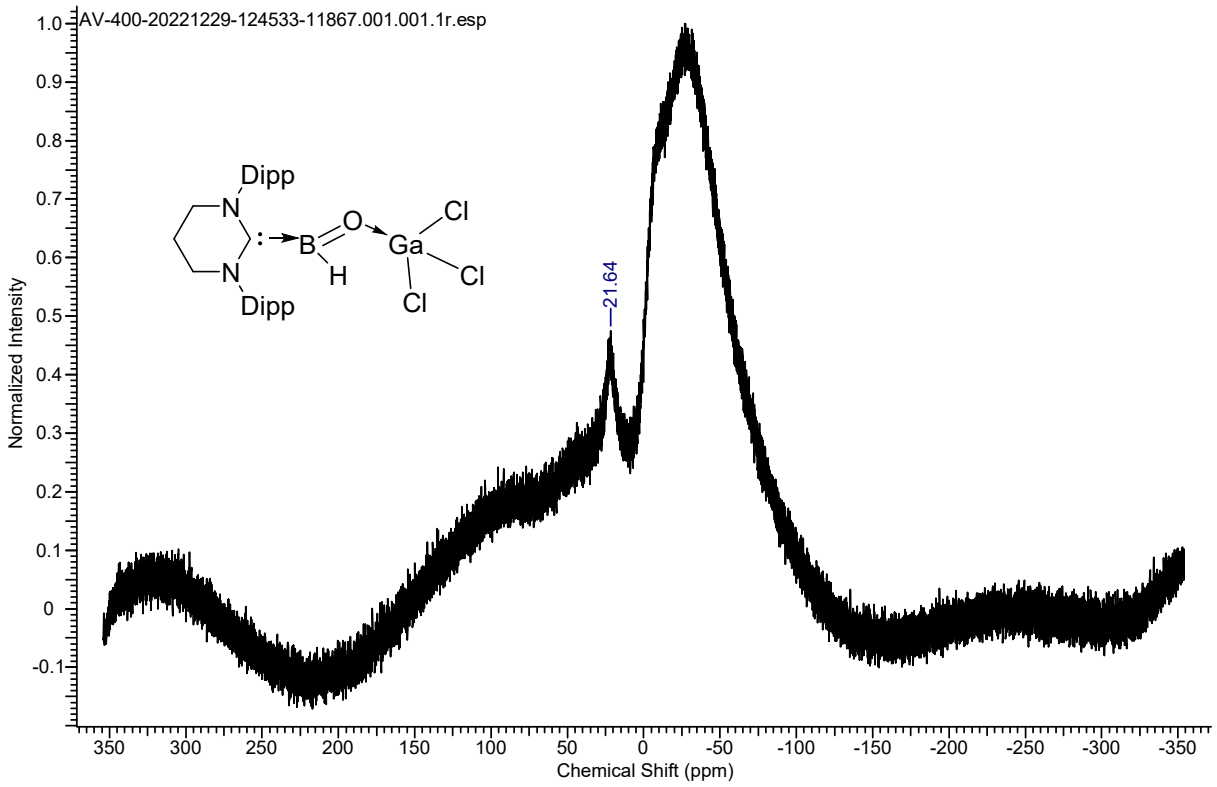



Figure S7. $^{11}$B NMR spectrum of **2**.

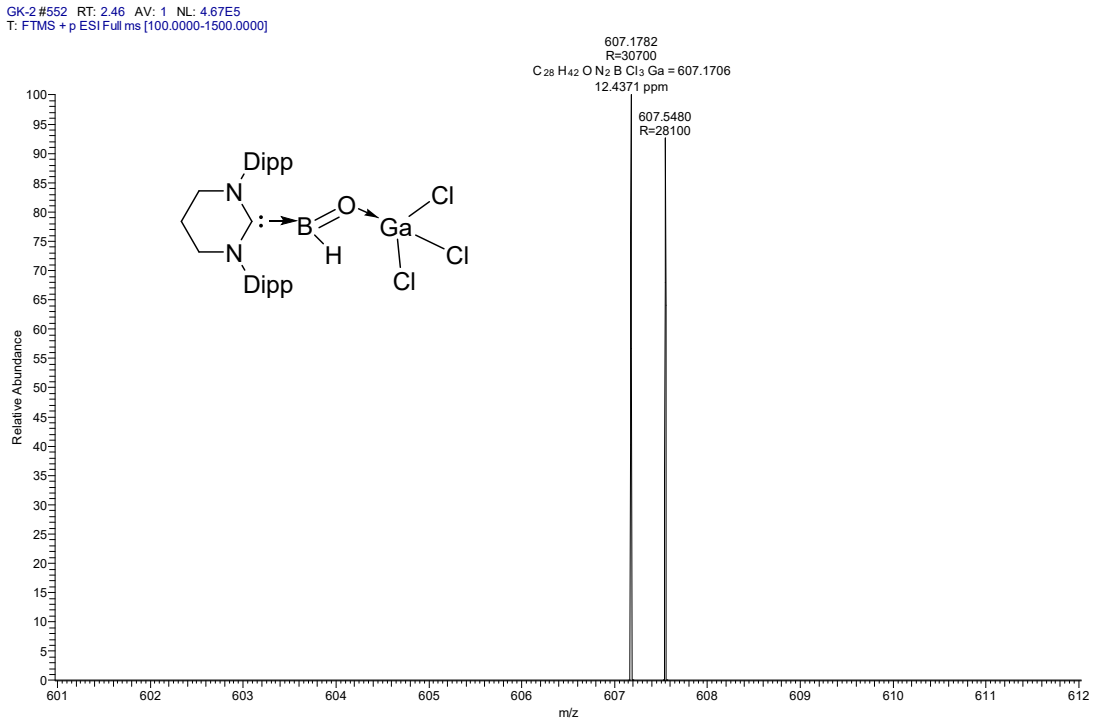



Figure S8. HRMS spectrum of **2**.

