Electronic Supplementary Material (ESI) for Chemical Science.

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

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Content

A) Spectroscopic Characterization

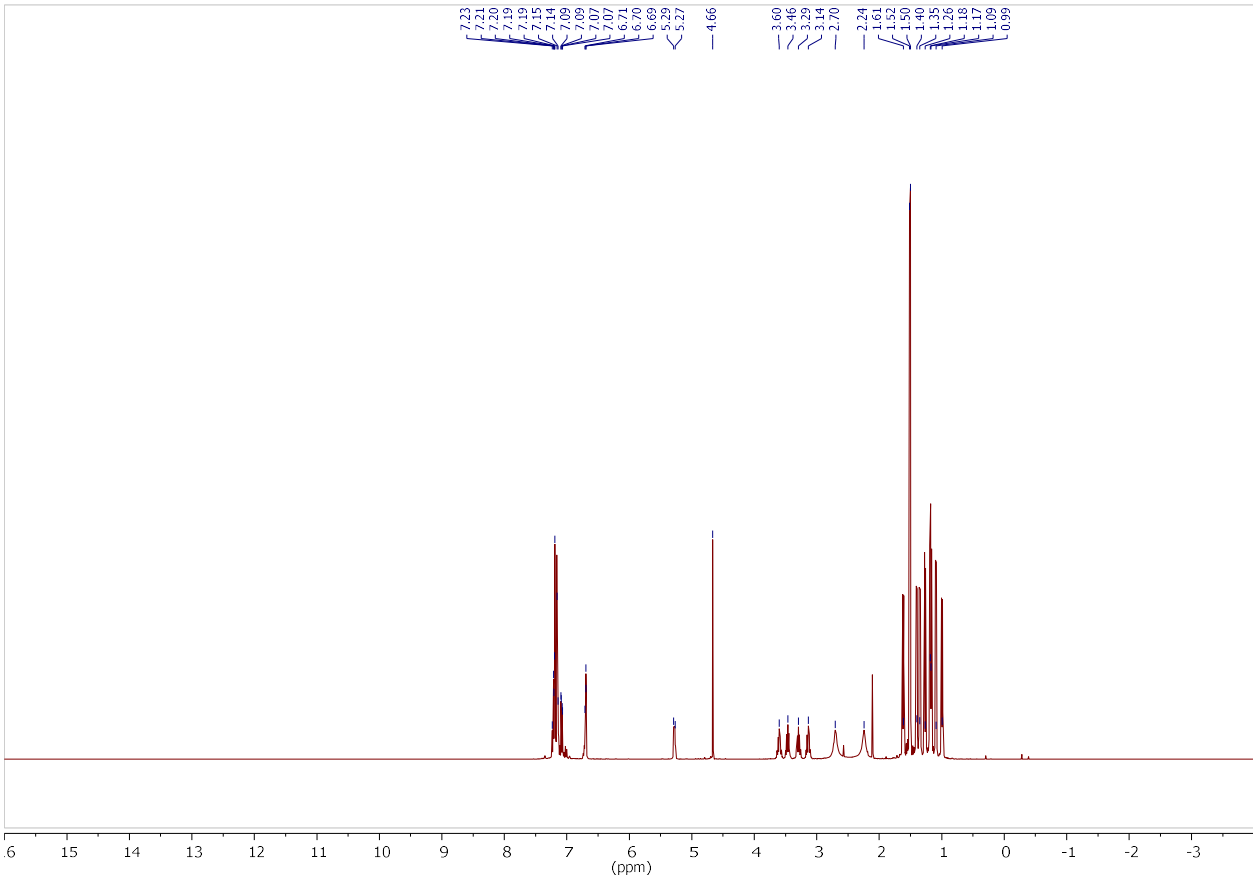

Fig. S1. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb]$_2$N-Ph (**1**).

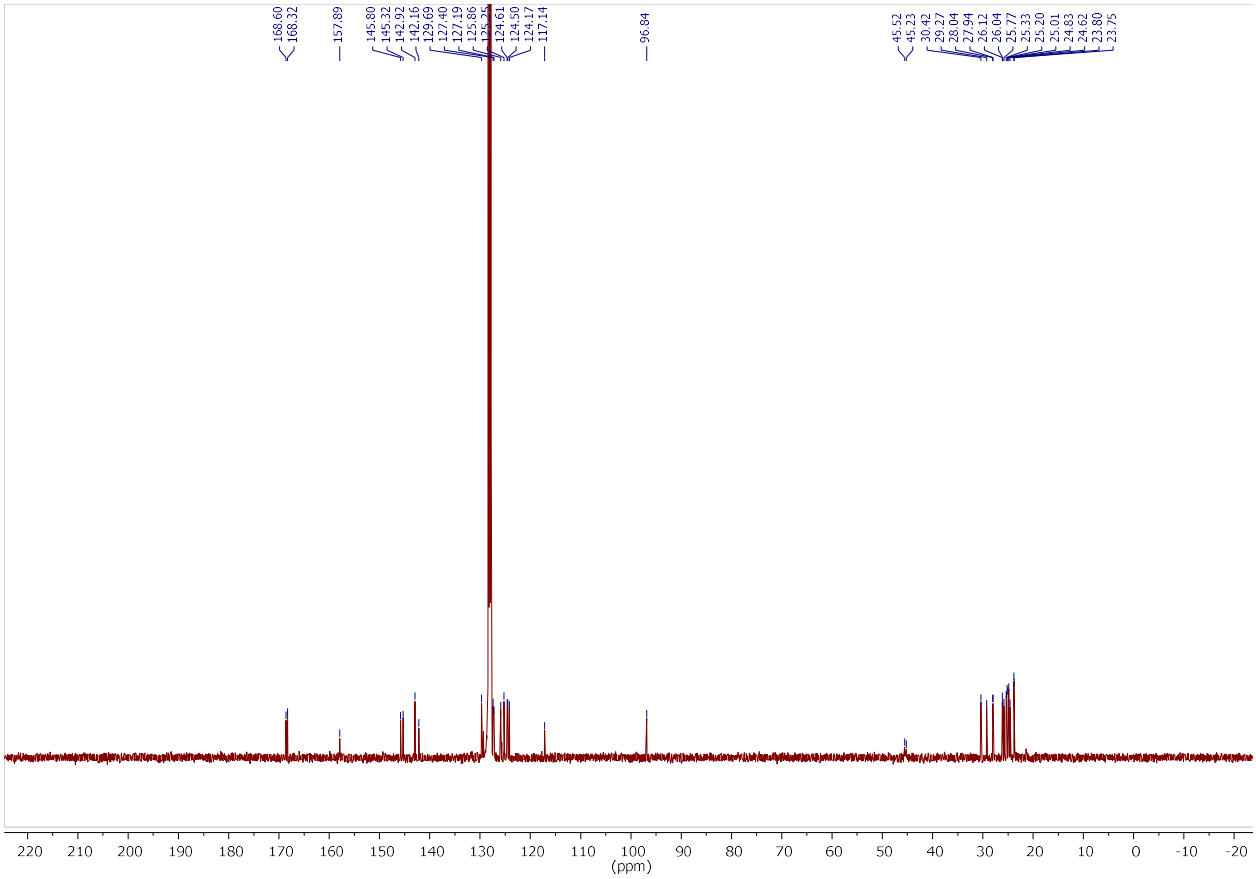

Fig. S2. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb]$_2$N-Ph (**1**).

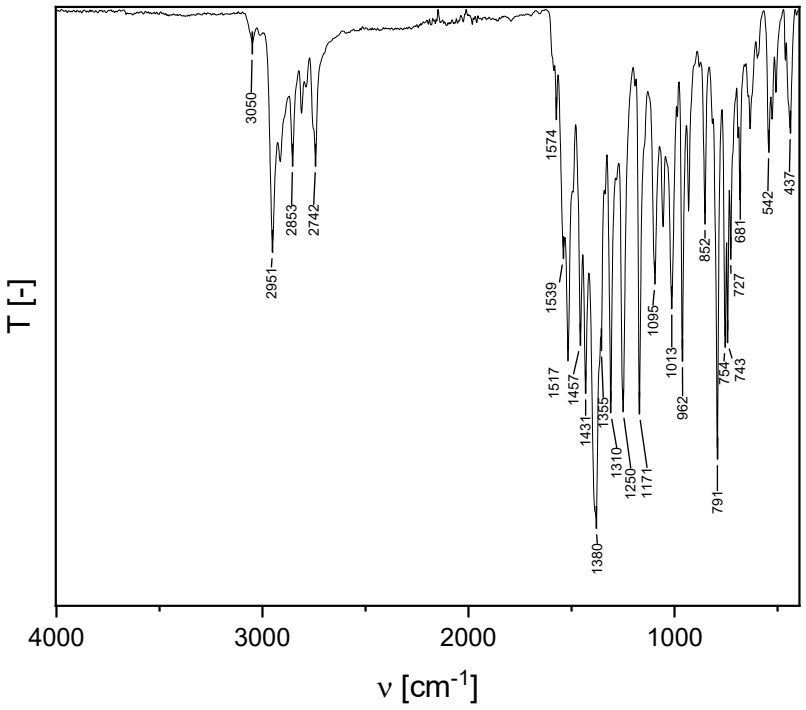

Fig. S3. ATR-IR spectrum of of [L(Me$_2$N)GaSb]$_2$N-Ph (**1**).

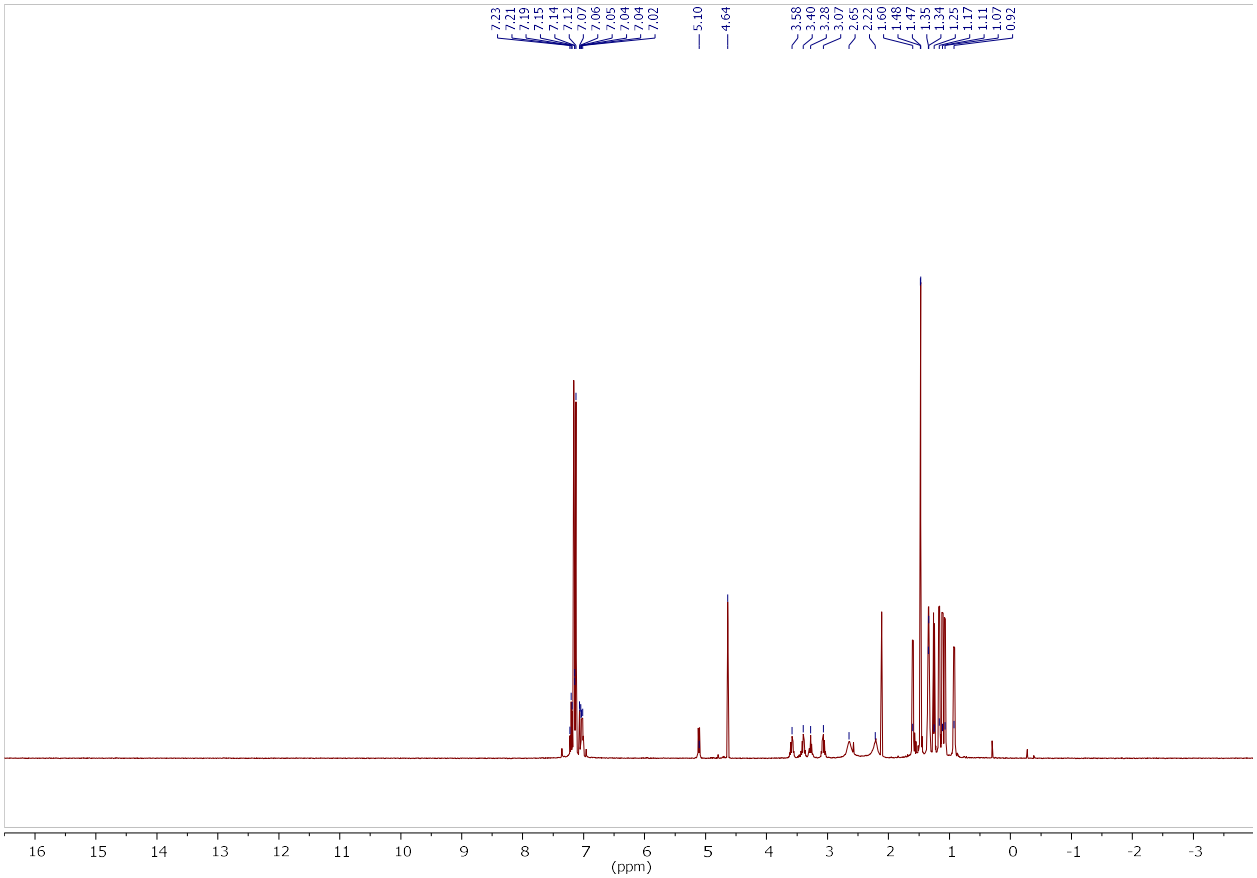

Fig. S4. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) [L(Me$_2$N)GaSb]$_2$N-p-CF$_3$-Ph (**2**).

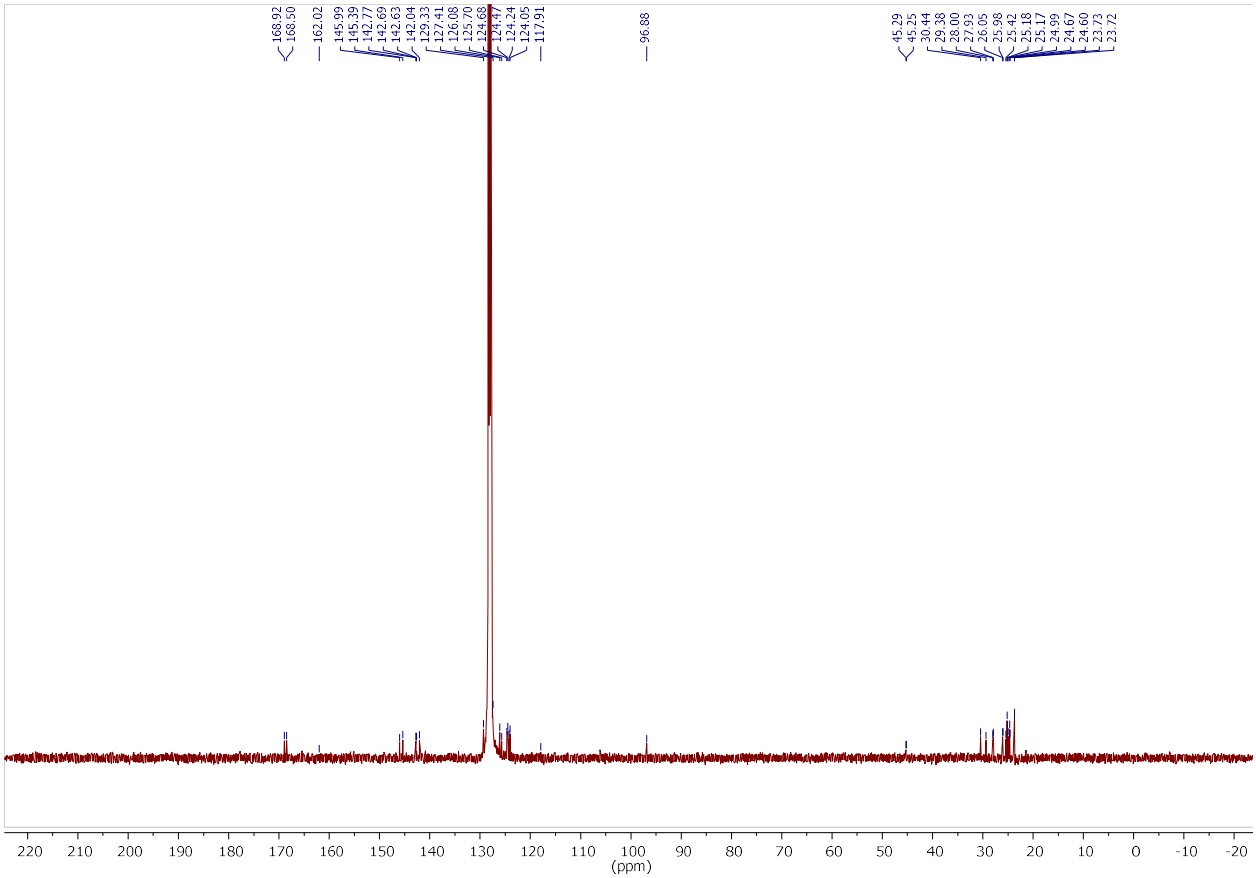

Fig. S5. ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of [L(Me_2N)GaSb]$_2$N-p-CF_3-Ph (**2**).

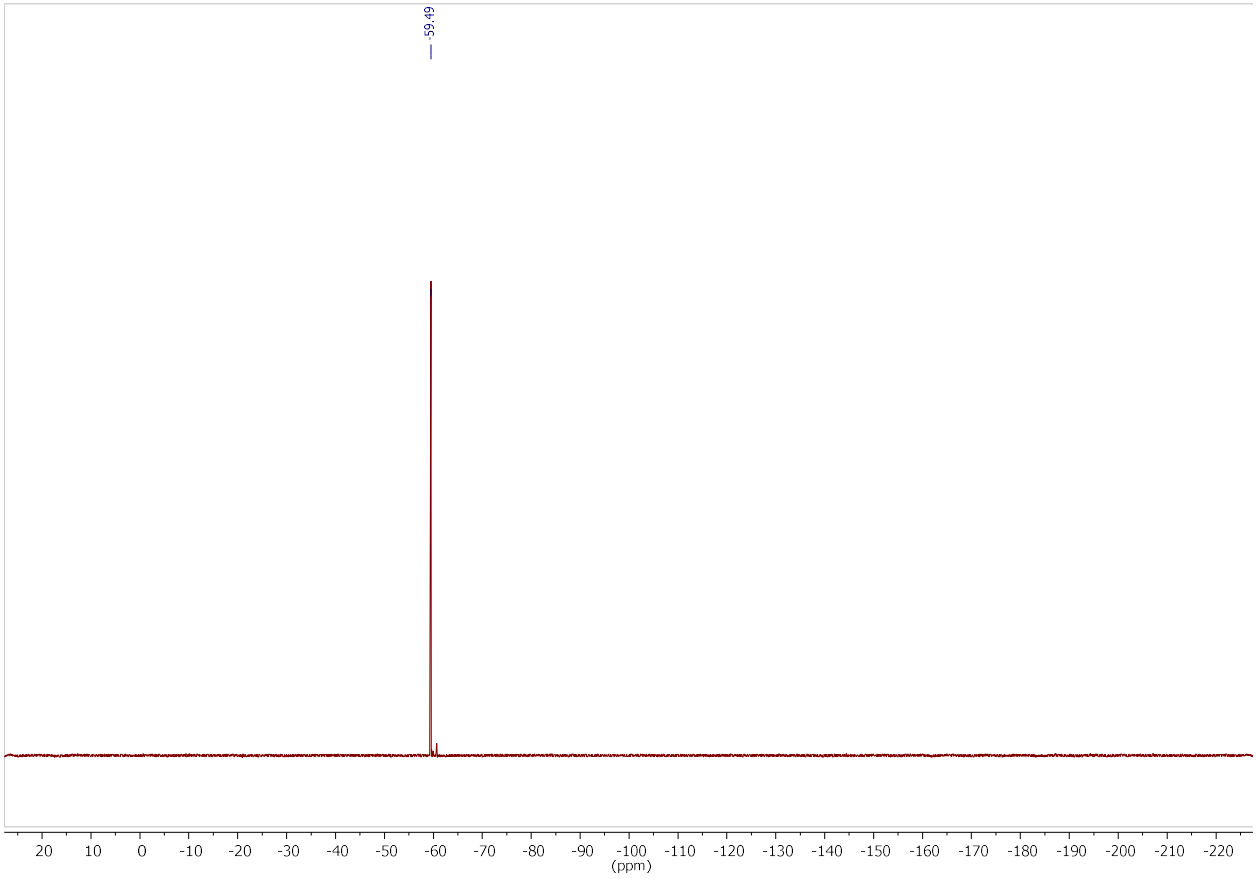

Fig. S6. ^{19}F NMR spectrum (376.5 MHz, C_6D_6, 25 °C) of [L(Me_2N)GaSb]$_2$N-p-CF_3-Ph (**2**).

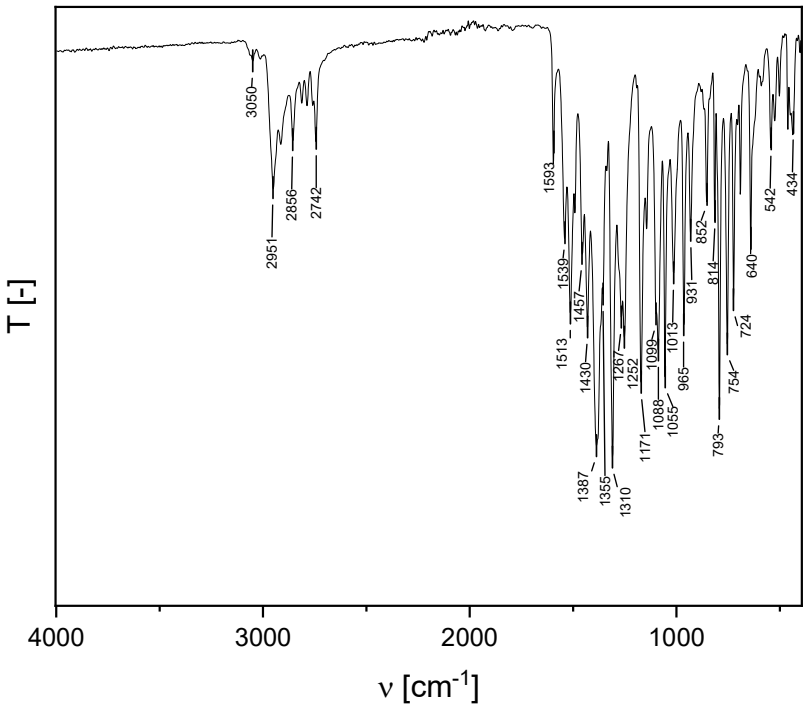

Fig. S7. ATR-IR spectrum of $[L(Me_2N)GaSb]_2N$-p-CF_3-Ph (**2**).

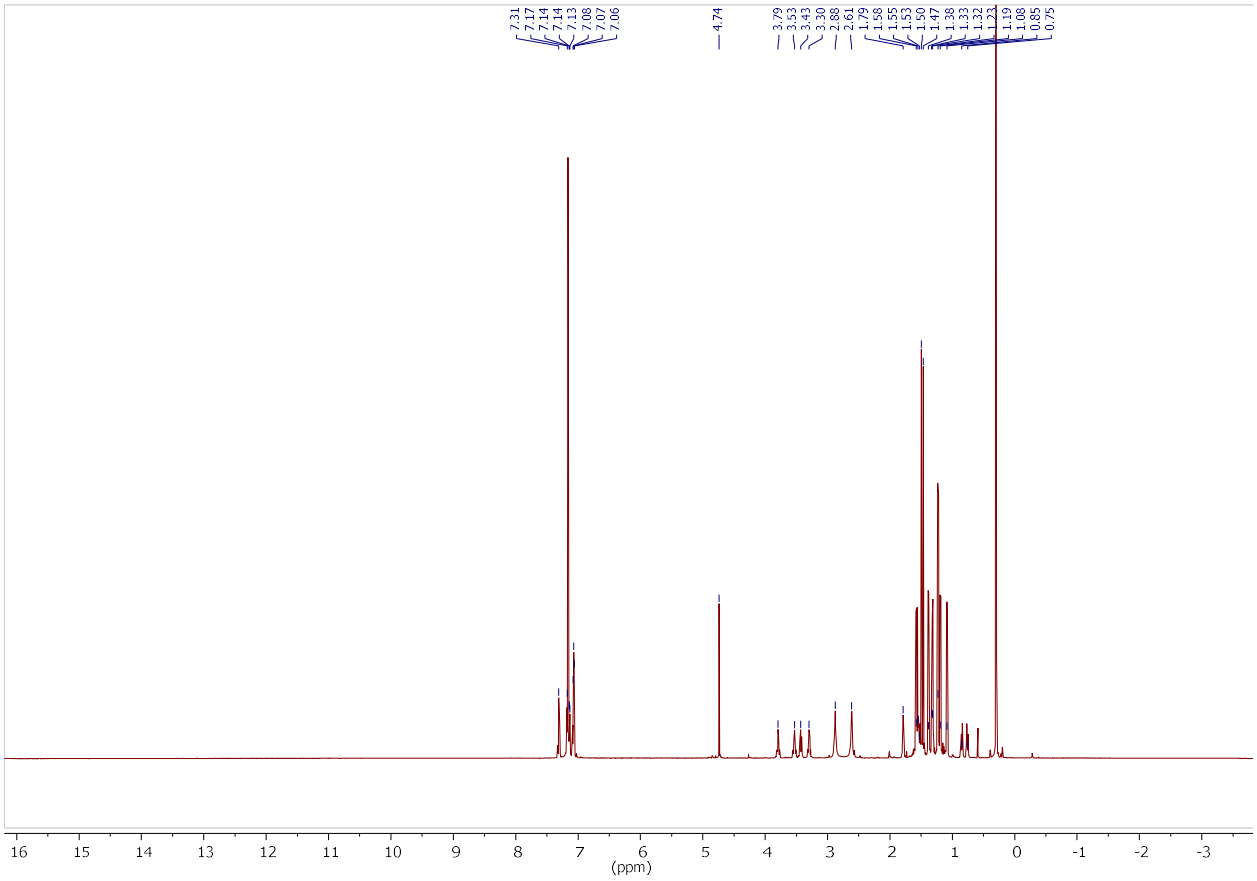

Fig. S8. ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2N$-ada (**3**).

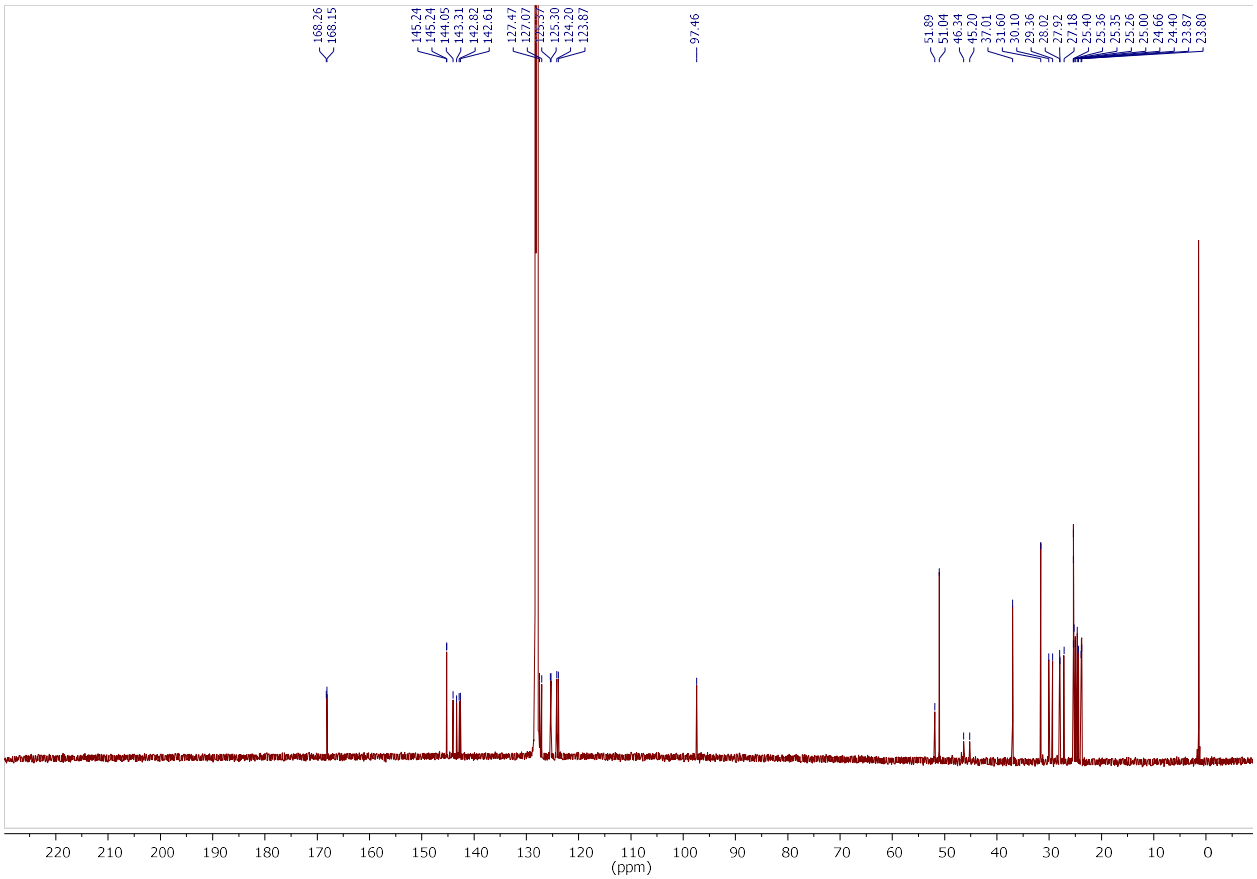

Fig. S9. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb]$_2$N-ada (**3**).

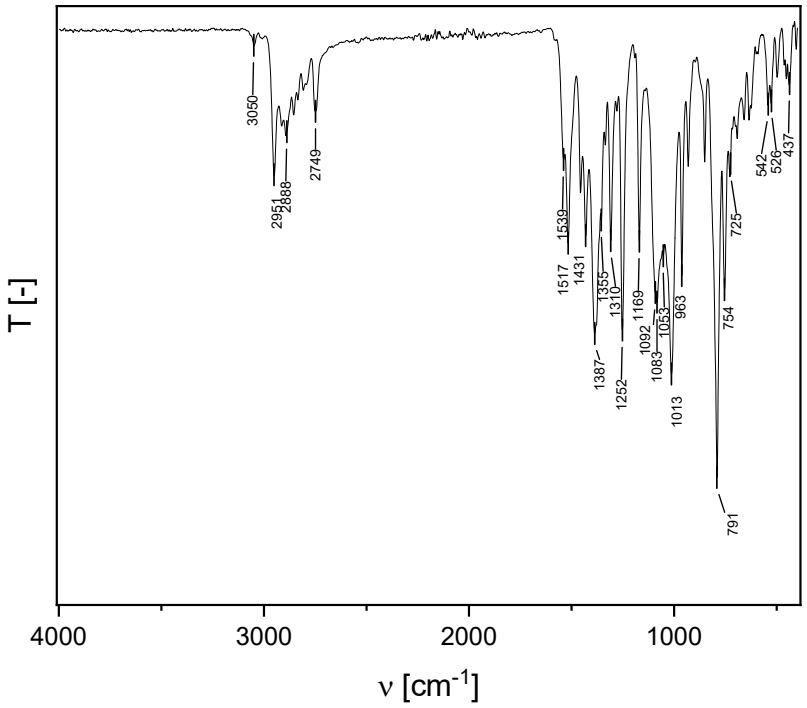

Fig. S10. ATR-IR spectrum of [L(Me$_2$N)GaSb]$_2$N-ada (**3**).

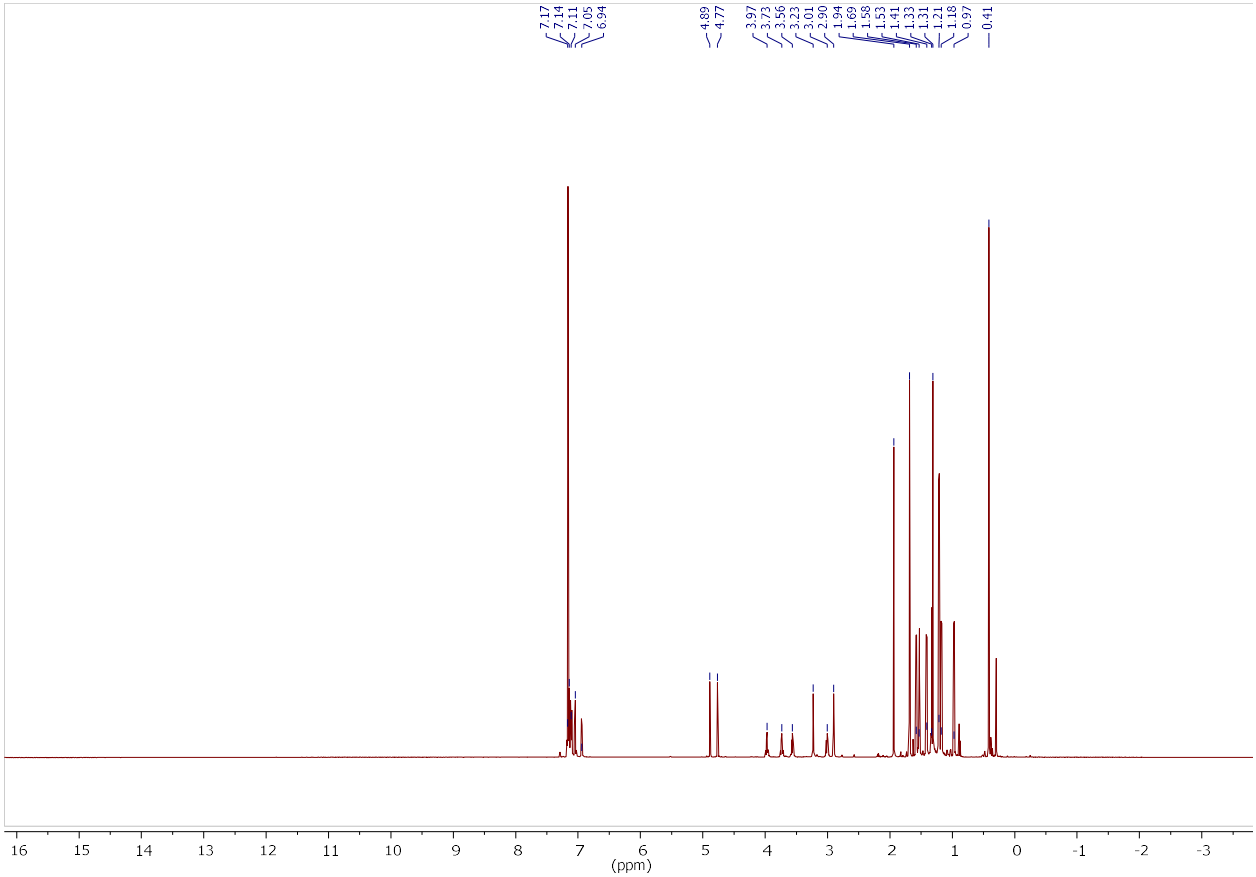

Fig. S11. ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**).

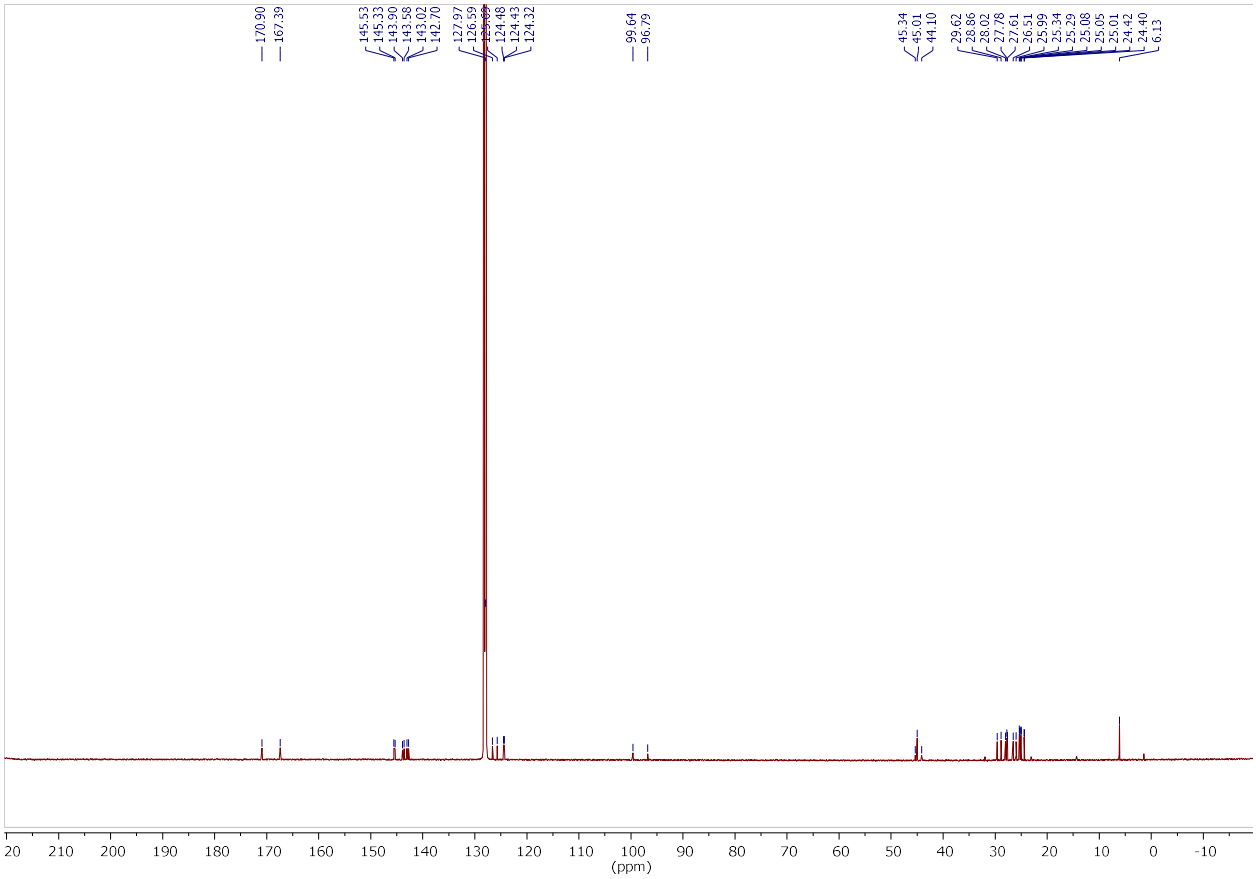

Fig. S12. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**).

