Synthesis of Distibiranes and Azadistibiranes by Cycloaddition Reactions of Distibenes with Diazomethanes and Azides

Hanns M. Weinert,† Christoph Wölper,† and Stephan Schulz*†#

†Institute for Inorganic Chemistry and #Center for Nanointegration Duisburg-Essen (Cenide), University of Duisburg-Essen, 45117 Essen, Germany
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A) Spectroscopic Characterization

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Fig. S26. DEPT $^{29}$Si NMR spectrum (119.2 MHz, C$_6$D$_6$, 25 °C) of [L(Me$_2$N)Ga]SbSb[N(SiMe$_3$)Ga(N(H)SiMe$_3$)L] (8).
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Fig. S29. $^{13}$C NMR spectrum (150.9 MHz, C$_6$D$_6$, 25 °C) of [L(Me$_2$N)GaSb][L(Me$_2$N)GaN(Ph)Sb]NPh (9).

Fig. S30. ATR-IR spectrum of [L(Me$_2$N)GaSb][L(Me$_2$N)GaN(Ph)Sb]NPh (9).
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Fig. S32. DEPTQ $^{13}$C NMR spectrum (150.9 MHz, C$_6$D$_6$, 25 °C) of [L(Me$_2$N)GaN(Ph)Sb]$_2$ (10).
**Fig. S33.** ATR-IR spectrum of [L(Me₂N)GaN(Ph)Sb]₂ (10).

**Fig. S34.** ¹H NMR spectrum (600 MHz, CD₆, 25 °C) of [L(Me₂N)GaSb]₂C(H)SiMe₃ (11).
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Fig. S36. $^{29}$Si NMR spectrum (79.5 MHz, C₆D₆, 25 °C) of [L(Me₂N)GaSb]₂C(H)SiMe₃ (11).
Fig. S37. ATR-IR spectrum of [L(Me₂N)GaSb]₂C(H)SiMe₃ (11).

Fig. S38. ¹H NMR spectrum (400 MHz, C₆D₆, 25 °C) of [L(EtO)GaSb]₂C(H)SiMe₃ (12).
Fig. S39. $^{13}$C NMR spectrum (100.6 MHz, C$_6$D$_6$, 25 °C) [L(EtO)GaSb]$_2$C(H)SiMe$_3$ (12).

Fig. S40. DEPT $^{29}$Si NMR spectrum (79.5 MHz, C$_6$D$_6$, 25 °C) of [L(EtO)GaSb]$_2$C(H)SiMe$_3$ (12).
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Fig. S42. $^1$H NMR spectrum (600 MHz, C$_6$D$_6$, 25 °C) of [L(Cl)GaSb]$_2$C(H)SiMe$_3$ (13).
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Fig. S44. DEPT $^{29}$Si NMR spectrum (79.5 MHz, C$_6$D$_6$, 25 °C) of [L(Cl)GaSb]$_2$C(H)SiMe$_3$ (13).
**Fig. S45.** ATR-IR spectrum of [L(Cl)GaSb₂C(H)SiMe₃] (13).

**Fig. S46.** ¹H NMR spectrum (300 MHz, C₆D₆, 25 °C) of the reaction of [L(Me₂N)GaSb]₂ with one equivalent Me₃SiN₃. Spektrum was recorded 5 min after addition of the azide.
Fig. S47. $^1$H NMR spectra (300 MHz, thf-d$_8$, –100 – +20 °C) of the reaction of [L(EtO)GaSb]$_2$ with PhN$_3$. Resonance marked with * and x are the N-C$_6$H$_5$ and L $\gamma$-H in 2 to 1 to 2 to 2 ratio, respectively. The low field shift of the ortho H of the phenyl ring was found to be characteristic of the azadistibiranes and having one resonance for the L(EtO)Ga excludes unsymmetrically species, i. e. imine or the [2+3] addition product.
Fig. S48. $^1$H NMR spectra (300 MHz, C$_7$D$_8$, –100 – +20 °C) of the reaction of [L(EtO)GaSb]$_2$ with 1.5 eq Me$_3$SiCHN$_2$.

Fig. S49. UV-vis spectra of azadistibirane 1–3 and 9 in toluene. Extinction coefficient is given in brackets, the wavelength refers to the inflection point.
Fig. S50. UV-vis spectra of distibenes 4–6, 8 and 10 in toluene. Extinction coefficient is given in brackets. The impurities with the highest concentration of 5 and 6 are 1 and 2 respectively. Due to their low adsorption in the visible region the spectra can be attributed almost purely to 5 and 6.

Fig. S51. UV-vis spectra of distibenes 4–6, 8 and 10 in thf. Extinction coefficient is given in brackets. The impurities with the highest concentration of 5 and 6 are 1 and 2 respectively. Due to their low adsorption in the visible region the spectra can be attributed almost purely to 5 and 6.
**Fig. S52.** UV-vis spectra of distibirane 11–13 in toluene. Extinction coefficient is given in brackets.

| Wavelength [nm] | Absorbance |
|-----------------|------------|
| 355 (33000)     |            |
| 355 (44000)     |            |
| 354 (46000)     |            |
Crystallographic Details.

Crystals were mounted on nylon loops in inert oil. Data of were collected on a Bruker AXS D8 Kappa diffractometer (1–4, 8–12) with APEX2 detector (monochromated MoKα radiation, λ = 0.71073 Å) and on a Bruker AXS D8 Venture diffractometer (6, 7, 13) with Photon II detector (monochromated CuKα radiation, λ = 1.54178 Å, microfocus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)\(^1\) and refined anisotropically by full-matrix least-squares on F\(^2\) (SHELXL-2017)\(^2\). Absorption corrections were performed semi-empirically from equiv. reflections on basis of multi-scans (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups.

The structure of 1 contains a toluene molecule highly disordered over a centre of inversion. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE\(^3\) run. The molecule was included in the sum formula for completeness. In 2 one half of the molecule and the p–Ph–CF\(_3\) moiety are disordered over two positions. The corresponding bond lengths and angles of the i-Pr groups were restrained to be equal (SADI) as well as those of the p–Ph–CF\(_3\) unit. The displacement parameters of all disordered atoms were refined with RIGU restraints. Additional SIMU and ISOR restraints were required for the fluorine atoms. Their disorder is more diffuse than the one of the remaining moiety and consequently an extra alternate position was used to model the electron density. Still, the displacement ellipsoids suggest further disorder, however no other alternate positions could be identified. Disordered atoms in proximity to its alternate positions were refined with common displacement parameters (EADP). Finally, the Ga2–N6 bond length of both alternate positions were restrained to be equal (SADI). The solvent molecule is disordered over a centre of inversion. The local symmetry was ignored in the refinement (negative PART). All its corresponding bond lengths and angles were restrained to be equal (SADI) and its atoms were restrained to lie on a common plane (FLAT). RIGU restraints were applied to the atoms’ displacement parameters. During the refinement ice formed on the crystal and the resulting reflections and ring patterns restrained to be equal to 1.54 Å (DFIX) and its bond angles to be equal (SADI). RIGU, SIMU and ISOR restraints were applied to the anisotropic displacement parameters of the respective atoms. The structure contains a highly disordered acetonitrile molecule. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE\(^3\) run. The molecule was included in the sum formula for completeness. The benzene molecules in 11 are highly disordered and were modelled with two alternate positions. No further alternate positions could be found although the anisotropic displacement parameters suggest that this is just a crude model. This can also be concluded from the unrealistically short bond lengths. All bond lengths and angles were restrained to be equal (SADI) and the atoms were restrained to lie on a mutual plane (FLAT). DFIX restraints were not suitable to improve the unrealistic bond lengths. The displacement parameters of the benzenes’ atoms were restrained with RIGU and SIMU. Two i-Pr groups are disordered over two positions. Their atoms’ displacement parameters were restrained with RIGU in both cases and additionally with SIMU in one case. The CHSiMe\(_3\) group is disordered over two positions. All its corresponding bond lengths were restrained to be equal (SADI) and RIGU restraints were applied to the displacement parameters. In 8 two i-Pr groups are disordered over two positions. Their corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints applied to the anisotropic displacement parameters of the respective atoms. The structure contains a highly disordered acetonitrile molecule. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE\(^3\) run. The molecule was included in the sum formula for completeness. The benzene molecules in 11 are highly disordered and were modelled with two alternate positions. No further alternate positions could be found although the anisotropic displacement parameters suggest that this is just a crude model. This can also be concluded from the unrealistically short bond lengths. All bond lengths and angles were restrained to be equal (SADI) and the atoms were restrained to lie on a mutual plane (FLAT). DFIX restraints were not suitable to improve the unrealistic bond lengths. The displacement parameters of the benzenes’ atoms were restrained with RIGU and SIMU. Two i-Pr groups are disordered over two positions. Their atoms’ displacement parameters were restrained with RIGU in both cases and additionally with SIMU in one case. The CHSiMe\(_3\) group is disordered over two positions. All its corresponding bond lengths were restrained to be equal (SADI) and RIGU restraints were applied to the displacement parameters. In 10 two i-Pr groups and the ipso-C atom of the phenyl ring common displacement parameters were used for both orientation (EADP). The model was refined as a two-component twin against HKLF5 data. The combination of twinning and a long axis led to serious problems with overlapping reflections and part of the frames could not be integrated successfully. Considering the low quality of the data, the twinning and the vast disorder quantitative results should not be discussed. The CHSiMe\(_3\) group and an i-Pr group of 13 are disordered over two positions. The corresponding bond lengths and angles of these groups were restrained to be equal (SADI) and RIGU restraints were applied to their atoms. For C12, C12’, C59 and C59’ additional SIMU restraints were used. Despite the rather large displacement ellipsoids no further alternate orientations could be identified. The solvent molecule is disordered over a centre of inversion and was crudely modelled with two alternate positions. Its bond lengths were restrained to be equal to 1.54 Å (DFIX) and its bond angles to be equal (SADI). RIGU, SIMU and ISOR restraints were applied to its displacement parameters. Due to their proximity C11_1 and C11_2 were refined with common displacement parameters (EADP). During the measurement ice formed on the crystal and the resulting reflections and ring patterns disturbed the integration leading to a rather high R\(_{int}\).

CCDC-2129215 (1 mw_124_1m_sq), -2129216 (2 mw_125_5), -2129217 (3 mw_097_3), -2129218 (4 mw_071_7), -2129219, (5 mw_130_4m_sq), -2129220, (6 mw_143_4), -2129221 (7 mw_130_1), -2129222 (8 mw_071_8m_sq), -2129223 (9 mw_145_1), -2129221 (10 mw_150_2), -2129212 (11 mw_089_1fs), -2129213 (12 mw_099_tw5), and -2129214 (13 mw_112_3f) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
Table S1a. Crystallographic data of [L(MeN)GaSb]2NPh (1), [L(Me2N)GaSb]2N-p-CF3-Ph (2), [L(Me2N)GaSb]2N(ada) (3) and [L(Me2N)Ga]SbSb[N(SiMe3)Ga(NMe3)L] (4) [L(Me2N)Ga]SbSb[N(Ph)Ga]N(Me2)2L] (5), [L(Me2N)Ga]SbSb[N(p-CF3-Ph)Ga]N(Me2)2L] (6), and [(L(Ph)Ga-kGa,kN)2-(μ,N⎦)2-(μ-1)] (7).