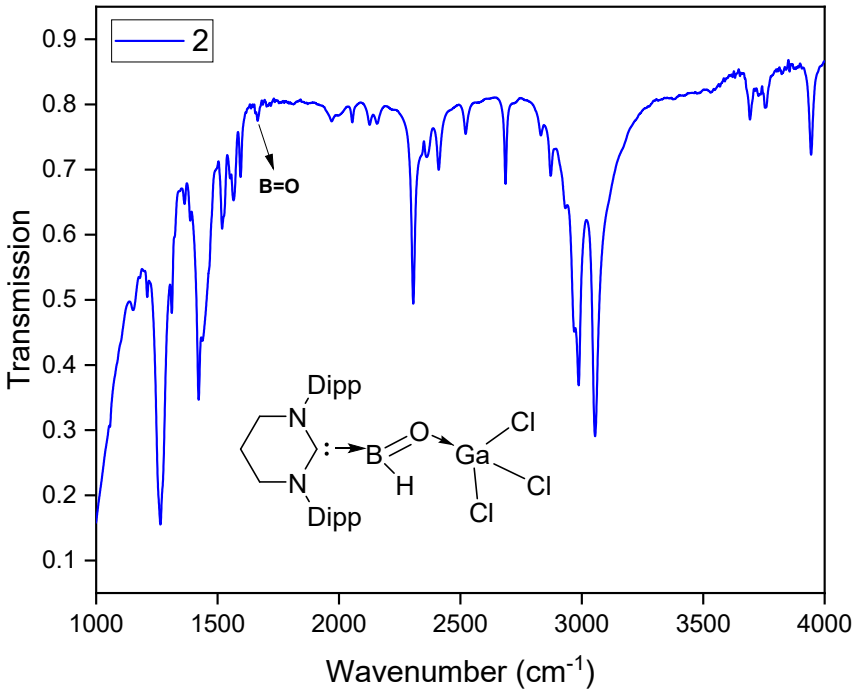
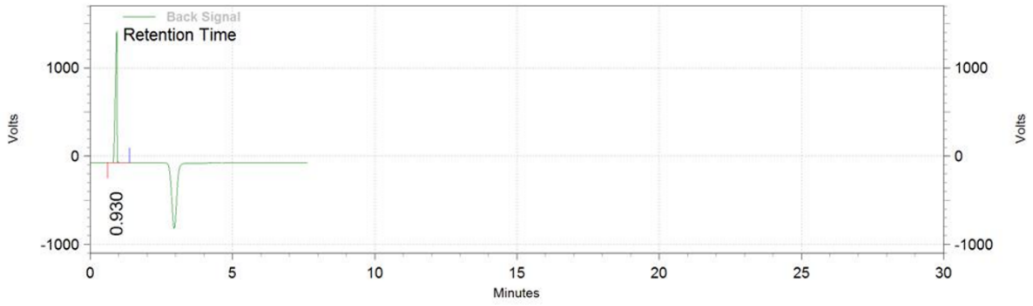



Figure S9. IR spectrum of **2**.




**Back Signal**
**Results**

| Retention Time | Area | Area % | Height | Height % |
|---|---|---|---|---|
| 0.930 | 48534314 | 100.00 | 11534638 | 100.00 |
| Totals | 48534314 | 100.00 | 11534638 | 100.00 |

Figure S10. Gas chromatogram and area % of hydrogen production of **2**.

**3**: 1.1 equivalent of degassed water (6.5 μL, 0.36 mmol) was added to a 10 ml toluene a solution of **2** (0.20 g, 0.33 mmol) at -30 °C in a Schlenk flask. Stirring the resultant mixture for further 3 hours at room temperature accessed a colorless solution. The toluene solution was dried completely and washed with hexane. 5 ml of toluene was added to dissolve the white precipitate and the toluene solution was filtered through the cannula filtration. Colorless crystals of **3** were isolated after keeping the solution at room temperature for 2-3 days with 62 % (0.13 g) yield.

$^{1}$H NMR (500 MHz, 298 K, $CDCl_3$): $\delta$ = 1.27 (d, $J$ = 6.9 Hz, 12 H, CH(C$H_3$)$_2$), 1.36 (d, $J$ = 6.6 Hz, 12 H, CH(C$H_3$)$_2$), 2.52 (quint, $J$ = 5.5 Hz, 2 H, NCH$_2$C$H_2$CH$_2$N), 2.97 (sept, $J$ = 6.8 Hz, 4 H, C$H$(CH$_3$)$_2$), 3.76 (t, $J$ = 6.1 Hz, 4 H, NC$H_2$CH$_2$C$H_2$N), 7.17 (d, $J$ = 7.4 Hz, 4 H, Ar-$H$), 7.48 (t, $J$ = 7.9 Hz, 2 H, Ar-$H$) ppm.

$^{13}$C{$^{1}$H} NMR (125 MHz, 298 K, $CDCl_3$): $\delta$ = 22.5 (CH$_2$$C$H$_2$CH$_2$), 26.2 (CH($C$H$_3$)$_2$), 28.8 ($C$H(CH$_3$)$_2$), 48.0 (N$C$H$_2$), 124.7 (Ar-$C$), 127.0 (Ar-$C$), 130.6 (Ar-$C$), 136.4 (Ar-$C$), 145.5 (Ar-$C$) ppm, N$C$N signal not observed.

$^{11}$B{$^{1}$H} NMR (128 MHz, 298 K, $CDCl_3$): $\delta$ = 23.6 (bs, 1 B, $B$(OH)OGa) ppm.

HRMS ($CH_3CN$): m/z Calcd. for $C_{28}H_{41}BCl_3GaO_2N_2$ [M+Na-Cl]$^+$ 614.1727, found 614.1696.

IR (ATR, cm$^{-1}$): 1697 ($\upsilon_{B=O}$), 3430 ($\upsilon_{OH}$).

Anal. Calcd for $C_{28}H_{41}BCl_3GaN_2O_2$: C, 53.85; H, 6.62; N, 4.49. Found: C, 51.27; H, 6.23; N, 4.21.