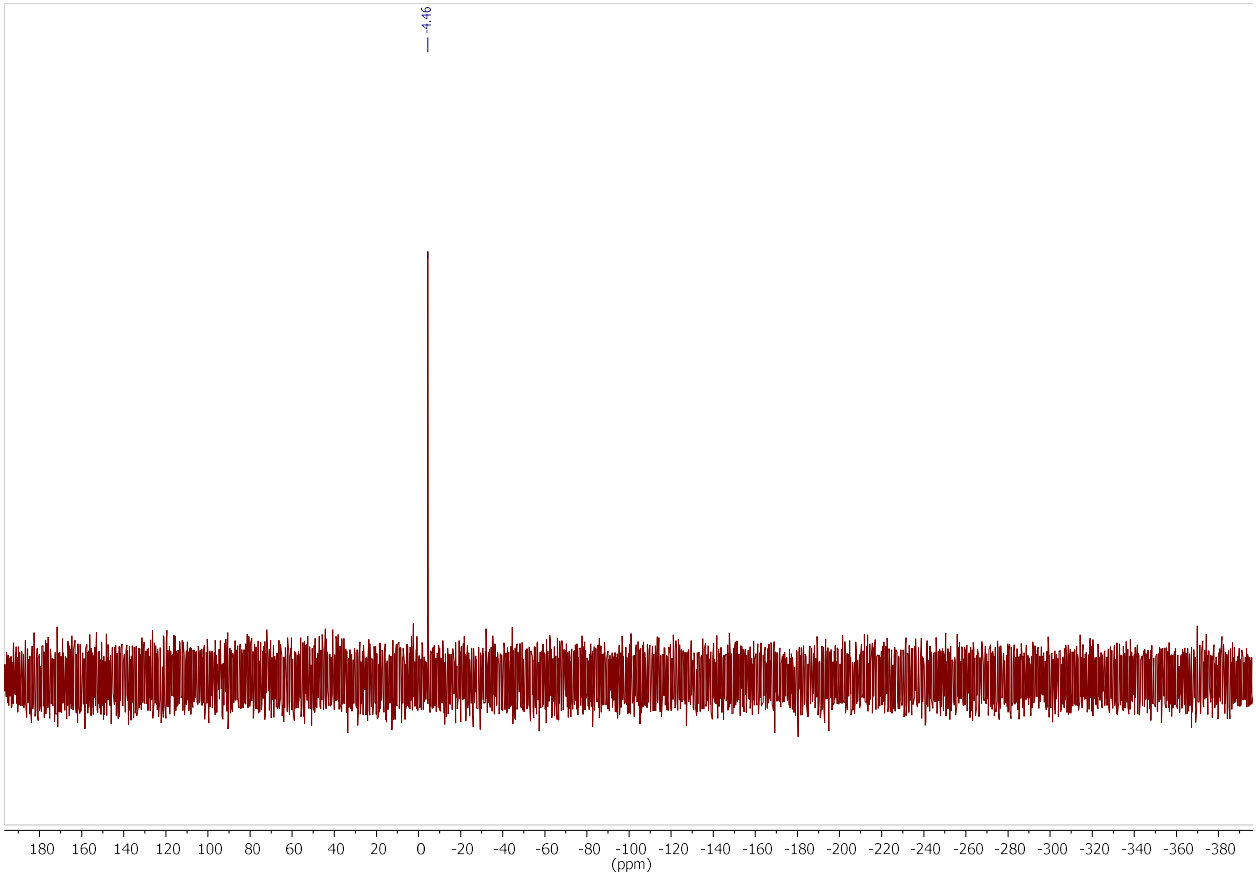

Fig. S13. DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**).

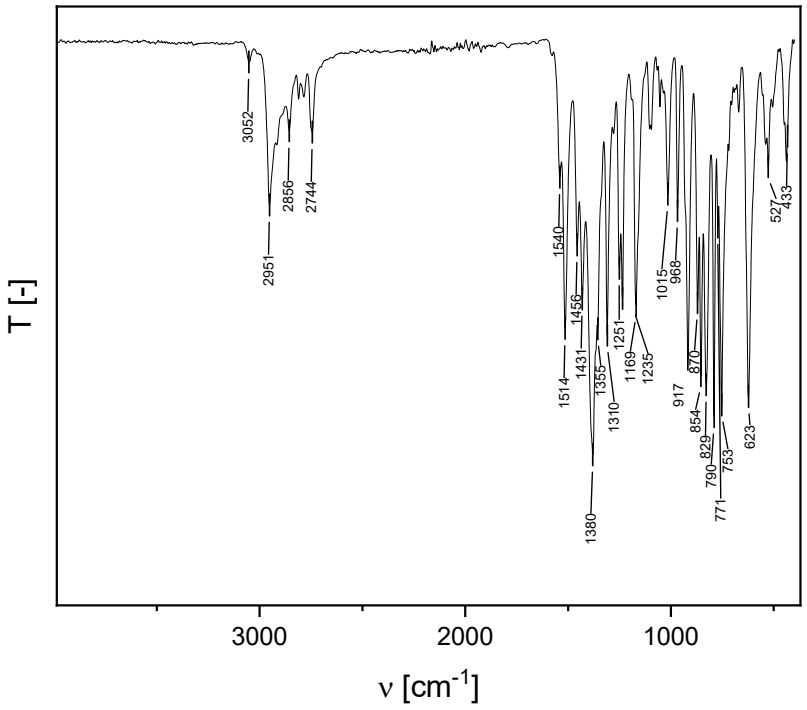

Fig. S14. ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**).

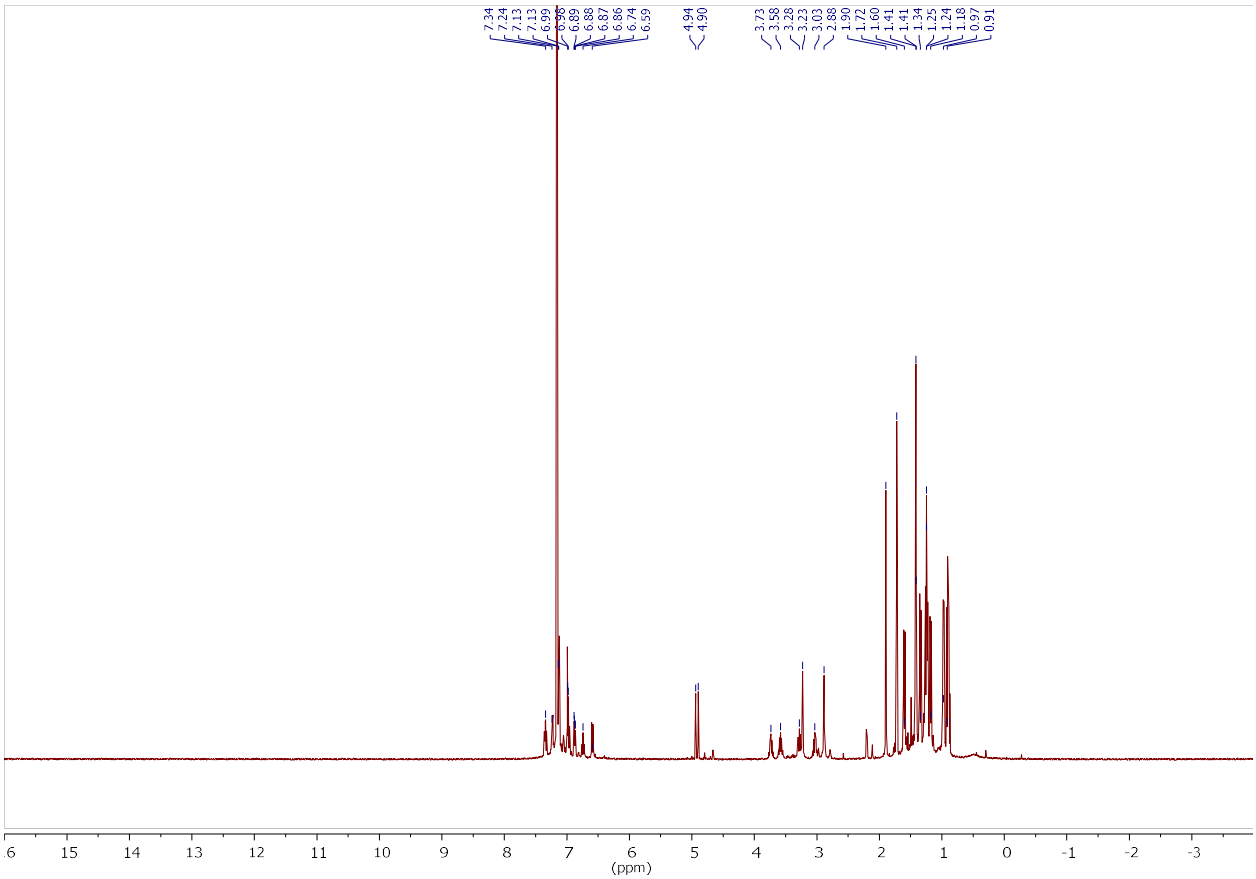

Fig. S15. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**).

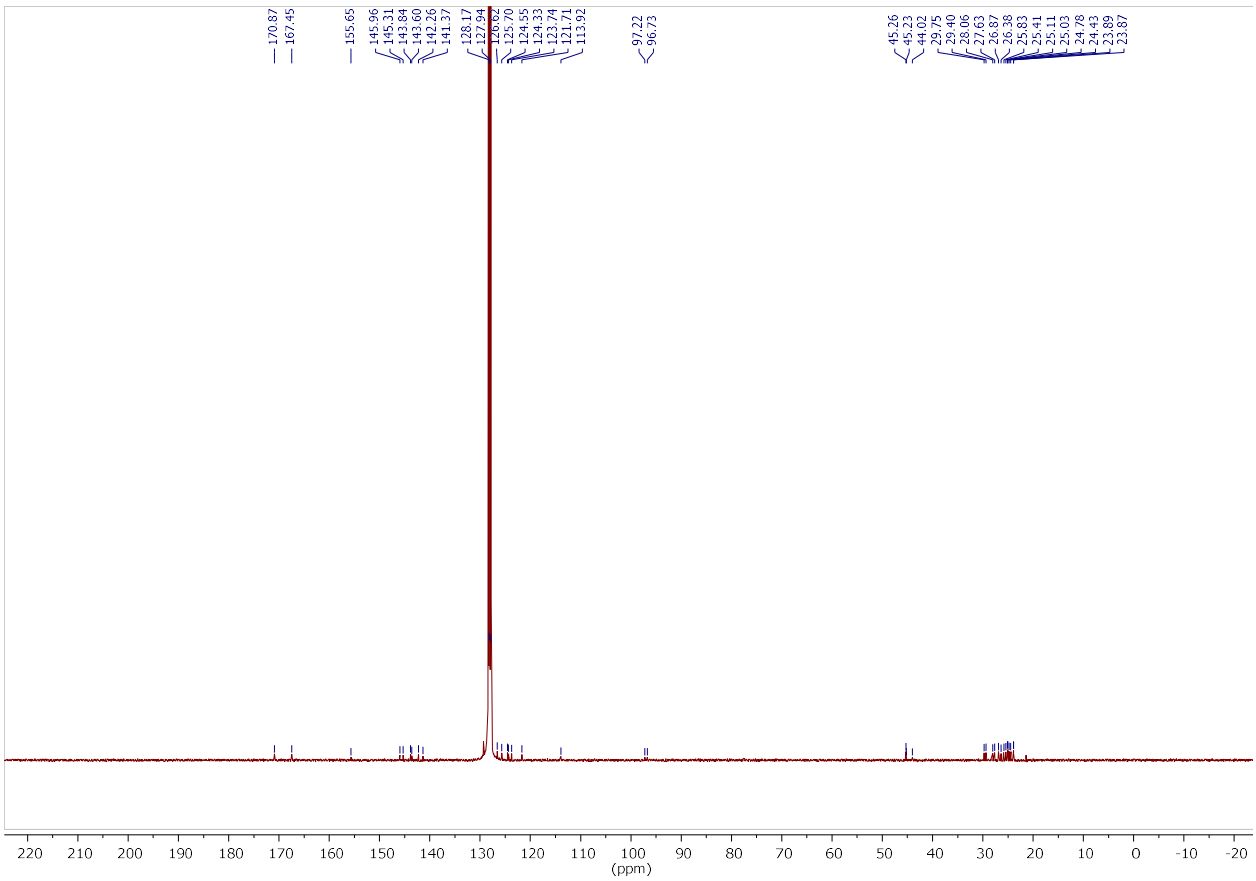

Fig. S16. ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**).

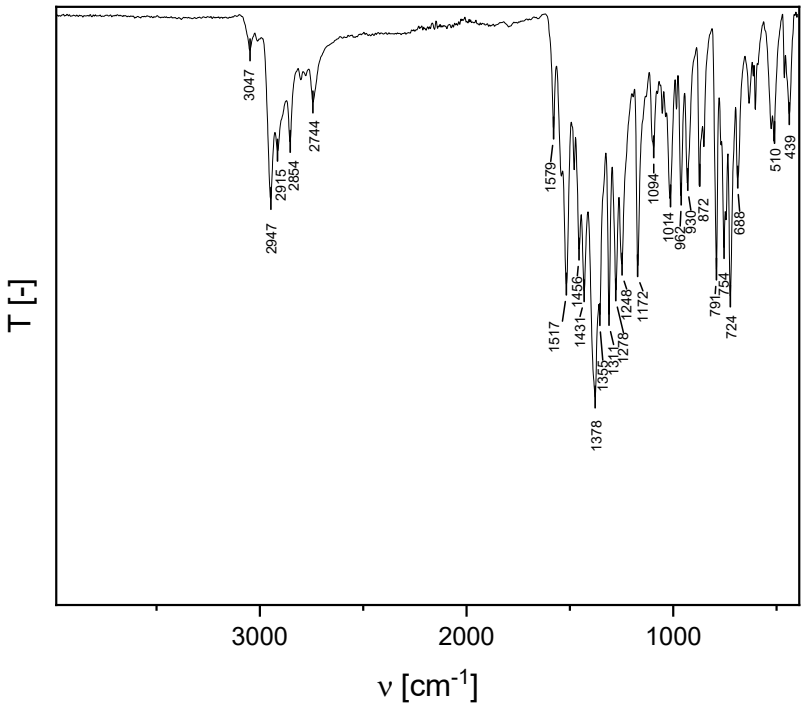

Fig. S17. ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**).

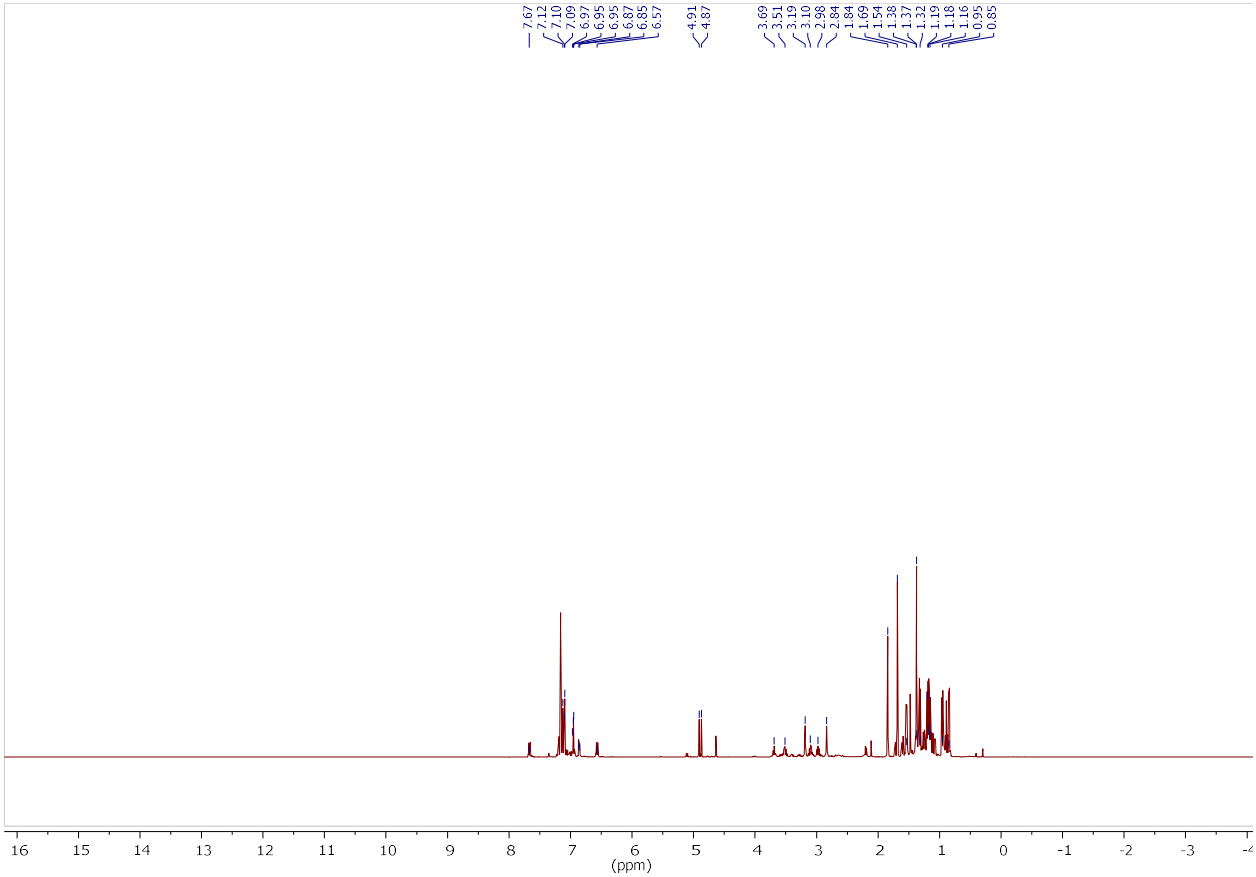

Fig. S18. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**).

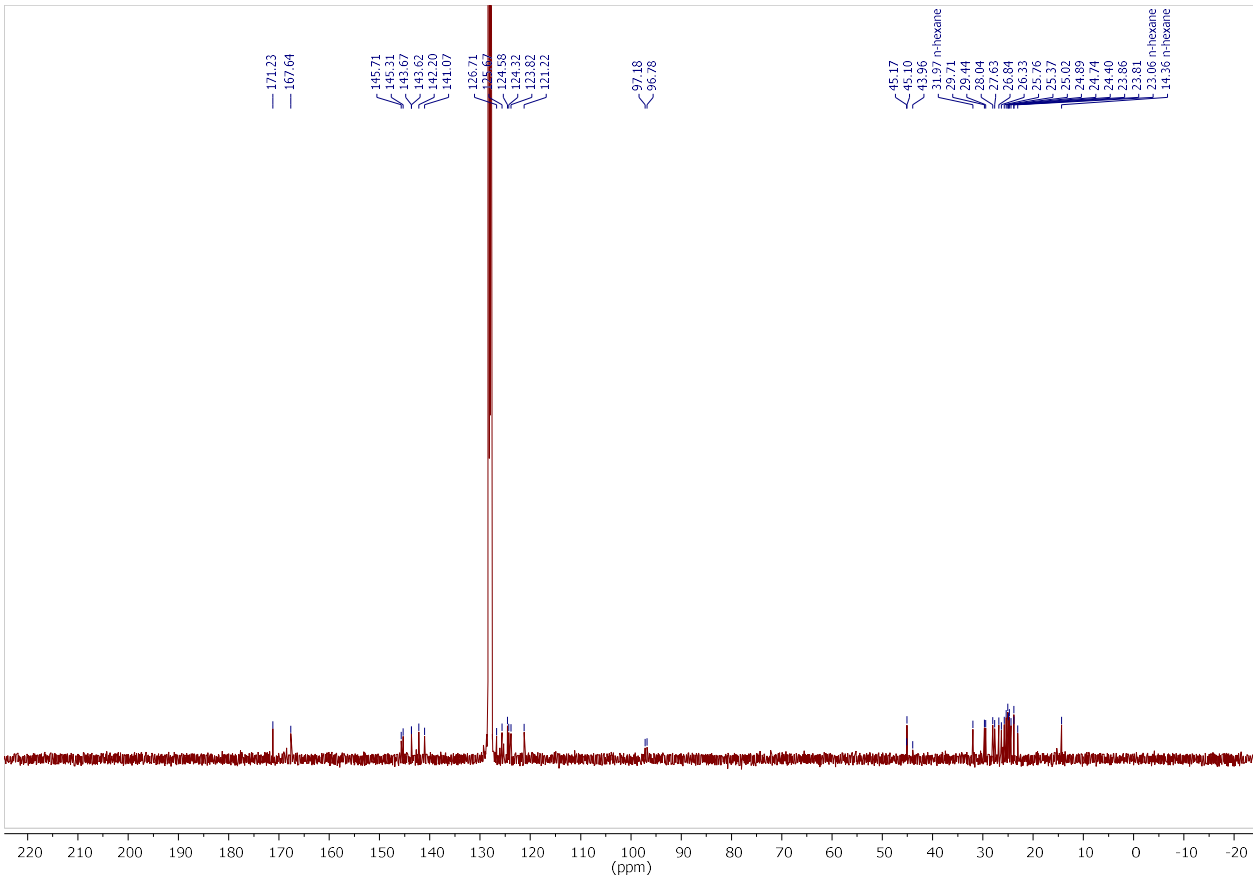

Fig. S19. ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**).

Fig. S20. ^{19}F NMR spectrum (282.4 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**).

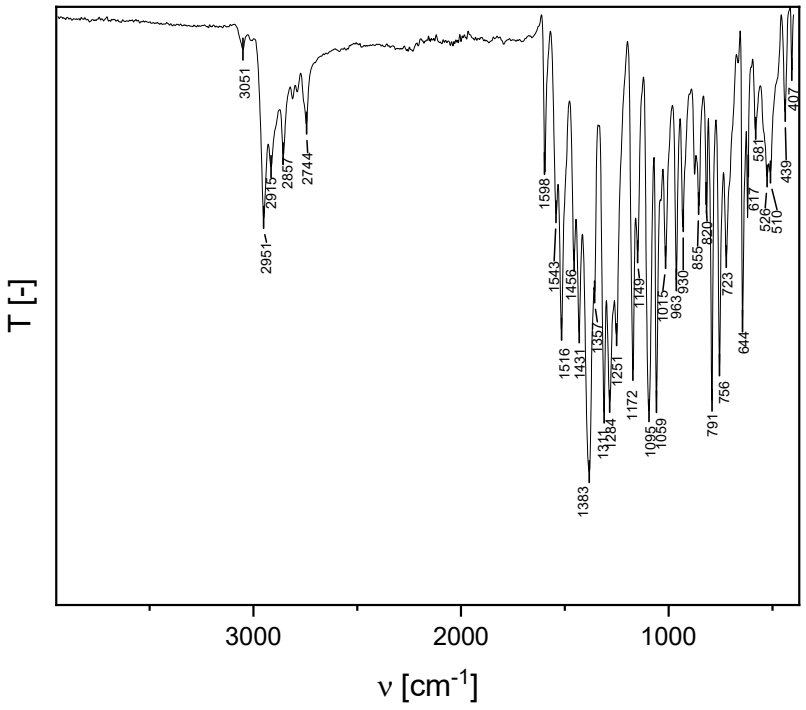

Fig. S21. ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**).

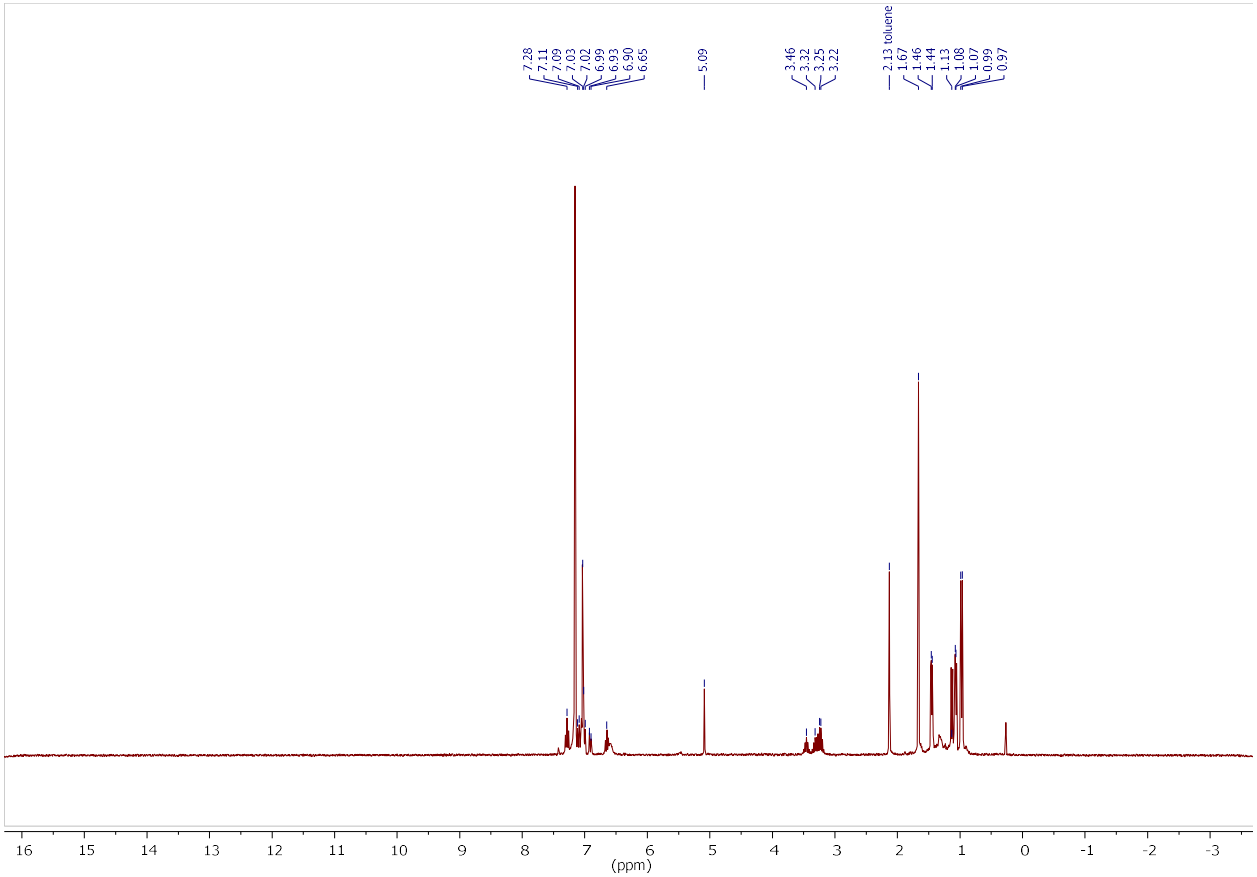

Fig. S22. ^{1}H NMR spectrum (300 MHz, C_6D_6, 70 °C) of [(L(PhN)Ga-κGa,κN)$_2$-(μ,$\eta^{1:1:1:1}$-Sb_4)] (**7**).

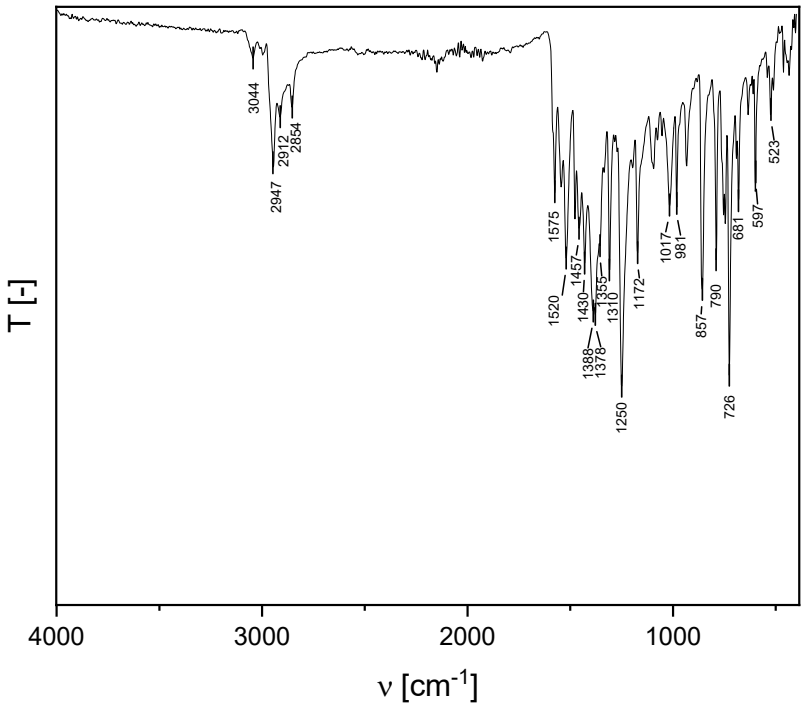

Fig. S23. ATR-IR spectrum of [(L(PhN)Ga-κ*Ga,*κ*N*)$_2$-(μ,η$^{1:1:1:1}$-Sb$_4$)] (**7**).

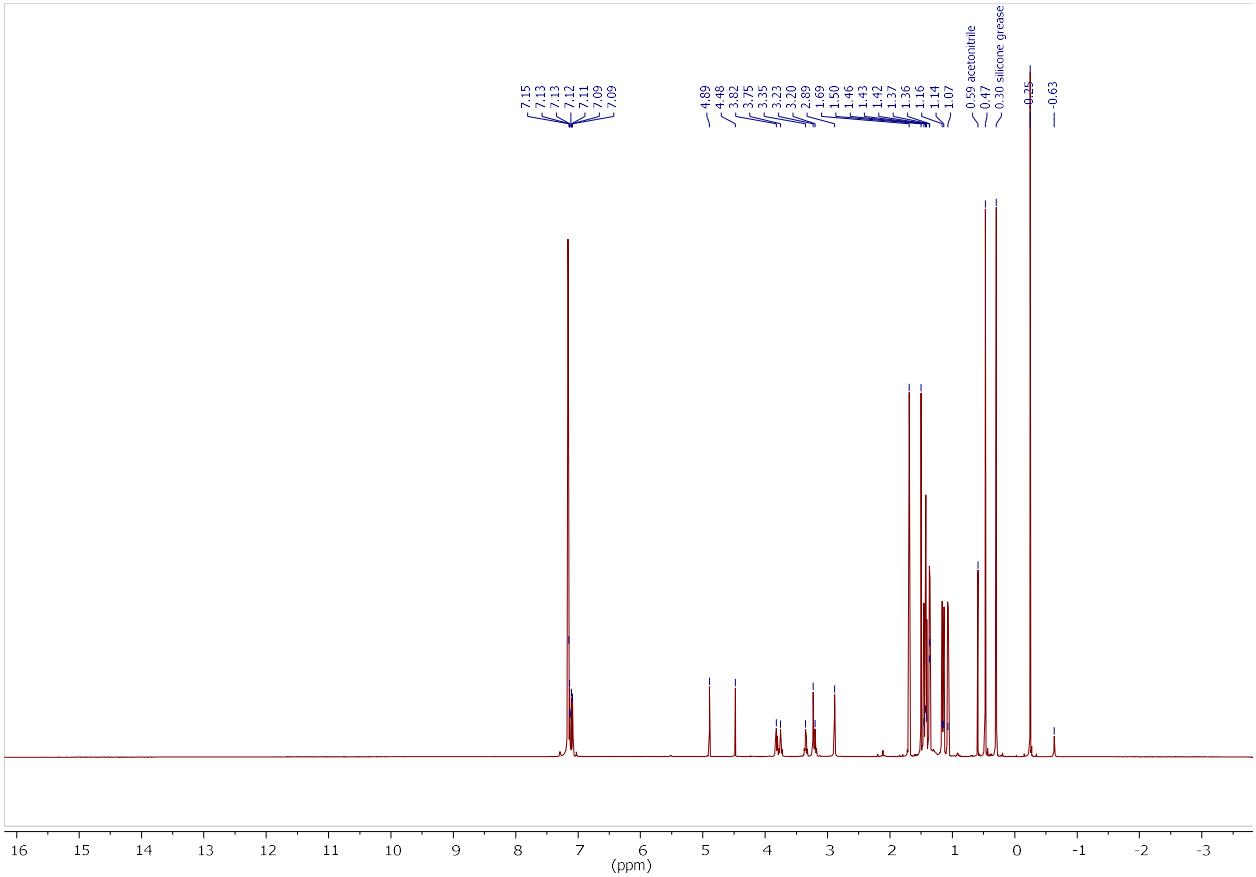

Fig. S24. ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**8**).

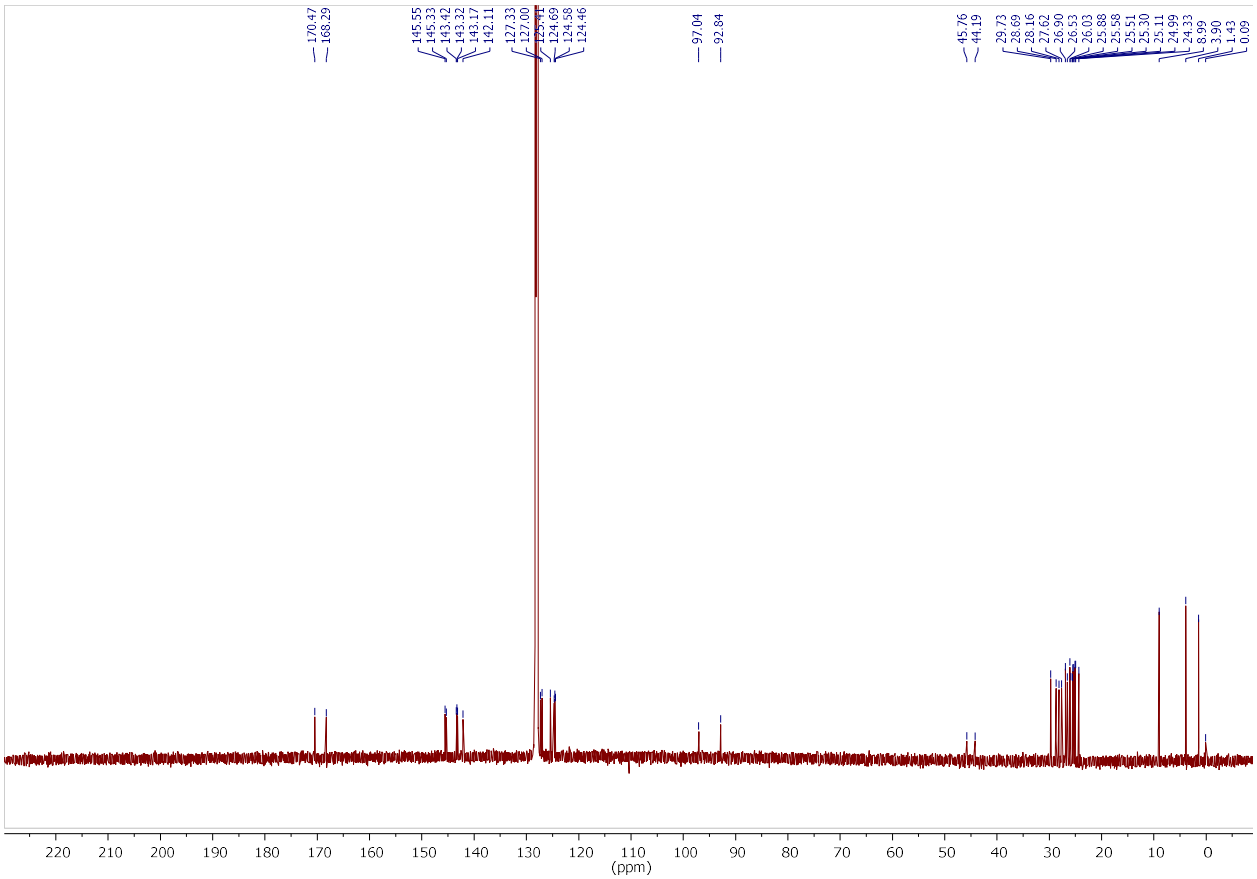

Fig. S25. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**8**).

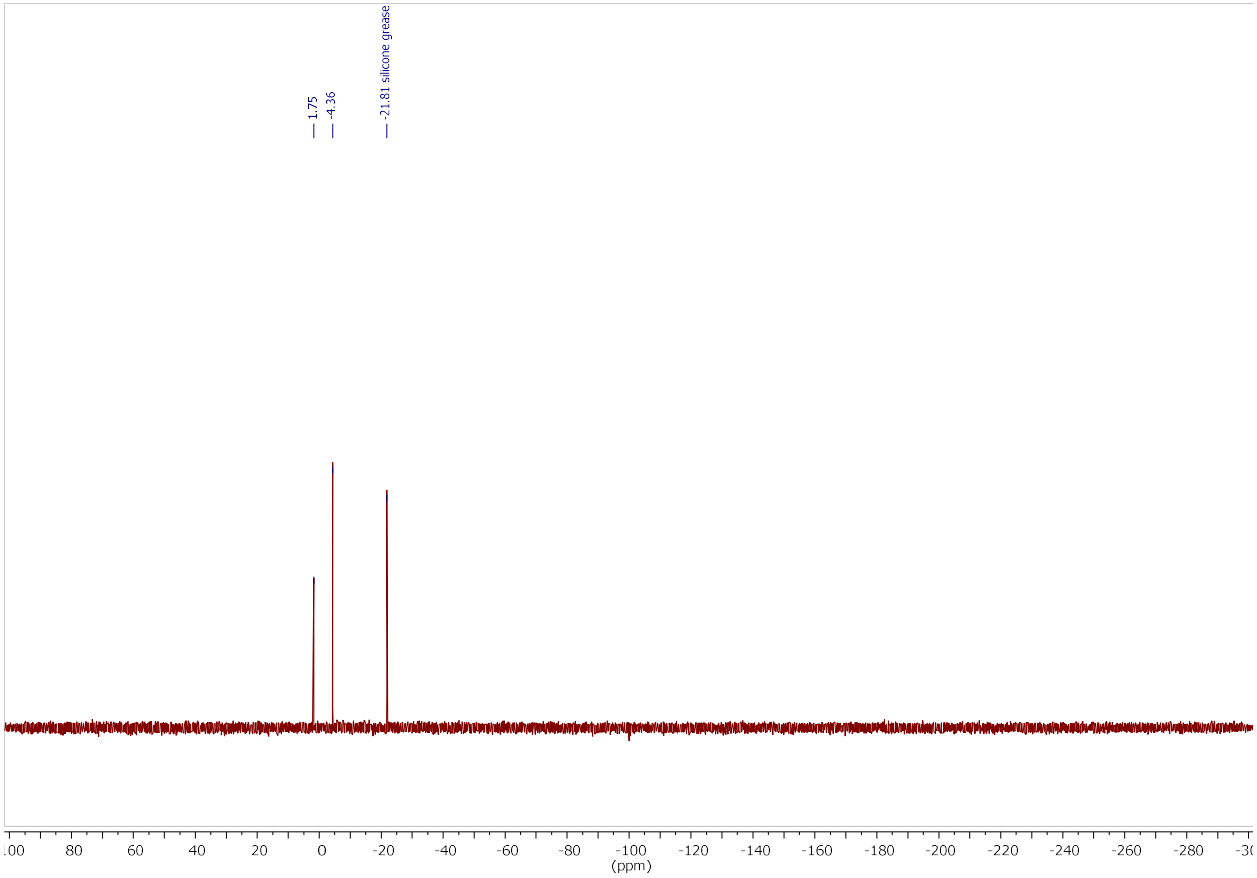

Fig. S26. DEPT ^{29}Si NMR spectrum (119.2 MHz, C_6D_6, 25 °C) of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**8**).