|   | 1       | 2       | 3       | 4       | 5       | 6       | 7       |
|---|---------|---------|---------|---------|---------|---------|---------|
| M | 1443.54 | 1511.54 | 1547.73 | 1393.57 | 1530.66 | 1594.73 | 1530.66 |
| Crystal size [mm] | 0.276 × 0.203 × 0.134 | 0.392 × 0.197 × 0.126 | 0.409 × 0.235 × 0.160 | 0.271 × 0.263 × 0.131 | 0.407 × 0.211 × 0.150 | 0.186 × 0.064 × 0.063 | 0.407 × 0.211 × 0.150 |
| T [K] | 100(2) | 100(2) | 100(2) | 100(2) | 100(2) | 100(2) | 100(2) |
| Crystal system | monoclinic | monoclinic | monoclinic | monoclinic | monoclinic | monoclinic | monoclinic |
| Space group | P21/c | P-1 | P21 | P21 | P21/c | P21/c | P21/c |
| a [Å] | 19.9634(10) | 10.6581(5) | 10.7967(11) | 13.6969(16) | 12.1758(10) | 12.1758(10) | 12.1758(10) |
| b [Å] | 12.5667(7) | 12.7136(6) | 45.894(5) | 21.163(3) | 28.763(3) | 28.763(3) | 28.763(3) |
| c [Å] | 29.4717(15) | 27.5744(13) | 15.2335(16) | 15.164(2) | 20.711(3) | 24.248(2) | 20.711(3) |
| α [°] | 90 | 90 | 90 | 90 | 90 | 90 | 90 |
| β [°] | 109.0277(16) | 92.993(2) | 94.502(5) | 96.979(3) | 94.587(5) | 99.805(3) | 94.587(5) |
| γ [°] | 90 | 90 | 90 | 90 | 90 | 90 | 90 |
| V [Å³] | 6989.7(6) | 3595.4(3) | 7643.8(13) | 3439.2(9) | 8133.4(17) | 7916.1(11) | 8133.4(17) |
| Z | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| Dcalc [g·cm⁻³] | 1.372 | 1.396 | 1.345 | 1.346 | 1.250 | 1.338 | 1.250 |
| μ(Mo-Kα) [mm⁻¹] | 1.572 | 1.537 | 1.442 | 1.611 | 1.355 | 6.527 | 1.355 |
| Transmissions | 0.75/0.67 | 0.75/0.55 | 0.75/0.66 | 0.75/0.64 | 0.75/0.62 | 0.75/0.54 | 0.75/0.62 |
| F(000) | 2980 | 1554 | 3216 | 1440 | 3168 | 3308 | 3168 |
| Index ranges | -33 ≤ h ≤ 33 | -16 ≤ h ≤ 16 | -16 ≤ h ≤ 16 | -16 ≤ h ≤ 16 | -15 ≤ h ≤ 14 | -21 ≤ h ≤ 21 | -21 ≤ h ≤ 21 |
| | -20 ≤ k ≤ 20 | -19 ≤ k ≤ 19 | -70 ≤ k ≤ 70 | -32 ≤ k ≤ 32 | -44 ≤ k ≤ 44 | -34 ≤ k ≤ 34 | -44 ≤ k ≤ 44 |
| | -49 ≤ l ≤ 49 | -42 ≤ l ≤ 42 | -23 ≤ l ≤ 23 | -23 ≤ l ≤ 23 | -32 ≤ l ≤ 32 | -30 ≤ l ≤ 30 | -32 ≤ l ≤ 32 |
| θmax [°] | 36.384 | 33.683 | 33.532 | 33.208 | 34.165 | 80.082 | 34.165 |
| Refl. collected | 369240 | 190515 | 368631 | 108278 | 285425 | 249345 | 285425 |
| Independent ref| 33974 | 28194 | 29384 | 26282 | 31986 | 17136 | 31986 |
| Rint | 0.0450 | 0.0415 | 0.0535 | 0.0441 | 0.0430 | 0.0710 | 0.0430 |
| Reff [I > 2σ(I)] | 0.0283 | 0.0457 | 0.0646 | 0.0323 | 0.0299 | 0.0322 | 0.0299 |
| wR2 [all data] | 0.0687 | 0.1266 | 0.1323 | 0.0689 | 0.0752 | 0.0893 | 0.0752 |
| x(Flack) | - | - | 0.131(7) | - | - | - | - |
| GooF | 1.084 | 1.132 | 1.368 | 1.036 | 1.060 | 1.051 | 1.060 |
| Δρfinal (max/min) [e·Å⁻³] | 1.133/-0.634 | 2.725/-1.306 | 1.745/-3.007 | 1.095/-0.509 | 0.899/-0.545 | 1.063/-0.593 | 0.899/-0.545 |

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| Table S1b. Crystallographic data of [L(Me₂N)Ga]SbBr[N(SiMe₃)Ga(N(H)SiMe₃)L] (8), [L(Me₂N)GaSb][L(Me₂N)GaN(Ph)Sb]N-Ph (8), [L(Me₂N)GaN(Ph)Sb]₂ (9), [L(Me₂N)GaSb]-C(H)SiMe₃ (10) and [L(EtO)GaSb]₂C(H)SiMe₃ (11), and [L(Me₂N)GaSb]₂(C(H)SiMe₃) (13). |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Empirical formula              | C₆₀H₁₁₆Ga₃N₃Sb₂Si₂ | C₆₁H₁₂₇Ga₃N₃Sb₂ | C₆₄H₁₆₃Ga₄N₅Sb₂ | C₆₉H₁₁₆Ga₅N₅Sb₂Si | C₆₈H₁₀₂Ga₅N₂O₂Sb₂Si | C₆₆₅H₈₈Cl₉Ga₃N₃Sb₂Si |
| M                               | 1478.75          | 1580.72         | 1488.59         | 1548.79         | 1394.54         | 1411.39         |
| Crystal size [mm]               | 0.483 × 0.182 × 0.144 | 0.185 × 0.071 × 0.045 | 0.184 × 0.182 × 0.116 | 0.321 × 0.316 × 0.107 | 0.451 × 0.429 × 0.344 | 0.338 × 0.053 × 0.040 |
| T [K]                           | 100(2)           | 100(2)          | 100(2)          | 100(2)          | 100(2)          | 100(2)          |
| Crystal system                  | monoclinic       | triclinic       | triclinic       | triclinic       | monoclinic      | monoclinic      |
| Space group                     | P2₁/n            | P-1             | P-1             | P-1             | C2/c            | P2₁/c           |
| a [Å]                           | 11.889(2)        | 11.6222(9)      | 10.4552(4)      | 10.919(2)       | 59.557(6)       | 19.7547(17)     |
| b [Å]                           | 18.460(4)        | 17.8727(14)     | 11.9732(4)      | 14.343(3)       | 11.8135(12)     | 10.5843(9)      |
| c [Å]                           | 33.366(7)        | 19.5796(16)     | 14.9227(5)      | 26.014(6)       | 21.011(2)       | 3.512(3)        |
| α [°]                           | 90               | 108.099(4)      | 93.2189(14)     | 83.994(15)      | 90              | 90              |
| β [°]                           | 96.360(11)       | 90.076(4)       | 97.3354(14)     | 78.718(10)      | 108.078(3)      | 96.970(4)       |
| γ [°]                           | 90               | 93.8174(7)      | 107.9954(14)    | 88.053(10)      | 90              | 90              |
| V [Å³]                          | 7278(2)          | 3856.2(5)       | 1753.06(11)     | 3972.9(16)      | 14053(3)        | 6955.1(10)      |
| Z                               | 4                | 2               | 1               | 2               | 8               | 4               |
| D₀ [g·cm⁻³]                     | 1.350            | 1.361           | 1.410           | 1.295           | 1.318           | 1.348           |
| μ(Mo-Kα) [mm⁻¹]                 | 1.543            | 1.431           | 1.569           | 1.401           | 1.578           | 8.131           |
| Transmissions                   | 0.75/0.58        | 0.75/0.68       | 0.75/0.65       | 0.75/0.59       | 0.75/0.46       | 0.75/0.48       |
| F(000)                          | 3064             | 1636            | 1168            | 1608            | 5760            | 2900            |
| Index ranges                    | -17 ≤ h ≤ 17    | -17 ≤ k ≤ 17   | -16 ≤ h ≤ 16    | -16 ≤ h ≤ 16   | -84 ≤ h ≤ 80   | -25 ≤ h ≤ 25   |
|                                 | -26 ≤ k ≤ 26    | -27 ≤ k ≤ 27   | -18 ≤ k ≤ 18    | -22 ≤ k ≤ 22   | 0 ≤ k ≤ 16     | -13 ≤ k ≤ 11   |
|                                 | -39 ≤ l ≤ 47    | -30 ≤ l ≤ 30   | -23 ≤ l ≤ 23    | -40 ≤ l ≤ 40   | 0 ≤ l ≤ 30     | -42 ≤ l ≤ 42   |
| θₘax [°]                        | 31.059           | 33.269          | 33.595          | 33.568          | 30.506          | 80.760          |
| Reflections collected           | 119071           | 311665          | 139632          | 238703          | 151709          | 273985          |
| Independ. reflections           | 22799            | 29569           | 13767           | 31007           | 25033           | 15129           |
| Rint                            | 0.0518           | 0.1010          | 0.0193          | 0.0652          | 0.0753          | 0.1275          |
| R₁ [I > 2σ(I)]                  | 0.0404           | 0.0393          | 0.0191          | 0.0402          | 0.0755          | 0.0359          |
| wR₂ [all data]                  | 0.0866           | 0.0856          | 0.0543          | 0.0942          | 0.1812          | 0.0902          |
| GoOF                            | 1.041            | 1.031           | 1.079           | 1.063           | 1.125           | 1.028           |
| Δρₘax (max/min) [e·Å⁻³]          | 2.358/-1.236     | 1.203/-0.884    | 0.928/-0.313    | 3.087/-3.509    | 2.377/-1.587    | 1.844/-1.943    |
**Fig. S53.** Molecular structure of \([\text{L(Me}_2\text{N)}\text{GaSb}]_2\text{N-p-CF}_3\text{-Ph} \) (2) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the \(\text{L(Me}_2\text{N)}\text{GaSb} \) and \(\text{p-CF}_3\text{-Ph} \) unit is displayed.

**Fig. S54.** Molecular structure of \([\text{L(Me}_2\text{N)}\text{GaSb}]_2\text{N-ada} \) (3) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.
**Fig. S55.** Molecular structure of $[\text{L(Me}_2\text{N)}\text{Ga}]\text{SbSb}[\text{N(SiMe}_3\text{)}\text{Ga(NMe}_2\text{)}\text{L}]$ (4) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

**Fig. S56.** Molecular structure of $[\text{L(Me}_2\text{N)}\text{Ga}]\text{SbSb}[\text{N(p-CF}_3\text{-Ph)}\text{Ga(NMe}_2\text{)}\text{L}]$ (6) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.
**Fig. S57.** Molecular structure of \([\text{L(Me}_2\text{N})\text{GaSb}]_2\text{C(H)SiMe}_3\) (11) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the CSiCMe\(_3\) unit is displayed.

**Fig. S58.** Molecular structure \([\text{L(Me}_2\text{N})\text{GaSb}]_2\text{C(H)SiMe}_3\) (13) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the CSiCMe\(_3\) unit is displayed.
C) Computational Details

The ORCA quantum chemistry package version (5.0.0)⁴ was used for the DFT calculations. The geometric parameters of the species were optimized in the gas phase employing the PBE0 density functional⁵ with the default "defgrid3" and "extremescf" with def2-SVP⁶ basis set on H, C, N, Si and def2-TZVP⁶ on Ga and Sb utilizing the atom-pairwise dispersion correction with Becke-Johnson damping scheme (D3BJ).⁷ Sill conversion to optimized structure was slow and 14”’ and 15”’ did not converge after the default number of steps (3 x number of atoms). In these cases, the optimization was restarted from the previous found minima and the maximum step size was reduced from 0.3 au (default) to 0.05 au in internal coordinates. A small effective core potential was employed on Sb.⁸ To accelerate the calculations the RIJCOSX⁹ (resolution of identity (RI-J) algorithm for the computation of the Coulomb terms and the ‘chain of spheres exchange’ (COSX) algorithm for the calculation of the exchange terms) approximation was utilized with the def-2J auxiliary basis sets.¹⁰ The structures used to estimate the ring strain (Table S3-8) were optimized analogous with def2-TZVP⁶ basis on H, C, N and def2-QZVP⁶ on Ga and Sb. Frequency calculations were carried out for all optimized structures. The Enthalpy and Gibbs free Energy derived from frequency calculation with the vibrational entropy being computed according to the quasi rigid-rotor-harmonic-oscillator approximation (QRRHO) of S. Grimme at 298 K in the standard manner by the ORCA quantum chemistry package version.¹¹ Single point calculations for the electron densities and frontier molecular orbitals were calculated with def2-TZVP⁶ basis set on H, C, N, Si and def2-QZVP⁶ on Ga and Sb. Electronic excitations were calculated analogous using the time-dependent DFT (TD-DFT) formalism taking solvent effects (toluene) into account utilizing the conductor-like polarized continuum model (CPCM).¹² Natural bond orbital analysis was performed using the NBO 7.0 program.¹³

In general, coordinated obtained from sc-XRD were used as the starting point for the geometry optimization, if possible. The imine structures ¹⁵ were obtained starting from the respective azadistibiranes by a rudimentary relaxed scan increasing the Sb-Sb-N angle. The starting point for the distibatriazoles were the imine structures adding a N₂ unit. Finally, for the closely related Me₃Si-N₃ and Me₃Si-CH-N₂ the starting point were the previously optimized structures replacing N with CH and vice versa.