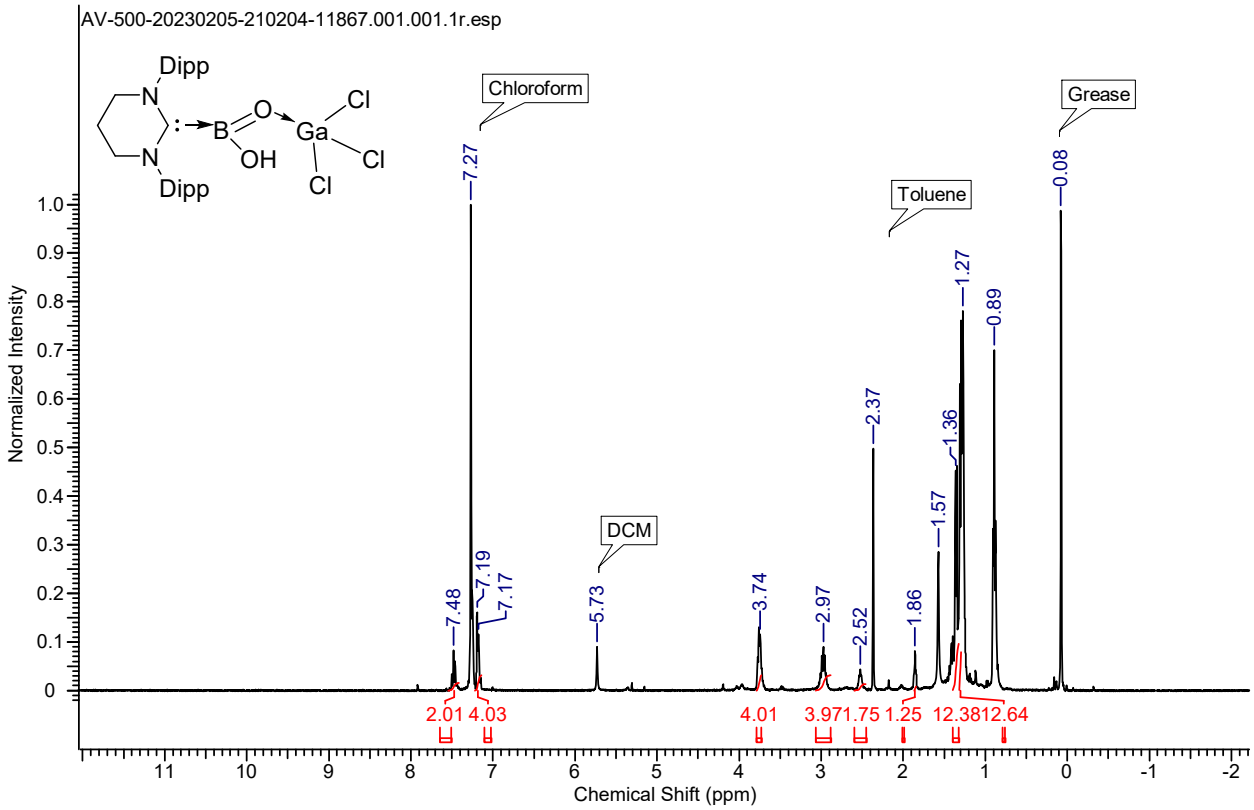



Figure S11. $^{1}$H NMR spectrum of **3**.

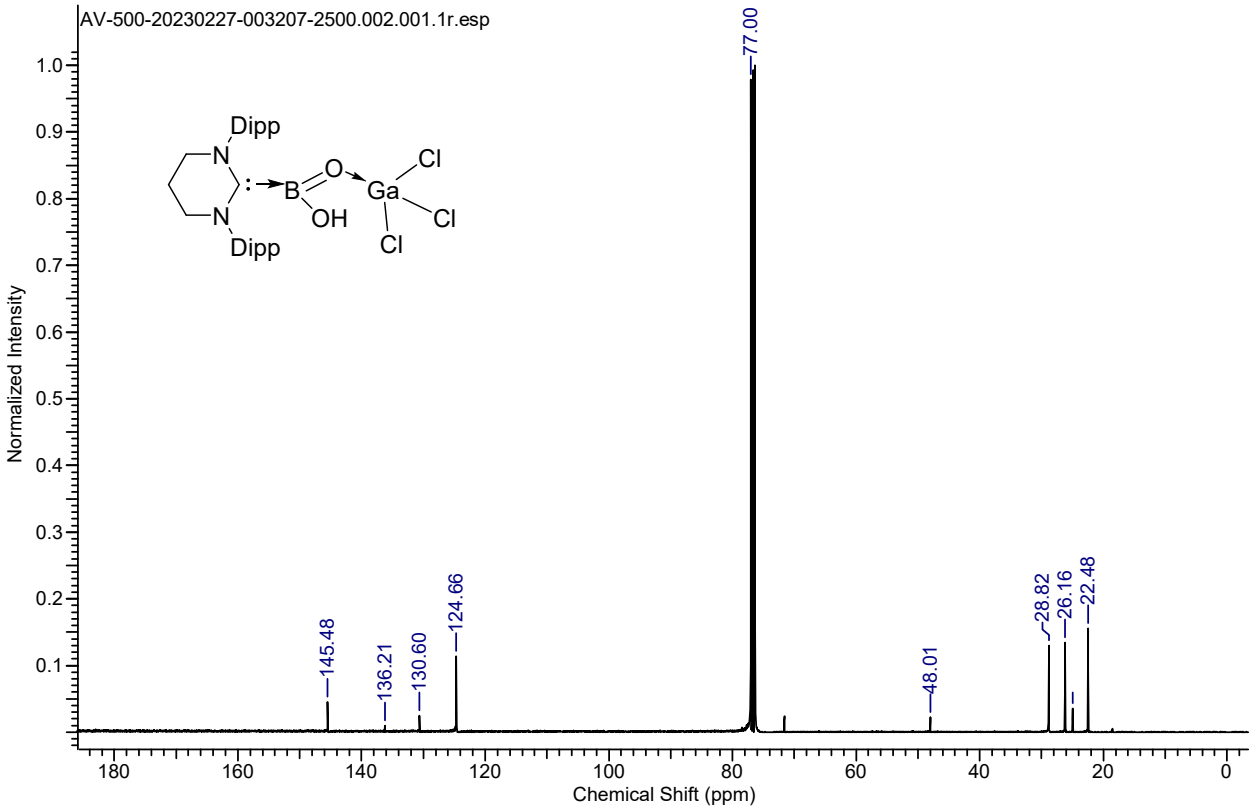



Figure S12. $^{13}C$ NMR spectrum of **3**.

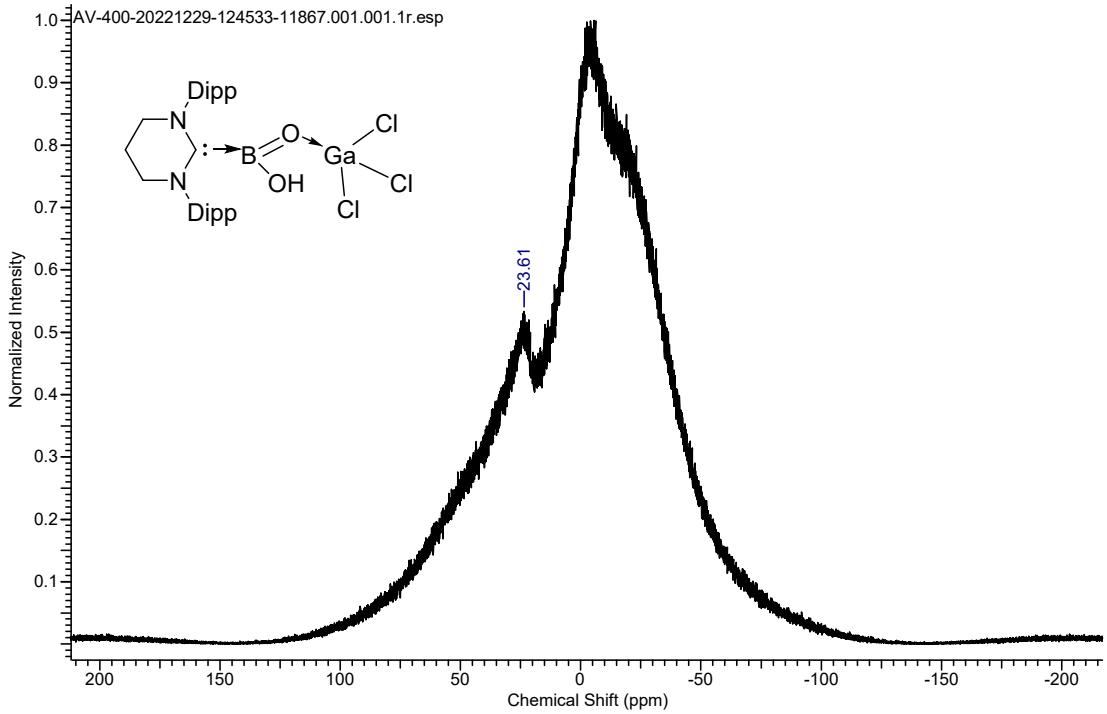


Figure S13. $^{11}B$ NMR spectrum of **3**.