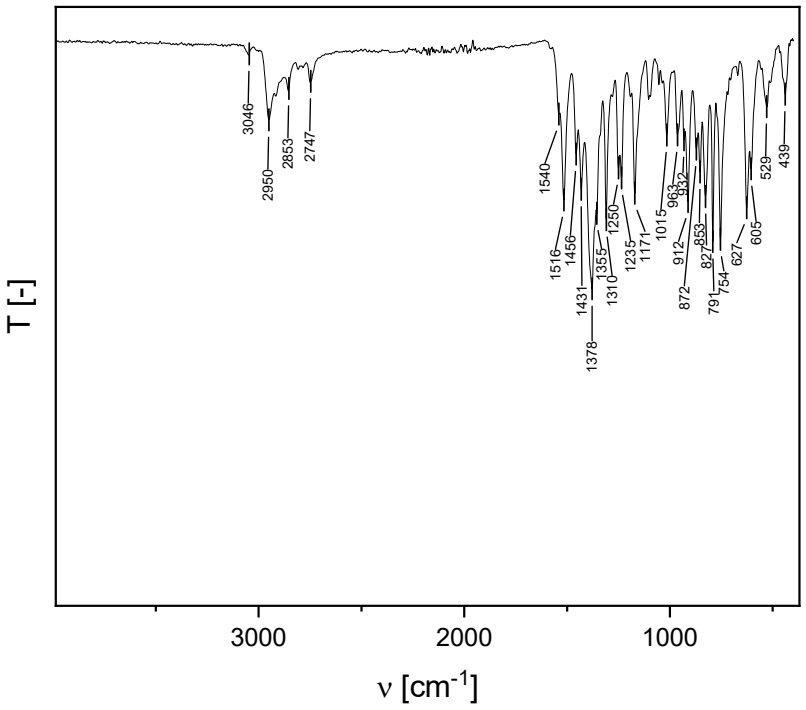

Fig. S27. ATR-IR spectrum of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**8**).

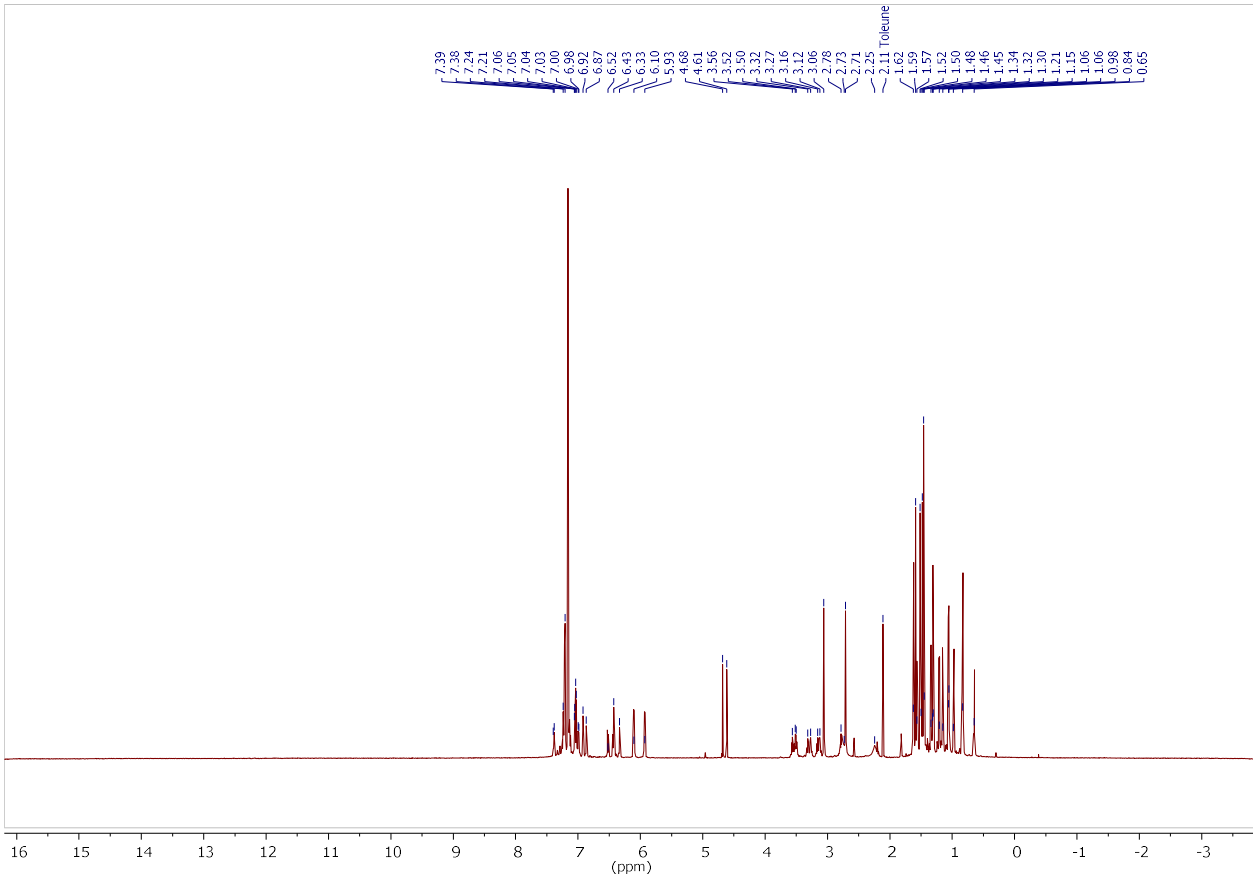

Fig. S28. ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of [L(Me_2N)GaSb][L(Me_2N)GaN(Ph)Sb]NPh (**9**).

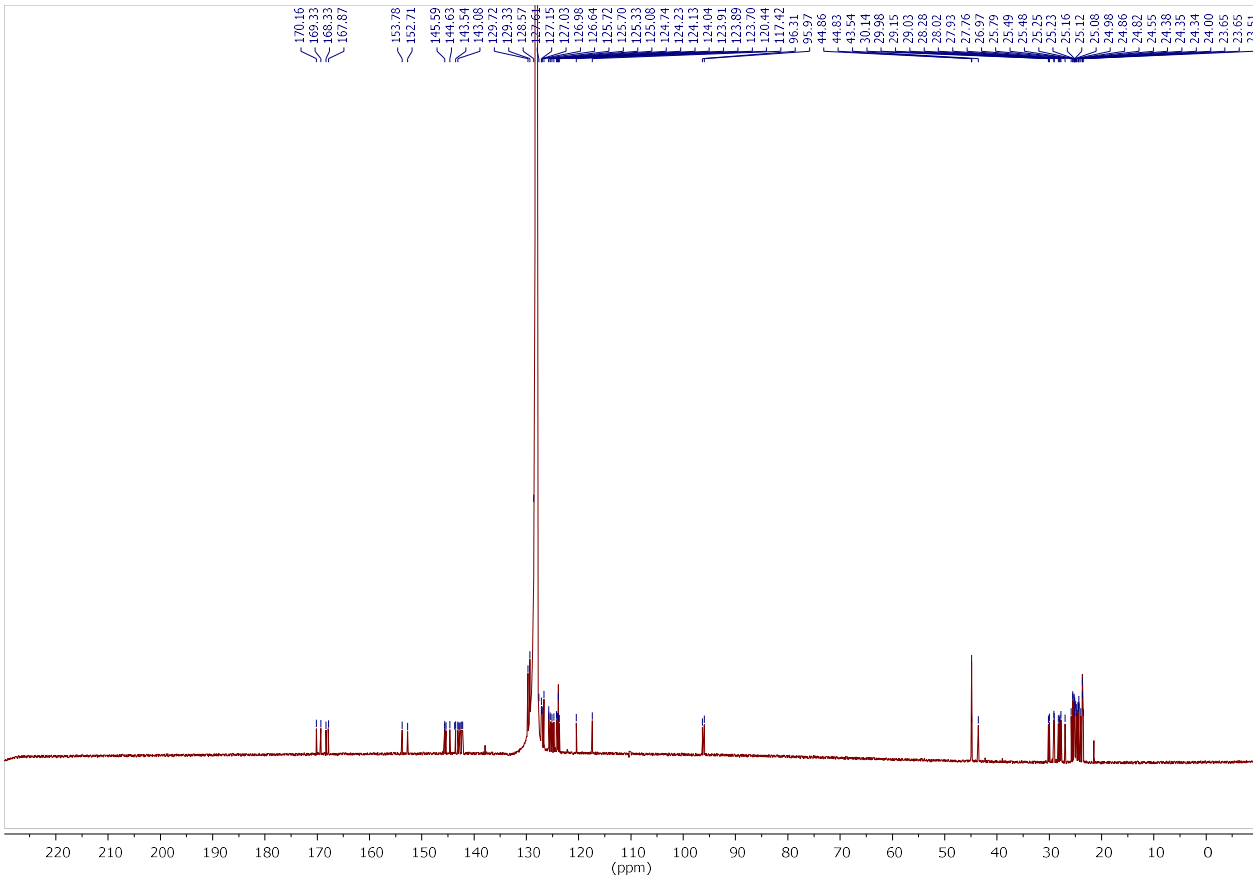

Fig. S29. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of [L(Me$_2$N)GaSb][L(Me$_2$N)GaN(Ph)Sb]NPh (**9**).

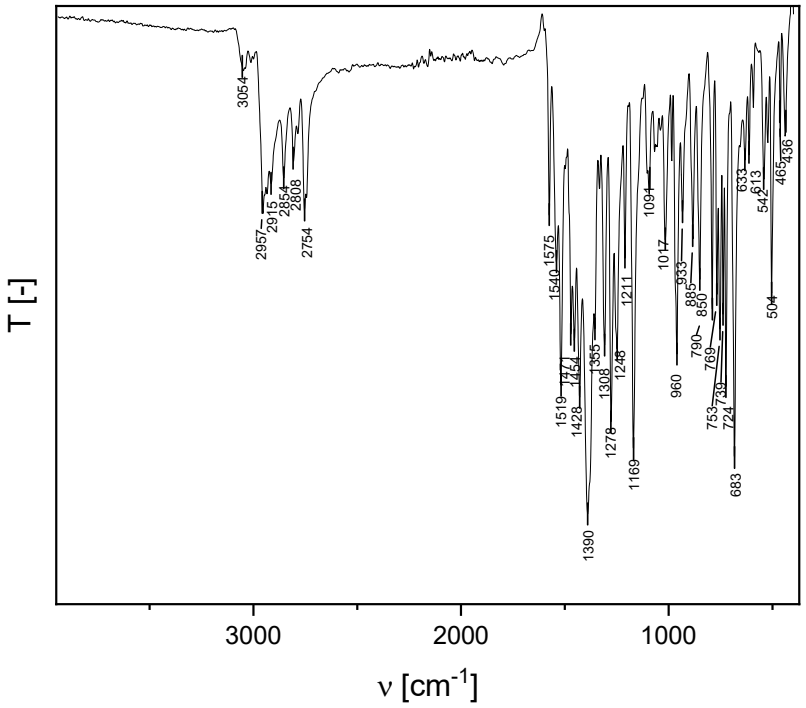

Fig. S30. ATR-IR spectrum of [L(Me$_2$N)GaSb][L(Me$_2$N)GaN(Ph)Sb]NPh (**9**).

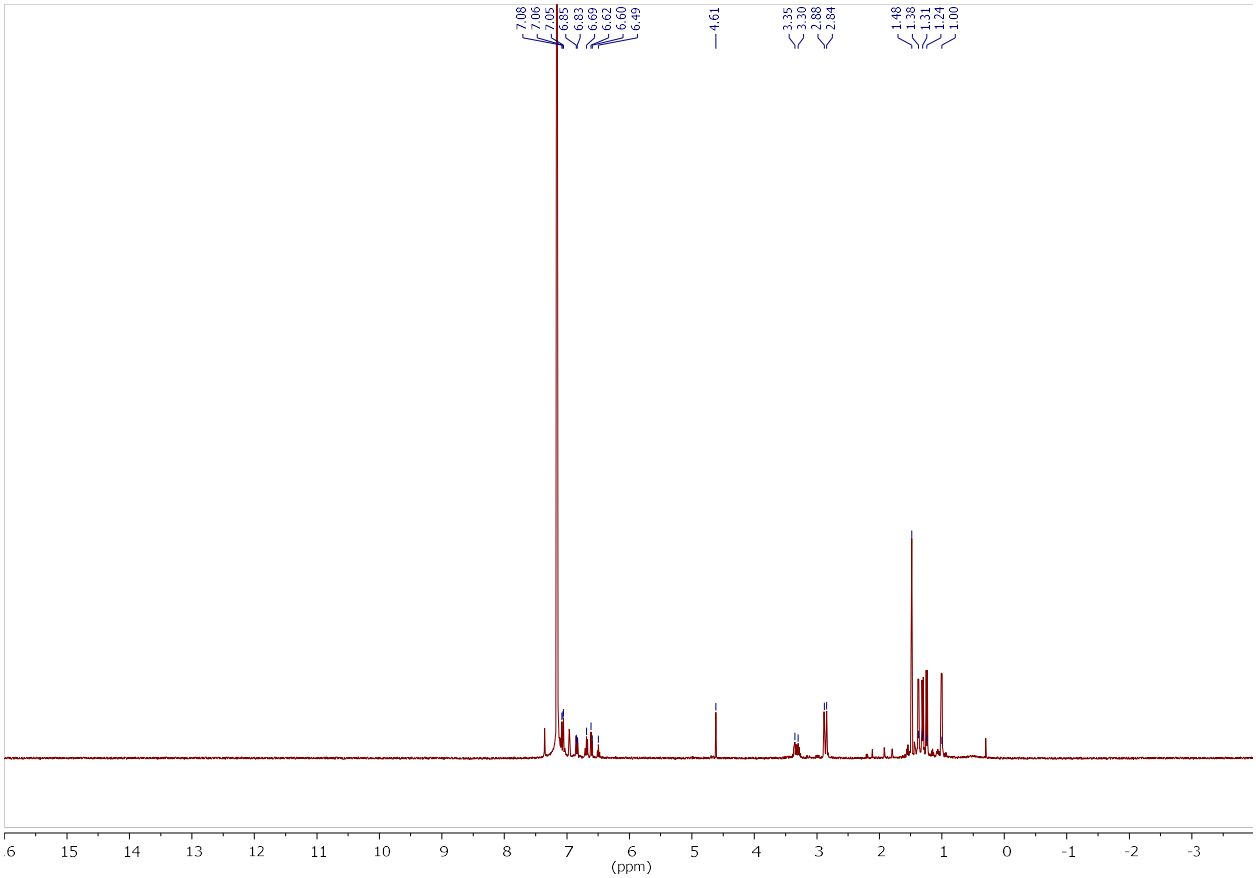

Fig. S31. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaN(Ph)Sb]_2$ (**10**).

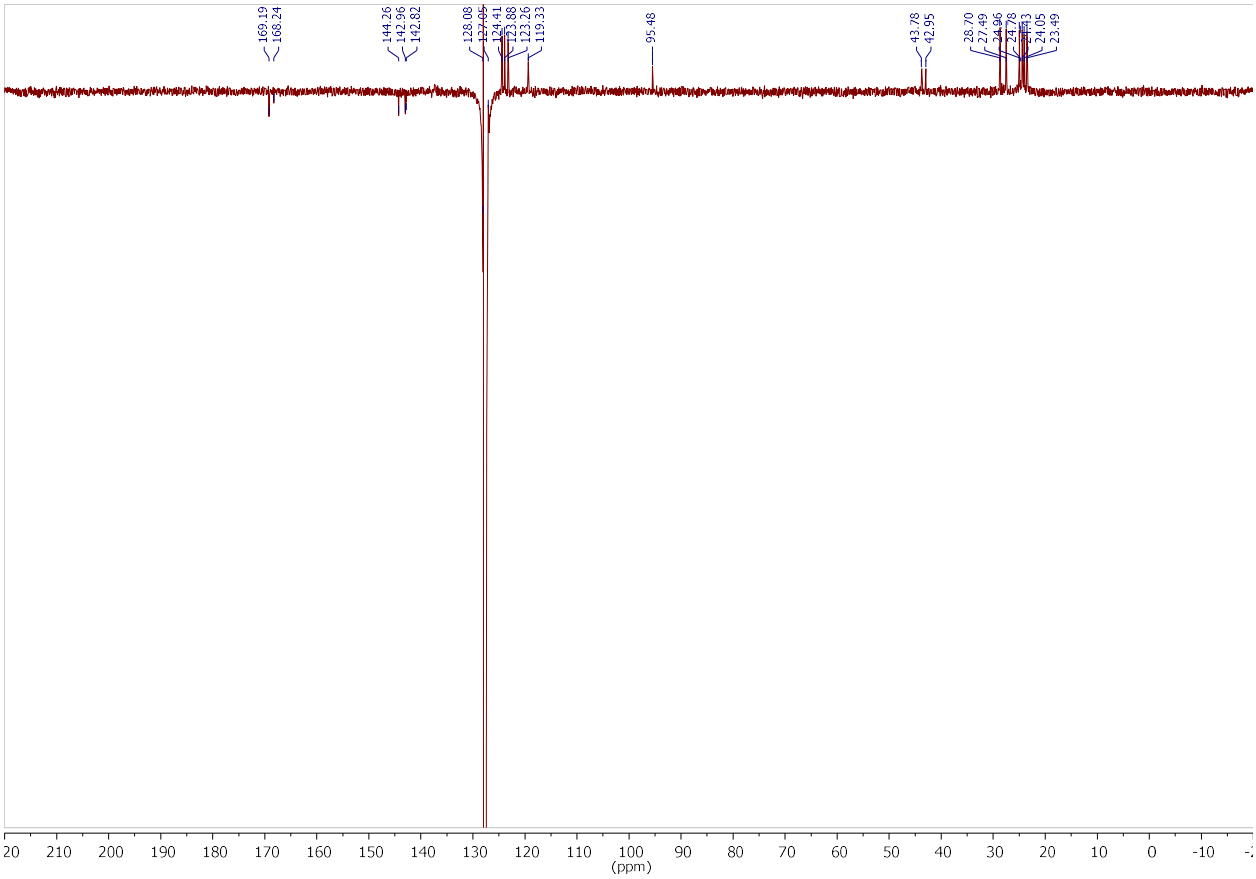

Fig. S32. DEPTQ ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaN(Ph)Sb]_2$ (**10**).

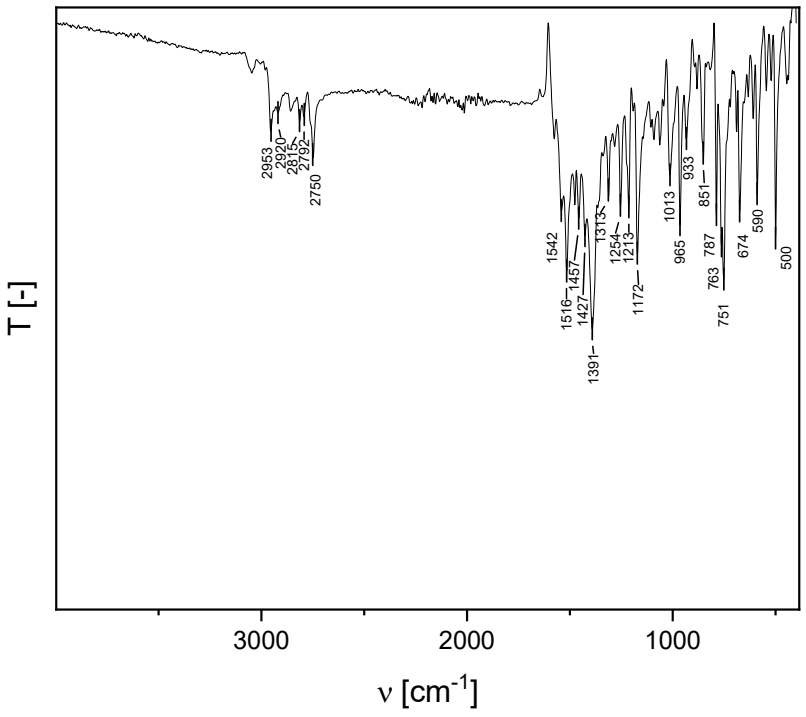

Fig. S33. ATR-IR spectrum of $[L(Me_2N)GaN(Ph)Sb]_2$ **(10)**.

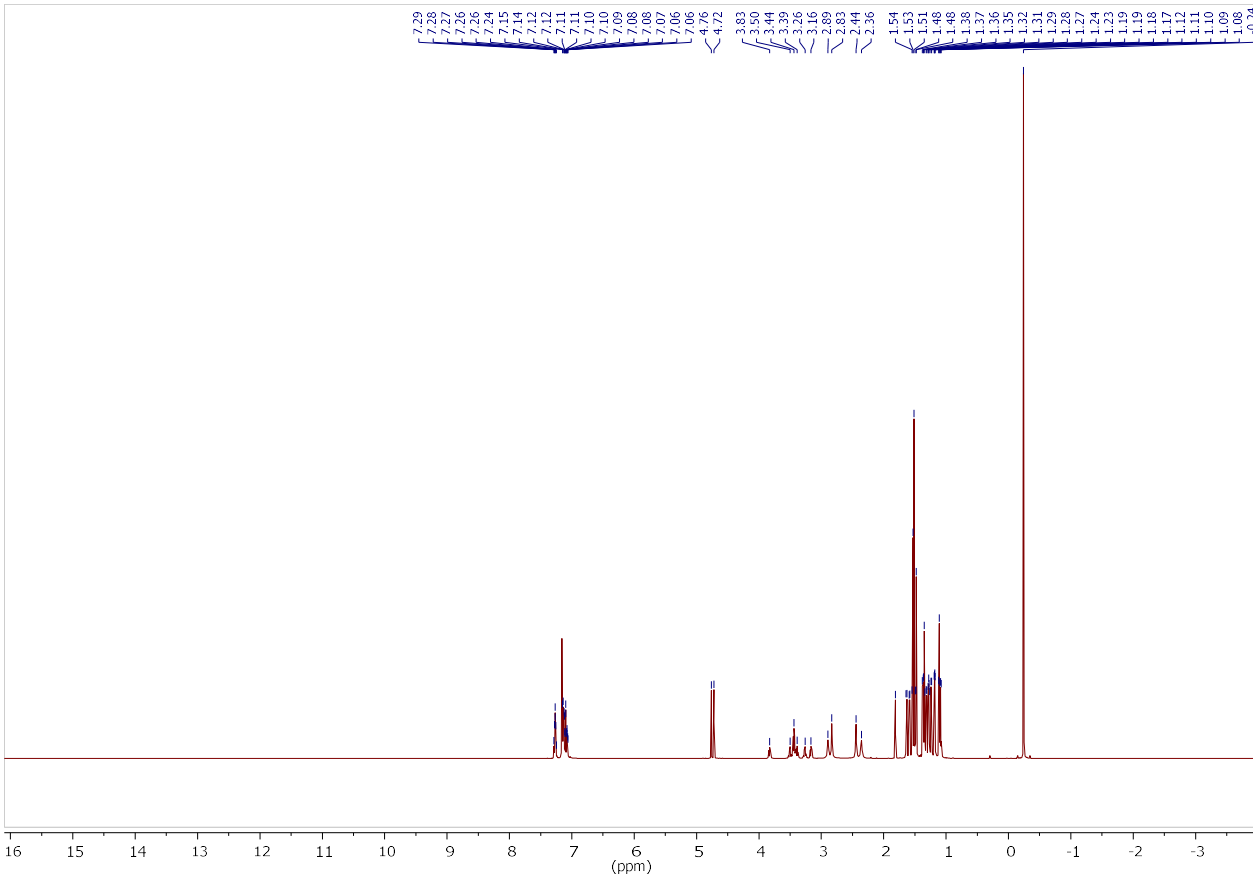

Fig. S34. ^{1}H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**).

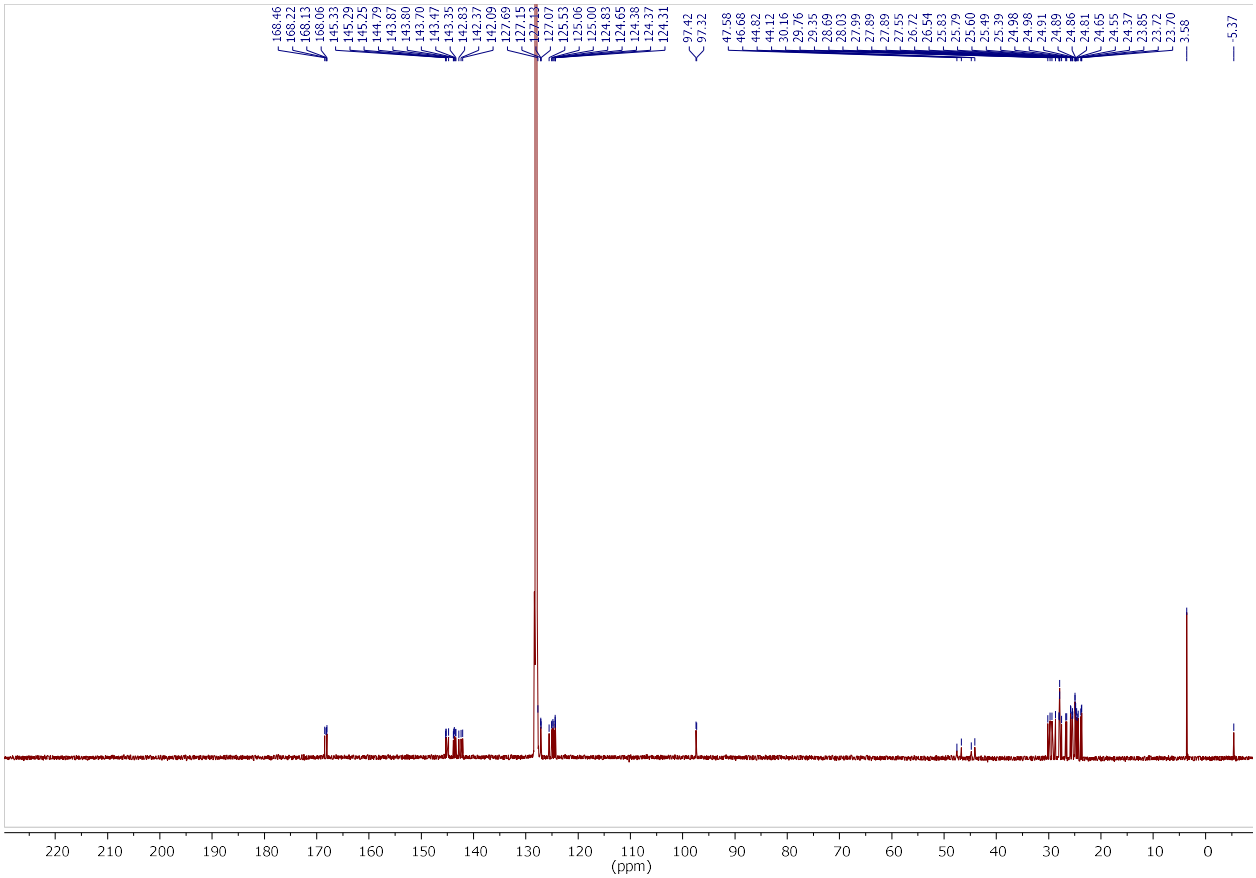

Fig. S35. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**).

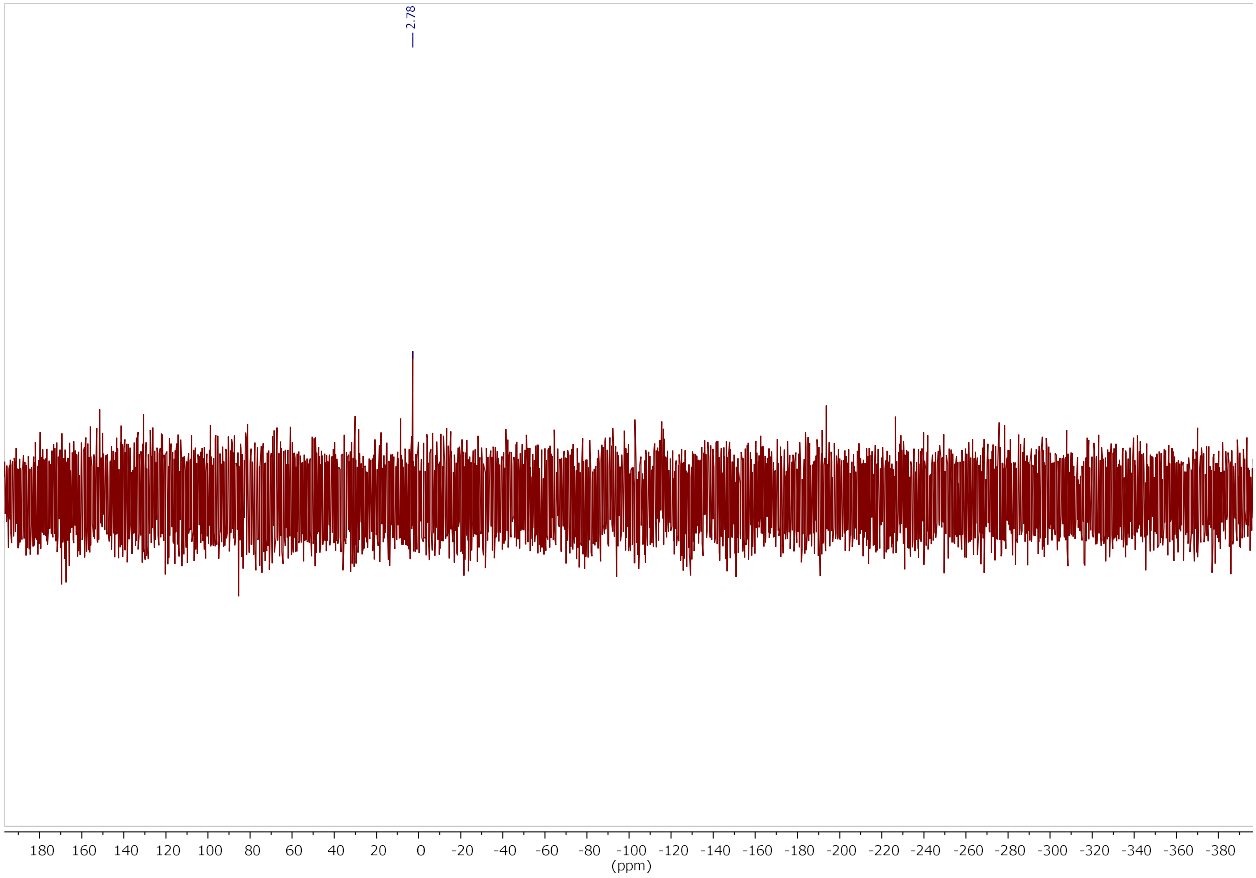

Fig. S36. ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**).

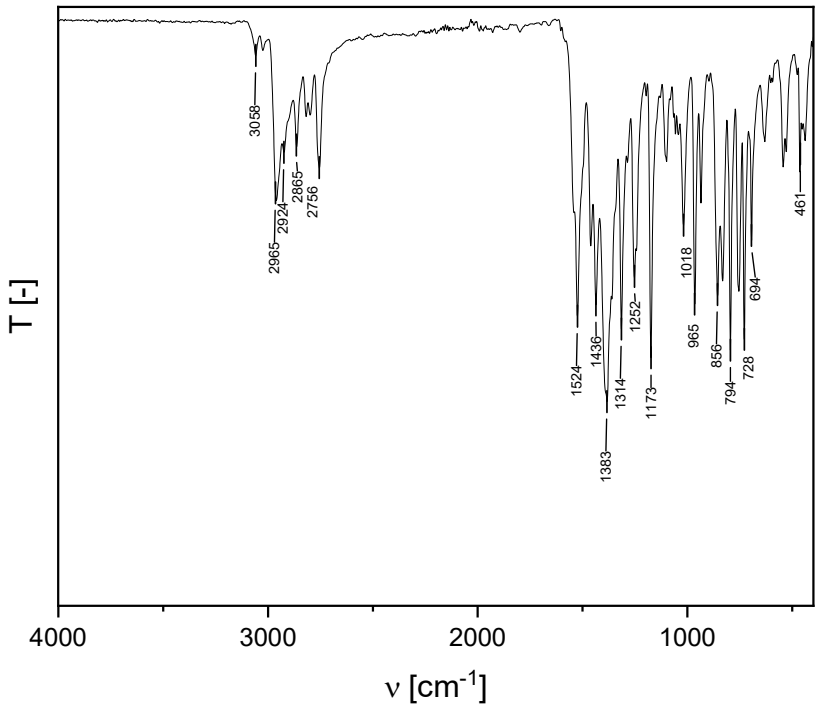

Fig. S37. ATR-IR spectrum of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**).

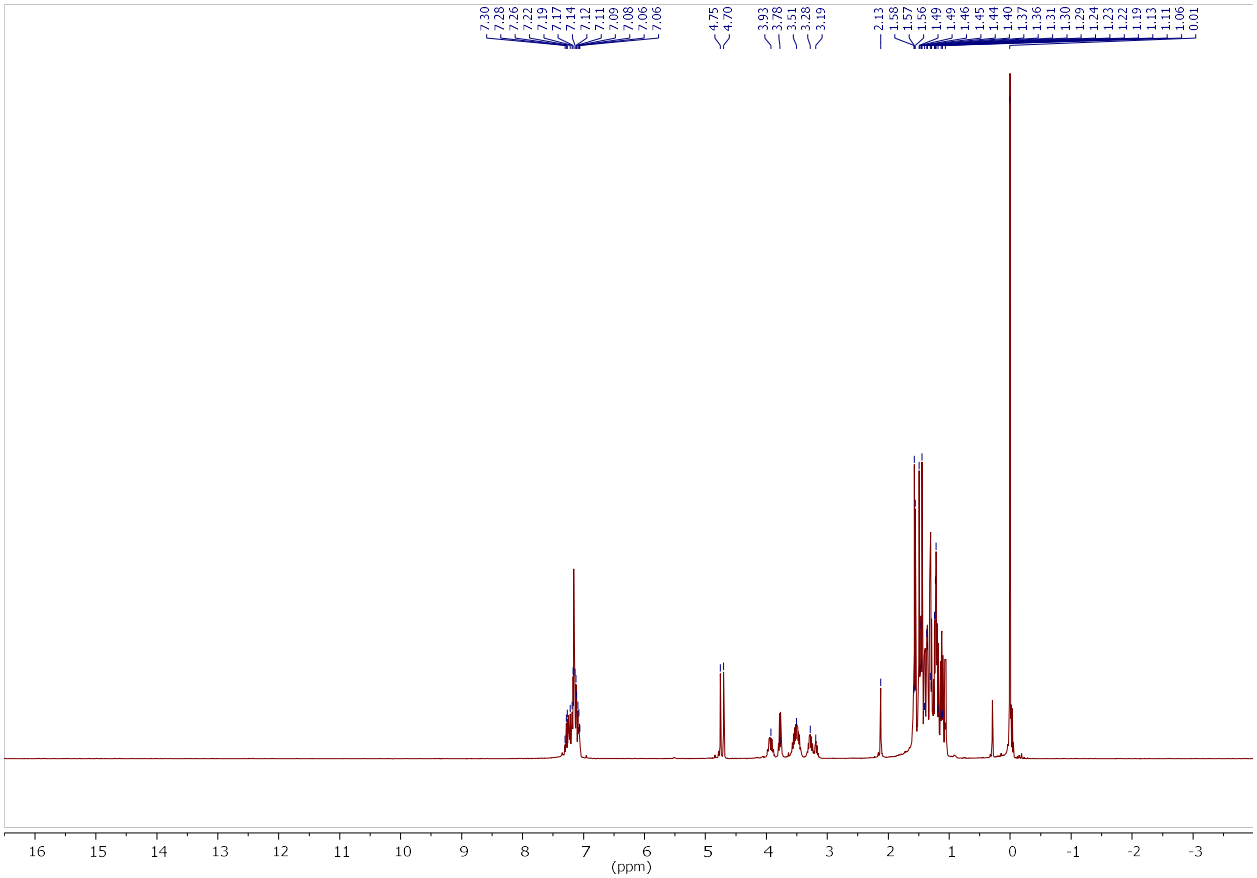

Fig. S38. ^{1}H NMR spectrum (400 MHz, C_6D_6, 25 °C) of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**12**).

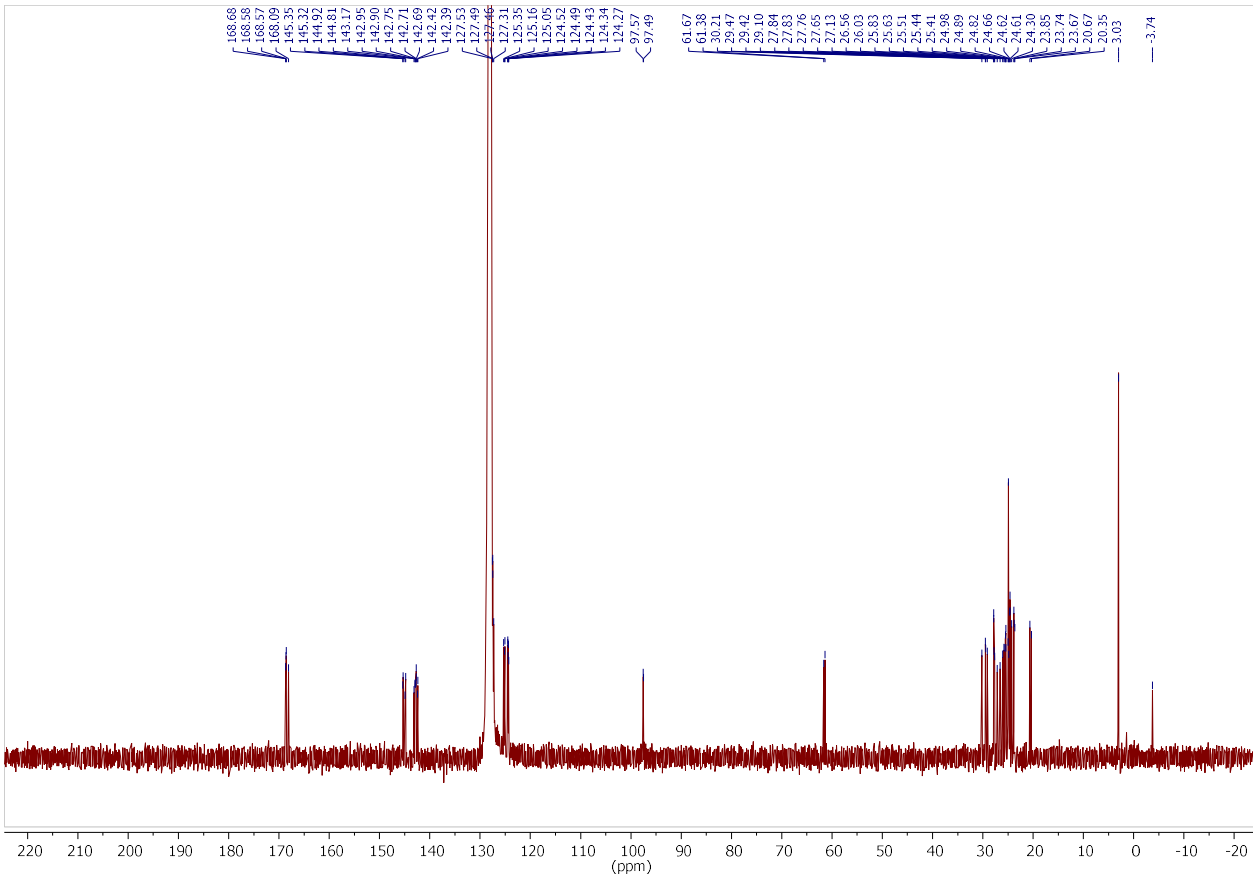

Fig. S39. ^{13}C NMR spectrum (100.6 MHz, C_6D_6, 25 °C) $[L(EtO)GaSb]_2C(H)SiMe_3$ (**12**).