Atoms in molecules (AIM)¹⁴ and electron localization function (ELF)¹⁵ computations were performed with the Multiwfn program 3.8¹⁶ replacing the inner-core density by a pseudo-potential.¹⁷ VMD was developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign (http://www.ks.uiuc.edu/Research/vmd/) and used to plot grid-data.¹⁸
**Fig. S 59.** Section of the MO diagram of \([\text{L(Me}_2\text{N})\text{Ga}\text{SbSb}[\text{N(SiMe}_3\text{)}\text{Ga(\text{NMe}_2\text{)L}}]\) (4) \([\text{L(Me}_2\text{N})\text{Ga}\text{SbSb}[\text{N(Ph)Ga(\text{NMe}_2\text{)L}}]\) (5) and \([\text{L(Me}_2\text{N})\text{GaN(Ph)Sb}]_2\) (10), isovalue 0.03.\(^{16}\)
Fig. S 60. UV-Vis spectrum of 4 in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions. 18

Fig. S 61. UV-Vis spectrum of 5 in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions. 18
**Fig. S 62.** UV-Vis spectrum of 10 in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions.\(^\text{18}\)
Table S2. Overview of most intense calculated UV-Vis transitions by TD-DFT for [L(Me₂N)GaSb]₂ (X)\textsuperscript{19} [L(Me₂N)Ga]SbSb[N(SiMe₃)Ga(NMe₂)L] (4) [L(Me₂N)Ga]SbSb[N(Ph)Ga(NMe₂)L] (5) and [L(Me₂N)Ga(N)Sb]₂ (10).

| Excited State | Excitation energy E [cm⁻¹] | Wavelength λ [nm] | Oscillator strength $f_{(electric/velocity)}$ | Transition orbital contribution (> 5%) |
|---------------|----------------------------|-------------------|----------------------------------------------|--------------------------------------|
| X             | 7                          | 23852.4           | 419.2                                        | 0.149/0.200                          |
|               |                            |                   |                                              | HOMO-4 → LUMO (7.1)                  |
|               |                            |                   |                                              | HOMO-3 → LUMO (71.1)                 |
|               | 2                          | 21815.7           | 458.4                                        | 0.043/0.044                          |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (49.6)               |
|               |                            |                   |                                              | HOMO → LUMO+1 (42.5)                 |
|               | 3                          | 23053.9           | 433.8                                        | 0.070/0.053                          |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (12.1)               |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (25.7)               |
|               |                            |                   |                                              | HOMO → LUMO+1 (33.5)                 |
|               |                            |                   |                                              | HOMO → LUMO+2 (22.9)                 |
| 4             | 4                          | 23776.9           | 420.6                                        | 0.042/0.019                          |
|               |                            |                   |                                              | HOMO-1 → LUMO (44.9)                 |
|               |                            |                   |                                              | HOMO → LUMO+2 (48.9)                 |
|               | 5                          | 24045.1           | 415.9                                        | 0.031/0.027                          |
|               |                            |                   |                                              | HOMO-1 → LUMO (37.4)                 |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (18.8)               |
|               |                            |                   |                                              | HOMO → LUMO+1 (11.3)                 |
|               |                            |                   |                                              | HOMO → LUMO+2 (26.6)                 |
|               | 3                          | 21607.6           | 462.8                                        | 0.056/0.018                          |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (85.3)               |
|               |                            |                   |                                              | HOMO → LUMO+1 (6.8)                  |
| 5             | 4                          | 21940.8           | 455.8                                        | 0.111/0.115                          |
|               |                            |                   |                                              | HOMO-1 → LUMO+1 (6.5)                |
|               |                            |                   |                                              | HOMO → LUMO+1 (77.3)                 |
| 10            | 1                          | 17748.4           | 563.4                                        | 0.166/0.157                          |
|               |                            |                   |                                              | HOMO-4 → LUMO (6.0)                  |
|               |                            |                   |                                              | HOMO → LUMO (87.1)                   |
Table S3. Calculated X–Y bond lengths (r, Å) (exp.), X and Y NPA atomic charges (q, |e|), Wiberg bond indices (WBI), occupation numbers (ON, |e|) of the σXY bonds according to NBO analysis, for the Ga$_2$Sb$_2$ skeleton of [L(NMe$_2$)GaSb]$_2$\cite{19} the N$_2$Sb$_2$ skeleton of 10 and the GaShSbN$_2$ skeleton for 4 and 5.

| X-Y     | r(X-Y) | q(X)/q(Y) | WBI | ON$[$a$]$ |
|---------|--------|-----------|-----|-----------|
| Ga$_2$Sb$_1$ | 2.60 (2.62) | 1.36/ -0.16 | 0.97 | 1.96 |
| Ga$_85$Sb$_84$ | 2.60 (2.62) | 1.38/ -0.16 | 0.96 | 1.96 |
| [L(Me$_2$N)GaSb]$_2$ | 2.62 (2.65) | -0.16/-0.16 | 1.82 | 0.501/0.499 |
| Sb$_1$–Sb$_84$ | 2.62 (2.65) | -0.16/-0.16 | 1.82 | 0.501/0.499 |
| Sb$_1$ lone-Sb$_84$ pair | | | | |
| N$_6$-Sb$_1$ | 2.07 (2.07) | -1.37/ 0.63 | 0.59 | 1.91 |
| N$_{101}$-Sb$_{96}$ | 2.07 (2.07) | -1.37/ 0.63 | 0.59 | 1.91 |
| 10 | | | | |
| Sb$_1$–Sb$_{96}$ | 2.66 (2.67) | 0.63/ 0.63 | 1.66 | 0.500/0.500 |
| Sb$_1$ lone-Sb$_{97}$ pair | | | | |
| Ga$_4$-Sb$_2$ | 2.59 (2.58) | 1.51/ -0.69 | 0.93 | 0.355/0.645 |
| Ga$_3$ | | | | |
| Sb$_1$-Sb$_2$ | 2.65 (2.65) | 1.08/-0.69 | 1.59 | 0.460/0.540 |
| 4 | | | | |
| Sb$_1$ lone-Sb$_2$ pair | | | | |
| N$_{10(NMe_3)}$-Sb$_1$ | 2.08 (2.09) | -1.97/ 1.08 | 0.49 | |
| N$_{11(NMe_2)}$-Sb$_1$ | 2.47 (2.47) | -0.96/ 1.08 | 0.22 | |
| 5 | | | | |
| Ga$_4$-Sb$_2$ | 2.60 (2.58) | 1.51/-0.66 | 0.92 | 0.354/0.646 |
| Ga$_3$ | | | | |
| Sb$_1$-Sb$_2$ | 2.65 (2.68) | 1.05/-0.66 | 1.60 | 0.458/0.542 |
| Sb$_1$ lone-Sb$_2$ pair | | | | |
| N$_{11(NPb)}$-Sb$_1$ | 2.10 (2.10) | -1.38/ 1.05 | 0.49 | 0.299/0.711 |
| N$_{9(NMe_2)}$-Sb$_1$ | 2.47 (2.40) | -0.96/ 1.05 | 0.21 | |

$[$a$]$: Squared polarization coefficients c$_X$ ($|c_X|^2$) of the σXY bond NBOs. The accepted Lewis structures of 4 and 5 consisted of multiple parts thus no ON could be given from the NBP analysis.
Table S 4. Calculated X–Y bond lengths (r, Å), X and Y NPA (AIM) atomic charges (q, |e|), Wiberg bond indices (WBI), occupation numbers (ON, |e|) of the σXY bonds according to NBO analysis, and AIM parameters at the bond (bcp) and ring (rcp) critical points (ρ(r_b), Δρ(r_b), |V(r_b)|/G(r_b), H(r_b), ε(r_b), atomic units) for the Sb2C skeleton of [L(Me_2N)GaSb]_2C(H)SiMe_3 11.

| X-Y   | r(X-Y) | q(X)  | q(Y)  | WBI  | ON^{[a]} | ρ(r_b) | Δρ(r_b) | |V(r_b)|/G(r_b) | H(r_b) | ε   |
|-------|--------|-------|-------|------|----------|--------|---------|---------|--------|------|-----|
| Sb1-C4 | 2.18   | 0.08  | -1.39 | 0.86 | 1.96     | 0.100  | 0.067   | 1.711   | -0.043 | 0.182|
| Sb20-C4 | 2.19   | 0.05  | -1.39 | 0.86 | 1.95     | 0.098  | 0.065   | 1.721   | -0.042 | 0.184|
| Sb1-Sb20 | 2.78   | 0.08  | 0.05  | 0.92 | 1.92     | 0.056  | 0.020   | 1.773   | -0.017 | 1.766|
| rcp    |        |       |       |      |          | 0.056  | 0.042   | 1.596   | -0.016 | -3.556|

[a]: Squared polarization coefficients c_X (|c_X|^2) of the σXY bond NBOs.

Table S 5. Calculated X–Y bond lengths (r, Å), X and Y NPA (AIM) atomic charges (q, |e|), Wiberg bond indices (WBI), occupation numbers (ON, |e|) of the σXY bonds according to NBO analysis, and AIM parameters at the bond and ring critical points (ρ(r_b), Δρ(r_b), |V(r_b)|/G(r_b), H(r_b), ε(r_b), atomic units) for the Sb2N skeleton of [L(Me_2N)GaSb]_2NSiMe_3 16.

| X-Y   | r(X-Y) | q(X)  | q(Y)  | WBI  | ON^{[a]} | ρ(r_b) | Δρ(r_b) | |V(r_b)|/G(r_b) | H(r_b) | ε   |
|-------|--------|-------|-------|------|----------|--------|---------|---------|--------|------|-----|
| Sb1-N12 | 2.09   | 0.26  | -1.66 | 0.67 | 1.96     | 0.108  | 0.215   | 1.451   | -0.044 | 0.045|
| Sb2-N12 | 2.08   | 0.33  | -1.66 | 0.62 | 1.96     | 0.109  | 0.228   | 1.435   | -0.044 | 0.059|
| Sb1-Sb2 | 2.75   | 0.26  | 0.33  | 0.94 | 1.92     | 0.057  | 0.016   | 1.818   | -0.018 | 0.876|
| rcp    |        |       |       |      |          | 0.056  | 0.056   | 1.525   | -0.016 | -2.570|

[a]: Squared polarization coefficients c_X (|c_X|^2) of the σXY bond NBOs.
Table S6. Cartesian coordinates of methane [Å] for the optimized geometry.

|          | Energy (PBE0/D3BJ/def2-T(Q)ZVP) | Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) | Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) | Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) |
|----------|---------------------------------|-----------------------------------------------|-----------------------------------|------------------------------------------|
| C        | -4.0507103396174               | 0.39299992642979                             | -40.47512126 Eh                  | -40.47512126 Eh                         |
| H        | -2.9614749598233               | 0.39299562860743                              | -40.42658194 Eh                  | -40.42658194 Eh                         |
| H        | -4.41389284390358              | 0.52846495896909                              | -40.48749999 Eh                  | -40.48749999 Eh                         |

Table S7. Cartesian coordinates of cyclopropane [Å] for the optimized geometry.

|          | Energy (PBE0/D3BJ/def2-T(Q)ZVP) | Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) | Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) | Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) |
|----------|---------------------------------|-----------------------------------------------|-----------------------------------|------------------------------------------|
| C        | -3.81482060044059               | 0.24686865910214                             | -117.79442036 Eh                  | -117.79442036 Eh                         |
| C        | -2.78481301377702               | -0.83348007109233                            | -117.70855551 Eh                  | -117.70855551 Eh                         |
| C        | -2.36498283820619               | 0.60348039642867                             | -117.73647728 Eh                  | -117.73647728 Eh                         |
| H        | -2.7219398021147               | -1.37888326726660                            | -117.70855551 Eh                  | -117.70855551 Eh                         |
| H        | -2.57204563579027              | -1.4283796367047                            | -117.73647728 Eh                  | -117.73647728 Eh                         |
| H        | -3.40187712360603              | 0.3856433767511                              | -117.70855551 Eh                  | -117.70855551 Eh                         |
| H        | -4.45101055526272              | 0.43568379061289                             | -117.73647728 Eh                  | -117.73647728 Eh                         |
| H        | -2.01618399266598              | 1.03445265103731                             | -117.70855551 Eh                  | -117.70855551 Eh                         |

Table S8. Cartesian coordinates of n-butane [Å] for the optimized geometry.

|          | Energy (PBE0/D3BJ/def2-T(Q)ZVP) | Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) | Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) | Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) |
|----------|---------------------------------|-----------------------------------------------|-----------------------------------|------------------------------------------|
| C        | -3.94910935878480               | 0.35834663911002                             | -158.31447698 Eh                  | -158.31447698 Eh                         |
| C        | -2.98813612556477               | -0.81823011388092                            | -158.17574760 Eh                  | -158.17574760 Eh                         |
| C        | -1.52926568926165               | -0.3973189668171                             | -158.21044423 Eh                  | -158.21044423 Eh                         |
| H        | -3.18988524827818              | -1.40291277911999                            | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -3.19216626475811              | -1.48870305973654                            | -158.21044423 Eh                  | -158.21044423 Eh                         |
| H        | -1.29306385251641              | 0.24819401872831                             | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -0.85991674777867             | -1.25949321881538                            | -158.21044423 Eh                  | -158.21044423 Eh                         |
| C        | -1.29531239752563              | 0.16147895447699                             | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -5.40798082390052              | -0.06255522503813                            | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -3.74506577231902             | 1.02881293051581                             | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -3.74736534369383             | 0.94301170707382                             | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -5.64190569620737            | -0.62140888147522                            | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -6.07731903130752             | 0.79963028562176                             | -158.17574760 Eh                  | -158.17574760 Eh                         |
| H        | -5.6442076409893             | -0.70801228884333                            | -158.17574760 Eh                  | -158.17574760 Eh                         |

Table S9. Cartesian coordinates of NMe₃ [Å] for the optimized geometry.

|          | Energy (PBE0/D3BJ/def2-T(Q)ZVP) | Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) | Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) | Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) |
|----------|---------------------------------|-----------------------------------------------|-----------------------------------|------------------------------------------|
| C        | -0.40651156977788              | 0.34330737478268                             | -174.32639160 Eh                  | -174.32639160 Eh                         |
| C        | 1.08884175363941              | 2.19270785397452                             | -174.19970764 Eh                  | -174.19970764 Eh                         |
| C        | 1.90765406684177              | -0.0271682460786                              | -174.2341508 Eh                   | -174.2341508 Eh                         |
| N        | 0.78873913416882              | 0.86288726423214                             | -174.19970764 Eh                  | -174.19970764 Eh                         |
| H        | -0.64159878111610            | -0.64010281766533                            | -174.2341508 Eh                   | -174.2341508 Eh                         |
| H        | -1.24941637949699            | 1.00776287820221                             | -174.19970764 Eh                  | -174.19970764 Eh                         |
| H        | -0.31154829050054            | 0.23823432661460                             | -174.19970764 Eh                  | -174.19970764 Eh                         |
| H        | 0.24684154399438            | 2.8582436579066                              | -174.19970764 Eh                  | -174.19970764 Eh                         |

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**Table S10.** Cartesian coordinates of [L'(Me2N)GaSb2]2NMe (L' = HC(CHMeNPh)) [Å] for the optimized geometry.