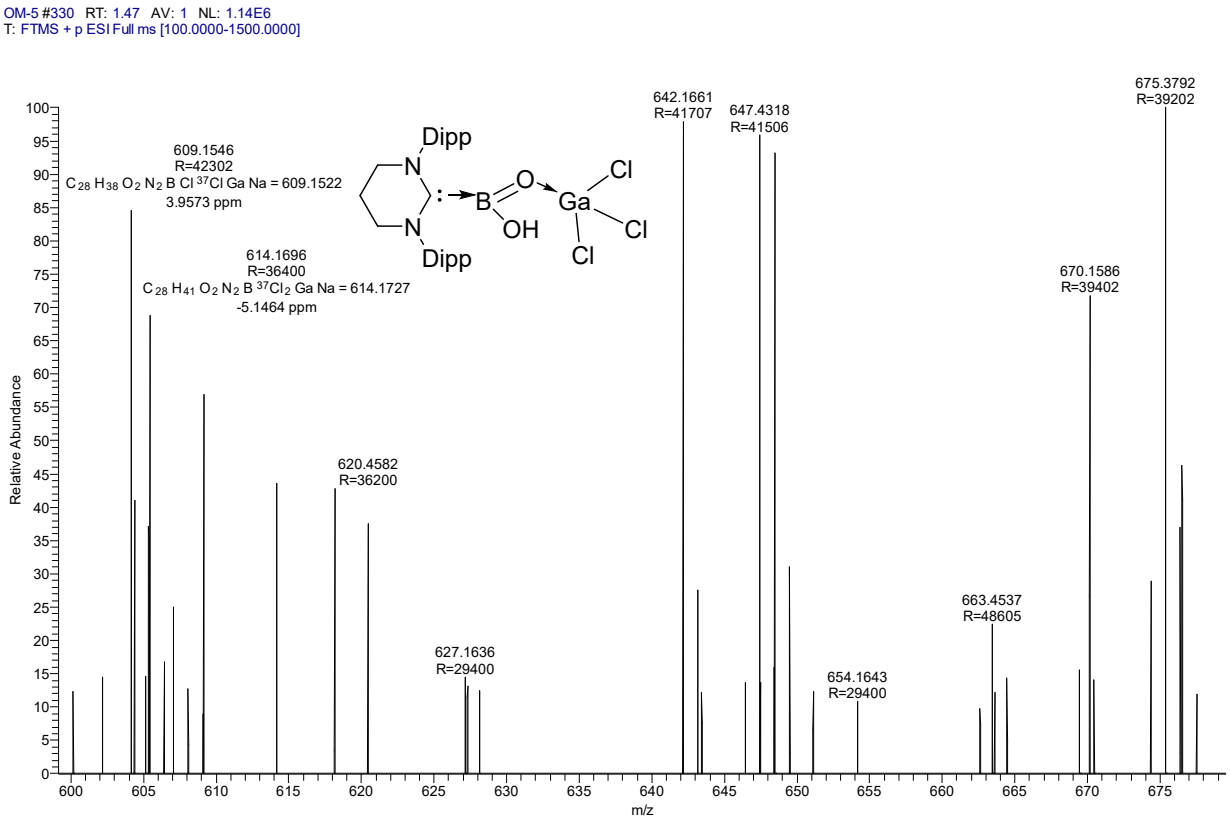



Figure S14. HRMS spectrum of **3**.

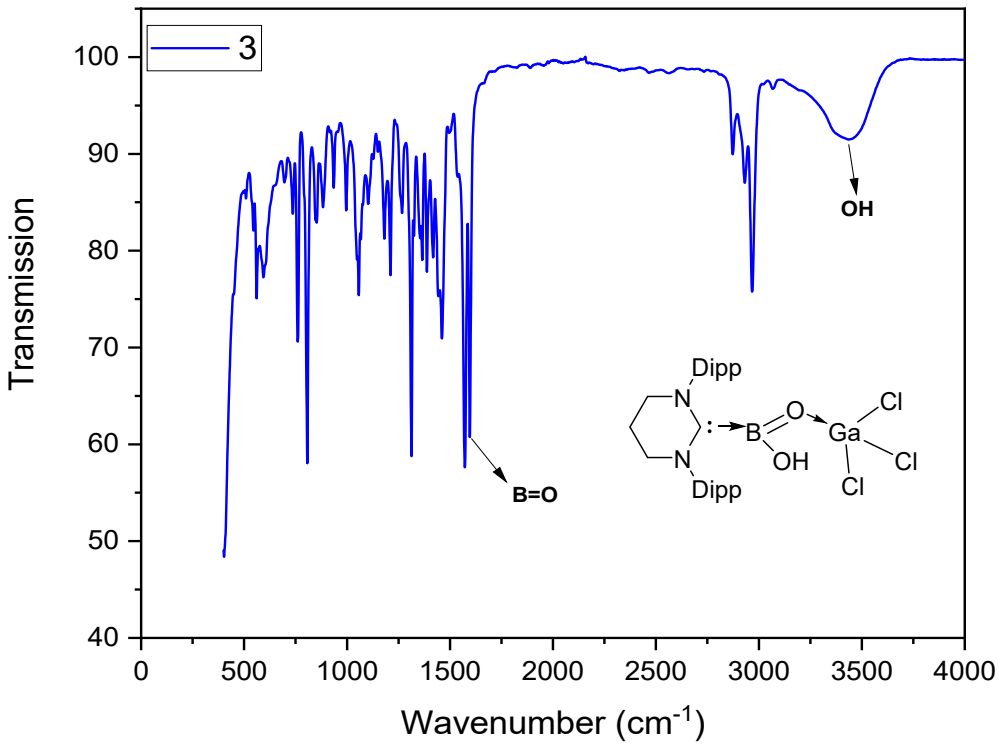



Figure S15. IR spectrum of **3**.