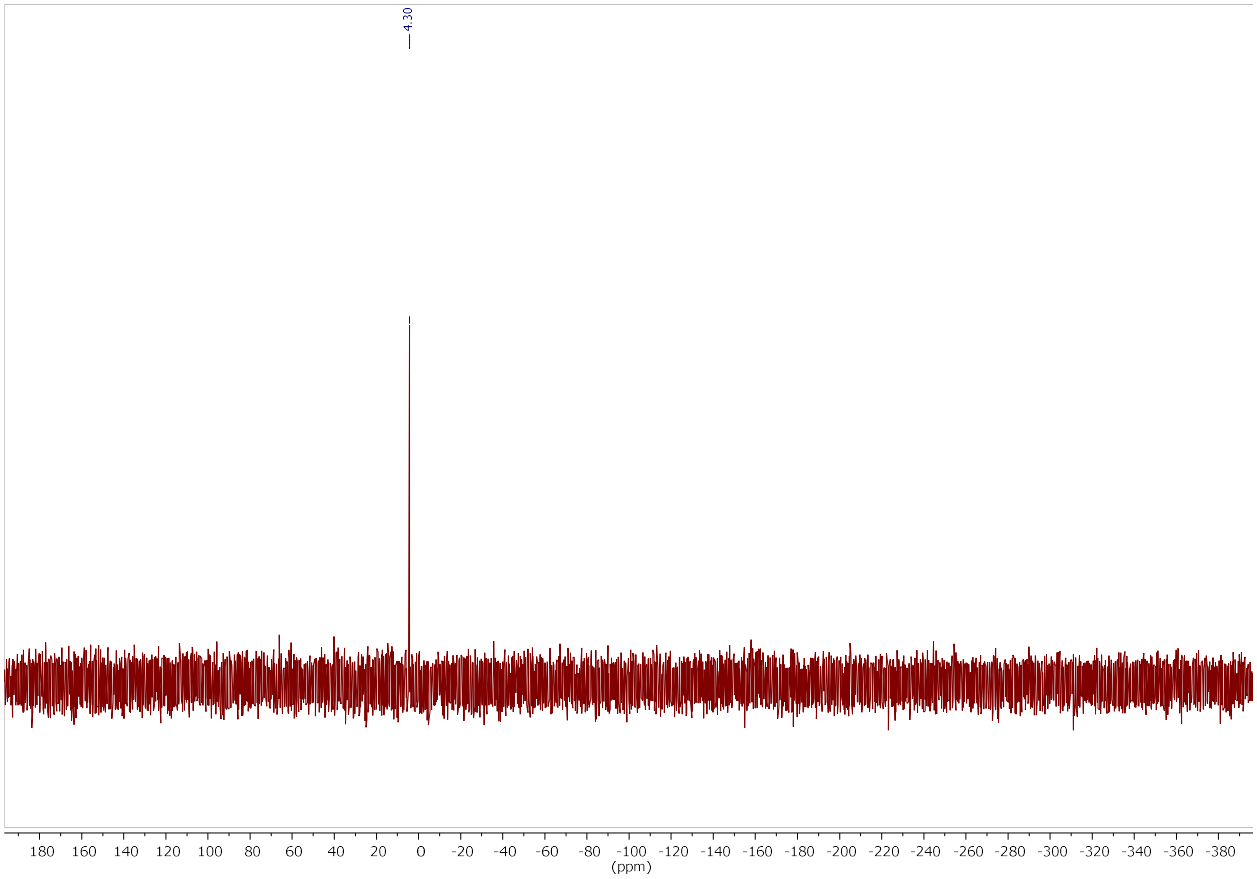

Fig. S40. DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**12**).

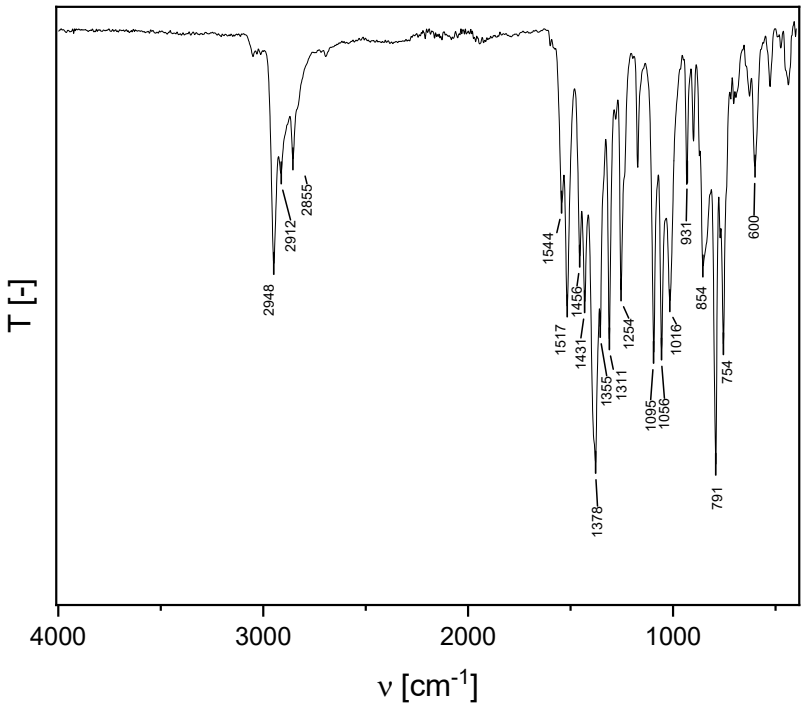

Fig. S 41. ATR-IR spectrum of $[L(EtO)GaSb]_2C(H)SiMe_3$ (**12**).

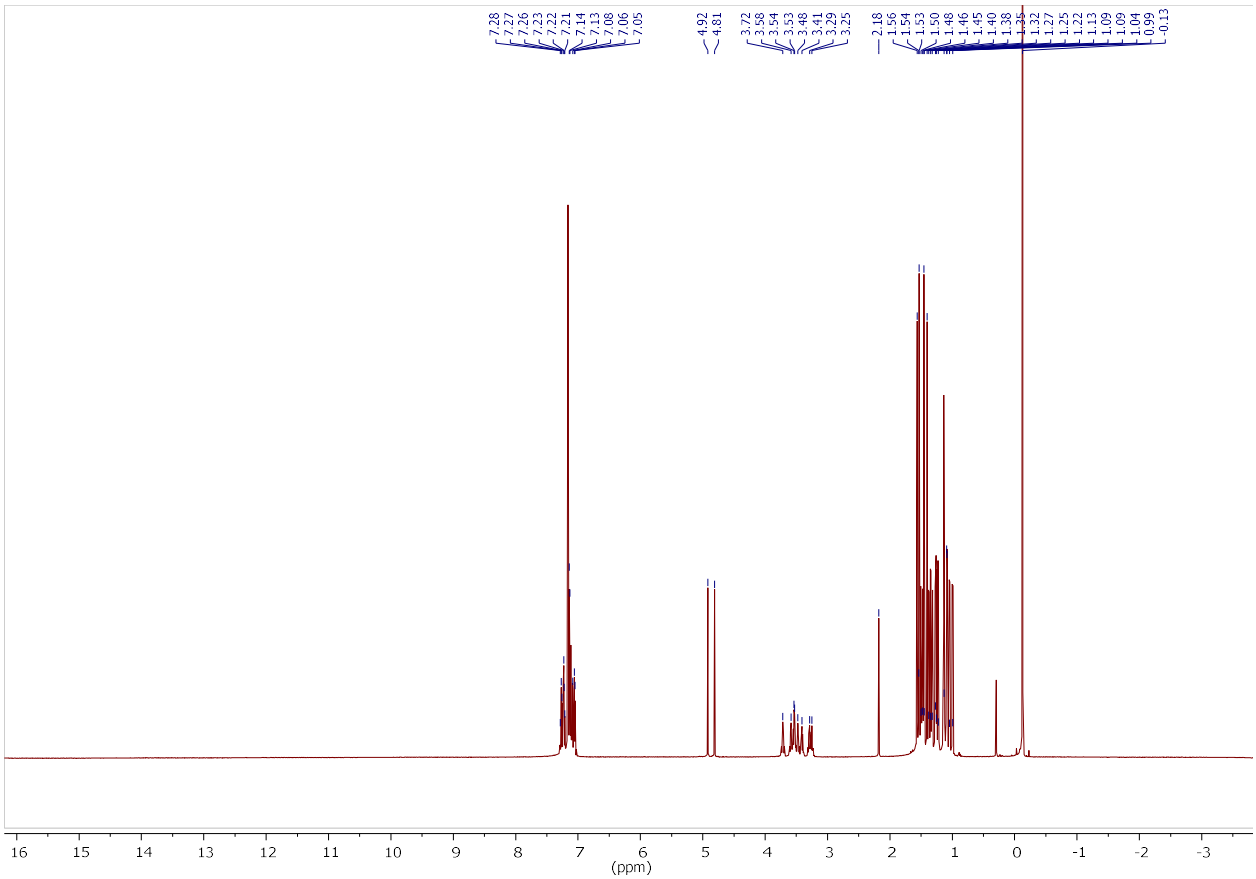

Fig. S42. ^1H NMR spectrum (600 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**13**).

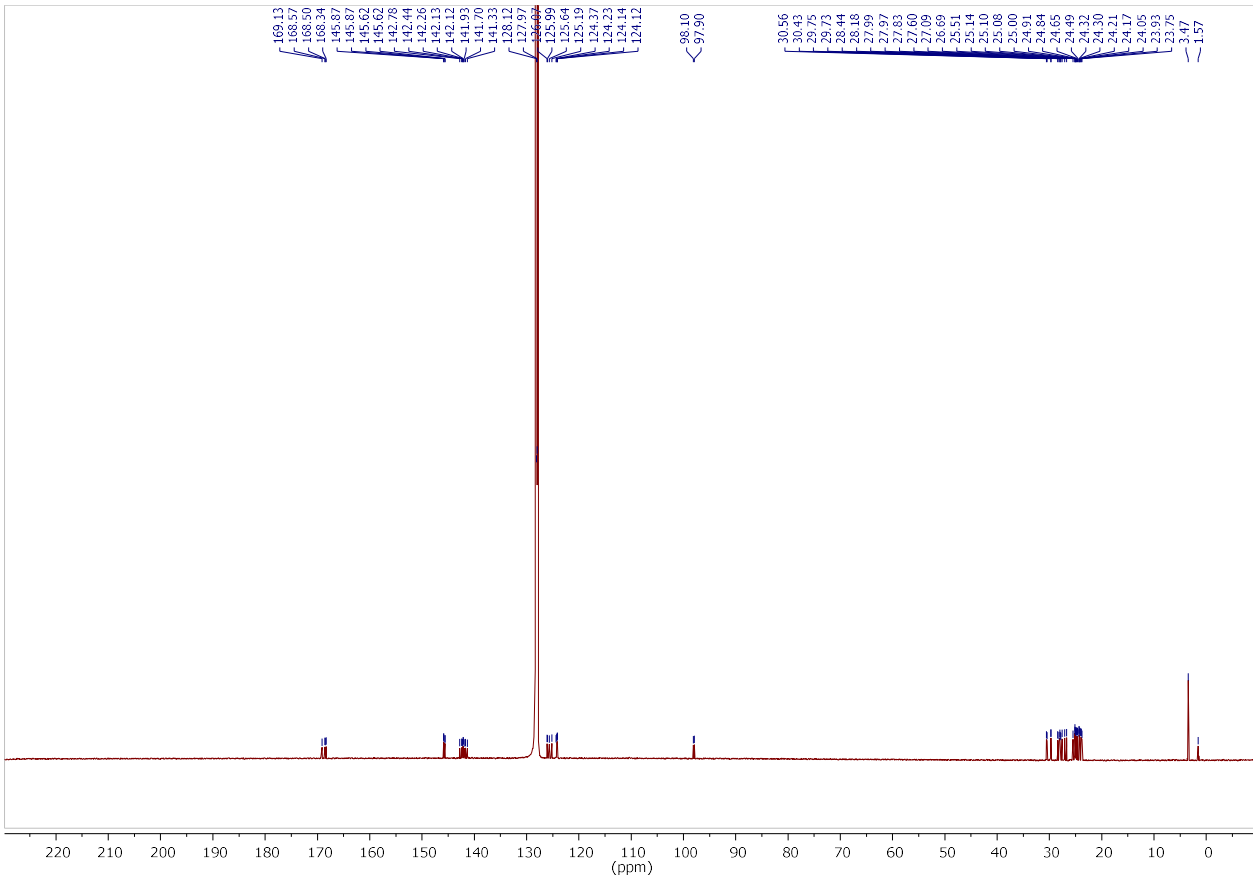

Fig. S43. ^{13}C NMR spectrum (150.9 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**13**).

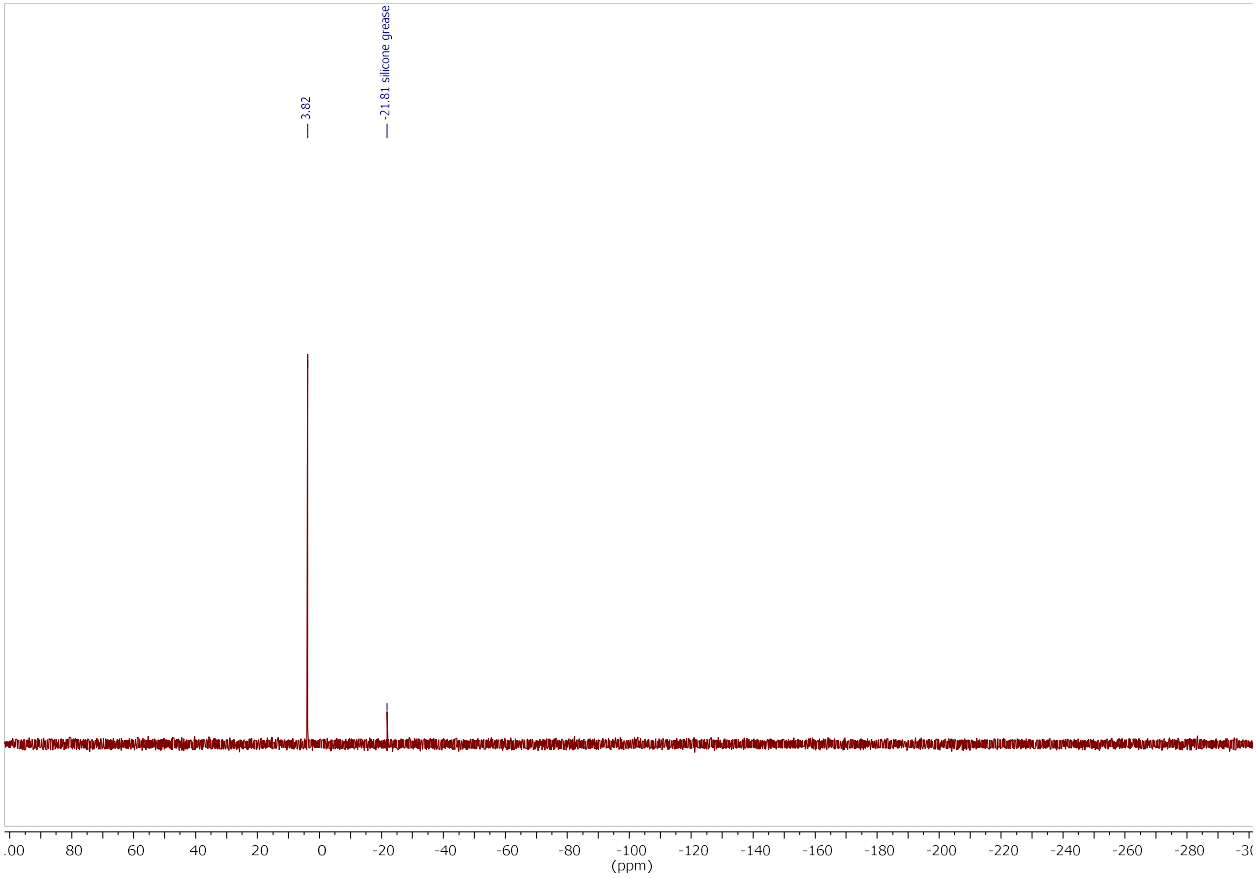

Fig. S44. DEPT ^{29}Si NMR spectrum (79.5 MHz, C_6D_6, 25 °C) of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**13**).

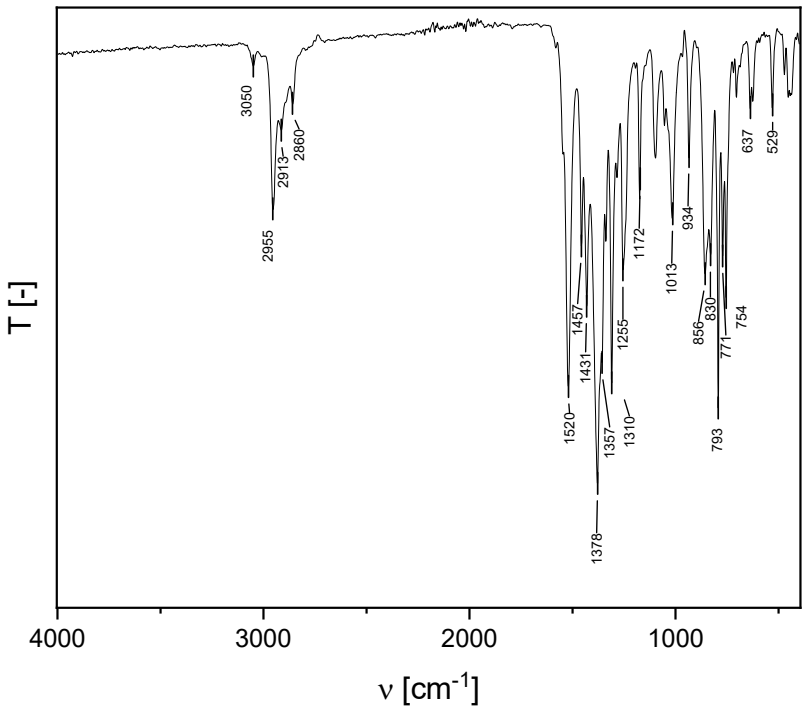

Fig. S45. ATR-IR spectrum of $[L(Cl)GaSb]_2C(H)SiMe_3$ (**13**).

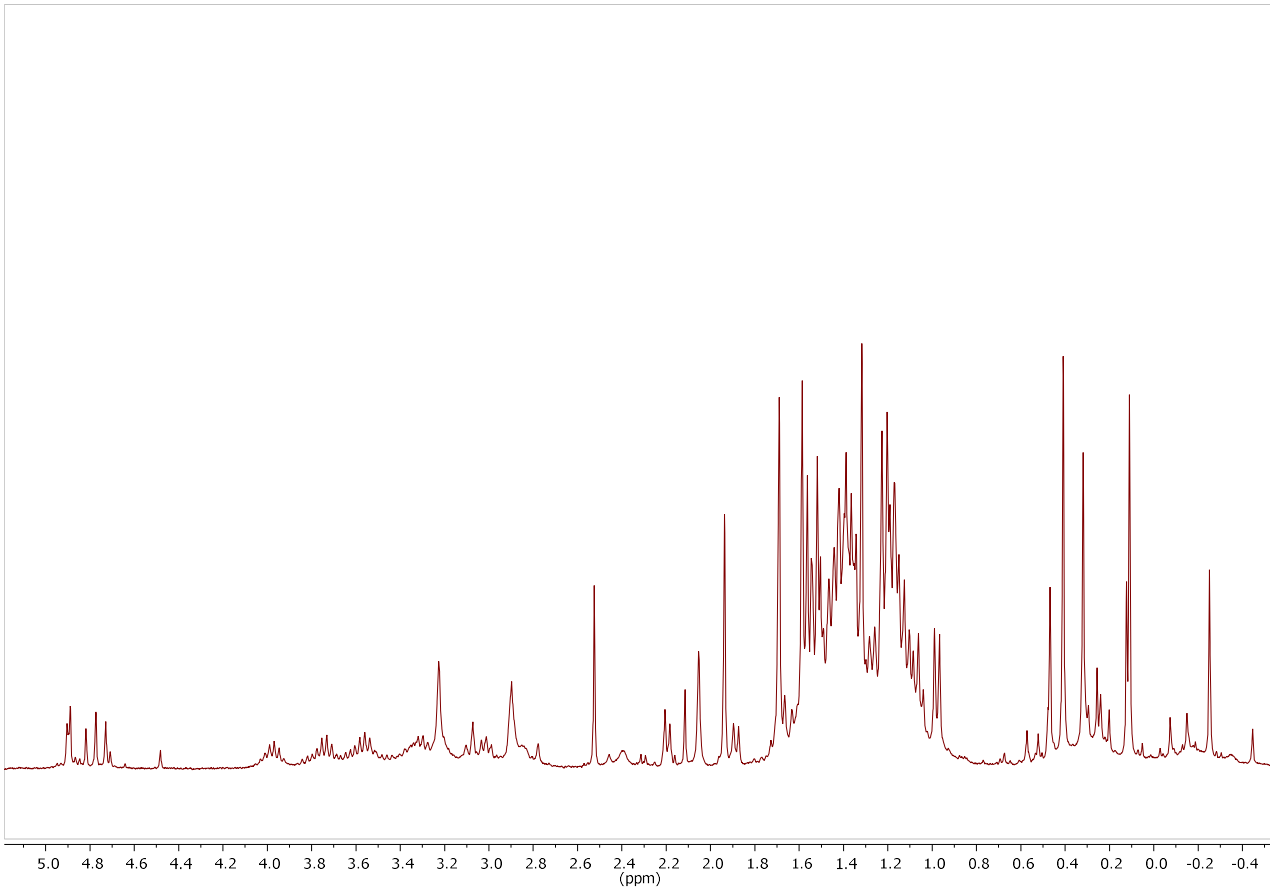

Fig. S46. ^{1}H NMR spectrum (300 MHz, C_6D_6, 25 °C) of the reaction of $[L(Me_2N)GaSb]_2$ with one equivalent Me_3SiN_3. Spektrum was recorded 5 min after addition of the azide.

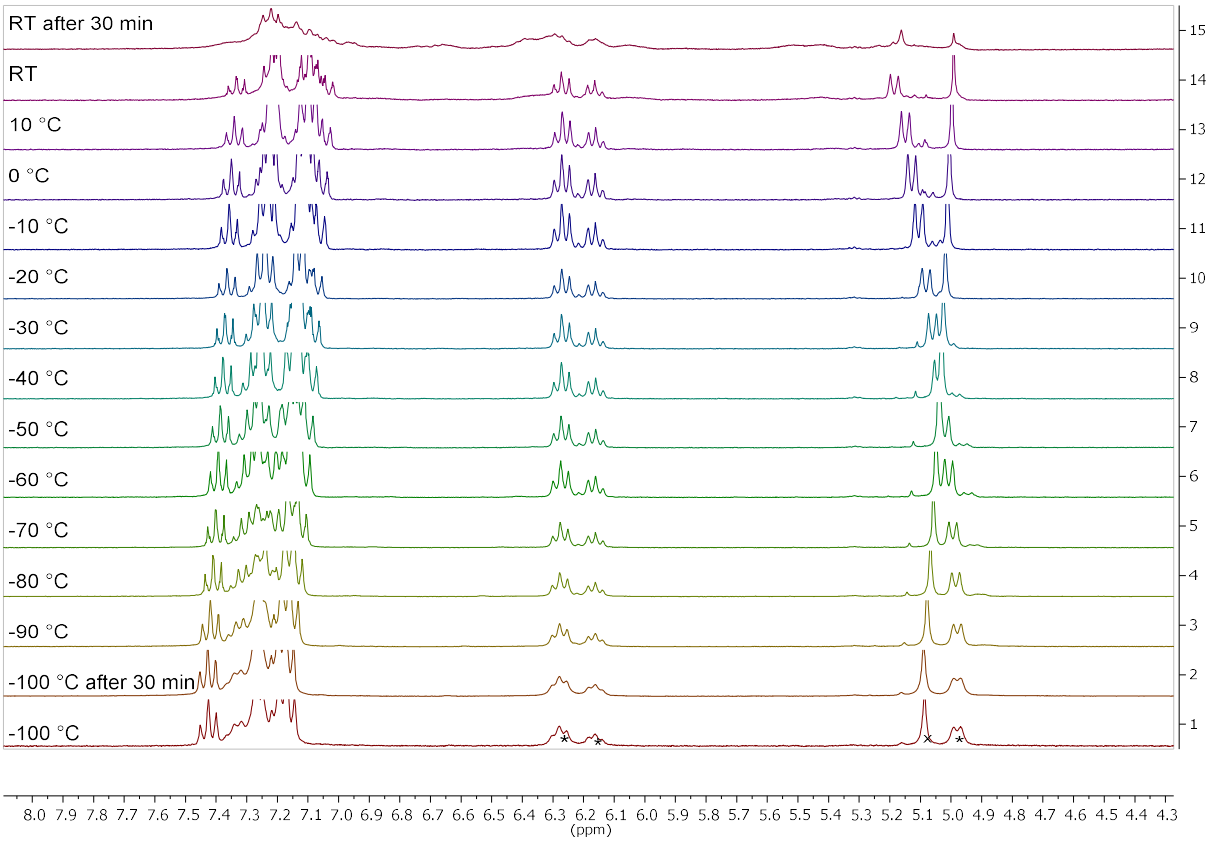

Fig. S47. ^{1}H NMR spectra (300 MHz, thf-d_8, –100 – +20 °C) of the reaction of $[L(EtO)GaSb]_2$ with PhN_3. Resonance marked with * and x are the N-C_6H_5 and L γ-H in 2 to 1 to 2 to 2 ratio, respectively. The low field shift of the ortho *H* of the phenyl ring was found to be characteristic of the azadistibiranes and having one resonance for the L(EtO)Ga excludes unsymmetrically species, i. e. imine or the [2+3] addition product.

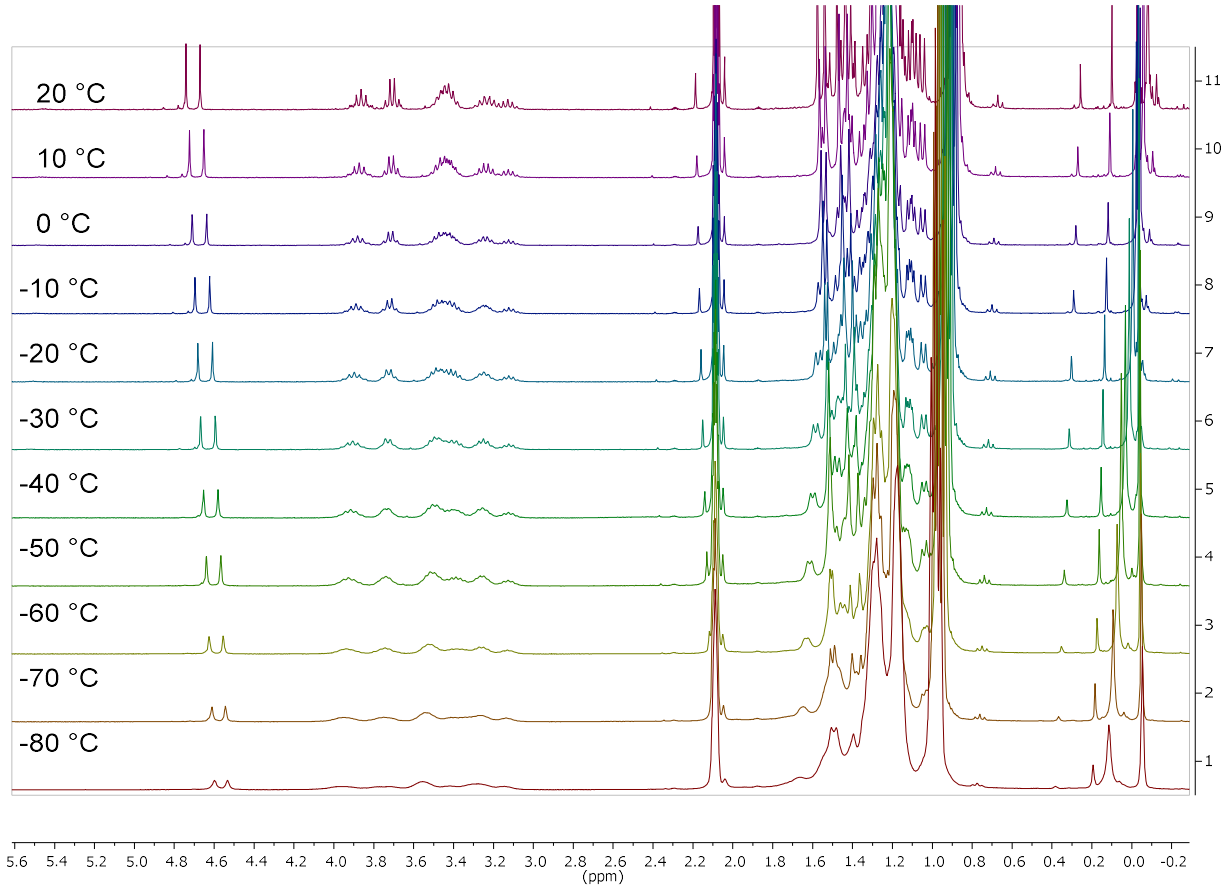

Fig. S48. ^{1}H NMR spectra (300 MHz, C_7D_8, –100 – +20 °C) of the reaction of $[L(EtO)GaSb]_2$ with 1.5 eq Me_3SiCHN_2.

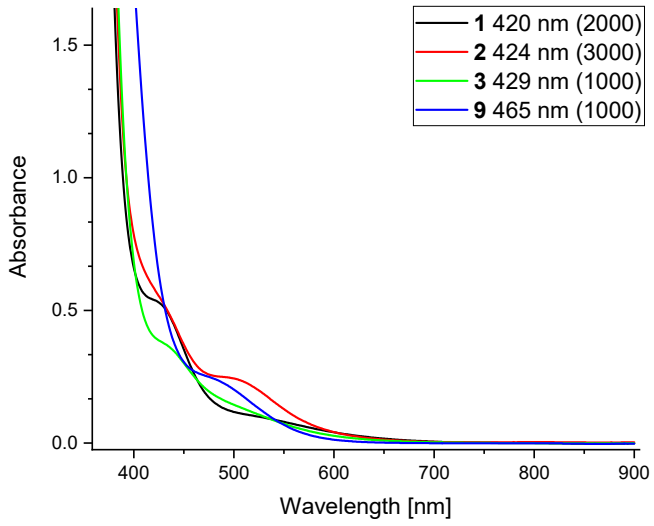

Fig.S49. UV-vis spectra of azadistibirane **1**–**3** and **9** in toluene. Extinction coefficient is given in brackets, the wavelength refers to the inflection point.

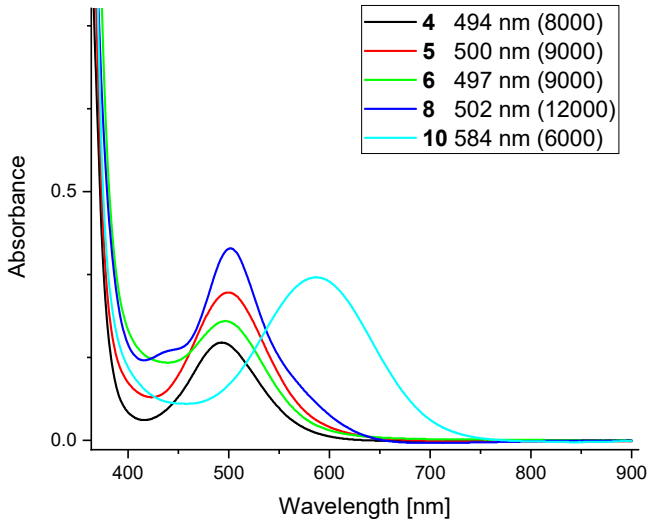

Fig. S50. UV-vis spectra of distibenes **4**–**6**, **8** and **10** in toluene. Extinction coefficient is given in brackets. The impurities with the highest concentration of **5** and **6** are **1** and **2** respectively. Due to their low adsorption in the visible region the spectra can be attributed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

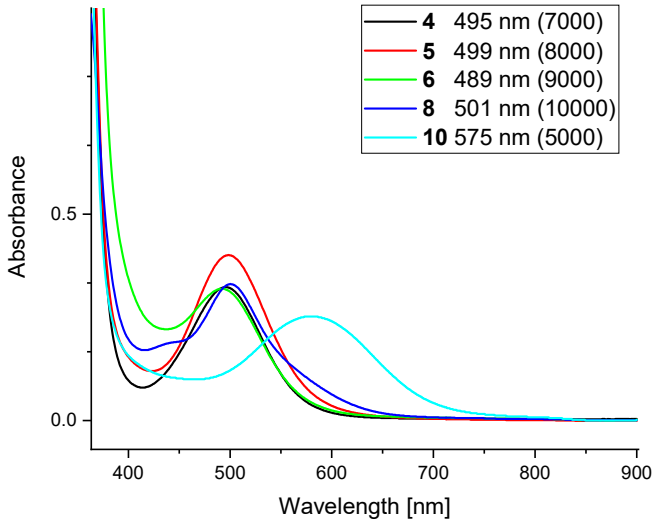

Fig. S51. UV-vis spectra of distibenes **4**–**6**, **8** and **10** in thf. Extinction coefficient is given in brackets. The impurities with the highest concentration of **5** and **6** are **1** and **2** respectively. Due to their low adsorption in the visible region the spectra can be attributed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

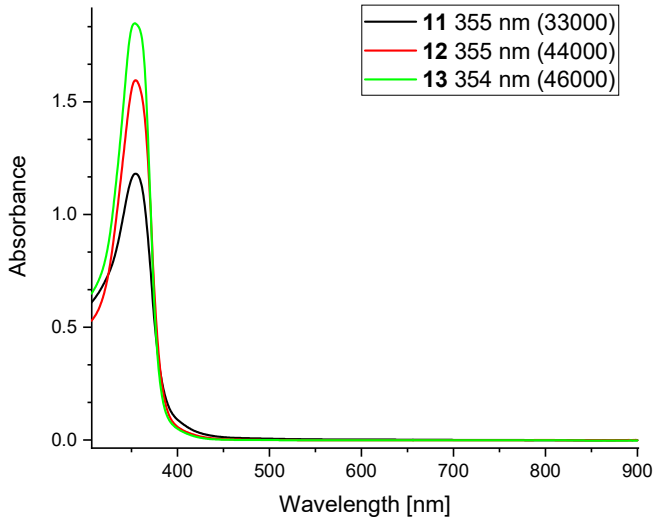

Fig. S52. UV-vis spectra of distibirane **11**–**13** in toluene. Extinction coefficient is given in brackets.

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 Mo_{Ka} radiation, λ = 0.71073 Å) and on a Bruker AXS D8 Venture diffractometer (**6**, **7**, **13**) with Photon II detector (monochromated Cu_{Ka} 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. Due to the long axis in **3** the integration of the intensities was hampered by overlap. The seven most disagreeable reflections were ignored in the refinement (OMIT). Since the intensities might be distorted due to the overlap quantitative results should be carefully assessed. The structure model of **4** was refined as a two-component inversion twin. The structure of **5** contains highly disordered solvent – likely a mixture of toluene and acetonitrile. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE[3] run. Since the nature and amount of the solvent is not clear it was not included in the sum formula. In **6** the bond lengths of the solvent molecules were restrained to be equal (SADI) and RIGU restraints were applied to their atoms' displacement parameters. One *n*-hexane molecule is disordered over a centre of inversion. Additional SIMU restraints were used for the refinement of the displacement parameters of this molecule. The local symmetry was ignored in the refinement (negative PART). The displacement ellipsoids suggest further disorder that could not be resolved. 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 restraint 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 **12** two *i*-Pr groups and a complete diisopropylphenyl moiety are disordered over two positions. All corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints were applied to the displacement parameters of the disordered atoms. For 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 it displacement parameters. Due to their proximity C1_1 and C1_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), -2129211 (**10** mw_150_2), -2129212 (**11** mw_089_1fs), -2129213 (**12** mw_099_tw5), and -2129214 (**13** mw_112_3fr) 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(Me_2N)GaSb]$_2$NPh (**1**), [L(Me_2N)GaSb]$_2$N-p-CF_3-Ph (**2**), [L(Me_2N)GaSb]$_2$N(ada) (**3**) and [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**) [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**), [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**), and [(L(NPh)Ga-κ*Ga*,κ*N*)$_2$-(μ,$\eta^{1:1:1:1}$-Sb_4)] (**7**).