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Sb      | 5.27612699586911  | 7.47744378301105  | 6.71762333465927  |
| Ga      | 4.82886198936814  | 6.73596018852156  | 2.9392960423595  |
| C       | 7.00009236212254  | 8.69238578730382  | 3.12901113550598  |
| N       | 3.02539207682472  | 9.12619842438155  | 5.4385628605086  |
| N       | 3.83819809295255  | 5.54192885137228  | 2.58225099529264  |
| N       | 4.75151308038372  | 7.34325676322830  | 1.04787065433530  |
| N       | 6.50432560490392  | 10.4556325728173  | 9.0675117635406  |
| N       | 6.79635143647703  | 7.57891180251978  | 10.05086378465813  |
| N       | 3.30893368198196  | 5.67447382092783  | 3.17361905238855  |
| N       | 8.81882797259454  | 8.74267885615243  | 7.9371131775985  |
| N       | 4.43297908919681  | 9.17513803092984  | 5.7881191190446  |
| C       | 6.78478261804768  | 5.15801905772599  | 1.38573032649994  |
| C       | 6.24988724084546  | 5.67212658117689  | 0.19655708538678  |
| H       | 6.62127067712407  | 5.22954232570343  | -0.71862463361590  |
| C       | 5.35769132835326  | 6.73573464092634  | 0.03807933517271  |
| C       | 7.86022789997599  | 4.11802929629102  | 1.26828479301258  |
| H       | 7.88642892026899  | 3.70452634766014  | 0.2617039666581  |
| H       | 7.70182423083700  | 3.31423318210045  | 1.9892687881519  |
| H       | 8.8390536593188  | 4.55187082035599  | 1.48555216448064  |
| C       | 5.07673872971548  | 7.17040124329391  | -1.37322441918292  |
| C       | 5.23520193202061  | 6.33516081698837  | -2.05426522399059  |
| H       | 5.74754795450752  | 7.9768679725771  | -1.6772279780713  |
| H       | 4.0557780440964  | 7.53738637353922  | -1.47993194010077  |
| C       | 7.01733951500988  | 5.10100095913516  | 3.77077047474695  |
| C       | 8.26147442727567  | 5.60012882573437  | 4.14517486499869  |
| C       | 8.78553613619444  | 5.29951089355551  | 3.5966601677335  |
| C       | 8.63743738902324  | 3.9990019379604  | 5.90325155305623  |
| C       | 6.30101440446574  | 4.29234815431764  | 4.65420793895945  |
| H       | 8.79158104357996  | 6.26315059125868  | 3.47054797452400  |
| H       | 5.30044876775667  | 3.93011353797196  | 4.36503840965058  |
| C       | 4.01161680968170  | 8.53257259397371  | 0.87728236403923  |
| C       | 4.59834825629993  | 9.68670039669261  | 0.3615430719007  |
| C       | 3.87543441780052  | 10.86574115662447  | 0.2889750227899  |
| C       | 4.34506802520960  | 11.7569520481551  | -0.1112851845577  |
| C       | 2.56567803837215  | 10.91434258582677  | 0.74537242474425  |
| H       | 2.00484110491324  | 11.83995613255776  | 0.69471620155113  |
| C       | 1.98679725161858  | 9.77390453001974  | 1.28182511058993  |
| H       | 0.96950520022791  | 9.8043111635316  | 1.65345006482542  |
| C       | 2.7201006345384  | 8.58871445390679  | 1.3512153690261  |
| C       | 5.97769408680996  | 10.64375918346334  | 10.26257607069753  |
| C       | 5.79629183288960  | 9.61840830766669  | 11.1998642395479  |
| C       | 5.32533490212999  | 9.90999738617343  | 12.12767701139170  |
| C       | 6.21775612004862  | 8.28875878743543  | 11.1239099694092  |
| C       | 5.53346212514693  | 12.01788454490274  | 10.67631100609854  |
| H       | 5.15536185516419  | 12.58259748229503  | 9.82939215217175  |
Table S11. Cartesian coordinates of \([\text{L' (Me}_2\text{N)}\text{GaSb(NMe}_2)]_2\) \((\text{L'} = \text{HC}[\text{C(Me)NPh}_2]_2)\) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -6401.8136228 \(E_h\)

Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.9289205 \(E_h\)
|     | Gibbs free energy (PBE0/D3BJ/def2-TQZVP) | Enthalphy (PBE0/D3BJ/def2-TQZVP) |
|-----|----------------------------------------|----------------------------------|
| Sb  | -2.35105783269888                     | -6400.978976 E_h                |
| Ga  | -1.77068631048936                     | -6400.82470381 E_h              |
| N   | -2.9209110722581                      | 0.23409846369268               |
| N   | -2.478219118727704                    | 2.78873738723842               |
| N   | 0.00858902771638                      | 3.45474560015187               |
| C   | -3.64302941273823                     | 4.10957457317875               |
| C   | -3.74347842555217                    | 4.55387690837734               |
| H   | -4.31618361849783                     | 5.37086462983685               |
| C   | -3.23707401964307                    | 6.27856148928390               |
| H   | -3.79602083822695                     | 4.98528448152905               |
| H   | -4.67807488346793                     | 6.0371105654839                |
| H   | -5.30548712023007                     | 4.39359163269589               |
| C   | -3.57571080311832                     | 6.1791675558923                |
| H   | -4.39785442161123                     | 5.83556560679715               |
| H   | -3.89783703537926                     | 7.1050368805165                |
| H   | -2.72439038108684                     | 6.36337467784742               |
| C   | -2.89991048018972                     | 2.6015280158846                |
| C   | -4.00383395977115                     | 1.8197140347016               |
| C   | -3.92450415660098                    | 0.91285171990807               |
| H   | -4.78653627143278                    | 0.3022872284984               |
| C   | -2.74403801442165                    | 0.76751967162564               |
| H   | -2.68393328646948                    | 0.05184305951652               |
| C   | -1.63935769377649                    | 1.5351897318472               |
| H   | -0.71027160160942                    | 1.42233159643209               |
| C   | -1.71371425794990                     | 2.44750507570482               |
| C   | -2.11920635252631                     | 3.88304079552790               |
| C   | -3.08091915604201                     | 3.5583132810733               |
| C   | -2.7051456216375                     | 3.278222264873                 |
| C   | -3.46126364045739                    | 3.0123362418206               |
| C   | -1.36693537332063                     | 3.30829698405302               |
| H   | -1.07372321120844                    | 0.30719935306547               |
| H   | -0.40723535597747                     | 0.61938096880274               |
| H   | 0.64198254914022                     | 3.63228582137528               |
| C   | -0.77730379740739                     | 3.90461633790901               |
| C   | 0.98784201361591                     | 2.32999984161726               |
| H   | 1.15625118929498                     | 2.38885935844011               |
| H   | 0.68489491910041                     | 1.30448862149328               |
| H   | 1.9670426911108                      | 2.49561337945367               |
| C   | 0.35341481110822                    | 4.62777687417986               |
| C   | 1.31687436526927                     | 6.9131065650520               |
| H   | -0.40495561376797                    | 4.82146837216066               |
| H   | 0.45131154677342                     | 3.26620057711513               |
| Sb  | -1.6535250573210                     | -3.5893789875013               |
| N   | -2.2920421940357                    | 5.85746085913385               |
| N   | -1.4503365149005                     | -3.07853301943663              |
| C   | -0.79237456146145                    | -4.74364296498614              |
| H   | -0.50401438431759                    | -5.4070997428051               |
| C   | -0.04886769836946                    | -6.3655463334357               |
| C   | -0.80388394975750                    | -4.9752831179837               |
| H   | -0.3169052182664                     | -5.41446448910740              |
| H   | -1.0271951832622                    | -5.26971800034398              |
| H   | -0.17489311746433                    | -6.48000253725294              |
| H   | 0.63818455593270                    | -4.9961520603721               |
| X                  | Y                  | Z                  |
|--------------------|--------------------|--------------------|
| 6.41771073706669   | -5.86060833081329  |
| 7.18183789229279   | -5.9756851926583   |
| 6.91199203132807   | -5.42346043875724  |
| 6.03216488974410   | -6.83917939713856  |
| 1.50781550918671   | -2.88537485657180  |
| 0.85323117386695   | -2.34978258541556  |
| -0.28361508515599  | -1.5770997689577   |
| -0.78062499699620  | -1.16043484730332  |
| -0.77358566767805  | -1.31937588343117  |
| -1.65840864314515  | -0.70766468698127  |
| -0.11730774468607  | -1.8194257268338   |
| -0.48786077226728  | -1.64198576767083  |
| 1.01831951531824   | -2.6195131164090   |
| 6.95963903769726   | -3.45714009826411  |
| 9.6495464244931    | -2.94551037057929  |
| 8.96260629173320   | -2.52870372677568  |
| 9.48577034909005   | -2.1135910406253  |
| 9.5955505098160    | -2.60974852139770  |
| 10.61543709834151  | -2.26225242048018  |
| 8.90224688657946   | -3.10110829574475  |
| 9.38442305370205   | -3.15248423024537  |
| 7.58552235311303   | -3.51757702545277  |
| 3.84773486404491   | -2.15083080708726  |
| 2.80549479042416   | -2.31227102665717  |
| 3.91218661212570   | -1.12267204024982  |
| 4.47385037869324   | -2.21447158705697  |
| 4.16351117850824   | -4.43970953975927  |
| 4.77512433909757   | -4.63502040753464  |
| 4.5123507012914    | -5.12438727941134  |
| 3.13126274746029   | -4.74139489802690  |
| 7.02416273970567   | -3.8766103973421   |
| 9.41609727037509   | -1.89300317558578  |
| 12.10809174394092  | 3.04127613987365   |
| 7.13752207404533   | -2.84765877138504  |
| 1.54413611162611   | -3.02421457585715  |
| 1.25897745438062   | -2.52089432629688  |
| 4.82041864471837   | 4.12769474314930   |
| 3.76684123715269   | 3.5022356947431    |
| 4.88528588200178   | -0.35432096438214  |
| 4.70776537869874   | 0.85291342709768   |
| 3.65241939450560   | 1.07198777727648   |
| 5.11782106093611   | 1.71666909486164   |
| 5.24863684397108   | 0.75899664784817   |
| 4.39243196365282   | -1.49427839540707  |
| 3.31576439132095   | -1.44155125610425  |
| 4.92285831460725   | -1.56455418158587  |
| 4.5722918658618    | -2.4220795418070   |
| 6.95769592128816   | 0.62589887130430   |
| 7.30187965058136   | -0.50963122533217  |
| 5.91916374990055   | 1.43395805173085   |
| 4.93582856709348   | 0.93400965131357   |
| 5.79160135600345   | 2.35142871294651   |
| 6.19042458600553   | 1.7174612103855    |
| 8.16859554891977   | -1.02502749772773  |
| 7.57160849226416   | -0.16684163345422  |
| 6.49470691553545   | -1.25074363264073  |

Table S12. Cartesian coordinates of N$_2$ [Å] for the optimized geometry.
Energy (PBE0/D3BJ/def2-S(TZ)VP) = -109.31560762 \text{E}_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 0.00576230 \text{E}_h
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -109.30654060 \text{E}_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -109.32893667 \text{E}_h

\begin{tabular}{ccc}
N & -1.45315231394315 & 1.04391077658411 \\
& 0.00000000000000 & 0.00000000000000
\end{tabular}

\begin{tabular}{ccc}
N & -0.35621768605685 & 1.00295922341589 \\
& 0.00000000000000 & 0.00000000000000
\end{tabular}

\textbf{Table S13.} Cartesian coordinates of [L(Me\textsubscript{2}N)GaSb\textsubscript{2}N\textsubscript{3}-Ph (14')] [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7467.92091380 \text{E}_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.55198463 \text{E}_h
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7466.27390470 \text{E}_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7466.48156992 \text{E}_h

\begin{tabular}{cccc}
Sb & -3.63075078361640 & 6.64557708400430 & 22.8168007525725 \\
& 4.72314938831901 & 24.75851742803625 \\
Ga & -1.37460782513996 & 5.17393094089000 & 25.9634002321803 \\
& 3.80367086672687 & 27.4070022071533 \\
N & -9.99336103540511 & 6.67834350696393 & 27.23188364865344 \\
& 0.29293871763483 & 6.72819525459886 & 22.14467080598133 \\
& -7.22736585539554 & 4.96966951321858 & 24.93787365511022 \\
& -2.75873422551918 & 7.90515598026993 & 24.34554491710905 \\
& -0.60845861538335 & 3.97386113598100 & 19.78414005148816 \\
C & -0.48368043146514 & 4.91218926632183 & 18.74439614504704 \\
& 0.01890603095403 & 4.58893775504958 & 17.84470413267658 \\
C & -1.04793050991395 & 6.1918181052929 & 18.66658049552877 \\
& -0.0505572155684 & 2.60132984525886 & 19.52054578341834 \\
H & -0.11695413919617 & 2.3413311104725 & 18.45674643863476 \\
& -0.54388679637928 & 1.82814451141219 & 20.12114216427624 \\
C & 1.01657972870001 & 2.60218373029336 & 19.7985441385280 \\
& -0.95249203898707 & 6.90896630418635 & 17.34517436563345 \\
H & -0.74919514298334 & 6.20486501211797 & 16.5294160319568 \\
& -0.12901147992055 & 7.63904168804837 & 17.38436491995091 \\
C & -1.86696460269988 & 7.47481638697250 & 17.1226374273104 \\
C & -1.56432066123192 & 3.19626039822619 & 21.83982645664982 \\
C & -0.75656991450412 & 2.79769753971669 & 22.92432430856692 \\
C & -1.22254602336111 & 1.77735168743613 & 23.76073318548351 \\
C & -0.60926286562618 & 1.46160174012545 & 24.60789368366285 \\
C & -2.4547791219729 & 1.17382749779606 & 23.5527258809663 \\
C & -2.80963741133036 & 0.39949667505617 & 24.2348414071255 \\
C & -3.24993551893155 & 1.58942234561806 & 24.9107756858979 \\
C & -4.22569016576080 & 1.12314771602554 & 22.33842446692248 \\
C & -2.82875642971464 & 2.60026664422004 & 21.6237353024400 \\
C & 0.59411556194278 & 3.42540157785751 & 23.203987331871 \\
H & 0.70282839636318 & 4.28764423377941 & 22.5308932839499 \\
C & 1.7145221701512 & 2.44397570442198 & 22.91713151105922 \\
H & 1.69087952671716 & 2.06232014499491 & 21.8865723918314 \\
H & 1.6864081288874 & 1.57423511822982 & 23.59249330377273 \\
H & 2.70890787120410 & 2.93042753220764 & 23.06226641985604 \\
C & 0.6828946983548 & 3.95389370685785 & 24.63456964821167 \\
H & 1.64899745781472 & 4.45400600114231 & 24.80039165161163
\end{tabular}
Table S14. Cartesian coordinates of $[\text{L(Me}_2\text{N)GaSb}_2\text{N}_3]^{-}\text{SiMe}_3$ (14") [Å] for the optimized geometry.