**S3. Crystallographic data for the structural analysis of compounds 1-3**

Single crystals of **1-3** were mounted on a Bruker SMART APEX II single crystal X-ray CCD diffractometer having graphite monochromatised (Mo-Kα = 0.71073 Å) radiation at low temperature 100 K. The X-ray generator was operated at 50 kV and 30 mA. The X-ray data acquisition was monitored by APEX2 program suit. The data were corrected for Lorentz-polarization and absorption effects using SAINT and SADABS programs which are an integral part of APEX2 package.[2] The structures were solved by direct methods and refined by full matrix least squares, based on $F^2$, using SHELXL Crystal structures were refined using Olex2-1.0 software. Anisotropic refinement was performed for all non-H atom. The C-H hydrogen atoms were calculated using the riding model.[3] The structures were examined using the ADSYM

subroutine of PLATON to assure that no additional symmetry could be applied to the models. The molecular weight of each structure mentioned herein has been calculated considering the solvent molecules trapped in the crystal. Crystallographic information is available at www.ccdc.cam.ac.uk/data or as part of Supporting Information.

| **Identification code** | **1** | **2** | **3** |
|---|---|---|---|
| Empirical formula | $C_{29}H_{45}BCl_5GaN_2$ | $C_{28}H_{41}BCl_6Ga_2N_2O$ | $C_{29}H_{43}BCl_5GaN_2O_2$ |
| Formula weight | 679.45 | 784.58 | 709.43 |
| Temperature/K | 100.0 | 100.0 | 100.00 |
| Crystal system | monoclinic | triclinic | monoclinic |
| Space group | $P2_1/m$ | $P$-1 | $P2_1/m$ |
| a/Å | 10.1202(5) | 10.613(4) | 10.6403(13) |
| b/Å | 16.2970(8) | 11.052(4) | 16.180(2) |
| c/Å | 10.7828(5) | 18.616(7) | 10.8244(12) |
| α/° | 90 | 76.655(13) | 90 |
| β/° | 107.539(2) | 88.743(12) | 111.793(4) |
| γ/° | 90 | 66.846(13) | 90 |
| Volume/Å$^3$ | 1695.72(14) | 1947.7(13) | 1730.3(4) |
| Z | 2 | 2 | 2 |
| $\rho_{calc}$g/cm$^3$ | 1.331 | 1.338 | 1.362 |
| μ/mm$^{-1}$ | 1.226 | 1.817 | 1.209 |
| F(000) | 708.0 | 800.0 | 736.0 |
| Crystal size/mm$^3$ | 0.14 × 0.1 × 0.05 | 0.14 × 0.13 × 0.08 | 0.15 × 0.11 × 0.05 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.22 to 49.986 | 4.186 to 62.198 | 4.122 to 55.11 |
| Index ranges | -12 ≤ h ≤ 12, -19 ≤ k ≤ 19, -12 ≤ l ≤ 12 | -15 ≤ h ≤ 15, -15 ≤ k ≤ 16, -26 ≤ l ≤ 26 | -13 ≤ h ≤ 13, -21 ≤ k ≤ 21, -14 ≤ l ≤ 14 |
| Reflections collected | 37086 | 115182 | 58209 |
| Independent reflections | 3091 [$R_{int}$ = 0.0890, $R_{sigma}$ = 0.0382] | 12343 [$R_{int}$ = 0.0651, $R_{sigma}$ = 0.0393] | 4107 [$R_{int}$ = 0.0654, $R_{sigma}$ = 0.0240] |
| Data/restraints/parameters | 3091/0/195 | 12343/0/373 | 4107/13/203 |
| Goodness-of-fit on $F^2$ | 1.028 | 1.038 | 1.128 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0394, w$R_2$ = 0.0932 | $R_1$ = 0.0530, w$R_2$ = 0.1313 | $R_1$ = 0.0711, w$R_2$ = 0.1884 |
| Final R indexes [all data] | $R_1$ = 0.0476, w$R_2$ = 0.0989 | $R_1$ = 0.0741, w$R_2$ = 0.1423 | $R_1$ = 0.0738, w$R_2$ = 0.1899 |
| Largest diff. peak/hole / e | 1.14/-0.86 | 2.05/-1.18 | 2.25/-0.96 |

| | | | |
|---|---|---|---|
| $Å^{-3}$ | | | |
| CCDC No | 2234583 | 2234584 | 2234585 |

## S4. Molecular structure of 2

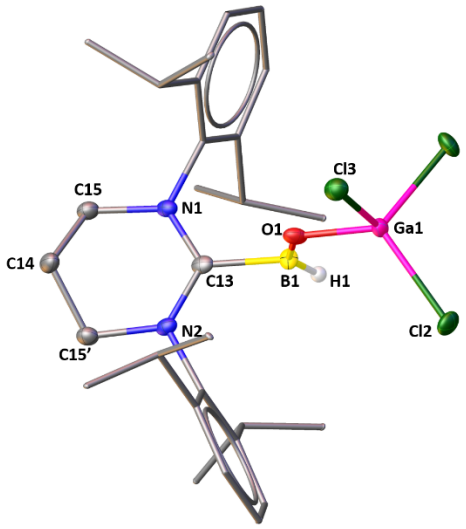
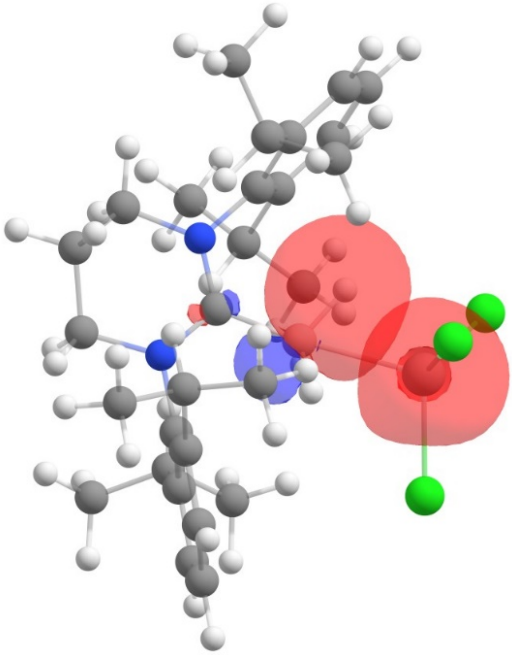



Figure S16. The molecular structure of **2**. Hydrogen atoms (Except the hydrogen attached with boron atom) are omitted for clarity.

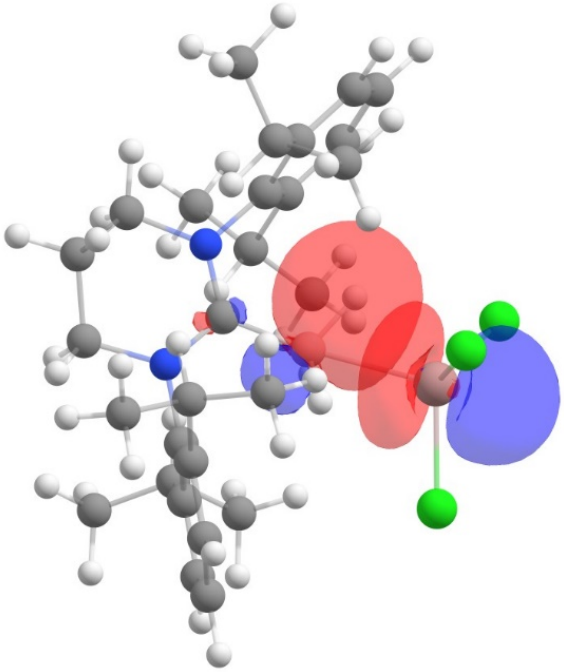
## S5. Computational details

All of the geometry optimizations in this study were performed using density functional theory (DFT) with the aid of the Gaussian 09 suite of programs,[4] employing the B3LYP functional[5] and empirical dispersion correction (DFT-D3).[6] The def2-TZVP basis set was used.[7] Additionally, NBO analysis[8] was conducted at the same level of theory using optimized geometries.