	1	**2**	**3**	**4**	**5**	**6**	**7**
Empirical formula	$C_{71.50}H_{103}Ga_2N_7Sb_2$	$C_{72.50}H_{102}F_3Ga_2N_7\ Sb_2$	$C_{79}H_{117}Ga_2N_7Sb_2$	$C_{65}H_{103}Ga_2N_7Sb_2Si$	$C_{77}H_{110}Ga_2N_8Sb_2$	$C_{78}H_{119}F_3Ga_2N_7Sb_2$	$C_{77}H_{110}Ga_2N_8Sb_2$
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	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	P-1	$P2_1/n$	$P2_1$	$P2_1/c$	$P2_1/n$	$P2_1/c$
a [Å]	19.9634(10)	10.6581(5)	10.9672(11)	10.7967(17)	13.6969(16)	12.1758(10)	13.6969(16)
b [Å]	12.5667(7)	12.7136(6)	45.894(5)	21.163(3)	28.763(3)	27.211(2)	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	102.129(2)	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	98.869(3)	90	90	90	90	90
V [Å^3]	6989.7(6)	3595.4(3)	7643.8(13)	3439.2(9)	8133.4(17)	7916.1(11)	8133.4(17)
Z	4	2	4	2	4	4	4
D_{calc} [g·cm-3]	1.372	1.396	1.345	1.346	1.250	1.338	1.250
μ(Mo/CuK_α) [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	-21 ≤ h ≤ 21	-15 ≤ h ≤ 14	-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
θ_{max} [°]	36.384	33.683	33.532	33.208	34.165	80.082	34.165
Refl. collected	369240	190515	368631	108278	285425	249345	285425
Independ. refl.	33974	28194	29384	26282	31986	17136	31986
R_{int}	0.0450	0.0415	0.0535	0.0441	0.0430	0.0710	0.0430
Refined parameters	736	1250	836	722	831	884	831
R_1 [$I > 2\sigma(I)$]	0.0283	0.0457	0.0646	0.0323	0.0299	0.0322	0.0299
wR_2 [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
$\Delta\rho_{final}$ (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

Table S1b. Crystallographic data of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(N(H)$SiMe_3$)L] (**8**), [L(Me_2N)GaSb][L(Me_2N)GaN(Ph)Sb]N-Ph (**8**), [L(Me_2N)GaN(Ph)Sb]$_2$ (**9**), [L(Me_2N)GaSb]$_2$C(H)$SiMe_3$ (**10**) and [L(EtO)GaSb]$_2$C(H)$SiMe_3$ (**11**), and [L(Me_2N)GaSb]$_2$C(H)$SiMe_3$ (**13**).

	8	**9**	**10**	**11**	**12**	**13**
Empirical formula	$C_{68}H_{110}Ga_2N_8Sb_2Si_2$	$C_{81}H_{112}Ga_2N_8Sb_2$	$C_{74}H_{104}Ga_2N_8Sb_2$	$C_{78}H_{116}Ga_2N_6Sb_2Si$	$C_{66}H_{102}Ga_2N_4O_2Sb_2Si$	$C_{64.50}H_{98}Cl_2Ga_2N_4Sb_2Si$
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	$P2_1/n$	P-1	P-1	P-1	$C2/c$	$P2_1/c$
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)	33.512(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	93.817(4)	107.9954(14)	88.053(10)	90	90
V [Å^3]	7278(2)	3856.2(5)	1753.06(11)	3972.9(16)	14053(3)	6955.1(10)
Z	4	2	1	2	8	4
D_{calc} [g·cm-3]	1.350	1.361	1.410	1.295	1.318	1.348
μ(Mo/CuK_α) [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	768	1608	5760	2900
Index ranges	-17 ≤ h ≤ 17	-17 ≤ h ≤ 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
θ_{max} [°]	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
R_{int}	0.0518	0.1010	0.0193	0.0652	0.0753	0.1275
Refined parameters	804	863	400	1048	827	838
R_1 [$I > 2\sigma(I)$]	0.0404	0.0393	0.0191	0.0402	0.0755	0.0359
wR_2 [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
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	2.358/-1.236	1.203/-0.884	0.928/-0.313	3.087/-3.509	2.377/-1587	1.844/-1.943

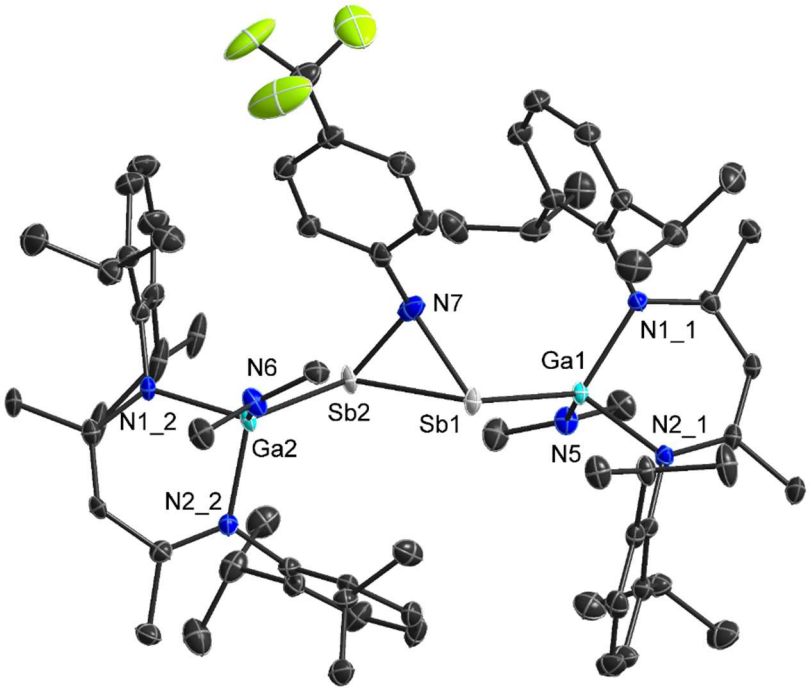

Fig. S53. Molecular structure of [L(Me$_2$N)GaSb]$_2$N-p-CF$_3$-Ph (**2**) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the L(Me$_2$N)GaSb and p-CF$_3$-Ph unit is displayed.

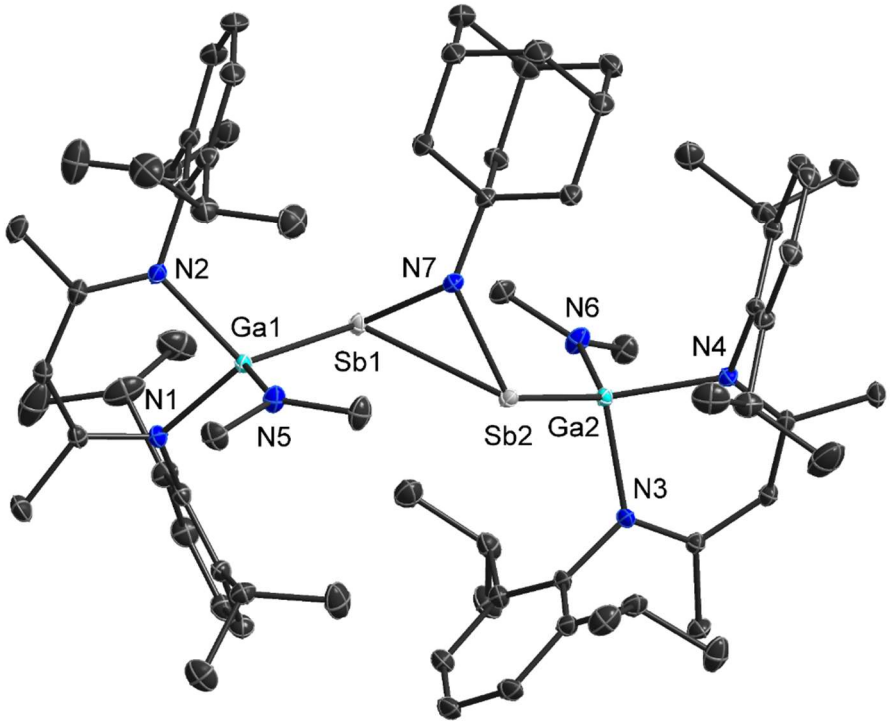

Fig. S54. Molecular structure of [L(Me$_2$N)GaSb]$_2$N-ada (**3**) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

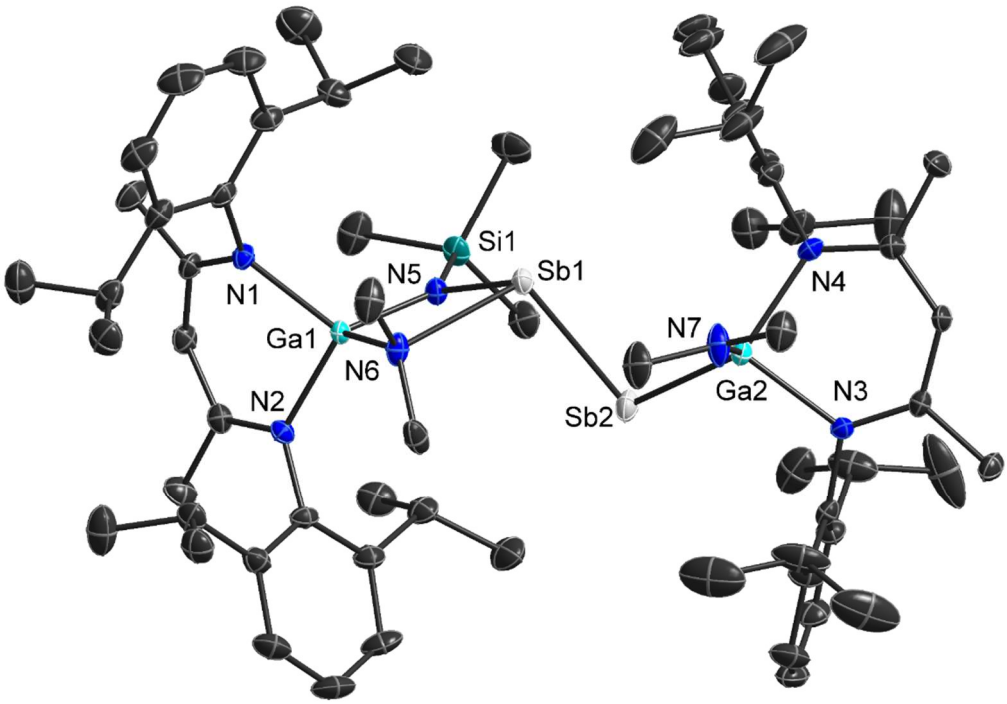

Fig. S55. Molecular structure of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**)in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

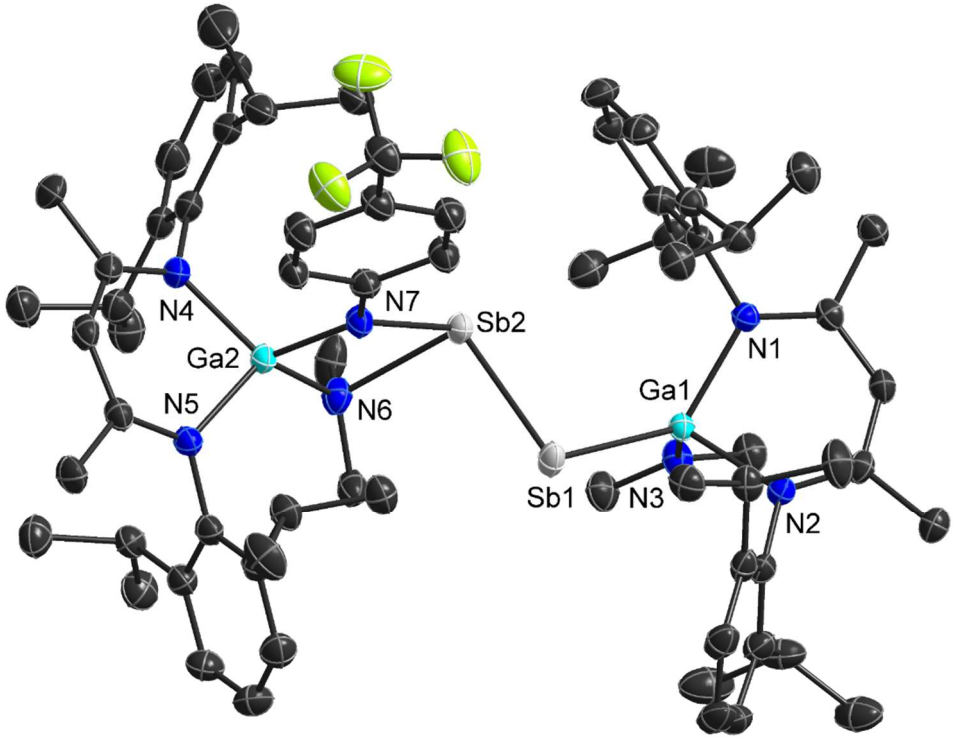

Fig. S56. Molecular structure of [L(Me_2N)Ga]SbSb[N(p-CF_3-Ph)Ga(NMe_2)L] (**6**) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

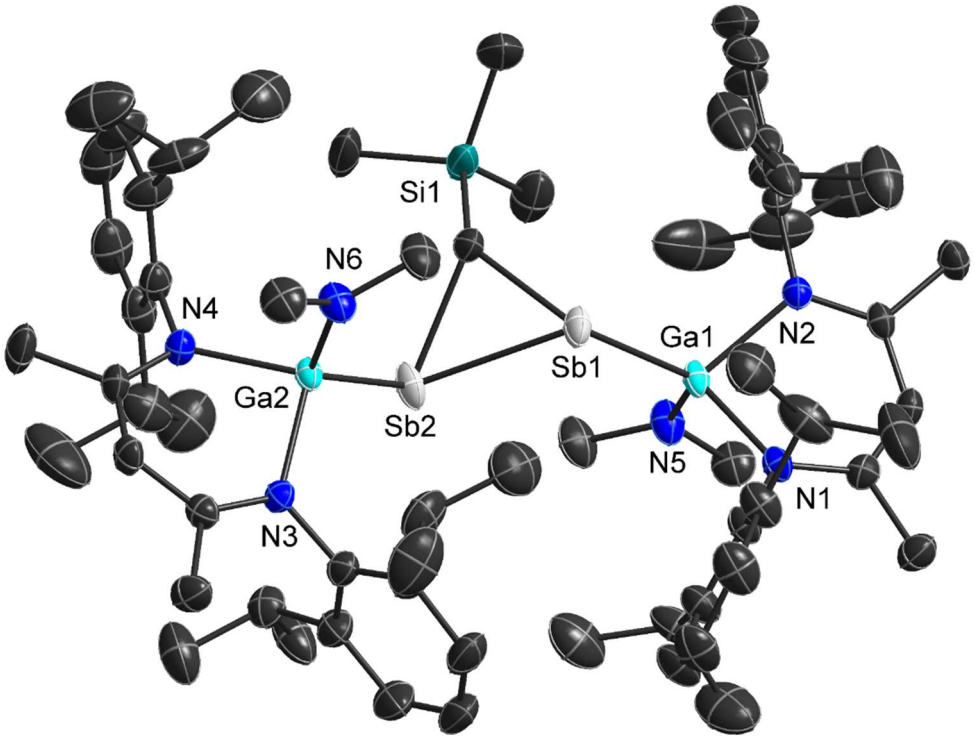

Fig. S57. Molecular structure of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the $CSiCMe_3$ unit is displayed.

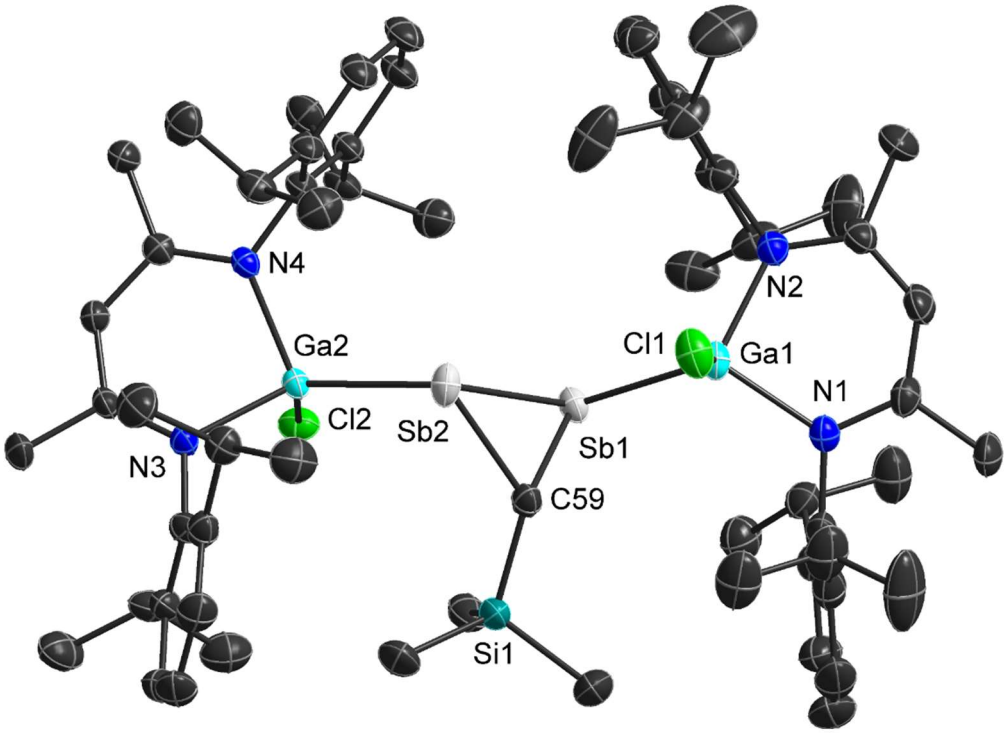

Fig. S58. Molecular structure $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**13**) in the crystal. H atoms and are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level. Only the major component for the disorder of the $CSiCMe_3$ unit is displayed.

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 functional[5] with the default "defgrid3" and "extremescf" with def2-SVP[6] basis set on H, C, N, Si and def2-TZVP[6] 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 RIJCOSX[9] (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-TZVP[6] basis on H, C, N and def2-QZVP[6] 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-TZVP[6] basis set on H, C, N, Si and def2-QZVP[6] 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 N_2 unit. Finally, for the closely related $Me_3Si\text{-}N_3$ and $Me_3Si\text{-}CH\text{-}N_2$ 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 3.8[16] 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]

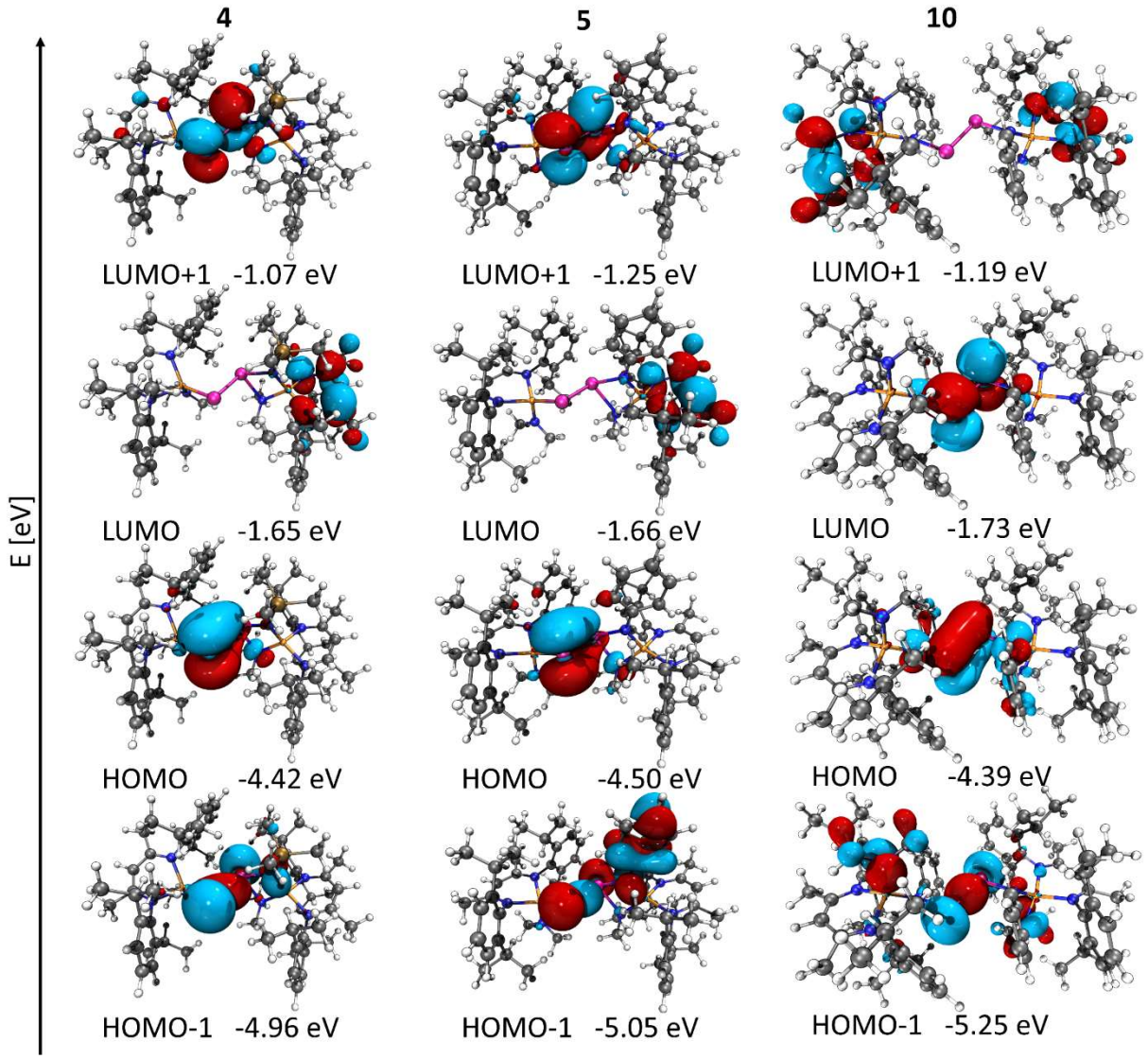

Fig. S 59. Section of the MO diagram of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**) [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**) and [L(Me_2N)GaN(Ph)Sb]$_2$ (**10**), isovalue 0.03.[18]

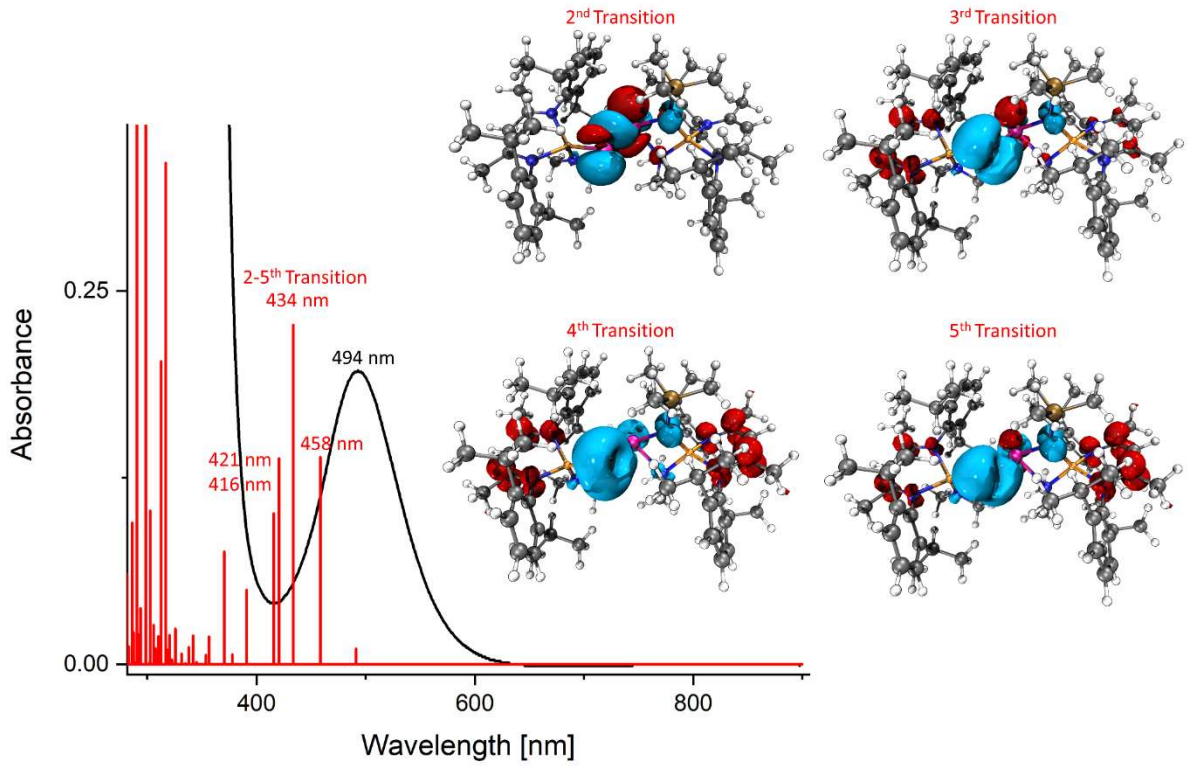

Fig. S 60. UV-Vis spectrum of **4** in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions. [18]

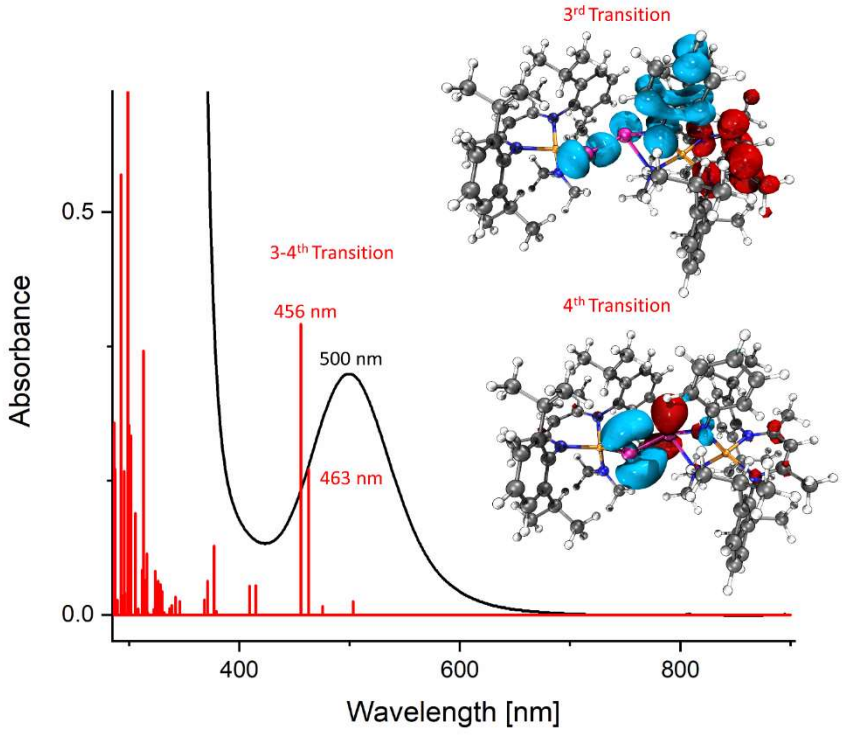

Fig. S 61. UV-Vis spectrum of **5** in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions. [18]

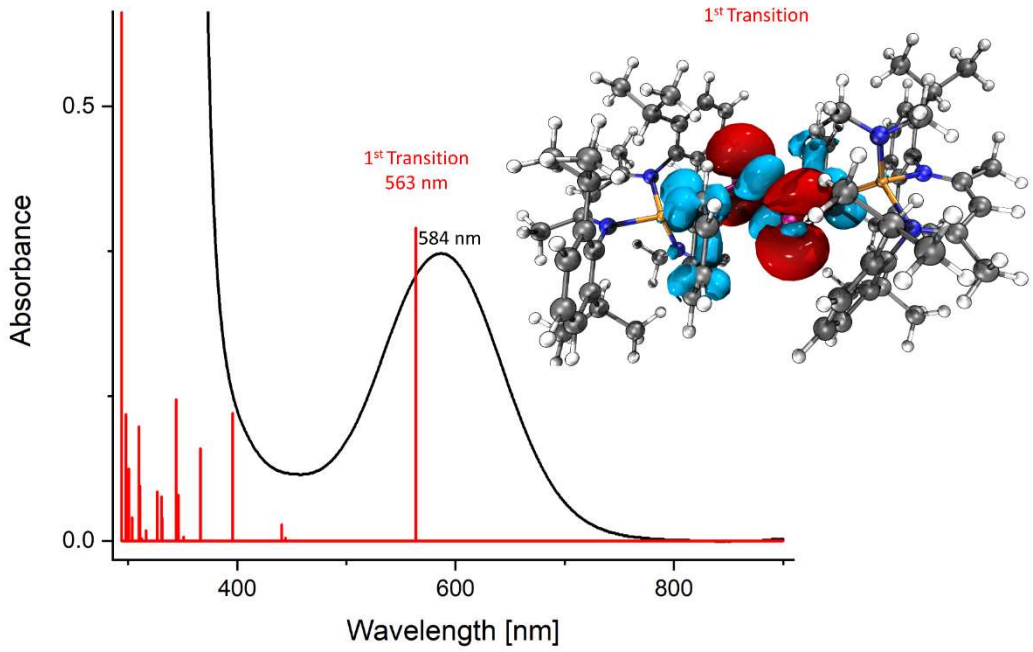

Fig. S 62. UV-Vis spectrum of **10** in toluene (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions. [18]

Table S2. Overview of most intense calculated UV-Vis transitions by TD-DFT for $[L(Me_2N)GaSb]_2$ (**X**),[19] $[L(Me_2N)Ga]SbSb[N(SiMe_3)Ga(NMe_2)L]$ (**4**) $[L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L]$ (**5**) and $[L(Me_2N)GaN(Ph)Sb]_2$ (**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)
4	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 (12.1) HOMO-1 → LUMO+1 (25.7) HOMO → LUMO+1 (33.5) HOMO → LUMO+2 (22.9)
	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)
5	3	21607.6	462.8	0.056/0.018	HOMO-1 → LUMO (85.3) HOMO → LUMO+1 (6.8)
	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_2Sb_2 skeleton of $[L(NMe_2)GaSb]_2$,[19] the N_2Sb_2 skeleton of **10** and the $GaSbSbN_2$ skeleton for **4** and **5.**

	X-Y	r(X-Y)	q(X)/q(Y)	WBI	ON[a]
$[L(Me_2N)GaSb]_2$	Ga2-Sb1	2.60 (2.62)	1.36/ -0.16	0.97	1.96 0.392/0.608
	Ga85-Sb84	2.60 (2.62)	1.38/ -0.16	0.96	1.96 0.390/0.601
	Sb1–Sb84	2.62 (2.65)	-0.16/ -0.16	1.82	σ 1.95 0.502/0.498 π 1.91 0.501/0.499
	Sb1 lone- Sb84 pair				1.94 1.93
10	N6-Sb1	2.07 (2.07)	-1.37/ 0.63	0.59	1.91 0.835/0.165
	N101-Sb96	2.07 (2.07)	-1.37/ 0.63	0.59	1.91 0.835/0.165
	Sb1–Sb96	2.66 (2.67)	0.63/ 0.63	1.66	σ 1.95 0.500/0.500 π 1.93 0.500/0.500
	Sb1 lone- Sb97 pair				1.91 1.91
4	Ga4-Sb2	2.59 (2.58)	1.51/ -0.69	0.93	1.90 0.355/0.645
	Ga3		2.06		
	Sb1-Sb2	2.65 (2.65)	1.08/ -0.69	1.59	σ 1.96 0.460/0.540 π 1.89 0.281/0.719
	Sb1 lone- Sb2 pair				1.89 1.90
	$N10_{(NSiMe3)}$-Sb1	2.08 (2.09)	-1.97/ 1.08	0.49	
	$N11_{(NMe2)}$-Sb1	2.47 (2.47)	-0.96/ 1.08	0.22	
5	Ga4-Sb2	2.60 (2.58)	1.51/ -0.66	0.92	1.90 0.354/0.646
	Ga3		2.03		
	Sb1-Sb2	2.65 (2.68)	1.05/ -0.66	1.60	σ 1.95 0.458/0.542 π 1.89 0.299/0.711
	Sb1 lone- Sb2 pair				1.89 1.90
	$N11_{(NPh)}$-Sb1	2.10 (2.10)	-1.38/ 1.05	0.49	
	$N9_{(NMe2)}$-Sb1	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.

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Table S 4. Calculated X–Y bond lengths (r, Å), X and Y NPA 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 ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|/ G(r_b)$, $H(r_b)$, $\epsilon(r_b)$, atomic units) for the Sb_2C skeleton of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ **11**.

X-Y	r(X-Y)	q(X)	q(Y)	WBI	ON[a]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert/G(r_b)$	$H(r_b)$	ϵ
Sb1-C4	2.18	0.08	-1.39	0.86	1.96 0.322/0.678	0.100	0.067	1.711	-0.043	0.182
Sb20-C4	2.19	0.05	-1.39	0.86	1.95 0.335/0.665	0.098	0.065	1.721	-0.042	0.184
Sb1-Sb20	2.78	0.08	0.05	0.92	1.92 0497/0.503	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 ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|/ G(r_b)$, $H(r_b)$, atomic units) for the Sb_2N skeleton of $[L(Me_2N)GaSb]_2NSiMe_3$ **16**.

X-Y	r(X-Y)	q(X)	q(Y)	WBI	ON[a]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert/G(r_b)$	$H(r_b)$	ϵ
Sb1-N12	2.09	0.26	-1.66	0.67	1.96 0.222/0.778	0.108	0.215	1.451	-0.044	0.045
Sb2-N12	2.08	0.33	-1.66	0.62	1.96 0.222/0.778	0.109	0.228	1.435	-0.044	0.059
Sb1-Sb2	2.75	0.26	0.33	0.94	1.92 0.506/0.494	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) = -40.47512126 E_h
Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.04472448 E_h
Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) = -40.42658194 E_h
Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -40.44874999 E_h

C	-4.05071033961748	0.39299992642979	-0.00000042731542
H	-2.96114749598233	0.39299562860743	-0.00000170451547
H	-4.41389284390358	0.52846495896909	1.01827930610203
H	-4.41389626534567	-0.55658997275859	-0.39182360517330

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

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -117.79442036 E_h
Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.08156021 E_h
Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) = -117.70855551 E_h
Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -117.73647728 E_h

C	-3.81482060044059	0.24686865910214	0.04749258100005
C	-2.78481301377702	-0.83348007109233	-0.06684078621815
C	-2.36498238820619	0.60348039642867	-0.06208729676691
H	-2.72119398021147	-1.37888326726660	-0.99998556261570
H	-2.57204563579027	-1.42837396367047	0.81242619130197
H	-4.30187712360063	0.38596433767511	1.00441618030968
H	-4.45101055526272	0.43563879061289	-0.80801786680060
H	-2.01618399266598	1.03445265103731	-0.99207246912808
H	-1.86692271004509	0.98487246717328	0.82037902891775

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

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -158.31447698 E_h
Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.13199235 E_h
Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) = -158.17574760 E_h
Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -158.21044423 E_h

C	-3.94910935878480		0.35834663911002
C	-2.98813612556477		-0.81823011388092
C	-1.52926568926165		-0.39731896861717
H	-3.18988524827818		-1.40291277911999
H	-3.19216626475811		-1.48870305973654
H	-1.29306385251641		0.24819401872831
H	-0.85991674777867		-1.25949321881538
H	-1.29531239752563		0.16147895447699
C	-5.40798082390052		-0.06255522503813
H	-3.74506577231902		1.02881293051581
H	-3.74736534369838		0.94301170707382
H	-5.64190569620737		-0.62140888147522
H	-6.07731903130752		0.79963028562176
H	-5.64420764809893		-0.70801228884333

Table S9. Cartesian coordinates of NMe_3 [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -174.32639160 E_h
Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.12028765 E_h
Enthalpy (PBE0/D3BJ/def2-(Q)ZVP) = -174.19970764 E_h
Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -174.23341508 E_h

C	-0.40651165977788	0.34330737478268	0.15041806946666
C	1.08884175363941	2.19270785397452	0.00325003603863
C	1.90765406684177	-0.02716872460786	-0.27973337214508
N	0.78873913416882	0.86288726423214	-0.46650169766020
H	-0.64159878111610	-0.64010281766533	-0.26283951628759
H	-1.24941637949699	1.00776287820221	-0.05246006693795
H	-0.31154829050054	0.23823432661460	1.24776489201316
H	0.24684154399438	2.85824436579066	-0.19985450578659

H	1.96486684605010	2.58345177985539	-0.51928341319601
H	1.29629465906253	2.22695799504945	1.08953489114960
H	2.17664960589355	-0.15992044661306	0.78528013925620
H	2.78432929119562	0.36188976193000	-0.80244215461132
H	1.67402821004522	-1.01087161154548	-0.69312330129949

Table S10. Cartesian coordinates of [L'(Me_2N)GaSb]$_2$NMe (L' = HC[C(Me)NPh]$_2$) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -6227.45917169 E_h

Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.80792285 E_h

Enthalpy (PBE0/D3BJ/def2-T(Q)ZVP) = -6226.59371280 E_h

Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -6226.73447620 E_h

Sb	5.27612699586911	7.47744378301105	6.71672333465927
Sb	5.86371835644656	8.71784363643609	4.34039087346502
Ga	4.82886198936814	6.73596018852156	2.93929620423595
Ga	7.00009239621254	8.69238578730382	8.31290113550598
C	3.02539270682472	9.12619842438155	5.43856286005086
N	6.38819809295255	5.54192885137228	2.58225099529264
N	4.75153180838727	7.34325676322830	1.04787065433530
N	6.50432560490392	10.45563257428173	9.06751176350460
N	6.79635143647703	7.75891180259178	10.05806378465813
N	3.30893386189186	5.67447382092783	3.17361905238855
N	8.81882797259454	8.74267885615243	7.93711313775985
N	4.43297908919681	9.17513803092984	5.78811991109446
C	6.78478261840783	5.15801905772599	1.38573703264994
C	6.24988724048456	5.67212658117689	0.19655780538678
H	6.62127067712407	5.22954232570343	-0.71682463361590
C	5.35769132385326	6.73573464092634	0.03807933517271
C	7.86022789997599	4.11802929629102	1.26828749301258
H	7.88642892026899	3.70452634766014	0.26170396965681
H	7.70182243083700	3.31423318210045	1.98929687881519
H	8.83905365593188	4.55187208355998	1.48555216448064
C	5.07673872791548	7.17040124329391	-1.37322441918292
H	5.23520193202061	6.33516081698837	-2.05426522399059
H	5.74754795450752	7.97686799725771	-1.67722779870813
H	4.05578780440964	7.53738637353922	-1.47993194100777
C	7.01733951500988	5.10100095913516	3.77077047474695
C	8.26147442727567	5.60012828573437	4.14517486499869
C	8.78535611361944	5.29951089355511	5.39166601677335
C	6.83743733890234	3.99900109379604	5.90235155350623
C	6.31001404046457	4.29234815431764	4.65420793895945
H	8.79158104357996	6.26315059152868	3.47054797452400
H	5.33044687675667	3.93011357397196	4.36503840965058
C	4.01161680968170	8.53257259397371	0.87728236403923
C	4.59834825628993	9.68670039669261	0.36154340719007
C	3.87543441780052	10.86574115662447	0.28897502277899
H	4.34506802520960	11.75695024841551	-0.11128518453577
C	2.56567803837215	10.91434258582677	0.74537242474425
H	2.00484110491324	11.83995613255776	0.69471620155113
C	1.98679725161858	9.77390453001974	1.28182511059893
H	0.96905020027291	9.80431111635316	1.65345006482542
C	2.70210036634584	8.58871445390679	1.35121536909261
C	5.97769406880996	10.64375918346334	10.26278670697538
C	5.79629183288960	9.61840380376669	11.19989642395479
H	5.32533439021299	9.90999738617343	12.12767701139170
C	6.21775612004862	8.28875878743543	11.12398099649029
C	5.53346212514693	12.01788454490274	10.67633100609854
H	5.15536185516419	12.58259748229503	9.82399215217175