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| Sb   | -6.4851833207110 | 9.2007969236816 | 5.74094143264128 |
| Sb   | 4.51643084778682 | 7.34624099875682 | 5.3295592367486 |
| Ga   | 4.8581469411502 | 6.46300015666474 | 2.84003170463874 |
| Ga   | 7.3273830011510 | 9.0589953691670 | 8.2939749514373 |
| Si   | 1.46871965996984 | 9.0231838434812 | 5.2434494171817 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7645.51002257 $E_h$

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.57381343 $E_h$

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7643.8304761 $E_h$

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7644.05042820 $E_h$
Table S15. Cartesian coordinates of [L(Me₂N)GaSb]₂N₂C(H)SiMe₃ (14”) [Å] for the optimized geometry.

| Atom | X          | Y          | Z          | E (Eh)         | ZPE (Eh)     | E_h (Eh)      | G (Eh)       |
|------|------------|------------|------------|---------------|--------------|---------------|--------------|
| Sb   | 6.943      | 6.562      | -2.887     | -7629.4892667 | 1.5833546    | -7627.9064252 | -7628.0200625 |
| Si   | 4.543      | 7.371      | 0.127      |               |              |               |              |
| Ga   | 5.072      | 6.418      | 0.198      |               |              |               |              |
| Si   | 7.375      | 8.430      | -2.887     |               |              |               |              |
| N    | 6.816      | 6.591      | 0.127      |               |              |               |              |
| N    | 4.042      | 7.124      | 0.198      |               |              |               |              |
| N    | 8.000      | 10.356     | 0.127      |               |              |               |              |
| N    | 6.021      | 8.364      | 0.127      |               |              |               |              |
| N    | 4.675      | 4.574      | 0.127      |               |              |               |              |
| N    | 8.714      | 7.162      | 0.127      |               |              |               |              |
| C    | 3.858      | 9.460      | 0.127      |               |              |               |              |
| C    | 6.840      | 6.307      | 0.127      |               |              |               |              |
| C    | 5.690      | 6.272      | 0.127      |               |              |               |              |
| C    | 5.846      | 5.948      | 0.127      |               |              |               |              |
| C    | 4.409      | 6.749      | 0.127      |               |              |               |              |
| C    | 8.139      | 5.992      | 0.127      |               |              |               |              |
| H    | 8.308      | 6.678      | 0.127      |               |              |               |              |
Table S16. Cartesian coordinates of $[\text{L(Me}_2\text{N})\text{GaSb(N-Ph)}]_2[\text{L(Me}_2\text{N})\text{GaSb}]$ (15') [Å] for the optimized geometry.

| Atom | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| C    | 2.7556288088215 | 9.8200994121532 | 7.4630679312495 |
| H    | 1.89890028722717 | 10.0520921200944 | 8.11443114517974 |
| H    | 3.5564181161638 | 10.548790258088 | 7.74058141695749 |
| H    | 3.13592197593375 | 8.8247602058137 | 7.30330791858989 |
| H    | 0.0462829362466 | 8.73902237252478 | 5.77598160940770 |
| H    | 1.3316778363592 | 7.06056376388184 | 5.70069850005844 |
| H    | 0.8375599241043 | 8.37080303879894 | 4.22166661044141 |
| C    | 1.59833528194507 | 11.49658783159356 | 5.1255113317146 |
| H    | 1.3087113779793 | 11.4746803469644 | 5.06510570030344 |
| H    | 2.3634772590425 | 12.27626910517674 | 5.25978205781482 |
| H    | 0.71010166738467 | 11.77391423167943 | 5.717585326392 |
| N    | 4.77719430135732 | 10.51878452155114 | 4.9085098374475 |
| N    | 5.88059323930625 | 10.48390683213074 | 5.39895681810169 |
| H    | 3.45708135087122 | 9.52753953609951 | 3.59125790442251 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7358.5846717 $E_h$

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.5415592 $E_h$

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7356.9512666 $E_h$

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7357.1568558 $E_h$
|     | x          | y          | z          |   |
|-----|------------|------------|------------|---|
| C   | -3.025161  | 128588004  | 6.850732   |  28.7492452339783 |
| C   | -6.035853  | 28985828   | 9.217953   |  27.333960148361 |
| H   | -6.733541  | 17953325   | 8.373437   |  27.4281843260527 |
| C   | -6.408390  | 93652812   | 10.265163  |  28.38391776186527 |
| H   | -5.800340  | 6886418    | 11.176711  |  28.27245890149110 |
| H   | -6.262564  | 0456564    | 9.897992   |  29.41083257722951 |
| H   | -7.463028  | 9053257    | 10.562106  |  28.27021594923447 |
| C   | -1.986966  | 69728672   | 9.783003   |  25.92414062817680 |
| H   | -5.898402  | 26372334   | 9.039692   |  25.17529919508968 |
| H   | -5.568814  | 48420909   | 10.673421  |  25.77519341528012 |
| H   | -7.244034  | 46677106   | 10.078143  |  25.74161208170896 |
| C   | -2.737912  | 97283003    | 5.383211   |  28.1029276541719 |
| H   | -3.474490  | 45073192    | 4.814098   |  27.512816310352 |
| C   | -2.949457  | 74353635   | 5.021960   |  29.5740563567012 |
| C   | -3.980454  | 51458519    | 5.213316   |  29.90129372156853 |
| H   | -2.274676  | 02843793    | 5.605729   |  30.22058922427127 |
| H   | -2.741083  | 32416694    | 3.953680   |  29.74428262454295 |
| C   | -1.361006  | 59034085    | 4.942756   |  27.62892573682087 |
| H   | -1.210365  | 61313473    | 5.189817   |  26.56982599313616 |
| H   | -1.258195  | 946651856   | 3.852923   |  27.72952629441157 |
| H   | -0.550879  | 791743081   | 5.403005   |  28.21707813055788 |
| C   | 1.090579   | 99558858   | 8.185876   |  20.9796123599333 |
| H   | 1.126752   | 85716407    | 7.455048   |  20.1567482696971 |
| H   | 2.019391   | 160542639  | 8.048408   |  21.57713795793074 |
| H   | 1.159249   | 95928994    | 9.195918   |  20.5258392042735 |
| C   | -0.216686  | 20344123    | 9.003438   |  22.81794328628076 |
| H   | -0.333706  | 65804703    | 10.033100  |  22.42388901827968 |
| H   | 0.673443   | 343094520   | 9.013246   |  23.47977172470151 |
| H   | -1.093644  | 428996644   | 8.807859   |  23.45213221520700 |
| C   | -8.304002  | 24536779    | 6.857675   |  25.6609856468463 |
| H   | -8.458953  | 96164130    | 7.956184   |  25.07827119530335 |
| H   | -8.337472  | 22439693    | 6.481122   |  26.6955059132465 |
| H   | -9.195238  | 28908636    | 6.444870   |  25.1362450868078 |
| C   | -6.973194  | 96292977    | 6.986066   |  23.67227232215615 |
| H   | -6.064816  | 60322577    | 6.596690   |  23.18902851347993 |
| H   | -6.914364  | 62040762    | 8.091888   |  23.61273457453347 |
| H   | -7.838438  | 40235263    | 6.677655   |  23.04897412711697 |
| C   | -3.712385  | 05113428    | 9.299012   |  23.37143776444445 |
| C   | -3.292183  | 17879629    | 10.501683  |  23.99474251265315 |
| C   | -3.369181  | 07164618    | 10.431201  |  25.0110867490498 |
| C   | -3.028947  | 38288896    | 12.626708  |  23.84620289142450 |
| C   | -3.882547  | 7175703    | 11.801493  |  22.0387208473417 |
| C   | -3.960063  | 47603805    | 12.765069  |  21.53040760675465 |
| C   | -4.299007  | 62106892    | 10.631296  |  21.40743877057969 |
| H   | -4.710710  | 64539199    | 10.669240  |  20.3968334549205 |
| C   | -4.202847  | 078416692   | 9.398758   |  22.0470187790423 |
| H   | -4.558752  | 25876911    | 8.493878   |  21.5447684181352 |

**Table S17.** Cartesian coordinates of $[L_{(Me_2N)}GaSb(N-SiMe_3)][L_{(Me_2N)}GaSb]$ (15°) [Å] for the optimized geometry.
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Sb      | 4.91156149009091 | 9.84574570219467 | 6.83561413943616 |
| Sb      | 4.53159257035483  | 8.13913904655557 | 4.88564679424705 |
| Ga      | 5.03238511135948  | 6.36400806737875 | 2.93618228784587 |
| Ga      | 7.09495698355508  | 9.21322344911904 | 8.18053021570157 |
| Si      | 1.38104196260665  | 9.01076682832086 | 4.84243119967392 |
| N       | 6.87362838077999  | 5.92784561600909 | 2.38765502541504 |
| N       | 4.52069210732321  | 7.12268750062646 | 1.17644652130662 |
| N       | 7.64048923273279  | 10.94226403608242 | 8.98741412519849 |
| N       | 6.38000235870511  | 8.42087891469325 | 9.88520792197525 |
| N       | 4.11346300272808  | 4.80181564090344 | 3.3142440238183 |
| N       | 8.51287172319875  | 12.8547642118614  | 7.65847812312637 |
| N       | 2.73754537959913  | 10.8908716023435  | 4.22461076275159 |
| C       | 7.10177358671215  | 5.5597594272068  | 1.1227054082937 |
| C       | 6.22421710751979  | 5.81469256145874 | 0.0651125400411 |
| H       | 6.52969037910713  | 5.43900947829788 | -0.90921232131906 |
| C       | 5.09180345687933  | 6.65086174686439 | 0.07175991920449 |
| C       | 8.38413969202979  | 4.84558639402378 | 0.78842355869088 |
| H       | 8.38704644929399  | 4.52101718663823 | -0.2589271127411 |
| H       | 8.51942138552330  | 3.97165617922696 | 1.4418935827988 |
| H       | 9.25474899117388  | 5.49393537835430 | 0.9616586651762 |
| C       | 4.52691803247731  | 7.01895695071518 | -1.27197003170178 |
| H       | 5.20311263204770  | 6.70761010160820 | -2.07648185084534 |
| H       | 4.34718122485262  | 8.10039400976711 | -1.34245624592071 |
| H       | 3.55155686281806  | 6.53442657157518 | -1.4221465032429 |
| C       | 8.00670289712639  | 5.93546593140016 | 3.25930426040589 |
| C       | 8.88183673397144  | 7.03974716919648 | 3.1942940851927 |
| C       | 10.08399316696457 | 6.97816114743045 | 3.90339548365276 |
| H       | 10.7799226628900  | 7.8189097482975  | 3.85062200952597 |
| C       | 10.41047521051292 | 5.86514066236519 | 4.6692103933972 |
| H       | 11.3593685447721  | 5.80366434469469 | 5.20974532563640 |
| C       | 9.50997780809748  | 4.81241020516665 | 4.7714602130187 |
| C       | 9.75309798011166  | 3.95545701365950 | 5.4040254728062 |
| C       | 8.29436004274161  | 4.82725601034535 | 4.08191955715055 |
| C       | 8.54813038959362  | 8.27980777064670 | 2.38589710485679 |
| H       | 7.57654782670520  | 8.10682320898761 | 1.90129069489285 |
| C       | 8.39177434330968  | 9.49365672885479 | 3.30002483753369 |
| H       | 8.08168261506993  | 10.37818691547186 | 2.72358068728170 |
| H       | 9.33642246413342  | 9.74628098454311 | 3.80657562195545 |
| H       | 7.63589021012612  | 9.31590550553881 | 4.0804407601204 |
| C       | 9.56752126642434  | 8.54763245452595 | 1.2797480149354 |
| H       | 9.64935809727833  | 7.6971622198435  | 0.5866703340452 |
| H       | 10.57003208705632 | 8.74233168500315 | 1.69258436849154 |
| H       | 9.27408302092634  | 9.43036649159755 | 0.69082349755154 |
| C       | 7.31756032247858  | 3.68303220075775 | 4.24778512041934 |
| H       | 6.52293443800370  | 3.82188824813044 | 3.5024685564066 |
| C       | 6.65834175595851  | 3.75516698744857 | 5.62561348536111 |
| H       | 6.14600746789126  | 4.7175777294586 | 5.76797352233721 |
**Table S18.** Cartesian coordinates of [(L(Me$_2$N)GaSb(CH-SiMe$_3$))(L(Me$_2$N)GaSb)] (15°) [Å] for the optimized geometry.