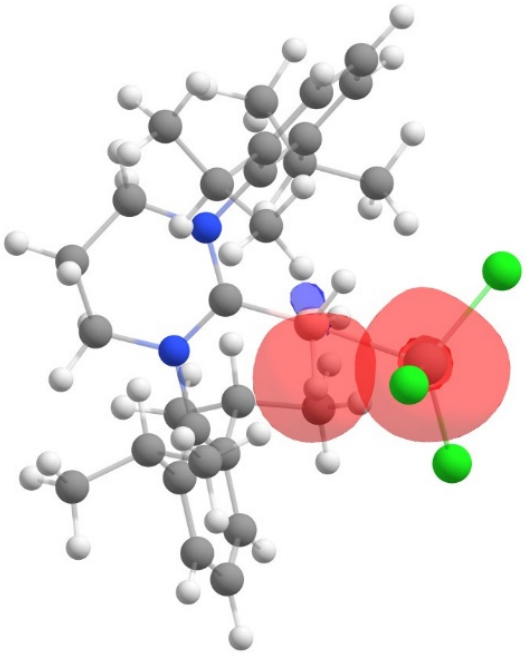
(i) NBO analysis of **1** and **3**



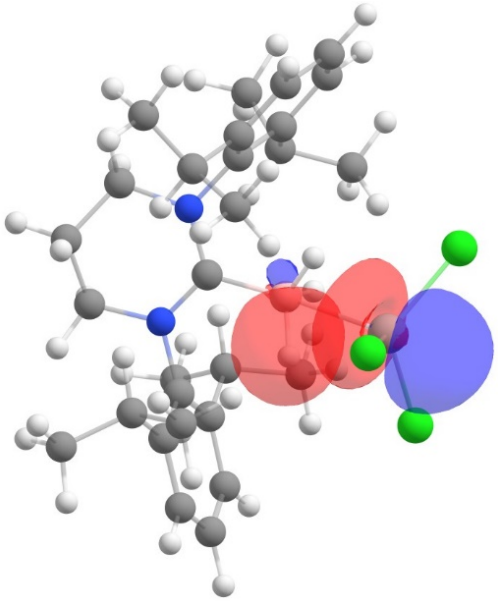
(a) BD (1) B (41) – H (43) ⟶ LP*(1) Ga (1) E(2) = 24.3 kcal/mol



(b) BD (1) B (41) – H (43) ⟶ LP*(4) Ga (1) E(2) = 27.6 kcal/mol

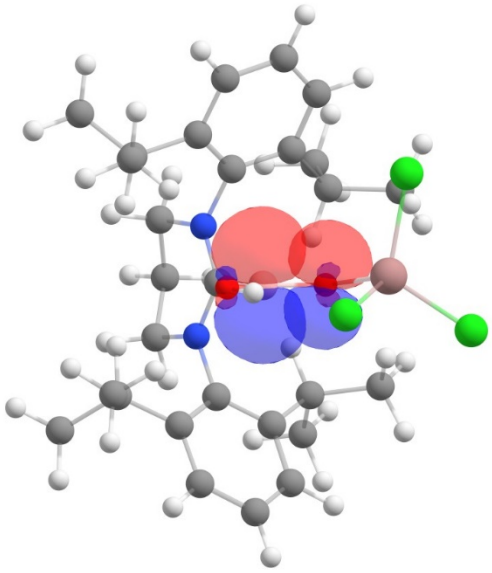


(c) BD (1) B (41) – H (77) ⟶ LP*(1) Ga (1) E(2) = 24.3 kcal/mol



(c) BD (1) B (41) – H (77) ⟶ LP*(4) Ga (1) E(2) = 27.6 kcal/mol

Figure S17. The NBO plots for the intra-molecular desired donor-acceptor interactions in compound **1** between the B-H bonds and gallium.



LP (3) O (4) ⟶ LP*(1) B (7) E(2) = 66.1 kcal/mol

Figure S18. The NBO plot of intra-molecular desired donor-acceptor interactions in compound **3** between oxygen and boron atoms.

**S6. References**


1. M. Iglesias, D. J. Beetstra, J. C. Knight, L.-L. Ooi, A. Stasch, S. Coles, L. Male, M. B. Hursthouse, K. J. Cavell, A. Dervisi and I. A. Fallis, *Organometallics,* 2008, **27**, 3279–3289.

2. APEX3, SAINT-Plus and SADABS; Bruker AXS Inc.: Madison, WI, USA, 2006. (b) Apex CCD and SAINT v8.30C; Bruker AXS Inc.: Madison, WI, USA, 2013.

3. (a) G. M. Sheldrick, *Acta Crystallogr. Sect. A*: 2008, **64**, 112–122; (b) L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Crystallogr.,* 2015, **48**, 3–10; (c) L. Krause, R. Herbst-Irmer and D. Stalke, *J. Appl. Crystallogr.,* 2015, **48**, 1907–1913.

4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota,

R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, S27 N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz and J. Cioslowski, D. J. Fox, Gaussian 09, rev. E.01; Gaussian, Inc., Wallingford, CT, 2013.

5. A. D. Becke, *J. Chem. Phys*. 1993, **98**, 5648-5652.

6. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.,* 2010, **132**, 154104 (1–19).

7. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys*., 2005, **7**, 3297–3305.

8. E. D. Glendening, A. E. Reed, J. E. Carpenter and F. Weinhold, NBO Version 3.1. Gaussian Inc., Pittsburgh. 2003.

## S7. B3LYP-D3/def2-TZVP optimized geometries of 1-3.

(a) **1**

78

| | | | |
|---|---|---|---|
| Ga | -2.728533 | 0.196853 | 0.000000 |
| Cl | -3.444179 | -0.808224 | 1.806783 |
| Cl | -3.003921 | 2.364291 | 0.000000 |
| N | 1.799073 | -0.052398 | 1.155624 |
| C | 1.128640 | -0.062909 | -0.000000 |
| C | 1.109666 | -0.095834 | 2.425307 |
| C | 0.734593 | -1.335118 | 2.960345 |
| C | 0.097938 | -1.333421 | 4.200390 |
| H | -0.219539 | -2.270880 | 4.636904 |
| C | -0.153049 | -0.149749 | 4.875253 |
| H | -0.661547 | -0.170988 | 5.830692 |
| C | 0.230718 | 1.062581 | 4.323167 |