H	6.36379567724217	12.58626035783525	11.10103134505522
H	4.75769300331814	11.94266890609789	11.43728033687350
C	6.01384040741290	7.43550203582912	12.34219331509262
H	6.93709927459287	6.91447429230546	12.60405581227847
H	5.26186188496184	6.66566174845139	12.15612596642307
H	5.69077924917183	8.04023596931903	13.18687034870927
C	6.83781603410363	11.53934315298199	8.21823956454291
C	7.80069941938956	12.47255724057699	8.59308225904267
C	8.16713989839599	13.48299451245605	7.71926673569391
H	8.91954786858660	14.20351602958401	8.01919317518351
C	7.58926107992158	13.56155105851869	6.45985064342883
H	7.88370605780242	14.34738589483561	5.77417843818430
C	6.64408758573243	12.61974705851532	6.08133160597649
H	6.19336965107515	12.66416581615055	5.09631840779458
C	6.26615204494324	11.60855143871997	6.95195601336985
C	7.16736851231223	6.39291316185761	10.03843095495684
C	8.51062069364578	6.03655493973084	10.11040911416824
C	8.87952423635096	4.70126217725550	10.06064438764286
H	9.92774852857185	4.43347568730974	10.12841783995804
C	7.91711880514122	3.71134592748663	9.91795644111965
H	8.20919243290695	2.66862202684694	9.87638099408793
C	6.58028318905511	4.06623244391057	9.81137728243217
H	5.82233958206760	3.30228240229739	9.68126532642709
C	6.20636486247085	5.39979038006539	9.86622030025909
C	2.72156773722163	5.34558745792920	4.44066311107628
H	1.62354785376129	5.29390657034314	4.37179398324023
H	2.97384087937304	6.08760157763616	5.19949253352613
H	3.05653696029767	4.36636873086502	4.82921837963916
C	3.05143103360569	4.66244287359502	2.18519330383572
H	3.46990150271285	4.94275320962608	1.21531906498306
H	1.97007547235654	4.50903439974982	2.04542682024236
H	3.47662028264035	3.67781029099621	2.45413091621501
C	9.35709036773079	8.69131020744266	6.60986696033889
H	9.60645837984464	9.69011959455434	6.21147045124864
H	8.64215411913069	8.23399132505922	5.92315778286687
H	10.28388214674088	8.09444388996076	6.57533939617430
C	9.71656858795027	9.34658125214636	8.87774218631255
H	10.00111426107400	10.37642418170967	8.59984410553051
H	10.65497033609231	8.77349037544675	8.96731215915753
H	9.26714782606402	9.39149256342159	9.87483681529890
H	2.78694197815914	9.96363495986776	4.77204224602754
H	2.41543559522073	9.23625995196396	6.34309080121950
H	2.70229969173039	8.20902193467638	4.92595498562763
H	5.63410075576789	9.65963634544977	0.04448813406911
H	2.26825935644503	7.69478899682028	1.78626731480136
C	8.07152423487570	4.50687294336185	6.27911464071255
H	9.74080999224181	5.71616967066073	5.68631988231815
H	8.46376725976884	4.30460224595992	7.26775385100702
H	6.26904700564765	3.38995425985484	6.59558002081761
H	8.27722347521233	12.38612910345924	9.56257865322715
H	5.52130992959965	10.87077065216337	6.65244368405403
H	9.25561375377441	6.81656099602081	10.20401328207278
H	5.16479353053882	5.68431436051213	9.76778724551089

Table S11. Cartesian coordinates of $[L'(Me_2N)GaSb(NMe_2)]_2$ (L' = HC[C(Me)NPh]$_2$) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -6401.81836228 E_h

Zero-point correction (PBE0/D3BJ/def2-T(Q)ZVP) = 0.92898205 E_h

Enthalphy (PBE0/D3BJ/def2-T(Q)ZVP) = -6400.82470381 E_h

Gibbs free energy (PBE0/D3BJ/def2-T(Q)ZVP) = -6400.97889769 E_h

Sb	-2.35105783269888	6.95307174674977	0.23409846369268
Ga	-1.77068631048936	7.07931925918134	2.78873738732842
N	-2.92019110722581	8.56489592096323	3.45474560015187
N	-2.47821911827704	5.78204568819245	4.10957457371875
N	0.00858902771638	7.38889594268786	3.26812220286277
C	-3.64302491273823	8.53117417045917	4.55387690837374
C	-3.74347842555217	7.39653515236671	5.37086462983685
H	-4.31618361849783	7.52131998373697	6.27856148928390
C	-3.23707401964307	6.11566868165774	5.14679204461956
C	-4.39484880191607	9.75649735474433	4.98528448152905
H	-3.79602083822695	10.65568221059519	4.83255977553871
H	-4.67807488346793	9.68154787582141	6.03371105654839
H	-5.30548712023007	9.87445987012759	4.39359163269589
C	-3.57571080311832	5.07315668495408	6.17491675558923
H	-4.39785442161123	4.43975717460539	5.83556560697715
H	-3.87938730537926	5.55034753397592	7.10503688805165
H	-2.72439308120864	4.41762804150672	6.36337467778472
C	-2.89991048018972	9.69284093259282	2.60152801588486
C	-4.00383389577115	10.02167222737280	1.81971403407163
C	-3.92450415660098	11.06540049352837	0.91285171990807
H	-4.78653627143278	11.30890341742283	0.30228272284984
C	-2.74403081442165	11.78135378402924	0.76751967162564
H	-2.68393328694684	12.59310120408683	0.05184305951652
C	-1.63935769377649	11.44536266311250	1.53518973184722
H	-0.71027160160942	11.99205822423500	1.42233159643209
C	-1.71371425794990	10.40384976476703	2.44750507570482
C	-2.11920635225631	4.42969259500668	3.88304079557290
C	-3.08019195604201	3.47508374875060	3.55831328107333
C	-2.70501456216375	2.17255750470585	3.27822222648737
H	-3.46126364045739	1.44327063805943	3.01233362418206
C	-1.36693537332063	1.80806391846612	3.30829698405302
H	-1.07372231210844	0.79229243954522	3.07199933056474
C	-0.40723535957747	2.75810218126759	3.61938096880274
H	0.64198254910422	2.48694534117485	3.63328582137528
C	-0.77730379740739	4.06379521780307	3.90461633790901
C	0.98784201361591	7.85532277691295	2.32999968416726
H	1.15625118924948	8.94623905428719	2.38885935844011
H	0.68489491910041	7.62757196745895	1.30448862149328
H	1.96704269211108	7.37877532879966	2.49561337945367
C	0.35341481110822	7.68770933271360	4.62777678417986
H	1.31687843526927	7.23423338911032	4.91234940517792
H	-0.40495561376797	7.30404183250357	5.31613016605620
H	0.45131154677342	8.77219755028486	4.82146837216066
Sb	-1.65535250573210	4.19943724521669	-0.11560343312037
Ga	-2.29204219410357	4.27050795326847	-2.66260057711513
N	-1.42682059168607	2.72415234316422	-3.58937989875013
N	-1.45033561459005	5.60265457714608	-3.85746085913385
N	-4.11321361314461	4.26836371760510	-3.07853301943663
C	-0.79237456146145	2.79521394383099	-4.74364296498614
C	-0.54001438431759	4.00113673755819	-5.40707997428051
H	-0.04886769836946	3.91560671109933	-6.36555465334357
C	-0.80388394975750	5.30358111120087	-4.97525831179837
C	-0.31690521820664	1.53846419409464	-5.41446448910740
H	-1.02711951832622	0.72351366983087	-5.26971800034398
H	-0.17489311746433	1.71164721250387	-6.48000253725294
H	0.63818455593270	1.21248160176617	-4.99651520603721

C	-0.32437744625382	6.41771073706669	-5.86060833081329
H	-1.09509926275563	7.18183789229279	-5.97568851926583
H	0.54565641676262	6.91199203132807	-5.42346043875724
H	-0.04510492476597	6.03216488974410	-6.83917939713856
C	-1.56327488236474	1.50781550918671	-2.88537485657180
C	-0.45716860354392	0.85323117386695	-2.34979825514556
C	-0.62586788613056	-0.28361508515599	-1.57707997689577
H	0.24264530101551	-0.78062493969620	-1.16043484730332
C	-1.89839556426656	-0.77358566767805	-1.31937588343117
H	-2.02811547765075	-1.65840864314515	-0.70766468689127
C	-3.00252792088360	-0.11730577446807	-1.84192457268338
H	-4.00128587338570	-0.48786007722678	-1.64198576767083
C	-2.83891201548520	1.01831951531824	-2.61951531164090
C	-1.57642104749778	6.95963903769726	-3.45714009826411
C	-0.48191057664620	7.64954564244931	-2.94551037075929
C	-0.62061338664082	8.96260629173320	-2.52870372677568
H	0.23279101302716	9.48577034909005	-2.11353910406253
C	-1.85211672859406	9.59555005908160	-2.60974852139770
H	-1.96356631792704	10.61543709834151	-2.26225240248018
C	-2.94706214974322	8.90224688657946	-3.10110829574475
H	-3.91650726167491	9.38442305307205	-3.15248423024537
C	-2.81609540295583	7.58552253511303	-3.51757702545277
C	-5.11951064864857	3.84773486404491	-2.15083080708726
H	-5.45308292744065	2.80549479402418	-2.31227102667517
H	-4.75267984010151	3.91218661212570	-1.12267204024982
H	-6.02351915819358	4.47385037869324	-2.21447158705697
C	-4.54020242266656	4.16535117850824	-4.44397059375927
H	-5.43796869299043	4.77512433909756	-4.63502020475346
H	-3.75795884292442	4.51235507102914	-5.12483727941134
H	-4.79681589523369	3.13126274746029	-4.74139489802690
H	-3.67031646015346	7.02416273970567	-3.87667103973421
H	-4.89786591170684	9.41609727037509	1.89300311755857
H	-0.85242721229370	10.12089174394092	3.04127613987365
H	0.46800850734157	7.13752207404533	-2.84765877138504
H	-3.69534456961299	1.54413611162611	-3.02421415785715
H	0.53268278146574	1.25897745438062	-2.52089432629868
H	-0.03461141342064	4.82041864471837	4.12769474314930
H	-4.12185543897992	3.76684123715269	3.50223565947431
N	0.30780105104273	4.88528588200178	-0.35432096432814
C	1.08337856128216	4.70776537869874	0.85291342707968
H	1.32439785132160	3.65241939450560	1.07198977727648
H	0.55725174711686	5.11782106093611	1.71666909408614
H	2.03412976103885	5.24863684397108	0.75899664784817
C	1.04112260757052	4.39423193665282	-1.49427839540707
H	1.27597739155506	3.31576439132095	-1.44155125160425
H	2.00225241469546	4.92285831460725	-1.56455541818587
H	0.49627574047377	4.57229218658161	-2.42207975418070
N	-4.37617071840366	6.95769592128816	0.62589887130430
C	-5.19763292351502	7.30189765058136	-0.50963122533217
C	-4.95343350947173	5.91916374990055	1.43395805173085
H	-5.00587273142602	4.93582856709348	0.93400965131357
H	-4.37757248707173	5.79160156500345	2.35142871294651
H	-5.98066907678026	6.19042458600553	1.71741621203855
H	-4.77834992636618	8.16859554891977	-1.02502749772773
H	-6.20658515753240	7.57160849226416	-0.16684163345422
H	-5.30631719834821	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 E_h
Zero-point correction (PBE0/D3BJ/def2- S(TZ)VP)			= 0.00576230 E_h
Enthalpy (PBE0/D3BJ/def2- S(TZ)VP)			= -109.30654060 E_h
Gibbs free energy (PBE0/D3BJ/def2- S(TZ)VP)			= -109.32893667 E_h
N	-1.45315231394315	1.04391077658411	0.00000000000000
N	-0.35621768605685	1.00295922341589	0.00000000000000

Table S13. Cartesian coordinates of [L(Me_2N)GaSb]$_2N_3$-Ph (**14'**) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP)			= -7467.92091380 E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP)			= 1.55198463 E_h
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP)			= -7466.27390470 E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP)			= -7466.48156992 E_h
Sb	-3.63075078361640	6.64557708400430	22.81680007525725
Sb	-3.37849563752933	4.72314938831901	24.75851742803625
Ga	-1.37460782513996	6.14283623501224	21.55987568807229
Ga	-5.67267415594724	5.17339309408900	25.96384020321803
N	-1.16001093887431	4.24753043200133	20.96257574854394
N	-1.63431958411928	6.80278865022652	19.69377388394914
N	-5.74535460468068	3.80367068672687	27.40700220721533
N	-5.99336103540511	6.67834350696393	27.23188364865344
N	0.29293871763483	6.72819525459886	22.14467080598133
N	-7.22736585539554	4.96966951321858	24.93787365511022
N	-2.75873452251918	7.90515598026993	24.34554491710905
C	-0.60845866158335	3.97386113598100	19.78414005148816
C	-0.48368043146514	4.91218926632183	18.74439614504704
H	0.01890680395403	4.55889375504958	17.84470413267658
C	-1.04793050991395	6.19811881052929	18.66658049552877
C	-0.05005572155684	2.60132984525886	19.52054578348134
H	-0.11695413919617	2.34113311104725	18.45674643863476
H	-0.54388679637928	1.82814451141219	20.12114216427624
H	1.01657972870001	2.60218373029336	19.79854411385280
C	-0.95249203898070	6.90896630418635	17.34517436563345
H	-0.74919514298334	6.20486501211797	16.52941603019568
H	-0.12901147992055	7.63904168804837	17.38436491995091
H	-1.86669462069988	7.47481638697250	17.12226374723104
C	-1.56432066123192	3.19626039822619	21.83982645664982
C	-0.75656991450412	2.79769753971669	22.92432430856692
C	-1.22254640233611	1.77735168746316	23.76073318548351
H	-0.60926286562618	1.46160174012545	24.60789368366285
C	-2.45477912197290	1.17387249779606	23.55272258809663
H	-2.80963741133036	0.39949667505617	24.23484144071255
C	-3.24993551893155	1.58942234461806	22.49107756685897
H	-4.22560916576080	1.12314771602554	22.33842446962248
C	-2.82875642971464	2.60026666422004	21.62337533024400
C	0.59411556194278	3.42540157785751	23.20393897331871
H	0.70282839636318	4.28764423377941	22.53089302839499
C	1.73145221701512	2.44397570442198	22.91713151105922
H	1.69087952671716	2.06232012449941	21.88657232918314
H	1.68648018288749	1.57423511822982	23.59249330377273
H	2.70890787120410	2.93042753220764	23.06226641985064
C	0.68289466983548	3.95389377068578	24.63456964821167
H	1.64899745781472	4.45400600114231	24.80039165161163

H	0.60381726614620	3.14118840196001	25.37382331429463
H	-0.11447461302051	4.68022911342877	24.85004928811966
C	-3.71498845910072	3.01371068528967	20.46320393036214
H	-3.33011823124663	3.97313672103506	20.08621010494865
C	-3.63810745539278	2.00773162721553	19.31331350597360
H	-4.26264623971008	2.33668050629426	18.46778512966027
H	-3.99828218514220	1.01741989939654	19.63556497139226
H	-2.61091627137047	1.88480441826782	18.94390371816742
C	-5.16289510742392	3.23242743746273	20.88851091443333
H	-5.75977897813318	3.60490715437978	20.04251592833031
H	-5.23585768723423	3.96451002806099	21.70506067825774
H	-5.63893046632263	2.30274346654060	21.23605301258431
C	-2.34386057513583	8.02871751739577	19.52068655494232
C	-1.66824786145504	9.26501534409610	19.57961871226465
C	-2.41141501275861	10.44002690443259	19.42749090634309
H	-1.89610136774006	11.40232192937872	19.47351731685779
C	-3.78483704543755	10.40586297514118	19.23746762250362
H	-4.34864559882643	11.33468262352754	19.12123886977960
C	-4.44501255807328	9.18175044557040	19.20815346596462
H	-5.52726889905028	9.16323254044974	19.07413415200151
C	-3.74931821746724	7.97826728094743	19.34845796679288
C	-0.17781021986790	9.36964555943961	19.82888846938241
H	0.22336195941783	8.34816981207558	19.86728080338391
C	0.54468746751955	10.12493538897317	18.71281435661841
H	0.34307638757933	9.69397698258698	17.72047227802144
H	1.63304507470608	10.10389297536206	18.87897805425176
H	0.23949326312310	11.18273402271880	18.67828472375463
C	0.09572848144657	10.01775671030024	21.18520709407103
H	-0.24711001355953	11.06378619122939	21.20641634387378
H	1.17467557063505	10.01233359104078	21.40545246101153
H	-0.42132758720154	9.48402790989994	21.99329746794293
C	-4.49410784065076	6.65563956280063	19.30054079199739
H	-3.97796585236409	5.98029449477692	20.00451696113674
C	-4.41730172655153	5.99431292984126	17.92274166849891
H	-4.99430413431582	5.05608473246137	17.91630939073091
H	-3.38646683093302	5.74584940532287	17.63806467313505
H	-4.83836887840844	6.65509040211880	17.14827308926768
C	-5.94709471394073	6.77092823354769	19.75141748673092
H	-6.56124181765648	7.31378241934784	19.01604096542690
H	-6.03215296239910	7.28616736601539	20.71971764639180
H	-6.38894688774649	5.77070925978922	19.86395948418446
C	-6.53537396517729	3.97563044951352	28.46133952052400
C	-7.12841518714490	5.20837660796762	28.78123658998897
H	-7.82852870023216	5.19919821215794	29.61563768349690
C	-6.81847920347683	6.47733278162923	28.25679267478750
C	-6.82587702611837	2.80679133443671	29.36053681359681
H	-7.41850752743123	2.05337118448542	28.82004484201817
H	-7.38027824927551	3.12040151671266	30.25280830435040
H	-5.89653786443742	2.30738151442754	29.66896987109176
C	-7.51158370394159	7.64848909364570	28.90145326242985

H	-6.93423611877661	8.57649168864510	28.81599948339519
H	-7.73539295604746	7.44977634071993	29.95691059826376
H	-8.47019203259391	7.80465102785932	28.38066209352361
C	-5.02757095367543	2.58394459338898	27.23708273715809
C	-5.62066373767827	1.48700703350472	26.58046899631240
C	-4.89015249215615	0.29875067495941	26.47467654565073
H	-5.34407764944808	-0.56330103311088	25.97923426719117
C	-3.59977339532708	0.19940777924866	26.97779787689829
H	-3.04761158759402	-0.74004088099287	26.89458097575141
C	-3.00177916721714	1.31044873255758	27.56346535498580
H	-1.97292646073335	1.24062442486618	27.92033354038666
C	-3.69081345358610	2.51842103610598	27.69479072892376
C	-6.98671327757795	1.58128993760934	25.93239908190204
H	-7.42103408776207	2.55010166335408	26.21391073429195
C	-7.94235182589565	0.47976881738225	26.38656632086259
H	-8.94051850563189	0.63355439204404	25.94796177369185
H	-8.05414811716609	0.45828478433815	27.48137248126295
H	-7.59645902726075	-0.51759188817124	26.07191142282095
C	-6.83621652241352	1.58561334628066	24.41039279077688
H	-6.42649084207578	0.62763573623178	24.05043396674940
H	-6.15969077227289	2.38891798721065	24.08612257669102
H	-7.81013673660031	1.74370457092960	23.92154673073780
C	-3.01143249821878	3.73152020966206	28.30150177021250
H	-3.44116894191884	4.61645873477953	27.80309158398251
C	-3.30656963264329	3.87258909933444	29.79582278107018
H	-4.37423708031990	4.04047783729371	29.99340854490039
H	-2.75723577133670	4.72974469763299	30.21442448195426
H	-2.99172077618025	2.96934624339787	30.34290770855248
C	-1.50889495019969	3.76722144561376	28.04329464777179
H	-1.28031989544296	3.58276663347403	26.98343368849629
H	-0.96712779874867	3.02344862313360	28.64948894975792
H	-1.11226005662088	4.76072422149408	28.29406163060914
C	-5.46711899471751	7.98563227671332	26.98185724160130
C	-6.04066795500983	8.82474698351940	26.00435455438762
C	-5.49021316621374	10.09688859112902	25.81313085972289
H	-5.92258995865522	10.75771168753261	25.05862529257673
C	-4.40574807222245	10.53469807373224	26.55746109856776
H	-3.98105613433387	11.52469985552755	26.37849226512664
C	-3.83795984494422	9.68942120271350	27.50350151361899
H	-2.96568059651717	10.02708466421887	28.06510812577149
C	-4.34178295383767	8.40741546522707	27.73136629914269
C	-7.26098197265665	8.42869369925913	25.19418133578809
H	-7.45425561954268	7.36186758039913	25.37864737129267
C	-8.49375751493900	9.22404985686037	25.62907830727151
H	-8.36491723164105	10.29863109624754	25.42146375360567
H	-8.68952264720445	9.12003354682746	26.70547813065311
H	-9.38835414968662	8.88154613779507	25.08512775956600
C	-7.02758497302425	8.59511764417783	23.69377858447870
H	-6.16953922060665	7.99680109268613	23.35246932082190
H	-6.83015763396059	9.64470054260359	23.42424454591449

H	-7.91328332394677	8.27040395710379	23.12647441414674
C	-3.68352834767494	7.50709159625259	28.76403843272386
H	-3.85999448214236	6.47321990128586	28.43157800370817
C	-4.30575698669616	7.66447222913968	30.15421980970537
H	-5.35822101830952	7.35833552376716	30.18535373478600
H	-4.24571201694681	8.71229719191778	30.49044503019484
H	-3.76411986380596	7.04470218473764	30.88592006166148
C	-2.17310137259410	7.70834171328817	28.86087161039436
H	-1.69625629436252	7.65288447920052	27.87443903340320
H	-1.73550187960637	6.92458777902048	29.49845995311473
H	-1.91929287746648	8.67391551287441	29.32709952445845
C	1.46219429182444	6.55742989533008	21.33321241453845
H	1.21078407418609	6.17620637825227	20.33191280096284
H	2.19038351084848	5.84198307266106	21.77829943746944
H	2.01731221968549	7.50973772978584	21.19282256938996
C	0.59388315354969	7.26310576918601	23.44016752923083
H	1.00220756976748	8.29370091903722	23.38824613507710
H	1.34961366065985	6.65375704387239	23.97662709193004
H	-0.29867603680558	7.29818769400191	24.07551942326281
C	-8.53230699723824	4.88327232249812	25.52429376244807
H	-9.15817344621317	5.78195317375574	25.31964816378365
H	-8.47859044833770	4.77166904540015	26.61702917044742
H	-9.10692037611792	4.01559432298552	25.13315401139593
C	-7.27190571320989	5.04577721331011	23.51016503909595
H	-6.26462832107735	5.18970837193304	23.09229092389233
H	-7.89111002406048	5.89305359578375	23.14697393461575
H	-7.69476719048646	4.12913663206518	23.04604656802414
C	-2.50321341209250	9.26512103020943	24.09358326581147
C	-1.54364500349694	9.98105571285617	24.82830486717009
H	-0.98662517703452	9.46511961814455	25.60926326661736
C	-1.32740655123083	11.32926794084804	24.57010887956016
H	-0.57635355910136	11.86723088787518	25.15429017900001
C	-2.05023513132504	11.99572199838853	23.57922769876706
H	-1.87525466357228	13.05562636668146	23.38224037736621
C	-2.98875257526473	11.28231348466914	22.83766832501897
H	-3.56043407623762	11.77464406005248	22.04813626182208
C	-3.21322919961551	9.93123150215265	23.08570610326441
H	-3.96270295197710	9.39498299654059	22.49874773481312
N	-2.27773570274604	7.42093863224259	25.47424650429251
N	-2.35561460334827	6.26887063932683	25.87586734666686

Table S14. Cartesian coordinates of [L(Me_2N)GaSb]$_2$$N_3$-$SiMe_3$ (**14″**) [Å] for the optimized geometry.

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) = -7643.83904761 E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7644.05042820 E_h

Sb	6.48581833207110	9.20079692367861	5.74094143264128
Sb	4.51643084778682	7.34264099875682	5.32955992367486
Ga	4.85814649411502	6.46300165664748	2.84003170463874
Ga	7.32738300115150	9.05899556491670	8.29397479541373
Si	1.46871965996984	9.02313838434812	5.24344694171817

N	6.75704976116523	6.12389170972828	2.30680958536420
N	4.39463045494293	7.25322526214653	1.06794832579181
N	7.73380330058116	10.89697586096651	8.93847434760402
N	6.40110738079190	8.46235733948329	9.95299102405900
N	3.95912959356762	4.80277376228875	2.82901523742537
N	8.86657319205883	7.96838256944060	8.09481777998427
N	3.25935834958830	9.11309026449859	5.31477008795246
C	7.00442783369833	5.74688336630375	1.04896810361793
C	6.17802054319846	6.06730373376041	-0.03628345620835
H	6.52502380378131	5.73658246801665	-1.01401963897568
C	5.03792272362976	6.89023975829032	-0.03575230548412
C	8.24091976025994	4.94234650728535	0.74825825722718
H	8.32384502186380	4.73555656355586	-0.32522374172644
H	8.19210227232660	3.98802104441619	1.29387404877841
H	9.15558879495673	5.44483701826606	1.08925048455008
C	4.54796467324540	7.35988551261082	-1.37804063467213
H	5.34019464454929	7.26908471483816	-2.13062668817229
H	4.20474082476944	8.40210719810105	-1.33454964629442
H	3.69045828379150	6.75493576405611	-1.70730308153794
C	7.86306070047995	6.07083761989599	3.20934442206164
C	8.81735595333225	7.11743397578638	3.15108766578784
C	10.00658154897027	6.96617557790839	3.86719105055698
H	10.76324127954708	7.75112822517430	3.81984352973210
C	10.24429186536410	5.83761557735367	4.64587551074948
H	11.18519100874483	5.73661413688695	5.19147286651194
C	9.25928089961540	4.86918164027037	4.76590192755601
H	9.42588591088980	4.00985506753573	5.42028201706067
C	8.05074240525068	4.96921053372590	4.06696007642466
C	8.57625323290708	8.37917662633815	2.33426246901186
H	7.48351271301248	8.52134289027108	2.30207058211700
C	9.19067458964592	9.61729873677651	2.98466819789566
H	8.81035785544734	10.52702494239772	2.49514795805801
H	10.28736719389008	9.63142718597422	2.88275455295875
H	8.93939940665010	9.68055601433463	4.05243372702007
C	9.07641405402946	8.27972491254313	0.88986450159185
H	8.51911850776787	7.54636436173510	0.29419601393587
H	10.14473156195021	8.00979123774053	0.86561612206631
H	8.96718128910701	9.25362957893470	0.38766277162499
C	6.99636721843942	3.89687723438747	4.26227778907210
H	6.13697231098479	4.14769055704812	3.62263471484679
C	6.50354440104375	3.89529303827061	5.71105168610255
H	6.09457289352014	4.87713409946734	5.99808277216652
H	7.31612728962709	3.66256592869759	6.41746762659271
H	5.70936639851225	3.14648144496595	5.85271306662515
C	7.48973324364954	2.50955391103532	3.85305436589697
H	7.82308403696691	2.48958451763740	2.80454499562525
H	6.68368093296381	1.76736554444218	3.96196775008163
H	8.33513927594956	2.17714330440447	4.47656919317914
C	3.26499791163759	8.11668357940449	0.97093315726548
C	3.43307126253503	9.47693744300015	1.31753625163296

C	2.33120110648821	10.32756775068017	1.20589063240291
H	2.44271237958613	11.38318972162239	1.45616415482815
C	1.09255595080699	9.85340380616294	0.78472759962851
H	0.24217966396003	10.53533403758583	0.71148385480313
C	0.94003723084643	8.51116480345349	0.46862499240270
H	-0.03758605549666	8.14100831785531	0.15122206358596
C	2.01400280581818	7.61728626890048	0.54837487319700
C	4.78278934438176	10.00633651279856	1.76735235030084
H	5.20842349951706	9.25121421443843	2.45385676435729
C	5.75546209425059	10.17009080149165	0.59636374423634
H	5.99957069888062	9.21717246983903	0.10951224137744
H	6.70131545057928	10.60792172063500	0.95062637794937
H	5.33515959167182	10.84904437509316	-0.16293332200948
C	4.69178777289130	11.31539868964288	2.53959741645971
H	4.41833042935388	12.15689971591422	1.88286023792029
H	5.67162634142301	11.55059038407029	2.97755680338367
H	3.96631598924853	11.26398492065908	3.36189249076705
C	1.78026469395388	6.15886253228712	0.19557966156905
H	2.75916187344133	5.66173074371571	0.15515856307505
C	1.10570645405130	5.99519348341764	-1.16766307174135
H	1.62523191704552	6.55270846019269	-1.96178770101540
H	0.06350042562225	6.35038124802581	-1.14890806433441
H	1.08095353046278	4.93284227357411	-1.45555824884554
C	0.97184902218804	5.44651047753836	1.27932741120042
H	-0.00570023377049	5.93101191397731	1.43175666092803
H	1.51786221061229	5.45024013485389	2.23085836142755
H	0.78840253247335	4.39894096646944	0.99308107313617
C	6.99513940651407	11.44199774893208	9.90706536279364
C	6.05797150018069	10.74187582151779	10.68004176456864
H	5.52811995577901	11.33589309295865	11.42306843337793
C	5.91912808597550	9.35094219314639	10.81572145764271
C	7.22644329898500	12.87649992502837	10.29644923126291
H	7.21423812122150	13.54178611494224	9.42704178101696
H	8.22274919454584	12.98748342759856	10.74933212936590
H	6.47321127466115	13.20802856060547	11.02043229449202
C	5.25460972307030	8.89419364046250	12.08703772005702
H	4.87994272515014	7.86679512104875	12.03183915416440
H	4.43071335228987	9.57386197565681	12.34340315464150
H	5.98562499671676	8.94268537007057	12.90847174288600
C	8.80864477852696	11.68955805809685	8.41715742897255
C	10.09260008269061	11.54488080086892	8.99582235888460
C	11.11094524045094	12.40187248783252	8.57142903100866
H	12.10540372708109	12.31050818643431	9.01005864439367
C	10.88557730984318	13.36752825303725	7.59639274245245
H	11.69455959260071	14.03337125033677	7.28655269332361
C	9.63582298563727	13.46219749820882	7.00373394429577
H	9.46687244599758	14.20098660816900	6.21676331146061
C	8.57930911524280	12.62800489526074	7.38812619602719
C	10.38366849469991	10.47848749073079	10.04061987679827
H	9.75343848467634	9.60765323311649	9.79548421276912

C	10.02386715056533	10.92643518259495	11.45920043796570
H	10.54078536717752	11.86409664673958	11.72069868787310
H	10.33159707481371	10.16117619503467	12.18875447668187
H	8.94378606100794	11.07969250711242	11.58784738885325
C	11.83420730749075	10.00387875505044	9.99637873497443
H	12.13969884601955	9.72722612505256	8.97673834117772
H	11.95956466496945	9.11872386231666	10.63533157833105
H	12.53295707099876	10.77047997241337	10.36733419844599
C	7.25653801545248	12.75728518355530	6.65711155183363
H	6.58674634967850	11.95479899165096	6.99865773063436
C	6.53293761143452	14.08182894295455	6.90863455702276
H	7.14930520987100	14.94121417290097	6.59830429852307
H	6.25691388750514	14.22891294449112	7.96161619286388
H	5.60078563468108	14.10477536609042	6.32415035682339
C	7.45646163754941	12.58747262614846	5.15068747366877
H	6.47639811051904	12.49635272905946	4.66193939342377
H	8.04105970703781	11.68782797966555	4.91280650115301
H	7.97770315918988	13.45359168884167	4.71250679967952
C	6.41570323207636	7.08125950353747	10.32914590250816
C	7.45773445011963	6.60253780467092	11.15092972214032
C	7.47407153455271	5.24427640022486	11.48479331648574
H	8.28051288540322	4.86105820517737	12.11461701990541
C	6.49129770428786	4.37980659442177	11.02979473303633
H	6.52074966109424	3.32082173039429	11.29682917714414
C	5.46285643110989	4.86821054041917	10.23140687586751
H	4.69350552957655	4.17939599916617	9.88411298762846
C	5.39559886555513	6.21594395363766	9.86606989333170
C	8.56570012783220	7.48524298601868	11.69262997338961
H	8.38870843312811	8.50991183596602	11.33535377448818
C	8.56392528877437	7.51229030239776	13.22275948354395
H	9.30365904320871	8.23820105125993	13.59495538965425
H	8.82904533935132	6.52853922202277	13.64129819427882
H	7.58142994543834	7.78801828237307	13.63281907978330
C	9.92936995937137	7.04531914144679	11.16177134584938
H	9.96226945542484	7.16741694359776	10.06914833193957
H	10.13899670113772	5.99446659648037	11.41605082106946
H	10.72796032091522	7.65562437796777	11.61026537889333
C	4.24756890714654	6.71450866208402	9.00345229616191
H	4.69617662924992	7.33221722475783	8.20271705113223
C	3.26029108728318	7.60593579757610	9.76175821571555
H	2.39926580736355	7.83580826732624	9.11925029392626
H	3.69765749234592	8.56594769600170	10.05840916778319
H	2.88096604625949	7.09892331468432	10.66345849104833
C	3.47551797591231	5.58368994097671	8.33231546377309
H	2.74757046663345	6.00141101486587	7.62298537062305
H	2.91459826650103	4.98607481057138	9.06885339183467
H	4.13237544172582	4.90999179635134	7.76321053022786
C	3.30871636473768	4.19890154446062	3.95407146571600
H	2.28054198188781	3.85723214777499	3.70659336045755
H	3.22446928736073	4.90000066747667	4.79852472442962

H	3.84825479386048	3.30262679571185	4.33207118742382
C	4.12968341138453	3.86527834913543	1.75613708064194
H	4.56069150874669	4.34040653250982	0.86395302048152
H	3.16498468595325	3.40618759443234	1.45396222195387
H	4.80153991121067	3.01863931124588	2.02653250762832
C	8.53044202092527	6.61486368496761	7.71932976893096
H	8.12449900584466	6.52817341622318	6.68638888993877
H	7.79042526814636	6.17625489873372	8.40460647517113
H	9.42669509297062	5.96421252825504	7.74808582853345
C	9.87972799846651	8.48887359762124	7.20914019310843
H	9.58500883768844	8.46987298536978	6.13733946693054
H	10.80913672098172	7.88854322052850	7.28180029411942
H	10.13922147398022	9.52839688013974	7.45433252917691
C	0.77991511071881	8.73075274074776	6.96544162239157
H	-0.32162757807517	8.75933075421128	6.95423904702333
H	1.13562364822600	9.50393742882566	7.66378171201348
H	1.08701516745249	7.74766919190684	7.35295164387712
C	1.05995006240954	7.58001832569708	4.13219011685169
H	-0.03111348000510	7.48614443991554	4.01282113696106
H	1.43327520155112	6.62546634442822	4.53415860879153
H	1.49487804935528	7.72825851249381	3.13366129875800
C	0.80996028287429	10.63660143876657	4.56643738736772
H	1.21257188243139	10.82298498298366	3.56112898729859
H	1.09974785040365	11.47294250541608	5.21919109782965
H	-0.28923186633766	10.60520320996599	4.49845017571373
N	3.71681520537888	10.29168341851994	5.69577435869884
N	4.86406689160552	10.61854679377496	5.94693861185590

Table S15. Cartesian coordinates of $[L(Me_2N)GaSb]_2N_2C(H)SiMe_3$ (**14'''**) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7629.48892667 E_h

Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.58383546 E_h

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7627.80694252 E_h

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7628.02006250 E_h

Sb	6.94365625888702	8.55634353353214	5.67914542517120
Sb	4.54372980987566	7.37124072572300	5.05715808152562
Ga	5.07295277117662	6.41861764818898	2.67438426755031
Ga	7.37501871128146	8.43074909949520	8.31650578787588
Si	2.27155085701894	9.82192079945964	5.65312056227372
N	6.81644394317753	6.59155294227547	1.69894567214900
N	4.04282333227568	7.12475223105059	1.12355143401350
N	8.00087465104820	10.30560448660735	8.79343466321226
N	6.02164149848901	8.36428422627257	9.74281954326180
N	4.67596058476140	4.57493301202141	2.76497299288998
N	8.71488908668893	7.16228796410770	8.56672098832521
C	3.85811912155175	9.46011504104639	4.64439554090766
C	6.84048781243343	6.30789911123773	0.40145327770268
C	5.69096258565215	6.27280140329999	-0.41183500042265
H	5.84684262282700	5.94813104829195	-1.44026583679474
C	4.40932425020297	6.74980710407081	-0.10252523747959
C	8.13914923463129	5.99251246747338	-0.29214595152986
H	8.30867949451181	6.67860235461374	-1.13372902805644

H	8.06973160061311	4.97735198054658	-0.71270596298040
H	9.00025110149353	6.03773013155503	0.38372275038474
C	3.40678669404320	6.81536530256343	-1.22143093075604
H	3.88349472874471	6.63788082671122	-2.19262793319015
H	2.88670771487058	7.78227336516815	-1.24437811818517
H	2.63331122779177	6.04822263047885	-1.06177618194659
C	8.01711767236912	6.97189820558804	2.36746033891993
C	8.58699414841977	8.23360463753374	2.08484705684901
C	9.75727999463803	8.60255321615591	2.75396349700524
H	10.20333622291511	9.57855976238140	2.54808812852281
C	10.35474773923431	7.76031849677972	3.68189195774318
H	11.26498619697223	8.06951637506361	4.20077278534638
C	9.77697890402329	6.52703183844338	3.95743949116309
H	10.24408923899015	5.87001595822216	4.69271764754764
C	8.60454182478290	6.11279367358671	3.32038115138711
C	7.96919958843896	9.21217348175201	1.10306759005177
H	7.05827834357973	8.75488376175521	0.69098236128842
C	7.55534194977362	10.50177995039986	1.80644241619617
H	7.05300426435668	11.18142725073915	1.10187574423127
H	8.43113152576682	11.03272456141972	2.20685579462421
H	6.87446859932387	10.30640686904236	2.64737637231409
C	8.90512912137618	9.52320173066457	-0.06585801018975
H	9.24302127543462	8.61151625004399	-0.57797423235275
H	9.80367750387865	10.06090501551493	0.27622765871745
H	8.39866500182381	10.16318126093405	-0.80550025669828
C	8.02788872488729	4.74454497177154	3.62244356112306
H	6.96813460237666	4.75431320996378	3.32517076709542
C	8.08352763270685	4.40000061140678	5.10795788290960
H	7.64897597124052	5.20371068172690	5.72107925813957
H	9.11416814953730	4.23258780101513	5.45860780893103
H	7.51939766249235	3.47702657977570	5.30882699453004
C	8.71650526279626	3.67170448045535	2.77662234355994
H	8.60989040965026	3.87881606856911	1.70164554248095
H	8.27962101551795	2.68008914990745	2.97384377622250
H	9.79399835870693	3.62227227325292	3.00417450736291
C	2.80683367610053	7.81320611072574	1.30185542588174
C	2.80104619755204	9.22875906450095	1.23250326494155
C	1.57745386452759	9.89220944927378	1.36162402349233
H	1.55019616919149	10.98115644216579	1.30582579171132
C	0.39152433423861	9.19293083320573	1.56298301249096
H	-0.55316803550150	9.73335046641767	1.65797180903309
C	0.41946496895468	7.80929637557300	1.66318759345902
H	-0.50913806561163	7.26282016413487	1.84523854006328
C	1.61721511284012	7.09542036190445	1.54336843380071
C	4.08407250779052	10.02039573915983	1.02408245356512
H	4.87389307683922	9.48506300871862	1.57893775970710
C	4.51474626477500	10.06502635771478	-0.44521899562029
H	4.78890163360470	9.07673908255224	-0.83513623350134
H	5.39605025457740	10.71472730794752	-0.56118709948462
H	3.71031362012208	10.47692596847904	-1.07553250809671