| Atoms | x        | y        | z        |
|-------|----------|----------|----------|
| Sb    | 5.01246684345640 | 9.90786272574718 | 6.6642523410343 |
| Sb    | 4.49215893976371 | 8.05012935860090 | 4.82446391686066 |
| Ga    | 5.12428226472651 | 6.33596303202340 | 2.89694806200026 |
| Ga    | 7.05671581885282 | 9.19159891209111 | 8.15096929621666 |
| Si    | 1.21412271953200 | 9.20207788686499 | 5.06000169785456 |
| N     | 6.96367206445657 | 5.95878495861922 | 2.32998015971334 |
| N     | 4.55878495861922 | 7.05147031059117 | 1.12743107218236 |
| N     | 7.63124156282582 | 10.93605289461678 | 8.93142181144798 |
| N     | 6.32653347246095 | 8.45061310006711 | 9.87760202547678 |
| N     | 4.19599066969192 | 4.75214840578697 | 3.19154732093398 |
| N     | 8.48488349784351 | 8.07178865241099 | 7.69813835458515 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7520.15096407 $E_h$

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.57324574 $E_h$

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.48076201 $E_h$

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.69231926 $E_h$
| C     | 2.58133085843949 | 8.18431190053085 | 4.32372813992520 |
| C     | 7.20522821586530 | 5.61271744809439 | 1.06017794652588 |
| C     | 6.31687059201276 | 5.49192675251081 | -0.97478476320935 |
| C     | 5.14421298738070 | 6.19655300053468 | 0.01580065366152 |
| C     | 8.52020480005333 | 4.97167913456817 | 0.71307022198899 |
| C     | 8.51435370463419 | 6.11195629688626 | -0.32218081231480 |
| C     | 8.73424782125761 | 4.13488267665301 | 1.39249486347245 |
| C     | 9.34944869391902 | 5.68304869958859 | 0.83412775295926 |
| C     | 4.54752619733800 | 6.96549836033368 | -1.31949103128568 |
| C     | 5.24971646622864 | 7.64219492731041 | -2.13107537769800 |
| C     | 4.26063324249332 | 8.02483849509776 | -1.36449183251996 |
| C     | 3.62774808909927 | 6.38516361530805 | -1.48337583117439 |
| C     | 8.09261658182003 | 5.97852827879005 | 3.21090825306100 |
| C     | 8.96587929414682 | 7.08628662334584 | 3.14478856290378 |
| C     | 10.15717099578264 | 7.03572174381208 | 3.87157611586133 |
| C     | 10.84983127175336 | 7.89745246302582 | 3.82300849369327 |
| C     | 10.47606788805094 | 5.93166659966665 | 4.65412408959635 |
| C     | 11.41727284245684 | 5.90554041408818 | 5.20773130614838 |
| C     | 9.57572504097785 | 4.88012969878974 | 4.75832663163094 |
| C     | 9.81124424968300 | 4.03187333443193 | 5.40573869394748 |
| C     | 8.36708170673155 | 4.88509824431221 | 4.05532604387680 |
| C     | 8.63452324551965 | 8.32421344604063 | 2.33106535390314 |
| C     | 7.70066721121153 | 8.12508794371650 | 1.78582061217948 |
| C     | 8.37946574601952 | 9.51622674144622 | 3.25298974420271 |
| C     | 8.09030056561826 | 10.40361301529916 | 2.66982438432812 |
| C     | 9.28008242757655 | 9.78018858190808 | 3.82913340343298 |
| C     | 7.57545266859874 | 9.30937526198609 | 3.97615551615931 |
| C     | 9.70605314913606 | 8.65407485800564 | 1.29312731208068 |
| C     | 9.88295603317881 | 7.81427112492208 | 0.60460415065087 |
| C     | 10.66726971395172 | 8.90607341368361 | 1.76813602832952 |
| C     | 9.39954816795587 | 9.52214020479614 | 0.68905442269553 |
| C     | 7.39940355313388 | 3.73181636886658 | 4.22378277068443 |
| C     | 6.53982661406011 | 3.91828313667673 | 3.56900271343893 |
| C     | 6.86686135884733 | 3.69222701524515 | 5.66074635485389 |
| C     | 6.34994586530915 | 4.62788464951964 | 5.91983803501891 |
| C     | 7.67749942066477 | 3.55017755860763 | 6.39297301327703 |
| C     | 6.15211594635880 | 2.86484254254680 | 5.78708482236903 |
| C     | 8.01373962232741 | 2.39119662676461 | 3.82769533123754 |
| C     | 8.37942311126126 | 2.40435467137367 | 2.78954902835232 |
| C     | 7.26659439254754 | 1.58649930570586 | 3.9097245549054 |
| C     | 8.86280892990997 | 2.12199972460403 | 4.47587882042259 |
| C     | 3.43764931447921 | 7.93224339208481 | 1.02304891290439 |
| C     | 3.65518820969311 | 9.31637610567528 | 1.20039036790823 |
| C     | 2.56359890225697 | 10.17816879910851 | 1.08024474634153 |
| C     | 2.71026528753367 | 11.25061224205051 | 1.21353794474868 |
| C     | 1.28918253713046 | 9.69344161271758 | 0.80876506888776 |
| C     | 0.44744516347755 | 10.3845427493895 | 0.72340824831502 |
| C     | 1.08758778860113 | 8.32750601610210 | 0.66937119363243 |
| C     | 0.08013279035099 | 7.94870308599164 | 0.48175917095577 |
Table S19. Cartesian coordinates of [L(Me2N)GaSb]2N-Ph (1) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = \(-7358.62915134\) E_h

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = \(1.54217813\) E_h

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = \(-7356.99388588\) E_h

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = \(-7357.19764448\) E_h
C  -1.50880610849780 0.15414505856949 22.53582260852182
H  -0.91974725298792 -0.53578391757402 23.1456697154005
C  -2.84380510505480 -0.12860015370101 22.28148532333418
H  -3.30194636327848 -1.03278078740458 22.68944187950983
C  -3.59473497552294 0.74443070004373 21.5009297254071
H  -4.64217700838307 0.51553762492694 21.29849865379115
C  -3.02858269922531 1.90180639669301 20.96118575456707
H  -3.59473497552294 0.74443070004373 21.5009297254071
C  -0.56135704330521 1.56469703563849 22.35849733407453
H  -0.85366140029059 2.49834455624757 21.85632467792360
C  -1.46473153769221 0.43698914387809 21.85632467792360
H  -1.31883301704217 0.23661419604321 20.7857062060691
H  -1.27103248940830 -0.50296132391752 20.96118575456707
H  -2.52379454201548 0.69386347970271 22.0149269627231
C  0.76254307321181 1.78342790940186 23.85664562330885
H  1.80890648631538 2.05317961498084 24.0688155148453
H  0.53311410155709 0.87081856266841 24.4308652741539
H  0.12266315260831 2.59739339075345 24.21850227931828
C  -3.83690908179381 2.79839364515483 20.04218603450410
C  -3.48151708576333 3.82922785454030 20.20742019132157
C  -3.56294988408563 2.46636714816129 18.57389228505386
H  -4.15813434695162 3.11183704998291 17.91218299086540
C  -3.83255459440050 1.41776048253327 18.35660546963287
H  -2.56062549122997 2.60207248760026 18.31066385013751
C  -5.33456776012310 2.76902629342619 20.3259818943670
H  -8.84529525808230 3.54413288340959 19.73599112601603
H  -5.55297176566607 2.95821036683078 21.38633040462184
H  -5.78552757389898 1.80341238176326 20.04726087546813
C  -1.73856847449818 7.53076823122568 20.2965289372757
C  -1.41476027489148 8.56093577608755 21.20556027586638
C  -2.07763159343956 9.78501069756064 21.08860800543306
H  -1.84535144111713 10.58774938174521 21.78966437083288
C  -3.03240705509375 10.00056223433231 20.10359941927662
C  -3.54478436873515 10.96255498785051 20.0385085999492
C  -3.36316477938432 8.97082539227795 19.23452472772026
C  -4.14485000044946 9.12986043298681 18.48764840043049
C  -2.74576006628717 7.72058775931260 19.32162499199308
C  -0.32982151673726 8.38684709269695 22.2497122826344
C  -0.27331593437877 7.31634802711367 22.50045252612995
H  1.0327073369296 8.78804783011591 21.6797571635966
H  1.30900985355394 8.17028839858327 20.8130988440238
C  1.02437188003579 9.84191905843033 21.3566385660472
C  -0.62001753307662 10.23047529314231 23.4203708168434
H  0.09635694125801 8.84015779848125 24.3242681969247
H  -1.63549250318911 8.9191638103399 23.9021026078790
C  -2.32501218248410 7.60376014338885 18.4133509860256
C  -2.55808926686665 5.74328739914854 18.52166528599775
H  -3.5256613540160 6.99813036795913 16.9364094820503
C  -3.51056954203498 6.13020976416464 16.30973558282085

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H  -2.27964647990173  7.38358096859726  16.59820278435317
H  -4.00123637141311  7.78036215588977  16.73568041297477
C  -4.62566977700332  6.1414263602755  18.849243714030
H  -5.35655124396530  6.96216061045598  18.77682763519675
H  -4.6278967789831  5.79057456972980  19.89183178481817
H  -4.98246417367742  5.31615004866802  18.2136983340362
C  -5.84466555346225  4.36702512284511  28.66726717504190
C  -6.4276842585766  5.43600805978291  29.36902349933839
H  -6.9295879816134  5.1772038912860  30.00388565071899
C  -6.32110128035376  6.81208709966241  29.09080209673361
C  -5.97814031264932  2.99513962831495  29.2690564609986
H  -6.944339755432  2.56890013755465  28.95281230051028
C  -5.97505708216120  3.03452627551587  30.3659260931060
C  -5.1895798669922  2.31653660731960  28.92154895326125
H  -6.84300848952119  7.75349799050028  30.14118186463497
H  -6.22908417323994  8.6609003901899  30.2161296562440
H  -6.891603434980  7.2688310051273  31.12145838568112
C  -7.8595481961696  8.0773624223443  29.87027157436518
C  -4.36394896457019  3.53871319786538  26.93280909581084
C  -4.85084559928423  2.62533246349635  25.97676903400263
C  -3.93128239063738  1.8270243921806  25.2882112401422
C  -4.28700624471375  1.13158186559541  24.52495047985233
C  -2.5699531343820  1.91261555426160  25.54104151504301
C  -1.87295821015705  1.29739872077473  24.9716150346418
C  -2.10323689517113  2.8418626580428  26.51983501998570
C  -1.03188506148703  2.943181297158  26.7214070365552
C  -2.97891188020310  3.60648136918924  27.2328402109345
C  -6.35010634774587  2.46148227790379  25.6954683916999
C  -6.85819204568734  3.25571003282108  26.24177607053122
C  -6.83221460354129  1.10864422684317  26.20614292346140
C  -7.9217992487721  1.0224586283062  26.06895595769294
H  -6.60892639351695  0.96170219525098  27.2725901621062
C  -6.35963273471302  0.28025331092611  25.65426983663936
H  -6.5486039227280  2.62893556085698  24.2148355271689
C  -6.21252911230676  1.8203205333292  24.31161785158335
H  -6.2692956928853  3.5842678750450  23.8446620614571
H  -7.74333926213011  2.6069510724247  24.05090420957936
C  -2.46008441761054  4.52187803564513  28.32856151202491
H  -3.127668456193  5.39885460131774  28.3540067887152
C  -2.55288755803227  3.84998923703302  29.7010217285330
H  -3.5808551577939  3.56624311637086  29.95670249409195
C  -2.1888554418096  4.52941646908991  30.4876516485916
C  -1.93584884733940  2.93749541104001  29.72581816839396
C  -1.0364858426845  5.01844756650288  28.0984258068828
H  -0.91989403538699  5.49953649157728  27.11648593759791
H  -0.30102784823068  4.20207920928188  28.1683088409224
H  -0.76901905403812  5.7558723613825  28.87051684168363
C  -5.59324490526283  8.70747011939021  27.81359786001328
C  -6.6358876016639  9.55344475455524  27.38235659493581
C  -6.36809348765333  10.91774174701251  27.22822629735656
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Sb      | 4.73859264137936 | 8.17882259457493 | 6.90543274303859 |
| Sb      | 5.9170267341003  | 8.68946659715297 | 4.4686544320799 |
| Ga      | 5.00495213864000 | 6.72921120694701 | 2.89864167057028 |
| Ga      | 6.86537817205024 | 8.9353683424663  | 8.35180481774364 |
| Si      | 2.77029569384425 | 10.15136545461158 | 5.12685612642757 |
| N       | 4.48730571543042 | 7.18225805987951 | 0.99570721098138 |
| N       | 6.96063783842453 | 10.72076038868592 | 9.17544219311848 |
| N       | 6.49317352292845 | 7.94714471749921 | 10.08672952987910 |
| N       | 3.82643938536892 | 5.37013474531412 | 3.3965352657427 |
| N       | 8.52453119184184 | 8.35492780848017 | 7.69766844969542 |
| N       | 4.41343184932305 | 9.68620337240397 | 5.50088363627071 |
| C       | 6.8057741589125  | 5.2619397741988  | 1.10454519062922 |
| C       | 5.9119161429375  | 5.4817976953018  | 0.0498661273641 |
| H       | 6.09427219665737 | 4.90919848026194 | -0.8594076082034 |
| C       | 4.90837847582809 | 6.46450026873982 | -0.03751636154590 |
| C       | 7.91270985828306 | 4.26984734160403 | 0.86963294667607 |
| H       | 7.9004758268707  | 3.90484965240992 | -0.16680183776463 |
| H       | 7.7922978056676  | 3.41357192146962 | 1.54753767266603 |
| H       | 8.89952942657426 | 4.7001699342488  | 1.08569334279431 |
| C       | 4.30143975480818 | 6.66532311092344 | -1.40066719188463 |
| H       | 5.03554193635205 | 6.44418735665499 | -2.18561635019302 |
| H       | 3.91539626971906 | 7.68311065103647 | -1.5367833029124 |
| H       | 3.45498670666732 | 5.97310059792767 | -1.53046508660605 |
| C       | 7.87881364618112 | 5.83215243291610 | 3.12555953395369 |
| C       | 8.88884147762098 | 6.80586849980781 | 2.9424893742643 |
| C       | 10.0750451964281 | 6.80658284379041 | 3.6700453105750 |
| H       | 10.86850420048297 | 7.41832165274880 | 3.5305479086305 |
| C       | 10.26696067077669 | 5.62951707295546 | 4.55940607142155 |
| H       | 11.20524529421803 | 5.54152298776484 | 5.11034405609888 |
| C       | 9.24232879197621 | 4.71629286300947 | 4.77364872952101 |
| C       | 9.37738057657860 | 3.9187443621625 | 5.50834621062770 |
| C       | 8.03223180282532 | 4.80580036777092 | 4.07945918943199 |
| C       | 8.72147316884608 | 7.94106638061901 | 1.9479927514333 |
| C       | 7.63866764606333 | 8.06678317467369 | 1.79238962800040 |
| C       | 9.2731161532088 | 9.2664726421479 | 2.4667869083012 |
| H       | 9.00975857392623 | 10.0808896689032 | 1.77470492210371 |
| H       | 10.37130113743913 | 9.2540337867104 | 2.54561942375015 |
| H       | 8.86146532505813 | 9.51446708941525 | 3.45651863199868 |
| C       | 9.33336082996920 | 7.60295783392864 | 0.58661056901440 |