| | | | |
|---|---|---|---|
| H | 0.014748 | 1.981713 | 4.852073 |
| C | 0.871607 | 1.116430 | 3.087994 |
| C | 1.258945 | 2.458942 | 2.490077 |
| H | 1.741504 | 2.275513 | 1.529300 |
| C | 2.269462 | 3.201310 | 3.376296 |
| H | 1.832328 | 3.459154 | 4.342724 |
| H | 2.585403 | 4.130381 | 2.897063 |
| H | 3.158116 | 2.595480 | 3.567147 |
| C | 0.023062 | 3.324154 | 2.207758 |
| H | -0.681982 | 2.815065 | 1.552058 |
| H | 0.317710 | 4.260631 | 1.728853 |
| H | -0.503440 | 3.572521 | 3.131183 |
| C | 0.998963 | -2.649309 | 2.245045 |
| H | 1.333064 | -2.422138 | 1.232430 |
| C | -0.268463 | -3.505247 | 2.117534 |
| H | -0.592975 | -3.882518 | 3.089035 |
| H | -0.072870 | -4.368874 | 1.478430 |
| H | -1.090833 | -2.935488 | 1.686878 |
| C | 2.124508 | -3.431977 | 2.939221 |
| H | 3.043610 | -2.845143 | 3.000364 |
| H | 2.342073 | -4.354322 | 2.395961 |
| H | 1.837689 | -3.701585 | 3.957705 |
| C | 3.266137 | -0.039178 | 1.234760 |
| H | 3.625412 | -1.066911 | 1.346054 |
| H | 3.539557 | 0.502158 | 2.138868 |
| C | 3.856425 | 0.613367 | -0.000000 |
| H | 4.941533 | 0.509350 | -0.000000 |
| H | 3.623919 | 1.680511 | -0.000000 |
| B | -0.452688 | -0.248759 | 0.000000 |
| H | -0.653575 | -1.435255 | -0.000000 |
| H | -0.928835 | 0.236854 | 1.006587 |
| N | 1.799073 | -0.052398 | -1.155624 |
| C | 1.109666 | -0.095834 | -2.425307 |
| C | 0.734593 | -1.335118 | -2.960345 |
| C | 0.097938 | -1.333421 | -4.200390 |

| | | | |
|---|---|---|---|
| H | -0.219539 | -2.270880 | -4.636904 |
| C | -0.153049 | -0.149749 | -4.875253 |
| H | -0.661547 | -0.170988 | -5.830692 |
| C | 0.230718 | 1.062581 | -4.323167 |
| H | 0.014748 | 1.981713 | -4.852073 |
| C | 0.871607 | 1.116430 | -3.087994 |
| C | 1.258945 | 2.458942 | -2.490077 |
| H | 1.741504 | 2.275513 | -1.529300 |
| C | 2.269462 | 3.201310 | -3.376296 |
| H | 1.832328 | 3.459154 | -4.342724 |
| H | 2.585403 | 4.130381 | -2.897063 |
| H | 3.158116 | 2.595480 | -3.567147 |
| C | 0.023062 | 3.324154 | -2.207758 |
| H | -0.681982 | 2.815065 | -1.552058 |
| H | 0.317710 | 4.260631 | -1.728853 |
| H | -0.503440 | 3.572521 | -3.131183 |
| C | 0.998963 | -2.649309 | -2.245045 |
| H | 1.333064 | -2.422138 | -1.232430 |
| C | -0.268463 | -3.505247 | -2.117534 |
| H | -0.592975 | -3.882518 | -3.089035 |
| H | -0.072870 | -4.368874 | -1.478430 |
| H | -1.090833 | -2.935488 | -1.686878 |
| C | 2.124508 | -3.431977 | -2.939221 |
| H | 3.043610 | -2.845143 | -3.000364 |
| H | 2.342073 | -4.354322 | -2.395961 |
| H | 1.837689 | -3.701585 | -3.957705 |
| C | 3.266137 | -0.039178 | -1.234760 |
| H | 3.625412 | -1.066911 | -1.346054 |
| H | 3.539557 | 0.502158 | -2.138868 |
| H | -0.928835 | 0.236854 | -1.006587 |
| Cl | -3.444179 | -0.808224 | -1.806783 |

(b) **2**

77

| | | | |
|---|---|---|---|
| C | -1.249139 | -3.028090 | 1.636880 |
| C | -0.001140 | -3.167562 | 2.496907 |

| | | | |
|---|---|---|---|
| C | 1.247016 | -3.028938 | 1.637000 |
| N | 1.157683 | -1.814626 | 0.817980 |
| C | -0.000474 | -1.281418 | 0.461951 |
| N | -1.159026 | -1.813731 | 0.818033 |
| C | 2.379716 | -1.173277 | 0.379811 |
| C | 2.902727 | -1.503736 | -0.879136 |
| C | 4.072994 | -0.859537 | -1.276078 |
| C | 4.687215 | 0.072991 | -0.456247 |
| C | 4.146311 | 0.381716 | 0.782163 |
| C | 2.979164 | -0.231395 | 1.229605 |
| C | 2.249306 | -2.527793 | -1.792620 |
| C | 3.060337 | -3.832950 | -1.812880 |
| B | -0.000016 | 0.027891 | -0.486704 |
| O | 0.000717 | 1.201352 | 0.084646 |
| Ga | 0.001172 | 2.814265 | -0.911646 |
| Cl | -1.837306 | 2.715825 | -2.111468 |
| C | 2.402196 | 0.129975 | 2.588534 |
| C | 3.316545 | -0.367260 | 3.719237 |
| C | -2.380638 | -1.171207 | 0.380420 |
| C | -2.904788 | -1.501551 | -0.878082 |
| C | -4.074807 | -0.856510 | -1.274384 |
| C | -4.687720 | 0.076704 | -0.454359 |
| C | -4.145633 | 0.385409 | 0.783543 |
| C | -2.978628 | -0.228463 | 1.230309 |
| C | -2.252751 | -2.526271 | -1.791812 |
| C | -3.065013 | -3.830664 | -1.811762 |
| C | -2.400343 | 0.132878 | 2.588696 |
| C | -3.313423 | -0.364717 | 3.720281 |
| Cl | 0.001829 | 4.384732 | 0.611647 |
| Cl | 1.839349 | 2.714653 | -2.111807 |
| C | 2.035225 | -1.990797 | -3.214194 |
| C | 2.126375 | 1.633993 | 2.719255 |
| C | -2.038774 | -1.989440 | -3.213464 |
| C | -2.124766 | 1.636928 | 2.719439 |
| H | 1.506206 | -1.038627 | -3.202436 |