C	4.00512423131177	11.44421250832233	1.57077020433840
H	3.31860452311265	12.06916691560095	0.97826011665877
H	4.99481869047488	11.91862036834415	1.51916591156418
H	3.68504938625543	11.47789123966875	2.62182348848367
C	1.59698952226019	5.58834672088486	1.70373844300818
H	2.60583381361457	5.21267943231506	1.48360011137323
C	0.61182977753712	4.91019618442635	0.75270126582419
H	0.80037050445394	5.18151715811647	-0.29732677818812
H	-0.43138117128615	5.18154082255409	0.97977939837407
H	0.69148809794748	3.81546802255943	0.83863831290817
C	1.30169182809448	5.21294202448955	3.15583671656258
H	0.30195131386441	5.55811995034507	3.46529487990255
H	2.03886415513133	5.66124817338800	3.83808364960716
H	1.34227699639195	4.12118428941389	3.28893992679774
C	7.09420180021769	11.14903677301132	9.24533302704804
C	5.77239935930919	10.76288439920163	9.58996232112337
H	5.08946459100906	11.58507551065611	9.80381655118619
C	5.31570567715347	9.49225162844964	9.93789853377743
C	7.41644215791303	12.59857202786013	9.47286605538637
H	6.87434472503880	13.21091249998326	8.73641960929631
H	8.48846035249191	12.80601816369197	9.38020340361971
H	7.07116010684444	12.90568552595719	10.46984547407816
C	3.96855304113989	9.39201088156351	10.59985769433792
H	3.36206855186190	8.61924163293602	10.10758294541481
H	3.43925272135586	10.35075378412376	10.55174772406274
H	4.05780619767937	9.08910306642326	11.65185535686516
C	9.34892793428034	10.68583347471644	8.50693194738075
C	10.37075684606330	10.23895460580209	9.37932757503442
C	11.70096896969956	10.50644320155086	9.05356375894971
H	12.49422188245869	10.16120746855240	9.71756875969012
C	12.03539493495201	11.21355111235903	7.90448010558394
H	13.08276306152686	11.41050320519573	7.66384960685046
C	11.02641932023658	11.67799922206785	7.07648916642908
H	11.28495854303375	12.25117443667805	6.18317327015857
C	9.67537003479155	11.43126800351491	7.35068623820852
C	10.03487741557561	9.57522028014296	10.69833260498814
H	9.16154902686694	8.92912117464876	10.52109067253453
C	9.64969086009082	10.64719540618405	11.72196323117245
H	10.47500783663293	11.36454099027013	11.85539701763490
H	9.42974723322609	10.20027495330043	12.70261775669967
H	8.76188581854800	11.21231228932613	11.40701912797233
C	11.15335439616071	8.69325943969102	11.24128962138094
H	11.50307441406686	7.97447845523747	10.48603954982237
H	10.79761030219112	8.12287514886042	12.11058584268607
H	12.01938936819661	9.28561292523383	11.57730438524750
C	8.65039499117225	12.00664846362848	6.39404135134093
H	7.64930588647099	11.65451855114166	6.68379139484566
C	8.64936343356546	13.53877419105751	6.41815041795944
H	9.59121444398276	13.93717965310887	6.00802754260540
H	8.53495744954080	13.95070569663577	7.42910557301360

H	7.82702532404763	13.92495630435308	5.79600792621541
C	8.88424092668240	11.53935790252582	4.96041166873631
H	8.04657907390343	11.86463869991129	4.32916300809200
H	8.94831837052652	10.44401244774662	4.88709615046458
H	9.81334345221299	11.96102717429161	4.54388327185418
C	5.67166214150853	7.23711416791426	10.54848270755181
C	6.06499881071228	7.22581004444424	11.90928505989688
C	5.62710228620733	6.17996111101315	12.72507054892602
H	5.90838158322826	6.17245058307902	13.78061972559181
C	4.85986563762120	5.13852007233437	12.21750817421835
H	4.52958797472504	4.32775658470182	12.87108203239064
C	4.53755847443788	5.12697369510017	10.86799134489608
H	3.95978524184844	4.29499638915141	10.45942253369131
C	4.92669844193373	6.16634320497363	10.01668022796710
C	6.99296992223430	8.27469957694951	12.49813066483487
H	7.40972828375967	8.84613774367056	11.65612351506435
C	6.27980511921937	9.26528735001852	13.41925935011967
H	7.00397893252082	9.97038996421902	13.85652957922192
H	5.77564237262755	8.74423584142299	14.24923786914300
H	5.52736187589884	9.85966683628499	12.88362840742101
C	8.15601661782177	7.60956496574835	13.23580661478933
H	8.68391499445555	6.89354158077258	12.58992584330555
H	7.81352818423287	7.06731168504805	14.13032550387337
H	8.88030397147561	8.36372758760788	13.57686874879933
C	4.58283545397369	6.07572471717505	8.54815564799371
H	4.78229824797004	7.05920253275905	8.09095922643498
C	3.11185629195127	5.74949624726395	8.30228028748934
H	2.89369025975859	5.80709840235002	7.22494705602290
H	2.44864887217395	6.45822127721302	8.82215016689762
H	2.85124497037226	4.73503512385814	8.64192393942176
C	5.50579674558053	5.05986490015933	7.87392605633786
H	5.28430851241173	4.98215812903542	6.79947026262566
H	5.38225116757054	4.06023509953309	8.32012605429291
H	6.56151619077821	5.35218285793273	7.98135241776201
C	4.47160555659801	3.87443463137251	3.99748411668302
H	3.60556374752185	3.18250192533198	3.93821481038079
H	4.26807509000676	4.56872293289952	4.82733361186405
H	5.34435502796871	3.25293897528866	4.29930740162187
C	4.87706128871653	3.66701455500543	1.67234770374731
H	4.93915995234570	4.19488606876930	0.71129285178776
H	4.04355065351751	2.93639820123751	1.59362194510317
H	5.80706995612384	3.06256698187308	1.77342408821564
C	8.80498540316055	6.19742447197668	9.62190663703895
H	8.85033746802474	5.15792041196440	9.23095862042996
H	7.93678422001320	6.24644313015132	10.29216431414898
H	9.71413383723734	6.33123992121792	10.24709248441138
C	9.82232691385337	7.09773923130101	7.65673689440209
H	9.94067514951206	6.08513661576379	7.21506890714132
H	10.78891399387922	7.34957181701711	8.14304616393675
H	9.69597448039400	7.80195799339519	6.81906468967713

C	2.75565288088215	9.82009994121532	7.46306798312495
H	1.89890028722717	10.05203921200944	8.11443114517974
H	3.55654181161638	10.54857980258088	7.66165930102741
H	3.13592197593375	8.82476020588137	7.74058141695749
C	1.00747938540134	8.47970664971089	5.30330791858989
H	0.04628829362466	8.73902237252478	5.77598160940770
H	1.33163778365392	7.50607367388184	5.70069895000584
H	0.83755992410430	8.37080303879894	4.22161666104141
C	1.59835328194507	11.49658783159356	5.12755113317146
H	1.30871137799793	11.47746803469446	4.06510570303044
H	2.36364772590425	12.27626910517674	5.25978205781482
H	0.71010166793867	11.77391423167943	5.71753985326392
N	4.77719401375320	10.51878452155114	4.90850983794475
N	5.88059323930625	10.48390683213074	5.39895681810169
H	3.54708135087122	9.52753953609951	3.59125790442251

Table S16. Cartesian coordinates of [L(Me_2N)GaSb(N-Ph)][L(Me_2N)GaSb] (**15′**) [Å] for the optimized geometry.
Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7358.58647817 E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.54155925 E_h
Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7356.95126669 E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7357.15685581 E_h

Sb	-3.03168002993993	6.47675701127969	23.43770729796930
Sb	-3.88430902203384	4.28284602939173	24.55649087236536
Ga	-1.20417987625709	6.56771448850112	21.53462229080696
Ga	-5.77785776420058	5.49304364302405	25.88702909521275
N	-0.21592506913753	4.86186184749348	21.53239565971882
N	-1.70915303551830	6.41149491747257	19.63507922424283
N	-6.67199881260067	3.91803086682953	26.74515377466163
N	-5.40262645241205	6.34207493660855	27.65753160209420
N	-0.09754493519955	8.03139370210018	21.76879799709632
N	-7.07692532951669	6.49960235581761	25.01419459347351
N	-3.70195310674186	8.14102302302455	24.10376107277073
C	0.52501483964368	4.57637292272095	20.45855467143102
C	0.24954954516088	5.08326438024804	19.18232800403118
H	0.91721438822710	4.76223767019397	18.38352763357543
C	-0.88053644802847	5.82437412280140	18.78024590459255
C	1.73953836001812	3.70310624818805	20.61194267465709
H	2.02665836565507	3.23651319233724	19.66174055510026
H	1.60227985427217	2.92899825164607	21.37667683487331
H	2.57483612095957	4.34206487635823	20.94332032597014
C	-1.11528697421315	5.94963694396226	17.30136793685486
H	-0.71862137732201	5.07543438522445	16.77044921600947
H	-0.59296564410265	6.84154575958196	16.92142394054387
H	-2.18029043510813	6.07199452706342	17.06707458464181
C	-0.18646707436210	4.01047957794241	22.67734276694713
C	0.53842786059177	4.37890814792837	23.82879067517998
C	0.52799949566994	3.51165482841441	24.92582412540376
H	1.08942262656832	3.78110194176181	25.82350130911651
C	-0.17989002516637	2.31856594351737	24.89462093922827
H	-0.17821368278582	1.65616016910254	25.76322832840866
C	-0.90516600058767	1.97599443002834	23.75858301429441

H	-1.47924780986008	1.04784409827573	23.75158206689704
C	-0.93381631755947	2.80668280022525	22.63612502963879
C	1.36113227648720	5.65130780412600	23.89794159814495
H	1.17661041771819	6.22159269878902	22.97572329842566
C	2.85684789047818	5.33811622848025	23.96457515864307
H	3.17777678379402	4.70826272274822	23.12183416707656
H	3.11241814503632	4.80160252387377	24.89239828866136
H	3.44826416729791	6.26689527643452	23.94148924655111
C	0.93947124317819	6.53879653012287	25.06747126648423
H	1.51822144507849	7.47442486525971	25.06900748776808
H	1.10806923262530	6.04266696041594	26.03571613252797
H	-0.12723931397038	6.80372647755201	25.01154743745106
C	-1.74243198717776	2.40103083113697	21.41243236454797
H	-1.98164033979357	3.32824420806942	20.86850483314844
C	-0.94267054991808	1.50417399317809	20.46310535818645
H	-1.56504958906790	1.21051255031604	19.60332525285830
H	-0.62244503186066	0.58390557608920	20.97778781303334
H	-0.04692927089655	1.99714345091359	20.06680630697314
C	-3.05955474728328	1.71156834871660	21.76220651897143
H	-3.65085533909959	1.54681802912010	20.84884713293375
H	-3.66392329453891	2.31012527629245	22.45890052528582
H	-2.89844720484035	0.72221660707956	22.21801678910210
C	-2.88698773072634	7.08811882589491	19.19740570694796
C	-2.80750859776702	8.39198767489924	18.66852968974522
C	-3.99784112902825	9.02034822771536	18.28826621941385
H	-3.95512418106970	10.02969891535572	17.87204743494507
C	-5.22790342686345	8.39765456291089	18.44804564292325
H	-6.14606053232688	8.91291514906079	18.15668885159999
C	-5.29026201250665	7.11737269380130	18.98939928688077
H	-6.26084420404289	6.63659742040333	19.11875681308405
C	-4.13051130636384	6.43711914774237	19.36685209639415
C	-1.49667041362875	9.14043413550007	18.51944735701997
H	-0.68298746145322	8.44764365997914	18.77723690877288
C	-1.27105983717098	9.62518917416692	17.08653426503864
H	-1.36485229893241	8.81176770919480	16.35141389565328
H	-0.26711812249153	10.06581486805717	16.98494210545817
H	-1.99743582599493	10.40424628049639	16.80696883724640
C	-1.41841135943141	10.30639304847612	19.50349496855381
H	-2.19642842967222	11.05706585320221	19.29697234517113
H	-0.44038375177686	10.80727477496001	19.42863652884162
H	-1.55682385860645	9.96188281831543	20.53623872740221
C	-4.20218181932474	5.01530852613462	19.89081033141728
H	-3.40910679118967	4.90887305138063	20.65119834360072
C	-3.90251320933199	4.01031436744797	18.77586209869159
H	-3.98941178996269	2.97966455344166	19.15102331769579
H	-2.88845617783571	4.13040797030446	18.37056216681416
H	-4.61700900869030	4.13009192392597	17.94605368464892
C	-5.52105922354657	4.67896572954956	20.57385562286724
H	-6.35199561554181	4.60604518532957	19.85429921224781
H	-5.78927843630433	5.42663271859197	21.33300558308049

H	-5.44244709246665	3.70925021083647	21.08597178483940
C	-7.34963088186817	4.04226686103376	27.88261584606763
C	-7.17191358121435	5.11825586816499	28.76159870951245
H	-7.79142533828025	5.11262549059475	29.65794741080872
C	-6.18315196268805	6.12386438040356	28.70719794359426
C	-8.37803637269253	3.00646873246014	28.24674978548490
H	-9.31909964357511	3.25057564447265	27.72701608174780
H	-8.57789616878680	2.99700459137215	29.32535300595243
H	-8.08280688116951	2.00148694180013	27.91863270419555
C	-6.04960322803247	6.98179085632924	29.93631734264870
H	-5.04296382980563	7.40674368970387	30.03399539438163
H	-6.29688635248224	6.40734943065481	30.83806288866793
H	-6.75649807916038	7.82354863233677	29.87100667679530
C	-6.57445900724451	2.67080874220818	26.06769667219660
C	-7.40551434313876	2.37551657439474	24.96847808750205
C	-7.21212507728458	1.16943406591185	24.28688375199555
H	-7.85327024042274	0.93211462398567	23.43417870301957
C	-6.22187101700229	0.27470913395760	24.66941410075456
H	-6.08424173152616	-0.66107145236932	24.12245605868647
C	-5.40197008280750	0.57849132467986	25.75100962527945
H	-4.61986745667484	-0.12455510242552	26.04407059951760
C	-5.55310337734908	1.77073848664824	26.46346710288001
C	-8.49228594652511	3.32347713465482	24.50798816738066
H	-8.43561012154582	4.21838642750776	25.14305918654883
C	-9.88252361884429	2.70817420241248	24.66770845958818
H	-10.66118567305466	3.43723652331141	24.39353224266306
H	-10.06786682305066	2.38458276830536	25.70288702792006
H	-10.00986346766693	1.82618722206690	24.01947080446161
C	-8.24812065780211	3.77574854350039	23.07046268278031
H	-8.32134815687178	2.93395175830946	22.36298590710350
H	-7.24848258328245	4.21993260937580	22.96742766449398
H	-8.99018174221421	4.53079908848324	22.76911274586612
C	-4.64753980468234	2.07306330582632	27.64392054665931
H	-4.64837643648579	3.16657918200865	27.77176076302952
C	-5.18668828384259	1.46337473696148	28.93980105167779
H	-6.18615167895812	1.84217382641390	29.19033605379217
H	-4.51990530960410	1.70146469653201	29.78342977857485
H	-5.25271972908692	0.36635308999000	28.85726778772386
C	-3.20428836273228	1.63344106348241	27.41426660685410
H	-2.79694349526420	2.05381576967013	26.48211216355036
H	-3.10933480670743	0.53704736502244	27.36917556997561
H	-2.57050394344710	1.97479936780496	28.24648967508280
C	-4.35330354474075	7.31112921675510	27.69709277432534
C	-4.63208442136704	8.68219697172849	27.53276444292141
C	-3.56000364493376	9.57982738017013	27.53201094537172
H	-3.76379273228874	10.64625321044996	27.40885635307146
C	-2.24984018311690	9.14289390695576	27.66165132314429
H	-1.42580228442019	9.86024865902057	27.64131331264559
C	-1.98869491191961	7.78551798553690	27.81562268256816
H	-0.95654434172031	7.44758517430689	27.91920593477733

C	-3.02516128588004	6.85073233163413	27.84942542339783
C	-6.03585328985828	9.21795363090293	27.33329960148361
H	-6.73335417953325	8.37343742097832	27.42831843206527
C	-6.40839039562812	10.26516538360688	28.38391776186527
H	-5.80033406886418	11.17671147540976	28.27245890149110
H	-6.26258640456546	9.89799227112603	29.41083257722951
H	-7.46302890532578	10.56210649275122	28.27201594923447
C	-6.19869669728672	9.78300380068412	25.92414062817680
H	-5.89840263723340	9.03969222055403	25.17529919508968
H	-5.56881448420909	10.67342142873401	25.77519341528012
H	-7.24403446771016	10.07814363308361	25.74161208170896
C	-2.73791272830037	5.38382113977726	28.10292976541719
H	-3.47444905073192	4.81409862314821	27.51282163610352
C	-2.94945743536035	5.02196092816890	29.57404563657012
H	-3.98045451458519	5.21331622533122	29.90129372156583
H	-2.27467602843793	5.60572893973763	30.22058922442712
H	-2.74108324166941	3.95368090027193	29.74428262454295
C	-1.36100659034085	4.94275608671602	27.62892573682807
H	-1.21036513134732	5.18981761987452	26.56928599313616
H	-1.25819496561856	3.85292300682418	27.72952629441157
H	-0.55087917438081	5.40300599633710	28.21707813055788
C	1.09057995588598	8.18587624638589	20.97961325399333
H	1.12675285716407	7.45504832807916	20.15674825696971
H	2.01939160542639	8.04840803944714	21.57717397593074
H	1.15924995928994	9.19591879713092	20.52583892042735
C	-0.21668620344123	9.00343863189757	22.81794328628076
H	-0.33370658047033	10.03310073630585	22.42389801827968
H	0.67344330495260	9.01324602945062	23.47977172470151
H	-1.09364432899644	8.80785921287526	23.45213221520700
C	-8.30400242536779	6.85767509616066	25.66098564684643
H	-8.45895396164130	7.95618431179105	25.70872119530335
H	-8.33747224939693	6.48112236323120	26.69550559132465
H	-9.19523829086936	6.44487024660615	25.13624650868078
C	-6.97319496292977	6.98606647692807	23.67227232215615
H	-6.06481603225778	6.59669016118992	23.18902851347993
H	-6.91436422040762	8.09188815522261	23.61273457453347
H	-7.83843840235263	6.67765511679997	23.04897124711697
C	-3.71238505113428	9.29901200292669	23.37143776444445
C	-3.29218317879629	10.50168342098337	23.99474251263513
H	-2.90211856375438	10.43120165777192	25.01108674904984
C	-3.36918107164618	11.72053882917275	23.33683602834310
H	-3.02894738928896	12.62670803222292	23.84620289142450
C	-3.88254717157503	11.80149338510432	22.03878208473417
H	-3.96006347603805	12.76509640988247	21.53040760675465
C	-4.29900762108692	10.63129626762819	21.40743877075969
H	-4.71071064539199	10.66924049592287	20.39683334549205
C	-4.20284708416692	9.39875820175032	22.04701187790423
H	-4.55875225876911	8.49387891374126	21.54476841881352

Table S17. Cartesian coordinates of [L(Me_2N)GaSb(N-$SiMe_3$)][L(Me_2N)GaSb] (**15''**) [Å] for the optimized geometry.

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) = -7643.83904761 E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7644.05042820 E_h

Sb	4.91156149009091	9.84574570219467	6.83561413943616
Sb	4.53159257035483	8.13919340965557	4.85654679424705
Ga	5.03238511153948	6.36400806737875	2.93618228874587
Ga	7.09495698355508	9.21322344911904	8.18053021570157
Si	1.38104196260665	9.01076682832086	4.84243119967392
N	6.87363288307799	5.92784561600908	2.38765502541504
N	4.52069210732321	7.12268750062646	1.17644652130662
N	7.64048923273279	10.94226403608242	8.98741412518949
N	6.38000235870511	8.42087891469325	9.88520792197525
N	4.11346300272808	4.80181564090344	3.31424405238183
N	8.51287172319875	8.12547642118614	7.65847812312637
N	2.73754537395913	8.10980716023435	4.22461076275159
C	7.10177358671215	5.55597594272068	1.12270504882937
C	6.22421179517894	5.81469256145874	0.06551125400411
H	6.52969037910713	5.43900947829788	-0.90921213231906
C	5.09180345687933	6.65086174686439	0.07175991920449
C	8.38414396920297	4.84558663940237	0.78842355869088
H	8.38704674492399	4.52101718663823	-0.25859271127411
H	8.51942138552330	3.97165617922696	1.44189358287988
H	9.25474889117388	5.49393537835430	0.96165836651762
C	4.52691803247731	7.01895695071518	-1.27197003170178
H	5.20311266320477	6.70761010160820	-2.07648185084534
H	4.34718182248526	8.10039400976711	-1.34245624592071
H	3.55155686281806	6.53442657175718	-1.42214165032429
C	8.00670289712639	5.93456931140016	3.25930426040589
C	8.88183673397144	7.03974716919648	3.19429405811927
C	10.08399316696459	6.97816114734035	3.90339548365276
H	10.77992226628900	7.81900970482975	3.85062200952597
C	10.41045721501292	5.86514066236519	4.66921039393972
H	11.35903685447721	5.83063644364698	5.20974753256340
C	9.50997780809748	4.81241020516665	4.77141602130187
H	9.75309798011166	3.95545701365950	5.40404254728062
C	8.29436004274161	4.82725601035435	4.08191955715055
C	8.54813038959362	8.27980777066470	2.38589710845679
H	7.57654782670520	8.10682320898761	1.90129069489285
C	8.39177434330968	9.49365672885479	3.30002483753369
H	8.08168261506933	10.37818691547186	2.72358068728170
H	9.33645224613342	9.74628098454311	3.80657562195545
H	7.63589021012612	9.31595055053881	4.08044076061204
C	9.56752126642434	8.54763245452595	1.27974780149354
H	9.64935809727833	7.69714622198435	0.58667033340452
H	10.57003208705632	8.74233168500315	1.69258436849154
H	9.27408302092634	9.43036649159755	0.69082384975514
C	7.31756032247858	3.68302320057759	4.24778512041934
H	6.52293443800370	3.82188824813044	3.50324685564066
C	6.65834175595851	3.75516698744857	5.62561348536111
H	6.14600747689126	4.71757772794586	5.76797352233721

H	7.39989971913860	3.65062549099781	6.43377505446124
H	5.91114474036879	2.95550738693967	5.74350877270568
C	7.95228560833640	2.31540943111764	4.00675461225109
H	8.43435252676622	2.25784819420980	3.01858804338360
H	7.18626077817992	1.52600091238761	4.05434324364995
H	8.71598391397473	2.07602306223657	4.76343206021646
C	3.42811195427740	8.03523245440200	1.02505927167681
C	3.67979340178213	9.41545182694803	1.15010379503925
C	2.62949274212025	10.30325493795307	0.90692432233760
H	2.80267366787306	11.37709682532096	0.99282218000210
C	1.36516365605859	9.84195480133881	0.55865402328412
H	0.55705597972188	10.55179915151817	0.36755116673373
C	1.12700060579339	8.47578745198467	0.48047904966984
H	0.12391421817708	8.11720804184946	0.23799909321562
C	2.14266111366557	7.54773387975751	0.72322528333523
C	5.05797925616074	9.93235298908736	1.51635462858865
H	5.52723290995635	9.16594001748830	2.15825012960875
C	5.95136701175027	10.08937285580561	0.28426499876838
H	6.12935494186004	9.13058436016901	-0.22279115147685
H	6.93284914920465	10.50093646405910	0.56682158154000
H	5.49308789782964	10.77964804357359	-0.44189061227659
C	5.01460785694934	11.22582653911613	2.32157085283724
H	4.67721045723604	12.07863796012731	1.71216025228472
H	6.01908409632224	11.47109210742403	2.69457685979072
H	4.34490284303867	11.13825256334388	3.18982369028748
C	1.82066346710940	6.06660663493210	0.72609203258145
H	2.77172684237400	5.51633136096791	0.76840594496281
C	1.06422104803711	5.60588706288407	-0.51846127054070
H	1.59148730131987	5.86104882706059	-1.45085233849850
H	0.06153809198024	6.05761371864960	-0.57416728858188
H	0.92661504691691	4.51369075539197	-0.49731023267449
C	1.04397605802111	5.72055460353715	1.99638773373564
H	0.03449020733999	6.15945673770110	1.96546132714756
H	1.55694166172029	6.11996226617688	2.88232685622671
H	0.93525316676535	4.62939086987475	2.10080885319401
C	6.86765037724294	11.42060623692381	9.96883393151463
C	5.96262650411559	10.64816551947650	10.70906389235872
H	5.40228487085006	11.18972349027971	11.47014445269623
C	5.87856567630801	9.23903129242387	10.79308637583819
C	6.99187966398171	12.86880672108936	10.35358842123973
H	6.67865866635784	13.51292772359010	9.52013217318956
H	8.03704134624028	13.12980438983422	10.57290022382147
H	6.37366223199531	13.09761708817294	11.22901494780322
C	5.24731229862514	8.70094017915626	12.04718568559181
H	4.98274526238615	7.64109741425180	11.96798049245971
H	4.35258783510591	9.28731145825584	12.29848144752578
H	5.95583321131485	8.81296860614118	12.88295570885138
C	8.69880454194638	11.76214594446600	8.48400729489655
C	9.99757731146848	11.58921804727737	9.02212862511877
C	11.02443227970835	12.41935678393590	8.56720616789395

H	12.02941011134332	12.30227303465276	8.97382336606656
C	10.79582011775776	13.38940748534246	7.59710630586406
H	11.61365447504410	14.02913679879929	7.25716676288516
C	9.52781714916195	13.52595924013196	7.05443471212538
H	9.35142340699687	14.27346157456270	6.27723407122530
C	8.46250990490056	12.72339842149677	7.47900390847517
C	10.28236865081410	10.51524792220295	10.05792795778761
H	9.66633240266228	9.64403724031740	9.77983502397462
C	9.87180947784462	10.94000806276537	11.46963989377493
H	10.39194610512070	11.86463230897266	11.76759836681702
H	10.13791797581535	10.15593132958365	12.19560019976693
H	8.79041221759374	11.10899383801451	11.55711265267377
C	11.73921925900523	10.06358095712815	10.05380774367413
H	12.06762521450330	9.75515025610858	9.05006230652466
H	11.87025345907200	9.20723891907161	10.73003517934997
H	12.41758918615502	10.85478199189514	10.40987973786701
C	7.11780217883884	12.90137454443222	6.80552582379208
H	6.39051057591863	12.26200728771323	7.33129784614231
C	6.60157877645404	14.33881731936081	6.86177643334403
H	7.23252570991644	15.02039745894541	6.26986744619044
H	6.56915364183921	14.73186113964094	7.88902414405186
H	5.58319277821151	14.39116180072585	6.44701772953262
C	7.18380914064180	12.41559607126383	5.35883565654059
H	6.19136375917151	12.46998556552532	4.88746045945675
H	7.51540538355929	11.36948861966849	5.30682988228804
H	7.88379113158391	13.02796282814321	4.76744542859214
C	6.40896919157294	7.00983597657864	10.11309906073764
C	7.54294529337825	6.43583289058329	10.72449198727065
C	7.57091095064119	5.05244301497751	10.92226271893021
H	8.44643984439765	4.60101508915435	11.39547910439456
C	6.51017286255735	4.24505233837018	10.53471225995432
H	6.54826918869051	3.16587924329321	10.70091050491639
C	5.39916876392448	4.82250235955422	9.93381436260870
H	4.56309010156227	4.18940406199914	9.62863356732742
C	5.32474429654679	6.19993717009935	9.70490609922243
C	8.72454675993039	7.26125743160261	11.18829157838906
H	8.52912166117325	8.30508472576824	10.90513963654313
C	8.87313458212868	7.21096494595833	12.70948786470158
H	9.69235290696157	7.86775424785448	13.04191578042933
H	9.10351653961532	6.19153972474439	13.05783737487403
H	7.95191437459697	7.53288977231746	13.21793879431672
C	10.00723732271787	6.82651562582991	10.48329198402198
H	9.90959234557027	6.99086599057659	9.40080799016658
H	10.22942586676556	5.76338946807625	10.66492187412549
H	10.86635748431189	7.40743110265510	10.84864904275589
C	4.08605360424811	6.76080163145830	9.03709586103901
H	4.30325618253116	7.80156234728996	8.74626933887063
C	2.87819356892882	6.78670764020544	9.97494116715324
H	2.00597689139725	7.21424903932948	9.45680119203153
H	3.06525582130011	7.39298903774096	10.87215193946881

H	2.61109609307157	5.77021368798912	10.30708938150730
C	3.74919509303840	6.00365089595415	7.75828748162359
H	2.94651263099023	6.51875883174992	7.21117761145215
H	3.40815630071751	4.97599085999467	7.95919719213532
H	4.62351092206790	5.93677464522919	7.09361894539626
C	3.28018792354113	4.55954593776592	4.45454196771876
H	2.27944082976173	4.18864821431535	4.15711115643453
H	3.11041273174556	5.48459445790269	5.02220709358766
H	3.70858249933841	3.80383409325251	5.14578626587418
C	4.20172963950391	3.68435493697448	2.41952997893394
H	4.85327490514309	3.90436300326259	1.55914850667467
H	3.21000660526388	3.39714238970268	2.00906771831509
H	4.60882467481165	2.77375571924151	2.91136158532405
C	8.11502171753899	6.84601927754323	7.13111565749462
H	7.87702599142497	6.86712809454181	6.04572708507312
H	7.23108213575622	6.45572156194713	7.65839786355613
H	8.91733539610012	6.09378586621213	7.25893553327430
C	9.66496243893525	8.65993555097004	6.98620696370748
H	9.52783421885630	8.76030068963495	5.89085594518984
H	10.54641572483544	8.00040646834263	7.12788921662060
H	9.93421935620161	9.65177442851390	7.37483310341628
C	1.04681655509067	8.66667565155897	6.67438263255070
H	0.18532123462446	9.26010080550117	7.02236329509032
H	1.91018412135719	8.91860695280828	7.30946900185095
H	0.80411547200516	7.60220474814665	6.82379061630290
C	-0.18304092879551	8.50017393227836	3.92699465578102
H	-1.03950884476905	9.09947162430934	4.27692934728845
H	-0.41560182818561	7.43856496028320	4.10161389716506
H	-0.07041284774542	8.65286768501711	2.84419828623379
C	1.60631613611199	10.87028316801409	4.59935414395319
H	1.73170565894873	11.09403301155790	3.52867788418956
H	2.49492203584954	11.23984780886427	5.13561483212176
H	0.73014534535106	11.42774932900291	4.96883718154195

Table S18. Cartesian coordinates of [L(Me_2N)GaSb(CH-$SiMe_3$)][L(Me_2N)GaSb] (**15‴**) [Å] for the optimized geometry.

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

Sb	5.01246684345640	9.90786722574178	6.66462532410343
Sb	4.49215893976371	8.05012935860090	4.82446391686066
Ga	5.12428226472651	6.33599630202340	2.89694806200026
Ga	7.05671558188528	9.19159898120911	8.15096929621666
Si	1.21412271795320	9.20207728846898	5.06000169785456
N	6.96637620446567	5.95878498586192	2.32998015917734
N	4.55878495640008	7.05174073105917	1.12743107218236
N	7.63124156282852	10.93605289461678	8.93142181144798
N	6.32653347246095	8.45061310006711	9.87760202534768
N	4.19599066696192	4.75214840578697	3.19154732093398
N	8.48488347948351	8.07178865241099	7.69813835458515

C	2.58133085843949	8.18431190053085	4.32372813992520
C	7.20522821586530	5.61271744809439	1.06017794652588
C	6.31687059201276	5.84269329625204	0.00294334673854
H	6.64215088178215	5.49192675251081	-0.97478476320935
C	5.14422129878307	6.61965530005368	0.01580065386512
C	8.52020204800533	4.97167913456817	0.71307022198899
H	8.51435370463419	4.61119562968866	-0.32218081231480
H	8.73424782125761	4.13488267653013	1.39249486347245
H	9.34944869391902	5.68304869958859	0.83412775295926
C	4.54752619733800	6.96549836033368	-1.31949101328568
H	5.24971646622864	6.74219492731041	-2.13102753776980
H	4.26063324249332	8.02483849509776	-1.36449183251996
H	3.62774808909927	6.38516361350805	-1.48337583117439
C	8.09261658182003	5.97875282787905	3.21090825306100
C	8.96587929414682	7.08628862334584	3.14478856290378
C	10.15717099578264	7.03572174381208	3.87157611586133
H	10.84983127175336	7.87945246302582	3.82300849369327
C	10.47606788805094	5.93166569966654	4.65412408995635
H	11.41727284256854	5.90554041408818	5.20773310614838
C	9.57572504097785	4.88012969878794	4.75832663163094
H	9.81124462496830	4.03187333443193	5.40573869394748
C	8.36708170673155	4.88509824431221	4.05532604387680
C	8.63452324551965	8.32421344640463	2.33106535390314
H	7.70066721211513	8.12508794371650	1.78582061217948
C	8.37946574601952	9.51622674144622	3.25298974420271
H	8.09030056561826	10.40361301529916	2.66982438432812
H	9.28008242757655	9.78018885019808	3.82913340343298
H	7.57545266859874	9.30937526198609	3.97615551615931
C	9.70605314913606	8.65407485800564	1.29312731208068
H	9.88295603317881	7.81427112492208	0.60460415065087
H	10.66726971395172	8.90607341368361	1.76813602832952
H	9.39954816795587	9.52214020479614	0.68905442269553
C	7.39940355313388	3.73181636686658	4.22738277068443
H	6.53982661406011	3.91828313636763	3.56900271343893
C	6.86686135884733	3.69222701524515	5.66074635485389
H	6.34994586530915	4.62788464951964	5.91983803501891
H	7.67749942066477	3.55017755860763	6.39279301327703
H	6.15211594635880	2.86484254254680	5.78708482236903
C	8.01373962232741	2.39119662766461	3.82769533123754
H	8.37942311126126	2.40435467137367	2.78954990283523
H	7.26659439254754	1.58649930570586	3.90972435549054
H	8.86280892909997	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
H	2.71026528753367	11.25061224205051	1.21353794474868
C	1.28918253713046	9.69344161271758	0.80876506888776
H	0.44744516347755	10.38454524793895	0.72340824831502
C	1.08758778860113	8.32750601610210	0.66937119336324
H	0.08013279035099	7.94870308599164	0.48175917095577

C	2.14711394055186	7.42088783405006	0.77665232508563
C	5.03593286423886	9.86279333975707	1.51216345550563
H	5.54435779123233	9.10525115720346	2.13408511591907
C	5.87991994829835	10.04241309260819	0.24842748987288
H	6.05889597549510	9.09080028401510	-0.27107983720472
H	6.86309004332528	10.46920481024451	0.50090801391664
H	5.38545481958110	10.72964176778223	-0.45653991591926
C	4.99603866251795	11.15249003036493	2.32325465962761
H	4.62293671226556	12.00116065983555	1.72873885232400
H	6.00776180439660	11.41375595654957	2.66326747041913
H	4.36179806567059	11.04729629101125	3.21609372991039
C	1.85423263562421	5.93592545910417	0.67247545192034
H	2.81579323812025	5.40348836795932	0.66813648157129
C	1.10249828213039	5.57441599000072	-0.60919774963912
H	1.61182065782943	5.94409110517350	-1.51211352905665
H	0.08515658245732	5.99574479843383	-0.61341545084012
H	1.00289949846400	4.48162841317308	-0.69873023099965
C	1.07744905925430	5.45575084519315	1.89905452890926
H	0.10480984580677	5.96684443159388	1.97742234218901
H	1.63933396109698	5.64787265829708	2.82223659200147
H	0.88581476461561	4.37297012149219	1.83666673132541
C	6.87928039216662	11.44023927717649	9.91588065724947
C	5.96152177601969	10.69838810077234	10.67125245206338
H	5.41892334183023	11.26238065884482	11.42889134338852
C	5.84394810873511	9.29395622139407	10.77281844843919
C	7.04763135754661	12.88573427414449	10.29567860627235
H	6.76345897252642	13.53765232063843	9.45864239090257
H	8.09919625255400	13.11219173780448	10.52318451235067
H	6.43095865606653	13.13749877497455	11.16591047595969
C	5.19946408688212	8.79027260617789	12.03537554998829
H	4.90640657248476	7.73682980504403	11.97242302638097
H	4.32072404297272	9.40381068233468	12.27820373936678
H	5.91080558010092	8.89547886931957	12.86959253187074
C	8.71620561842645	11.72387148881523	8.43128902715435
C	10.00623353191170	11.51007972672116	8.97778188343023
C	11.06222290142868	12.30989530320739	8.53579367362733
H	12.05926754246750	12.15942505843356	8.95081216789648
C	10.87266563779924	13.29131719644089	7.56914345901962
H	11.71240548116357	13.90765469517792	7.23942539626377
C	9.61397251629640	13.46851216175796	7.01768262212578
H	9.46673529145698	14.22543193969947	6.24349866750522
C	8.51985982551220	12.69766458432097	7.42867401112278
C	10.25369271810116	10.42625667693555	10.01292192936065
H	9.60624441713774	9.57725336367207	9.73752378721770
C	9.86402838756486	10.86914164207261	11.42505958817873
H	10.41688499086803	11.77636137218186	11.71785299372399
H	10.10610168641228	10.07889557331194	12.15275158173272
H	8.78934275327037	11.07552885023351	11.51616499982409
C	11.69374178622061	9.92296092937967	10.00415896111914
H	12.00784334968829	9.60566411324989	8.99863142326920