**Table S20.** Cartesian coordinates of [L(Me\(2\)N)GaSb]\(2\)N-SiMe\(3\) (16) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7536.24119054 \(E_h\)
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.56269284 \(E_h\)
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7534.58233655 \(E_h\)
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7534.79231493 \(E_h\)
Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -7539.1480564 \(E_h\)
Table S21. Cartesian coordinates of $\text{[L(Me}_2\text{N)GaSb]_2}$ (11) [Å] for the optimized geometry.

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Sb      | 5.66507803460978 | 6.06637369834588 | 10.98291520046017 |
| H       | 11.01503967131364 | 7.74675204545337 | 10.519065809382 |
| C       | 4.39843655326050 | 5.81522611265552 | 9.72650162662206 |
| H       | 11.30200598843819 | 6.90017572205782 | 9.58007170070185 |
| C       | 3.51344910205309 | 5.38359313798910 | 10.90012379648881 |
| H       | 2.46180646741894 | 5.64385583475496 | 10.70266557293366 |
| H       | 3.80779420638516 | 5.8506294796282 | 11.8401737044775 |
| H       | 3.56397461291811 | 4.2920221490404 | 11.0414282405727 |
| C       | 9.2161942369813 | 5.10581906175465 | 8.45870063649882 |
| H       | 2.06822865321660 | 5.2395961684267 | 4.5789753851954 |
| C       | 3.42549797100396 | 6.39537406016465 | 5.30485462309644 |
| H       | 3.47056565614632 | 3.6511662793368 | 5.22870113741916 |
| C       | 3.63151435585590 | 2.20580415118322 | 2.58335238268406 |
| H       | 1.43006842325691 | 4.30537470566622 | 1.6074099165124 |
| H       | 2.55074256973693 | 4.00495605057353 | 2.38641703359553 |
| H       | 4.03228422267366 | 3.2818309133382 | 3.0520200317155 |
| C       | 8.49659563929064 | 7.02450227742329 | 7.1469501335815 |
| H       | 8.17243263879994 | 6.99137861452732 | 6.0873895800401 |
| H       | 7.8224779343323 | 6.36231929047497 | 7.71759381990391 |
| H       | 9.50055931230491 | 5.6573194160878 | 7.1809809092989 |
| C       | 9.37795201652242 | 9.21238186773933 | 6.91855708193208 |
| H       | 9.06539892803818 | 9.29386882368701 | 5.85393902673762 |
| H       | 10.41672346850392 | 8.82316929056116 | 6.90666771535845 |
| H       | 9.41665208297523 | 10.2308667186244 | 7.32881622790354 |
| C       | 1.88334212984553 | 10.51357149916076 | 6.75211106145413 |
| H       | 0.8799774021473 | 10.9263619883190 | 6.5583748922949 |
| H       | 2.43828411709221 | 11.2377620701574 | 7.36726111902006 |
| H       | 1.75767929035852 | 9.59275697569194 | 7.3441171220054 |
| C       | 1.81876250331983 | 8.81132974655150 | 4.22244792755676 |
| H       | 0.78551171128143 | 9.12344956433195 | 4.00217313129002 |
| H       | 1.77732571507148 | 7.88719798389276 | 4.81877449851823 |
| H       | 2.30143611767395 | 8.57568301025566 | 3.2628005963610 |
| C       | 2.76769539303069 | 11.70649045479226 | 4.0665506469106 |
| H       | 3.29837867843327 | 11.53279637722741 | 3.1198276375834 |
| H       | 3.23739227704905 | 12.55968221856106 | 4.5781675203003 |
| H       | 1.73185095798009 | 11.98548471753007 | 3.8137881165907 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) $= -7520.22183531 \text{E}_h$

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) $= 1.57348089 \text{E}_h$

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) $= -7518.55169516 \text{E}_h$

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) $= -7518.76217520 \text{E}_h$

Energy (PBE0/D3BJ/def2-T(Q)ZVP) $= -7523.09516169 \text{E}_h$
H  5.98201382286831  9.808589798393194  4.09991219809858
C  4.21257698848048  7.20521236284187  2.928094727537908
H  4.53077912093266  7.84462705049495  2.09144601213760
H  3.16336108792408  7.45680622681770  3.1490497742620
H  4.24602447021574  6.15779109415691  2.5868519228583
C  7.04122784797728  6.89258035649236  2.928094727537908
H  7.04159323683814  5.82895364649710  3.71989420929283
H  7.72549281217846  7.0083476875180  4.86041545666397
H  7.43844239641674  7.47420611966568  3.1624147028538
C  4.60051425273985  6.46667933731183  5.86007387139399
H  3.58215982210046  7.79689834692411  6.1106337451377
H  5.22481785116943  6.5626097671314  7.5820477309058
H  4.55391981535570  5.39780077061564  5.5999467118568
N  5.15487701635113  10.38634094841797  10.25511241736984
Ga  4.88441707910090  9.01793818301843  8.8196521553333
Sb  3.45070632784750  10.37741699024679  5.00609361569681
C  5.94954931273302  8.7082809032282  11.86492292987151
H  6.12964839643309  8.6205266578447  12.92674295201726
N  6.20269413297117  7.76034774283499  9.69366034329522
Ga  4.00848558118022  12.30739285331034  3.30903832393253
N  3.22347542909400  8.20940825000905  9.0674128076984
C  7.25825676627871  6.70176403136338  11.6456611827607
H  6.59865189780521  5.88658853222527  11.9782550592942
H  7.77882470364589  7.09111780092971  12.52950410762636
H  7.98907219526909  6.26740858694534  10.95223187641355
N  3.1281435229507  11.90820040837288  1.5468904399756
C  5.12873868171730  10.99458308479374  12.6298831204834
N  5.6536411711892  11.95670794036022  12.4753133072163
H  5.43199377058260  10.58020786724236  13.5986083399989
H  4.05116965604603  11.21593575103205  12.6573553873718
N  2.91697673590168  13.96232868970972  3.5616027413129
C  6.43743732725014  7.78608531387185  10.9994052514212
N  5.75581638637486  12.82944151369908  2.8957120395362
C  5.001054647219  11.7802016195089  9.9971628752877
C  4.79238602782893  14.55108923753320  9.7767563511336
C  4.7096456528663  15.63903825660948  9.72051195091990
C  6.04404170948130  13.94496435201765  9.75910611322321
H  6.94033989273057  14.56263808005447  9.6683687320006
C  6.1740741664935  12.55813997985200  9.8437780752452
C  3.64876444145766  13.76701962182145  9.3682994375518
C  2.6668112407316  14.2428955204503  9.80349801136504
C  3.7268241436295  12.37502822459214  9.9434485824747
C  7.5513541660078  11.91897008291939  9.79691008161544
H  7.3963819642079  10.8522733121337  9.5728596362762
C  8.41284052362252  12.5056789255196  8.68016651087440
H  7.8907688485755  12.47017345258086  7.7124343624622
H  9.35009436587551  11.3574810073273  8.8465233446487
H  8.69953604748468  13.55204167786117  8.8812433524839
C  8.28416924886223  11.9968634719948  11.1373804935280
H  9.28965441869047  11.5577723196505  11.05164067293832

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H  3.27427739518564  12.30026850083192 -1.22418380284972
H  1.94144788565545  13.4883821707863 -1.16551483071518
H  1.66307871366116  11.7681478278960  -0.76006055549132
C  2.59096701034078  14.4486793276787  4.8624559667175
C  1.28562972580721  14.2292802914244  5.35748050660655
C  0.92759583428321  14.8099288974023  6.57670456794309
H  -0.08504487688884  14.6634382368815  6.96138920712871
C  1.8371207973321  13.5732975659620  7.30301735535176
H  1.5310575171526  16.0363964667569  8.2455937897831
C  3.13051117720264  15.7304093931223  6.8312657722832
H  3.85082438526150  16.3067739428830  7.41569907149581
C  3.5380844341999  15.1693816964715  5.61781585055981
C  4.97234869356026  15.34936526698214  5.16145823597897
H  5.0856830870044  14.8248845496793  4.20199408765409
C  5.33393246462014  16.8184825627681  4.94528258924870
H  6.36542069258214  16.9079617955094  4.57032673060224
H  5.2704886888229  17.3940340176957  5.88281810305906
H  4.66929188540897  17.3028724778167  4.21389691398119
C  5.92938184557975  14.6910508872878  6.154620284919
H  6.5629627622004  13.6242168087588  6.2901293015174
H  5.87039050411850  15.1645094361027  7.1459053017384
H  6.9698069564562  14.7708756519251  5.8047833495778
C  3.05013411134664  10.5748535887701  1.03926473481354
C  1.89104994217219  9.81461167855951  1.3134271493720
C  1.7513475246712  8.5629967274380  0.69498060767556
H  0.85614640099740  7.9745187272507  0.88404272675751
H  2.73382755170970  8.06986525344012  -0.1516547014680
H  2.60262714672784  7.09648173811098  -0.6296573240647
C  3.89902363040133  8.7971895597966  -0.35455632891815
H  4.68937821646231  8.38359690912173  -0.9855372981233
C  4.088572446617385  10.0415398390959  0.23929082575287
C  0.80627225520408  10.33540188669206  2.23894181806525
H  1.30154121186198  11.0156341993397  2.9511091526519
H  -0.24690712471316  11.1569852243720  1.4935182518005
H  0.18215417762693  12.05853781223580  1.0344969201227
H  -1.03861562906299  11.48566430210728  2.18503510551670
H  -0.72070489937097  10.55869378588003  0.69685730206250
C  0.14987281556188  9.2241606802070  3.05270572896349
H  -0.47108643119811  8.5647283486647  2.42662467665518
H  -0.50800972871395  9.65517380619364  3.8208061165570
H  0.90120736339785  8.60553439742698  3.56587700183815
C  2.7921666291002  7.7986840629083  10.37189930159890
H  2.00733826078927  8.46618172365786  10.79495483935265
H  3.62558319901649  7.7927059356155  11.09022456790814
H  2.3553349165531  6.77824341001564  10.36415662033761
C  2.16799544674993  8.1896854310838  8.09993194523942
H  2.50022394648482  8.6112146663604  7.13940245782003
H  1.28553620553597  8.7821424574074  8.42156967806163
H  1.79607294616375  7.1609108081453  7.9020566677910
C  6.04199380015522  13.78731184572709  1.8685565301987

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Table S22. Cartesian coordinates of [(L(Me₂N)Ga)SbSb[N(Ph)Ga(NMe₂)L] (5) [Å] for the optimized geometry.