| | | | |
|---|---|---|---|
| H | 1.451034 | -2.703890 | -3.799335 |
| H | 2.984019 | -1.840834 | -3.731717 |
| H | 1.262551 | -2.763114 | -1.390366 |
| H | 2.564239 | -4.584437 | -2.430975 |
| H | 3.185519 | -4.242277 | -0.808185 |
| H | 4.056448 | -3.661424 | -2.225738 |
| H | 3.048906 | 2.214470 | 2.668126 |
| H | 1.657788 | 1.843970 | 3.683158 |
| H | 1.459885 | 1.983235 | 1.934122 |
| H | 1.441595 | -0.376207 | 2.695362 |
| H | 4.499100 | -1.079343 | -2.245478 |
| H | 5.584965 | 0.576062 | -0.791588 |
| H | 4.626057 | 1.126807 | 1.402366 |
| H | 2.142079 | -2.947700 | 2.251349 |
| H | 1.373283 | -3.893192 | 0.977994 |
| H | -0.000924 | -2.389777 | 3.263249 |
| H | 3.496725 | -1.442842 | 3.653300 |
| H | 2.869438 | -0.154427 | 4.692498 |
| H | 4.287052 | 0.131158 | 3.681307 |
| H | -0.000476 | -0.204406 | -1.660513 |
| H | -1.508667 | -1.037872 | -3.201920 |
| H | -1.455706 | -2.703173 | -3.798947 |
| H | -2.987669 | -1.838333 | -3.730473 |
| H | -1.266055 | -2.762530 | -1.389966 |
| H | -2.569842 | -4.582616 | -2.430034 |
| H | -3.190183 | -4.239855 | -0.807011 |
| H | -4.061120 | -3.658234 | -2.224246 |
| H | -3.047514 | 2.217189 | 2.669891 |
| H | -1.654820 | 1.846733 | 3.682714 |
| H | -1.459482 | 1.986605 | 1.933480 |
| H | -1.439501 | -0.373060 | 2.694432 |
| H | -4.501775 | -1.076238 | -2.243425 |
| H | -5.585360 | 0.580324 | -0.789168 |
| H | -4.624358 | 1.131043 | 1.403875 |
| H | -2.144223 | -2.946478 | 2.251140 |

| | | | |
|---|---|---|---|
| H | -1.375796 | -3.892183 | 0.977729 |
| H | -3.493276 | -1.440366 | 3.654569 |
| H | -2.865484 | -0.151701 | 4.693121 |
| H | -4.284155 | 0.133337 | 3.683223 |
| H | -0.001464 | -4.132457 | 3.003417 |

(c) **3**

78

| | | | |
|---|---|---|---|
| Ga | -1.417325 | -2.498576 | -0.891517 |
| Cl | -3.526068 | -1.900873 | -0.880568 |
| Cl | -1.012464 | -4.326891 | 0.228372 |
| O | -0.476525 | -1.113681 | -0.041148 |
| N | -0.219142 | 2.059276 | 0.835289 |
| O | 0.224103 | 0.299970 | -1.895406 |
| B | 0.057455 | -0.036537 | -0.583363 |
| C | 0.620547 | 1.130374 | 0.401375 |
| C | 0.232273 | 3.198111 | 1.646324 |
| H | -0.606986 | 3.522777 | 2.256033 |
| H | 0.495656 | 4.024376 | 0.979685 |
| C | 1.421643 | 2.783305 | 2.495309 |
| H | 1.100177 | 2.052064 | 3.239396 |
| H | 1.825437 | 3.644811 | 3.026883 |
| C | -1.632277 | 1.952089 | 0.536406 |
| C | -2.136661 | 2.638751 | -0.574924 |
| C | -3.508230 | 2.556017 | -0.811228 |
| H | -3.933907 | 3.068340 | -1.663632 |
| C | -4.330149 | 1.814617 | 0.020458 |
| H | -5.389916 | 1.747725 | -0.189321 |
| C | -3.799746 | 1.129573 | 1.103142 |
| H | -4.451640 | 0.523415 | 1.715402 |
| C | -2.438730 | 1.177904 | 1.389131 |
| C | -1.871638 | 0.420579 | 2.580810 |
| H | -0.814783 | 0.239189 | 2.388459 |
| C | -1.984267 | 1.256009 | 3.867066 |
| H | -1.472529 | 2.216342 | 3.784901 |
| H | -1.551939 | 0.715115 | 4.711848 |

| | | | |
|---|---|---|---|
| H | -3.031456 | 1.461402 | 4.098795 |
| C | -2.513001 | -0.956221 | 2.783462 |
| H | -3.541790 | -0.875992 | 3.139910 |
| H | -1.950726 | -1.515588 | 3.533123 |
| H | -2.518152 | -1.531495 | 1.861383 |
| C | -1.250659 | 3.461788 | -1.495542 |
| H | -0.210337 | 3.246881 | -1.246267 |
| C | -1.433292 | 3.084111 | -2.970786 |
| H | -1.258026 | 2.020099 | -3.119326 |
| H | -0.723300 | 3.638673 | -3.588091 |
| H | -2.436513 | 3.325332 | -3.326246 |
| C | -1.486836 | 4.964525 | -1.276242 |
| H | -2.511522 | 5.237141 | -1.537142 |
| H | -0.812449 | 5.554992 | -1.900438 |
| H | -1.327279 | 5.249544 | -0.234161 |
| H | -0.042906 | -0.422146 | -2.494405 |
| N | 1.906684 | 1.149857 | 0.726285 |
| C | 2.491130 | 2.177058 | 1.601852 |
| H | 3.273900 | 1.700051 | 2.188082 |
| H | 2.962867 | 2.941645 | 0.978970 |
| C | 2.772722 | 0.077741 | 0.281869 |
| C | 3.465259 | 0.221498 | -0.929078 |
| C | 4.291495 | -0.829901 | -1.321247 |
| H | 4.838006 | -0.759621 | -2.252007 |
| C | 4.417568 | -1.969327 | -0.541287 |
| H | 5.054543 | -2.779914 | -0.871986 |
| C | 3.730056 | -2.078535 | 0.657173 |
| H | 3.836362 | -2.974444 | 1.253959 |
| C | 2.895969 | -1.054849 | 1.101778 |
| C | 2.192943 | -1.177529 | 2.444085 |
| H | 1.508523 | -0.335063 | 2.547505 |
| C | 3.208134 | -1.091829 | 3.595457 |
| H | 3.800776 | -0.175258 | 3.551182 |
| H | 2.693837 | -1.119571 | 4.558384 |
| H | 3.902480 | -1.933573 | 3.562865 |

| | | | |
|---|---|---|---|
| C | 1.345824 | -2.450600 | 2.549241 |
| H | 1.964145 | -3.348960 | 2.509098 |
| H | 0.809867 | -2.463321 | 3.500815 |
| H | 0.616913 | -2.505907 | 1.745272 |
| C | 3.370415 | 1.479919 | -1.774571 |
| H | 2.514409 | 2.057827 | -1.423969 |
| C | 3.125511 | 1.182215 | -3.258428 |
| H | 2.248218 | 0.551562 | -3.384865 |
| H | 2.959306 | 2.114432 | -3.802077 |
| H | 3.982518 | 0.685634 | -3.716923 |
| C | 4.630999 | 2.341516 | -1.591363 |
| H | 5.514396 | 1.812050 | -1.954414 |
| H | 4.543349 | 3.274741 | -2.152130 |
| H | 4.804734 | 2.587253 | -0.541758 |
| Cl | -0.624403 | -2.561748 | -2.975980 |