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Sb      | 3.6291713181556  | 23.46636438542158  | 7.83175894299146  | 1.15642116885291 |
| Sb      | 1.55861151087495  | 24.73029912510697  | 6.75653258423900  | 2.27627818367127 |
| Ga      | 3.53806150068520  | 20.37905880974398  | 7.98758156297777  | 1.28069346158645 |
| Ga      | 3.15578731072583  | 26.57989126828297  | 5.88135961648900  | 5.1461754323125  |
| N       | 4.96355170865099  | 19.50931445878630  | 9.02284374279720  | 14.74728728566097 |
| N       | 2.49042047844445  | 18.77100915215630  | 7.6908393877862  | 14.0329769233811 |
| N       | 2.07153301035226  | 28.23225369868553  | 5.54648589874501  | 12.45993266245541 |
| N       | 4.44795958680398  | 27.57753547563255  | 7.04980790488430  | 12.145614332125  |
| N       | 3.95001269780010  | 21.45746396216916  | 6.42783938649810  | 12.86496799520976 |
| N       | 4.13724653604107  | 26.2391763454259  | 4.30996735215322  | 12.08069346158645 |
| N       | 2.76449961612884  | 21.84415995904685  | 8.83933773510100  | 12.08069346158645 |
| C       | 4.70372642363798  | 18.3956911717204  | 9.70079293148613  | 17.62663109177645 |
| C       | 3.53704707937108  | 17.62663109177645  | 9.53319179999785  | 17.89014534326435 |
| H       | 3.44559984664022  | 16.76411437263904  | 10.19178488901184 | 17.75683248257922 |
| C       | 5.67147951205650  | 17.89014534326435  | 10.73348652771932 | 17.75683248257922 |
| H       | 5.76247481624411  | 16.79777254724036  | 10.6699064446872  | 16.79777254724036 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7358.65076302 $E_h$
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.54393203 $E_h$
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7357.01417187 $E_h$
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7357.21762931 $E_h$

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -7361.55393990 $E_h$
Table S23. Cartesian coordinates of $[\text{L(Me}_2\text{N)}\text{Ga}]{\text{SbSb[NSiMe}_3\text{Ga(NMe}_2\text{L)]}}(4)$ [Å] for the optimized geometry.

|      |                    |                             |                             |
|------|--------------------|-----------------------------|-----------------------------|
|      |                    | Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7536.2767127 $E_h$ | Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.56419145 $E_h$ |
|      |                    | Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7534.61669845 $E_h$ | Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7534.82585016 $E_h$ |
|      |                    | Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -7539.17537521 $E_h$ |                             |

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Sb      | 7.14999785 | 11.45254977 | 245778       |
| Sb      | 8.70623029 | 9.44238051 | 152256       |
| Ga      | 7.81586330 | 10.95993159 | 585553       |
| Ga      | 6.91662033 | 10.19670487 | 691733       |
| Si      | 8.65349022 | 12.32948001 | 128059       |
| N       | 7.56901989 | 9.62460675 | 899353       |
| N       | 6.15604326 | 9.03576510 | 494803       |
| N       | 6.30016274 | 11.87410412 | 524276      |
| N       | 6.35477946 | 10.48717991 | 335248      |
| N       | 8.86744678 | 10.37779263 | 630118      |
| C       | 8.20673385 | 10.25006738 | 114927      |
| C       | 7.47558249 | 12.41517865 | 493010      |
| C       | 7.13018884 | 11.64165408 | 213554      |
| C       | 7.30836763 | 10.06643382 | 367522      |
| C       | 8.46514019 | 13.64847349 | 705129      |
| H       | 9.16486238 | 14.34098333 | 227226      |
| H       | 8.48010328 | 13.38279307 | 544325      |
| H       | 7.50474485 | 14.16783254 | 489458      |
| C       | 6.86095527 | 9.09697534 | 488587      |
| H       | 6.13537906 | 8.37290363 | 337593      |
| H       | 6.42660210 | 9.63448669 | 22182      |
| C       | 7.71600863 | 8.50955165 | 04122      |
| C       | 9.69169972 | 13.20673677 | 593916      |
| C       | 11.02117324 | 12.96070950 | 596561      |
| C       | 12.03347756 | 13.81064619 | 082977      |
| H       | 13.06226950 | 13.63410289 | 097344      |
| C       | 11.75938799 | 14.86761351 | 545762      |
| H       | 12.56479144 | 15.51781671 | 801792      |
| H       | 10.45218426 | 15.08946386 | 141345      |
| C       | 10.23716873 | 15.91953892 | 043161      |
| C       | 9.39910919 | 14.27780735 | 939906      |
Table S24. Cartesian coordinates of [L(Me$_2$N)Ga]SbSb[CH(SiMe$_3$)Ga(NMe$_2$)L] (17) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) =  -7520.21610791 \ E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) =  1.57459498 \ E_h
| Element | Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) | Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) |
|---------|----------------------------------|---------------------------------------------|
| Sb      | -7518.54538584 $E_h$            | -7518.75505712 $E_h$                        |
| Sb      | 7.03461884703783               | 11.46526160314096                           |
| Sb      | 5.8663793235097               | 9.43882944427222                           |
| Ga      | 7.7753129234760               | 10.9272926750987                           |
| Ga      | 6.9512353860020               | 10.19827714454319                           |
| Si      | 4.6601491046516             | 12.34681421202372                           |
| N       | 7.6303579249443              | 9.06536253223131                           |
| N       | 6.22534267807681             | 9.0406755150138                            |
| Sb      | 6.3003579249443              | 11.8727867592112                           |
| Ga      | 6.0966360184222              | 11.24191936335396                           |
| Ga      | 8.82453838036140             | 10.34867187125892                          |
| N       | 8.81790955098786             | 10.2887267015962                           |
| Sb      | 8.2258398468543             | 12.45051989312475                           |
| C       | 7.50590294752536             | 11.45835873322900                          |
| H       | 7.1736751214792             | 11.73171342742575                           |
| Sb      | 7.33907319168461             | 10.10412405989859                           |
| N       | 4.8909016210851             | 13.71066637847487                           |
| C       | 9.21186552646636             | 14.37221378122542                           |
| H       | 8.83918555231021             | 13.48150419291026                           |
| C       | 7.5355875422002             | 14.25042881804466                           |
| C       | 6.83992296319234             | 9.19242156734887                            |
| H       | 5.80078833771685             | 8.90129638686673                           |
| H       | 6.87255932932277             | 9.68756265141363                           |
| C       | 7.42089034339456             | 8.26153990249332                            |
| C       | 9.70810776015329             | 13.17410429230368                           |
| C       | 11.03301762309891            | 12.9088942031307                           |
| C       | 12.05988557264794            | 13.73813678494258                           |
| H       | 13.08495369552901            | 13.54814472429123                           |
| C       | 11.80592700087029            | 14.79027637798136                           |
| C       | 12.62258541808256            | 15.4244746082036                           |
| C       | 10.50479645988084            | 15.0252793241282                           |
| H       | 10.30665381626119            | 15.84809179465357                           |
| C       | 9.43821944573539             | 14.23523598242770                           |
| C       | 11.39090886169381            | 11.76499230709027                          |
| H       | 10.50624524737521            | 11.1800989011922                           |
| C       | 11.74981639536976            | 12.2661808052875                           |
| H       | 12.65154251797428            | 12.89586827425113                           |
| H       | 11.95533172247018            | 11.4193366826144                           |
| H       | 10.9429563380340            | 12.86291827735205                           |
| C       | 12.53438379273128            | 10.91922421309167                          |
| H       | 12.30076015876464            | 10.52600081974093                          |
| H       | 12.74084848062829            | 10.06738231675529                          |
| H       | 13.4671914943607            | 11.49771452641546                          |
| C       | 8.03496091075963            | 14.58411853733616                           |
| H       | 7.42168837552315            | 13.67088285119423                          |
| C       | 7.4197481415003            | 15.63621425864718                          |
| H       | 8.01118067307347            | 16.5623460090901                           |
| H       | 7.38373420520277            | 15.2972459125050                           |

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Table S 25. Cartesian coordinates of [L(Me₂N)GaN(Ph)Sb]₂(10) [Å] for the optimized geometry.

| Atom | x          | y          | z          |
|------|------------|------------|------------|
| Sb   | 1.99261000606432 | 5.6562084037422 | 6.3273258039876 |
| Ga   | 1.71357695919004  | 4.0896309234678  | 3.4158775152125 |
| N    | 0.75265332026892  | 2.77607646792375  | 2.292324694082163 |
| N    | 0.84679496040734  | 5.66296476246967  | 2.57879320412835 |
| N    | 3.52608931194215  | 4.08785091227173  | 2.9913400980580 |
| N    | 1.30847803829523  | 4.02673806304107  | 5.25813470641101 |
| C    | 0.35438022890024  | 3.10879519168155  | 1.0660861818995 |
| C    | 0.29621061480472  | 4.42807561806157  | 0.58736092454075 |
| H    | -0.02497151592742  | 4.5423447508685  | -0.4469256240467 |
| C    | 0.42379635451976  | 5.62081807916181  | 1.32183335376879 |
| C    | -0.09531260497200  | 2.03040310811780  | 0.12017491915856 |

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7644.53075775 \ E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.63905760 \ E_h
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7642.79257570 \ E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7643.00911482 \ E_h
Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -7648.04917981 \ E_h
| H          | 2.26530140884398 | 8.94460940462436 | 0.87807607674919 |
|------------|------------------|------------------|------------------|
| C          | 4.26081324616018 | 7.56232154973015 | 3.37930115179448 |
| H          | 5.14924156809974 | 7.3498333228730 | 2.76443969987199 |
| H          | 4.15108382213304 | 6.75965377326666 | 4.12134293179810 |
| H          | 4.44780254846692 | 8.49866630415921 | 3.92784941775341 |
| C          | -1.5202629299157 | 5.98726244923116 | 4.1697686603118 |
| H          | -1.09822882222646 | 5.05619080566284 | 3.76585342819368 |
| C          | -2.64987707801179 | 6.4253616235865 | 3.23566323661398 |
| H          | -2.29761370700617 | 6.5506029462695 | 2.20152521972858 |
| H          | -3.07996264285120 | 7.38583454355000 | 3.56251267368539 |
| H          | -3.45857051236598 | 5.67807270799231 | 3.2244088986757 |
| C          | -2.04910074402419 | 5.67618753681035 | 5.56561204058427 |
| H          | -2.57631407733658 | 6.53324729284584 | 6.01295799274897 |
| H          | -1.22944386287979 | 5.38725130552328 | 6.23975868493274 |
| H          | -2.76536026655686 | 4.84193465229257 | 5.52313508844986 |
| C          | 3.99791430011039 | 4.22247107656972 | 1.63902412953368 |
| H          | 4.59274249746570 | 3.35884822746050 | 1.30330919851195 |
| H          | 4.61396390297844 | 5.12322474753149 | 1.49096766840606 |
| H          | 3.13128634943626 | 4.30771821574583 | 0.94012674450225 |
| C          | 4.59042723734211 | 3.9888966588004 | 3.9465223810987 |
| H          | 5.21709795505854 | 3.08233495486612 | 3.8017044126309 |
| H          | 4.19843563860770 | 3.95629643929147 | 4.97495659753557 |
| H          | 5.28575080813874 | 4.85229778364115 | 3.8948529917736 |
| C          | 1.25998556447698 | 2.80002063412151 | 5.93507084250550 |
| C          | 2.17697222644057 | 1.76369104777646 | 5.67684325654225 |
| H          | 2.94710091671952 | 1.92092480535970 | 4.91975940670666 |
| C          | 2.11173203503837 | 0.5505725266662 | 6.35902711037678 |
| H          | 2.82948919317424 | -0.2367681969418 | 6.11610804533031 |
| C          | 1.14461599615789 | 0.34184747125141 | 7.33901478060891 |
| H          | 1.09395847441504 | -0.60855067642215 | 7.87512155966751 |
| C          | 0.23515263822031 | 1.36323349274625 | 7.62035791757047 |
| H          | -0.53651912083599 | 1.2158309758212 | 8.38038094589343 |
| C          | 0.28894484614870 | 2.56978349120481 | 6.93098832568750 |
| H          | -0.43094333303531 | 3.36201830522162 | 7.14623625322221 |
| Sb         | 2.85949734636203 | 4.23080388228786 | 8.39687806539972 |
| Ga         | 3.13731282932347 | 5.79798016631480 | 11.30822663449453 |
| N          | 4.09790297153837 | 7.1117038321576 | 12.43182490193951 |
| N          | 4.00368105469163 | 4.22475631711431 | 12.14601412079126 |
| N          | 1.32464768450778 | 5.79973079233703 | 11.73211967558881 |
| N          | 3.54323569028481 | 5.86044950108708 | 9.46613473823497 |
| C          | 4.49576015758660 | 6.77922539993292 | 13.65829616522689 |
| C          | 4.55365851975161 | 5.45934020101110 | 14.13714517484190 |
| H          | 4.87436365106110 | 5.34597803399761 | 15.1715294306495 |
| C          | 4.42620592190060 | 4.26714748443925 | 13.40311145678014 |
| C          | 4.944945662849956 | 7.85783524408082 | 14.60419732862893 |
| H          | 5.49040549093849 | 7.43179637061547 | 15.45427100820993 |
| H          | 5.58075996208441 | 8.5947247932401 | 14.09527718249461 |
| H          | 4.07240377534682 | 8.40462168398868 | 14.9907182052984 |
| C          | 4.79203574023179 | 2.99147157124397 | 14.10879799824694 |
| H          | 3.88011552372920 | 2.53600670469714 | 14.52639380777913 |
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