H	11.79551903826188	9.06049370070746	10.67709257493161
H	12.40122731670922	10.68814951419153	10.36056549797001
C	7.19011708995946	12.93348362410083	6.74245960959010
H	6.43925345202569	12.29368054032414	7.23345078877488
C	6.71058524955618	14.38187661918214	6.84232411908111
H	7.37009026232132	15.06549918643503	6.28474231900346
H	6.67045274698135	14.74203331275122	7.88104251343510
H	5.70121756210624	14.47610089829028	6.41299032887114
C	7.26600362809256	12.50405229853175	5.27826423748841
H	6.28174084363434	12.60316817362052	4.79685939605909
H	7.56834538502461	11.45189443846636	5.19042597497122
H	7.98913087178620	13.12264433273597	4.72216286753663
C	6.31729245359273	7.04464049202247	10.13408187069494
C	7.42233917818701	6.45290970852169	10.78071187152507
C	7.40705544010755	5.07412166169378	11.01026540050125
H	8.26046189580338	4.60948484705225	11.51041763151916
C	6.33141329985019	4.28799876339438	10.62082370648889
H	6.33542251893167	3.21232179326388	10.81236031805224
C	5.24921029313063	4.88266349199707	9.98508515228449
H	4.40115118435058	4.26628357494739	9.67901232239612
C	5.21896512240585	6.25583978389521	9.72304466616232
C	8.61960238658586	7.25320878051646	11.24827314411616
H	8.45785881119547	8.29688782538270	10.94441606951135
C	8.74616205585868	7.22372752033947	12.77207867717262
H	9.57750564394643	7.86472255820077	13.10533178886326
H	8.94573123813509	6.20465263086630	13.14002311860371
H	7.82701838548953	7.57743476368959	13.26271564297698
C	9.89907514690574	6.76977091752301	10.56926907731296
H	9.82964504369380	6.93838281020441	9.48499452846720
H	10.07661254734091	5.69896904131004	10.75498430244108
H	10.77191339759321	7.31707186136627	10.95362204659584
C	4.00805050491945	6.83898241056851	9.02341332769294
H	4.26884570220889	7.85529959194431	8.68622405034742
C	2.80219909456377	6.95175486934021	9.95765341920605
H	1.94416288265422	7.38324870595381	9.42028538122316
H	3.01064291737436	7.59451128644574	10.82404519876540
H	2.50245666550651	5.96187657220655	10.33920308150459
C	3.64349516316958	6.03606146724988	7.77955284598648
H	2.87479531352794	6.56115401135171	7.19454969698931
H	3.24968075276794	5.03788542203913	8.02842619414061
H	4.52099166317418	5.89384389823748	7.13072562223075
C	3.52438487317848	4.36841790575706	4.39770834446044
H	2.49193390590217	4.01498160202432	4.19795708927156
H	3.43955095030735	5.21674370849026	5.09142376536835
H	4.04088690889087	3.54579358018800	4.93461846758393
C	4.27687578413834	3.69255153161469	2.22703467701003
H	4.77526279471657	4.02383712438314	1.30264589224877
H	3.27224061664862	3.31622435128586	1.94143494563060
H	4.84303898729334	2.81056226235579	2.60083841618459
C	8.08531842884537	6.78071475266411	7.20195209174729

H	7.81058189620423	6.78486392429151	6.12406542189941
H	7.22559913931128	6.38556342924694	7.76444340913826
H	8.90282008219012	6.04091351130651	7.30925613921045
C	9.60715503752295	8.59792039454820	6.96999545834465
H	9.42646456023271	8.67388112610014	5.87833692160166
H	10.49650788405877	7.94494667725790	7.09002757200196
H	9.88674059784744	9.59885183504760	7.32661868027093
C	1.03597630828834	8.89833514399735	6.91309603086805
H	0.27976890294890	9.57303619067771	7.34592969911665
H	1.98992840389436	9.07702561534679	7.43374671662045
H	0.72036000192647	7.86094472834382	7.10556671278119
C	-0.39363201035429	8.68363938364937	4.21689863317632
H	-1.25256824122969	9.24575745997438	4.61750714350054
H	-0.58611995413386	7.60991854601721	4.37201414062324
H	-0.33826845077016	8.86436546871762	3.13253334005664
C	1.49538929036546	11.04435465667629	4.76326311052749
H	1.56007549074032	11.25270958026364	3.68429881199602
H	2.43837433079181	11.36804998705493	5.23219604382143
H	0.67596279326869	11.64724877874358	5.18752123788242
H	2.33672102510775	7.61301345513374	3.42239140391873

Table S19. Cartesian coordinates of [L(Me_2N)GaSb]$_2$N-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

Sb	-3.74855737065017	5.21910768870670	22.90389561338931
Sb	-3.12970110082980	6.51766296073685	25.26374049015896
Ga	-1.31387517708840	5.02472542245234	21.88968193930455
Ga	-5.49995738095781	6.14373977429179	26.36302247351389
N	-1.11396779065125	3.39482833553025	20.73534411216997
N	-1.06114672566872	6.27513620114637	20.35583367930062
N	-5.22060528479099	4.52140330461431	27.50819517666236
N	-5.80591208153983	7.30470511788823	27.96903958811041
N	0.23408076564823	4.98622776042051	22.94640897346191
N	-7.12205858605500	5.95435474908729	25.47293100745495
N	-3.61032025419584	7.25199781501687	23.39475170782519
C	-0.34754191168374	3.42285854826654	19.65371000923460
C	0.14046221053488	4.61159053235227	19.07976069055244
H	0.81740961833420	4.48534193699962	18.23488787048436
C	-0.26793689007355	5.92917535981383	19.34268542110041
C	0.06095376728213	2.14210759504269	18.97695590225766
H	0.11214424214185	2.27819162281973	17.88893448651422
H	-0.61899780861387	1.31360066873195	19.21032906659021
H	1.06691430169601	1.85667791930541	19.32225491992635
C	0.20144289207992	6.97586209183992	18.36782684044973
H	1.20291471183169	6.71645539200282	17.99869622071554
H	0.22109054120219	7.97555099868378	18.81896340205716
H	-0.46894943440450	7.02190628949996	17.49725809164411
C	-1.66826391925110	2.18218213163345	21.23610335157795
C	-0.89724597425701	1.30773574951062	22.03222817320101

C	-1.50880610849780	0.15414505856949	22.53582260852182
H	-0.91974725298792	-0.53578391757402	23.14566597154005
C	-2.84380510505480	-0.12860015370101	22.28148532333418
H	-3.30194636327848	-1.03278078740458	22.68944187950983
C	-3.59473497552294	0.74443070004373	21.50092907254071
H	-4.64217700838307	0.51553726492694	21.29849865379115
C	-3.02858269922531	1.90180639669301	20.96118575456707
C	0.56135704330521	1.56469703563849	22.35849733407453
H	0.85366614002905	2.49834455624757	21.85898657894398
C	1.46473153769221	0.43698914387809	21.85632467792360
H	1.31883301704217	0.23366141960432	20.78570620260691
H	1.27103248940830	-0.50296312391752	22.39719048790209
H	2.52379454201548	0.69386347970271	22.01492649627231
C	0.76254307321181	1.78342790940186	23.85664562330885
H	1.80890648631538	2.05317961498084	24.06881755148453
H	0.53311410155709	0.87081856266841	24.43086527241539
H	0.12266315260831	2.59739339075345	24.21850227931828
C	-3.83690908179381	2.79839364515483	20.04218603504410
H	-3.48151708576333	3.82922875454030	20.20742019132157
C	-3.56294988408563	2.46366714816129	18.57389228505386
H	-4.15813434695162	3.11183704998291	17.91218299806540
H	-3.83254559440050	1.41776048253327	18.35660546963287
H	-2.50602549112997	2.60320487600262	18.31066385013751
C	-5.33456776012310	2.76902629432619	20.32529818943670
H	-5.84529528508230	3.54413288340959	19.73591162016013
H	-5.55297176566607	2.95821036683078	21.38633040462184
H	-5.78552757389898	1.80343218736269	20.04720687548813
C	-1.73856874498418	7.53076823122568	20.29656289372757
C	-1.41476027489148	8.56093577680755	21.20556027586638
C	-2.07763159343956	9.78501069756064	21.08860800543306
H	-1.84535144111713	10.58774938714521	21.78966437083288
C	-3.03240705509375	10.00065622343321	20.10359941927662
H	-3.54478436837515	10.96255498785051	20.03850805999492
C	-3.36316477993842	8.97082539227795	19.23452472772026
H	-4.14485000044946	9.12986043298681	18.48764840040349
C	-2.74576006628717	7.72058775931260	19.32162499199308
C	-0.32982151673726	8.38688470926965	22.24974122826344
H	-0.27331595347878	7.31634802711367	22.50045252612995
C	1.03270733369296	8.78807483011591	21.67975716135966
H	1.30900985355394	8.17028839858237	20.81308988440238
H	1.82249201092452	8.67093553843222	22.43855211255719
H	1.02437188003579	9.84191905843033	21.35663857660472
C	-0.62001753307662	9.13985345749787	23.54426322265528
H	-0.52721249890680	10.23047529314231	23.42030780168434
H	0.09635694125801	8.84015779848125	24.32426819692473
H	-1.63549250318911	8.91916381083399	23.90210226078790
C	-3.23501218248410	6.60376014333885	18.41335039860256
H	-2.55808926608665	5.74328739914854	18.52166528599775
C	-3.25266163540160	6.99813036795913	16.93640494820503
H	-3.51056954203498	6.13020297641646	16.30973558282085

H	-2.27964647990173	7.38358096895726	16.59820278435317
H	-4.00123637141311	7.78036215889787	16.73568041297477
C	-4.62566977700332	6.14142436302755	18.84924317414030
H	-5.35655124396530	6.96216061045598	18.77682763519675
H	-4.62278967789831	5.79057456972980	19.89183317848187
H	-4.98246417367742	5.31615004866802	18.21369863340362
C	-5.84466555436225	4.36702512284511	28.66726717504190
C	-6.42765842585766	5.43600805978291	29.36902349893389
H	-6.92956879816134	5.17727038912860	30.30088565071899
C	-6.32110101205376	6.81208709662641	29.09080209673361
C	-5.97841031269342	2.99513962831495	29.26905646409986
H	-6.94433939755432	2.56890013755465	28.95282130051028
H	-5.97505708261210	3.03456267551587	30.36592609831060
H	-5.18915978669922	2.31653660731960	28.92154895326125
C	-6.84300848952119	7.75349799050028	30.14181186463497
H	-6.22908417232994	8.66069003901899	30.21612996562440
H	-6.89160334534980	7.26288310051273	31.12145838568112
H	-7.85954189169696	8.07736242343443	29.87027157436518
C	-4.36394896450719	3.53871319786538	26.93282009581084
C	-4.85084559928423	2.62533246349635	25.97676903400263
C	-3.93128239063738	1.82720439241806	25.28822112401422
H	-4.28700624471375	1.13158186559541	24.52495047985231
C	-2.56995331343820	1.91261555462160	25.54130415154031
H	-1.87295821015705	1.29739872077473	24.97166150934641
C	-2.10323688951713	2.78418626580427	26.51983501998570
H	-1.03188500641870	2.83431881297158	26.72140170365552
C	-2.97891180202310	3.60648136918924	27.23284021009345
C	-6.33010634774587	2.46148227790379	25.69584683916999
H	-6.85819204568734	3.25571003282108	26.24177607053122
C	-6.83221460354129	1.10864422684317	26.20614292341640
H	-7.92179924387721	1.02245086283062	26.06895595769294
H	-6.60892639359165	0.96170219525098	27.27259016121062
H	-6.35963273471302	0.28025331092611	25.65426983663396
C	-6.65486039227280	2.62893556085698	24.21483535271689
H	-6.21252911230676	1.82032053335292	23.61107188153335
H	-6.26922956928853	3.58426788750450	23.83446620614571
H	-7.74333926213011	2.60695150724247	24.05090420959736
C	-2.46008441761054	4.52187803564513	28.32856151202491
H	-3.12766684556193	5.39885460131774	28.35400067887152
C	-2.55288755803227	3.84998923703302	29.70102172285330
H	-3.58088551577939	3.56624311637086	29.95670249401958
H	-2.18885554418096	4.52941646908991	30.48765161485916
H	-1.93584887433940	2.93749541104001	29.72581818683396
C	-1.03648584268453	5.01844756650288	28.09848258068828
H	-0.91989403538699	5.49953649157728	27.11648549375971
H	-0.30102784823068	4.20207920298188	28.16830884009224
H	-0.76901905043812	5.75548723613825	28.87051684168363
C	-5.59324940526283	8.70747011939021	27.81359786001328
C	-6.63585876016639	9.55344475455524	27.38235659493581
C	-6.36809348765333	10.91774174701251	27.22822629735656

H	-7.17062549118986	11.58060789447579	26.89561689302232
C	-5.10630421626772	11.43988060773582	27.47255437419831
H	-4.91685009619667	12.50801604575473	27.34251479378043
C	-4.07863883753917	10.59213432564184	27.87244838068647
H	-3.08454526832639	11.00483810825249	28.05033813230934
C	-4.29598220187333	9.22365828748493	28.04926302822895
C	-8.02033067130598	9.03975469513177	27.04428766173820
H	-8.03427159449766	7.96126568128444	27.25426408601457
C	-9.11153127457723	9.70824799994962	27.88137069959439
H	-9.19552117846694	10.78160612101207	27.64848978167244
H	-8.92159713997090	9.62294798426630	28.96168380180283
H	-10.09039112945371	9.25004196907632	27.67028649446416
C	-8.30167673290695	9.21966470851804	25.55344602728720
H	-7.50547554357118	8.77687559891357	24.94220516983574
H	-8.36762970730414	10.28639435789905	25.28670873151432
H	-9.25754741888564	8.74675516227162	25.27894175300125
C	-3.16357495259477	8.32326275229002	28.50525028218911
H	-3.33982400508136	7.34269717856712	28.03442642990690
C	-3.18250843265151	8.09418840588939	30.01753515846218
H	-4.10771830944414	7.60318866069905	30.34825493357640
H	-3.08882885864015	9.04898517809840	30.55932912440502
H	-2.34138549135842	7.44980069600051	30.31895023788978
C	-1.79005134529451	8.80829553721300	28.05309118130043
H	-1.76908898264085	9.02499981833346	26.97427549565505
H	-1.03262923443291	8.03660969892274	28.25183974820374
H	-1.47736668743688	9.71694463245320	28.59112037283483
C	1.52930109458672	5.11745520698813	22.34177018290680
H	1.49906040217697	4.88500297782652	21.26709420100861
H	2.26444466157447	4.42588562811699	22.80635491658950
H	1.95924643135620	6.13785188901250	22.44198755901962
C	0.25883251144977	5.24083216770849	24.35474489295589
H	0.47481806866667	6.30147919598787	24.61661028595114
H	1.03649031502824	4.63197898537714	24.86014528499709
H	-0.70485085087057	4.98304560746211	24.81592941066420
C	-8.30274307746269	5.51266776114796	26.15311888111991
H	-9.13737934794271	6.24253630413707	26.06921452629659
H	-8.11617490712598	5.35786972961185	27.22745556903357
H	-8.69589235066999	4.55391055596384	25.74808862775123
C	-7.32770150614575	6.18109318915139	24.07226634628539
H	-6.42298396409713	6.58274893003582	23.59707990113504
H	-8.13454365330069	6.91653937447078	23.88070631325769
H	-7.61081130269451	5.25826070827795	23.52453912922422
C	-4.49452702546526	8.26917232196017	23.11399147063746
C	-4.62759150462487	9.37437076218081	23.98339725790153
H	-4.06872338289595	9.38514388332345	24.92493183649009
C	-5.45352604201261	10.44517500929913	23.66122439294210
H	-5.52554036330561	11.28173016700222	24.36045418459078
C	-6.20024773475042	10.44485743459737	22.48214125014304
H	-6.85900480484259	11.28132618109631	22.23946686252671
C	-6.10405608590256	9.34252660500131	21.63183980019270

H	-6.68891471032537	9.31102632752680	20.70823732860142
C	-5.26971981165015	8.27499413853994	21.93835237029853
H	-5.19255857778442	7.42378993226886	21.26014588556130

Table S20. Cartesian coordinates of [L(Me_2N)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) = -7539.14180564 E_h

Sb	4.73859264137936	8.17882259457493	6.90543274303859
Sb	5.91702267341003	8.68946659715297	4.46865644320799
Ga	5.00495213864000	6.72921120694701	2.89864167057028
Ga	6.86537817205024	8.93534683424663	8.35180481774364
Si	2.77029569384425	10.15136545461158	5.12685612642757
N	6.72905727577554	5.88619132291991	2.28046452118848
N	4.48730751543042	7.18225805987951	0.99570721098138
N	6.99603783842453	10.72076038868592	9.17544219311848
N	6.49317352292845	7.94714471749921	10.08672952987910
N	3.82643983583692	5.37013474453142	3.39655352657427
N	8.52453119184184	8.35492780848017	7.69766844969542
N	4.41343814932050	9.68620337240397	5.50088363627071
C	6.80577415891259	5.26193977471988	1.10454519026922
C	5.91191691429375	5.48179769503108	0.04896661273641
H	6.09427219656737	4.90919848026194	-0.85940670680234
C	4.90837847582809	6.46450026873982	-0.03751636154590
C	7.91270985828306	4.26984734160403	0.86693239466702
H	7.90047598268707	3.90484965240992	-0.16680183776463
H	7.79229278056676	3.41357192146962	1.54753767266603
H	8.89952942657426	4.70016993642488	1.08569334279431
C	4.30143975488018	6.66533211092344	-1.40066719188463
H	5.03554193635205	6.44418735665499	-2.18561635019302
H	3.91539626971906	7.68311065103647	-1.53678333029124
H	3.45498670666732	5.97310059797267	-1.53046508660605
C	7.87881364618112	5.83215243291610	3.12555953395369
C	8.88884147762098	6.80586849980781	2.94244893742643
C	10.07540541964281	6.68065284379041	3.67004531305750
H	10.86850420048297	7.41832165274880	3.53305479086305
C	10.26609660707766	5.62951707295546	4.55940067142155
H	11.20524529421809	5.54152298776484	5.11034405506988
C	9.24232879197621	4.71629286300947	4.77364872952101
H	9.37738075675860	3.91871443621625	5.50834621062770
C	8.03223180282532	4.80580036777092	4.07945918943199
C	8.72147316884608	7.94106638061901	1.94797927514333
H	7.63866764606333	8.06678317467369	1.79238962800040
C	9.27311611532088	9.26644726421479	2.46678690833012
H	9.00975985739263	10.08088966689032	1.77470492210371
H	10.37130113743913	9.25403373876104	2.54561942375015
H	8.86146532505813	9.51446708941525	3.45651863199868
C	9.33336082996920	7.60295783392864	0.58661056901440

H	8.83733954798342	6.74501570626532	0.11286853646644
H	10.40513125730892	7.36722479380741	0.68730526152126
H	9.23899900810214	8.45797154661862	-0.10088779130820
C	6.91657181294987	3.83135860731483	4.39363074934347
H	6.11028881741381	4.00640570874586	3.66714076847668
C	6.34893303773539	4.13414851624793	5.77998300853228
H	5.99975505709226	5.17603706489489	5.83792083730453
H	7.10704172062313	3.99126383845105	6.56687696246161
H	5.49778312400033	3.47485697368095	6.00749246682572
C	7.34767064164792	2.37023933627417	4.28474075031739
H	7.76878160130289	2.13753903255839	3.29475252904741
H	6.48586194518076	1.70494773388791	4.44923975351242
H	8.10963288734578	2.11183394113352	5.03702808791740
C	3.54116021348931	8.23104969925916	0.80311891554587
C	4.01992932883758	9.56178010563083	0.76694200380135
C	3.09789782396383	10.59840011995841	0.61221815493313
H	3.45102586909578	11.63025007965311	0.57535344276030
C	1.73520958769920	10.33911347467082	0.50552917994676
H	1.02775065102476	11.16430767357948	0.39654429148963
C	1.28097042941030	9.02849217478282	0.53615644857938
H	0.21021406683340	8.82850766506497	0.45000659602518
C	2.16388248924840	7.95209335050906	0.67758696631488
C	5.50759214304958	9.85042423211068	0.82878549796628
H	5.95152402345668	9.06831752021728	1.46552195951970
C	6.15463991754266	9.72465568725482	-0.55171094448026
H	6.04871919931730	8.71254844483298	-0.96524798087907
H	7.23137364953339	9.94847147526129	-0.49477508887871
H	5.69782158673461	10.43264946325599	-1.26161773185796
C	5.84815606658685	11.19501612651232	1.45904217271030
H	5.54724006257550	12.04072529964137	0.82089908762080
H	6.93423627569354	11.27424152885576	1.61316488862342
H	5.36678476339669	11.31940829217710	2.43913790686554
C	1.60444182655439	6.54170738296818	0.68150108016802
H	2.45439554114603	5.84540861978005	0.69519291105710
C	0.77531483080691	6.25938286756540	-0.57318761171348
H	1.32138423812865	6.50492965211672	-1.49603741191280
H	-0.15749267928199	6.84490080966745	-0.57910160586357
H	0.49246843853965	5.19592450835481	-0.61395667146660
C	0.78358064044811	6.26544347592690	1.93944435525276
H	-0.05763567263298	6.97050649727617	2.03192399215562
H	1.40813383823066	6.35590353077052	2.83618984268255
H	0.36662797760030	5.24651845301745	1.90948037552742
C	6.22585099052095	10.97632142103442	10.23591473460763
C	5.58895051819178	9.99142219942240	11.00080902383556
H	4.97553738309883	10.36539413922328	11.82089152092298
C	5.86503395261657	8.60591874061362	11.04572709274848
C	6.07171039800702	12.39455622155780	10.71523152986988
H	6.14925701454159	13.11766105599300	9.89404881498229
H	6.86323128109040	12.63840328032827	11.43919137536264
H	5.10669225260562	12.51602316160146	11.22452682650100

C	5.43115337515261	7.91447079139366	12.31021252660750
H	5.78391298907330	6.87876367446394	12.36642301161079
H	4.33247878357004	7.92040010863100	12.37161262044516
H	5.80489212831707	8.46832929217532	13.18281881988889
C	7.87411674636308	11.74014904012772	8.70231526836675
C	9.02538017355306	12.06679408256707	9.45104772090840
C	9.85620348748649	13.09209864986692	8.98841256488707
H	10.74825898957326	13.35566272231054	9.56214178196198
C	9.58128815319076	13.76335200732314	7.80572469740915
H	10.24258048090551	14.56060166583504	7.45820404698679
C	8.46902364535612	13.40075662161006	7.05427972531358
H	8.26915157764685	13.91541904520910	6.11381057597225
C	7.60073190378853	12.39228864442714	7.47925585412157
C	9.45268811587644	11.29007047319913	10.68207056146273
H	8.65801199293598	10.57013546230104	10.92872410456248
C	9.67773396024460	12.17874987486619	11.90481866481756
H	10.52307441129241	12.86850530761421	11.75432688533758
H	9.91027967714212	11.56324031027770	12.78773703056255
H	8.79443200372190	12.78947983464707	12.14306364918079
C	10.71505460886316	10.48996333731884	10.35915830669736
H	10.53917615909200	9.79573845016678	9.52567644061499
H	11.04135289088983	9.90683859818392	11.23341758611946
H	11.54355206167035	11.15800369738398	10.07624164636838
C	6.38575420769881	12.02964737392936	6.65412980416980
H	6.23848069329958	10.93691963478446	6.71598403743972
C	5.11621156811570	12.66619387787305	7.21724410509377
H	5.21417693256349	13.76294591639297	7.26508401038857
H	4.88314267600600	12.29535852526640	8.22441210069312
H	4.26270911766905	12.42041226165978	6.57225736317847
C	6.53075302607322	12.36176154077432	5.17524371609245
H	5.68181994779142	11.92453310398530	4.63379180744438
H	7.45632781228267	11.94388463078728	4.75121398668683
H	6.52316794839566	13.44776127877031	4.98882480611330
C	6.83129413520069	6.56460646754091	10.21627851657763
C	8.17444580381552	6.22722161299964	10.50792487385428
C	8.53164272944560	4.87889185213209	10.56066283434981
H	9.56510315957647	4.60904050804943	10.78186220658688
C	7.59918557172543	3.87311905286326	10.33615283270854
H	7.89954668440308	2.82349434265333	10.37725267390983
C	6.28296665930374	4.21417021545405	10.06614353726121
H	5.54750476297603	3.42403597523428	9.89918654392718
C	5.86855448971638	5.54996341394364	10.00100217851706
C	9.20480862708978	7.29525801811824	10.81555274231414
H	8.92930444488833	8.18119720232689	10.22542492274939
C	9.16083554214946	7.66161613748491	12.30049744109215
H	9.89646523981835	8.44717405813295	12.53338664454341
H	9.39118698500675	6.78571558621761	12.92840945672333
H	8.17073508528352	8.03446063120591	12.59848070332044
C	10.61346090350616	6.90111795404034	10.38674780450516
H	10.63453789358917	6.61264374585910	9.32583364577658

H	11.01503967131364	6.06637369843588	10.98291520046017
H	11.30200598843819	7.74675204545337	10.51906580609382
C	4.39843655326050	5.81522611265552	9.72650162662206
H	4.26939692360520	6.90017572205782	9.58007170070185
C	3.51344910205309	5.38359313798910	10.90012379648881
H	2.46180646741894	5.64385583475496	10.70266557293366
H	3.80779230683516	5.85062497946282	11.84801737044775
H	3.56397461291811	4.29230221490404	11.04142832405727
C	3.92161942369813	5.10581906175465	8.45867006364982
H	2.90598489457662	5.43328651570681	8.19013478013329
H	3.89274564931033	4.01425908290157	8.60136848268942
H	4.57273157985254	5.31149718958153	7.59987928253555
C	3.17568701317181	5.27713490210690	4.66838421922098
H	2.06822865321660	5.23955961684267	4.57897953851954
H	3.42549797100396	6.13953740601645	5.30485462403964
H	3.47056565614632	4.36511662793368	5.22870113741916
C	3.63151435585590	4.20590415118322	2.58335238268406
H	4.13006842325691	4.30537470566622	1.60740910156124
H	2.55704596973693	4.00495760505735	2.38641703335955
H	4.03228422267366	3.28183093913382	3.05820090317155
C	8.49659563992064	7.02450227774239	7.14965013355815
H	8.17243263879994	6.99137861452732	6.08738958000401
H	7.82247793743323	6.36423192904749	7.71759381990391
H	9.50055931230491	6.55733194160878	7.18098099092989
C	9.37795230165242	9.21238186773933	6.91855708193208
H	9.06539892803818	9.29386882368701	5.85339309267372
H	10.41672346850392	8.82316929065116	6.90666771535845
H	9.41665208297523	10.23088677186244	7.32881622790354
C	1.88334212984553	10.51357149916076	6.75211106145413
H	0.87995774021473	10.92636198831901	6.55837489822949
H	2.43828411709221	11.23776207105741	7.36726111902006
H	1.75767929035852	9.59275697569194	7.34411711220054
C	1.81876250331983	8.81132974655150	4.22244729775567
H	0.78551171128143	9.12344956433195	4.00217313129002
H	1.77732571507148	7.88719798389276	4.81877449851823
H	2.30143621176395	8.57565830102556	3.26280059063610
C	2.76769539303069	11.70649045479226	4.06655906469106
H	3.29837867843327	11.53279637722741	3.11998276375834
H	3.23739227704905	12.55968221856106	4.57816750230003
H	1.73185095798009	11.98548471753007	3.81378811665907

Table S21. Cartesian coordinates of $[L(Me_2N)GaSb]_2C(H)SiMe_3$ (**11**) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7520.22183531 E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.57348089 E_h
Enthalphy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.55169516 E_h
Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.76215720 E_h
Energy (PBE0/D3BJ/def2-T(Q)ZVP) = -7523.09516169 E_h

Sb	5.66507803460978	10.40226385574637	6.68500430936089
C	5.41094507346289	10.02555220551102	11.51334826661856
Si	5.29780939099186	7.46567161160285	4.44248607973482
C	5.34725359948886	9.29314689970844	4.83464223717975

H	5.98201382286831	9.80858979893194	4.09991219809858
C	4.21257698848048	7.20521236284187	2.92809272537908
H	4.53077911209326	7.84462705049495	2.09144601213760
H	3.16336108792408	7.45680622681770	3.14690497742620
H	4.24602447021574	6.15779109415691	2.58668819228583
C	7.04122784797728	6.89258035649236	4.00843185771611
H	7.04159323683814	5.82899836464710	3.71989420929283
H	7.72549281217846	7.00834767865180	4.86041459666397
H	7.43844423964176	7.47472061196568	3.16124417028538
C	4.60051425273985	6.46667933731183	5.86007387139399
H	3.58251958221004	6.79869834692411	6.11106337451377
H	5.22481785116943	6.56260907671314	6.75820477309058
H	4.55391981535570	5.39780077061564	5.59994467118568
N	5.15487701635113	10.38634094841797	10.25511241736984
Ga	4.88441707910090	9.01793818301843	8.81396521553333
Sb	3.45070632784750	10.37741699024679	5.00609361569681
C	5.94954931273302	8.78282809322818	11.86492292987151
H	6.12964389643309	8.62025266578447	12.92674295021726
N	6.20269413297117	7.76034774283499	9.69336603432952
Ga	4.00848581180223	12.30739285310346	3.30903832393523
N	3.22347542098400	8.20940825000905	9.06741280786984
C	7.25825676627871	6.70176403136338	11.64566711827607
H	6.59865189780521	5.88568853522527	11.97872550599249
H	7.77882470364589	7.09111780092971	12.52950410762636
H	7.98907219526909	6.26740858694534	10.95223187641355
N	3.12814135229507	11.90820040837288	1.54689040399756
C	5.12873868171730	10.99458308487934	12.62988312040834
H	5.63563411711892	11.95670794036022	12.47537133072163
H	5.43199377058260	10.58020786722436	13.59860883399989
H	4.05116965604603	11.21593575103205	12.65735535873718
N	2.91697673590168	13.96232868997092	3.56160274213129
C	6.43743732725014	7.78608531387185	10.99949052514212
N	5.75581638637486	12.82944151369908	2.89571203953626
C	5.00105046474219	11.78020161695089	9.99791628752877
C	4.79238602782893	14.55108923753320	9.77675563511336
H	4.70964565288633	15.63903825609048	9.72051195091990
C	6.04404170948130	13.94494635021765	9.75916011322321
H	6.94033989273057	14.56263808004547	9.66863877320006
C	6.17407416664935	12.55813979985200	9.84837780752452
C	3.64876344145766	13.76701962182145	9.83682994375518
H	2.66668112407316	14.24289952204503	9.80349801136504
C	3.72628414362955	12.37502822459214	9.94344845824747
C	7.55135416660078	11.91897008291939	9.79691038161544
H	7.39633819642079	10.85227331213373	9.57285996362762
C	8.41284052362252	12.50567897255196	8.68016651087440
H	7.89076088485755	12.47017345258086	7.71243439624622
H	9.35009436587551	11.93574810073273	8.58465233446487
H	8.69095360474846	13.55204167786117	8.88121433524839
C	8.28416924886223	11.99686347199486	11.13738049352802
H	9.28965441869047	11.55577723196505	11.05164067293832

H	7.75347869886912	11.45242710230431	11.93024530066343
H	8.40146894154396	13.04382884518101	11.46106612075031
C	2.44968886922031	11.55995946095395	9.98216052046396
H	2.73245812041022	10.50381884240614	10.10036121479183
C	1.54629084584577	11.94179400685732	11.15391543910379
H	1.18677458378281	12.97973156914140	11.06799671269376
H	2.06565232417504	11.85090062361540	12.12005467007522
H	0.66154929759849	11.28692910274016	11.18470274779787
C	1.70810571318929	11.68994625921181	8.65204887328681
H	2.33460810785616	11.34285066295757	7.81693276502866
H	1.43475356124445	12.73549471790871	8.44222712703961
H	0.78473994637886	11.09073735095162	8.65723309395091
C	6.79032295142064	6.74211386266823	8.88724523203133
C	7.91099627715827	7.08111115666586	8.09459108614699
C	8.47433977181755	6.09598067387967	7.28150583168766
H	9.34514456736050	6.33812192811579	6.66993573853871
C	7.94476631150129	4.81046512536224	7.23707841843240
H	8.39239158118868	4.05618186483284	6.58595155149471
C	6.84620996526198	4.49203880153410	8.02294970475367
H	6.43244460900784	3.48156521833162	7.98358152594819
C	6.25010831234662	5.43821730290869	8.86362580904785
C	8.52831007930391	8.46409236278673	8.17524719641608
H	7.70742181348643	9.16382228774809	8.40177726349241
C	9.52282211510813	8.55739809661625	9.33381013790581
H	10.34218584946811	7.83228334719208	9.20414195100794
H	9.04360623145956	8.35794833662115	10.30242165836229
H	9.96529776018142	9.56460621011023	9.38318818017849
C	9.16697637245942	8.92847320172733	6.87159960549550
H	8.46835706286281	8.84204138676745	6.02633815557540
H	10.07583918403659	8.35624509946165	6.62720051629749
H	9.45959760159082	9.98569429146944	6.95343238807464
C	5.05419504050144	5.02320254030095	9.70142771080982
H	4.81691997431671	5.85307138840055	10.38143467049774
C	5.35621102142335	3.78516319377611	10.54825262783053
H	5.47424203781424	2.88721003696370	9.92166626039934
H	4.52747865228068	3.58765277382070	11.24581737943530
H	6.27989936809045	3.89760707574119	11.13536127023819
C	3.81454739993704	4.79285031514058	8.83840370237406
H	3.52266255530097	5.71910001151706	8.32838641776410
H	2.97089150020941	4.45949067935545	9.46295093728727
H	3.99608161493163	4.01838910986438	8.07645274090416
C	2.55102181338101	14.69807701773395	2.51368008392430
C	2.54516734456220	14.22306617033704	1.19309940995332
H	2.25751822142398	14.94233489960098	0.42826083740039
C	2.70674745590411	12.89538402020579	0.76040004884492
C	2.08991009768502	16.11280777635893	2.73276662272993
H	1.86739686663825	16.60634874411701	1.77956809925504
H	2.86207725095298	16.68498829290548	3.26669595559286
H	1.19420121765348	16.14542966571020	3.36811161128191
C	2.37003247977949	12.60552936320966	-0.67715283723878

H	3.27427739518564	12.30026850083192	-1.22418380284972
H	1.94144788565545	13.48838821707863	-1.16551483071518
H	1.66307871366116	11.76814788278960	-0.76006055549132
C	2.59096701034078	14.44867932767871	4.86245598667175
C	1.28565297528071	14.22928029142441	5.35748050660655
C	0.92759585342831	14.80992828974023	6.57670456794309
H	-0.08504487688884	14.66343823688154	6.96138920712871
C	1.83371207097332	15.57352975659620	7.30301737535176
H	1.53105775717526	16.03639646675693	8.24555937897831
C	3.13051117720264	15.73040939312231	6.83126557722832
H	3.85082438526150	16.30677394428830	7.41569907149581
C	3.53805804434199	15.16938169864715	5.61781585055981
C	4.97234869356026	15.34936526698214	5.16145582359789
H	5.08568308700044	14.82488454967983	4.20199408765409
C	5.33393246462014	16.81848256276814	4.94528285924870
H	6.36542069258214	16.90796179550946	4.57032673060224
H	5.27048806688229	17.39404301769579	5.88281810305906
H	4.66929188540897	17.30287247781673	4.21389691398119
C	5.92938184557975	14.69105088728784	6.15456202824919
H	5.69526972622004	13.62421680875884	6.29012293015174
H	5.87039050411850	15.16450943361027	7.14590530717384
H	6.96980699564562	14.77087565192519	5.80476833495778
C	3.05013411134664	10.57485435887701	1.03926473481354
C	1.89104994217219	9.81461167855951	1.31341274193720
C	1.75134759246712	8.56929967274380	0.69498060767556
H	0.85614460099740	7.97451872725074	0.88404272675751
C	2.73382755170970	8.06986525344012	-0.15165647014680
H	2.60262714672784	7.09648173811098	-0.62965673240647
C	3.89902363040133	8.79718955957966	-0.35455632891815
H	4.68937821646231	8.38359690912173	-0.98555372981233
C	4.08572446517385	10.04915398309598	0.23929082575287
C	0.80627225520408	10.33540188669206	2.23894181806525
H	1.30154121186198	11.01565341993397	2.95110915025619
C	-0.24690172417136	11.15698522437203	1.49351802518005
H	0.18215417762693	12.05853781223580	1.03443969201227
H	-1.03861652960299	11.48566430210728	2.18503510551670
H	-0.72074989337097	10.55869378588003	0.69865703206250
C	0.14987281556188	9.22416068020707	3.05270572896349
H	-0.47108864311981	8.56472834836647	2.42662647665518
H	-0.50800972871395	9.65517380619364	3.82080601165570
H	0.90120736339785	8.60553439742698	3.56587700183815
C	2.79216566291002	7.79868406290832	10.37189301359890
H	2.00733826078927	8.46618172365786	10.79495483936265
H	3.62558319901649	7.79270593536155	11.09022456790814
H	2.35533943165513	6.77824341005164	10.36415662033761
C	2.16799544674993	8.18968541301833	8.09993194523942
H	2.50022239464842	8.61121416663604	7.13940245782003
H	1.28553462055397	8.78214241574078	8.42156967806163
H	1.79607294616375	7.16091080081453	7.90205566677910
C	6.04199380015522	13.78731184572709	1.86855656301987

H	6.81348103240615	13.42150045573658	1.15642116885291
H	6.43296773354124	14.74728728566097	2.27627818367127
H	5.14561154332125	14.03297962933811	1.28069346158645
C	6.92358390130204	12.45993266245541	3.63778197011565
H	7.65710545820064	11.88967999520976	3.02801680714605
H	6.66847685955546	11.84306117816841	4.51212829383813
H	7.46746230813170	13.34456764320318	4.03016495544442
C	0.26648262258340	13.39186927785716	4.60642973609455
C	-0.19150103439257	12.20083006962716	5.44719840687310
H	0.76399737961219	12.99523799164026	3.70947229270688
C	-0.93252560296605	14.21779129430698	4.13932854389340
H	-0.62980115274194	15.04530176117160	3.48154520227749
H	-1.47873747137469	14.65023193388598	4.99279519012790
H	-1.63925571261746	13.58805644794733	3.57666801248967
H	-0.90797129164035	11.58407042339845	4.88358602492151
H	-0.69232844785534	12.52598653327016	6.37239075555205
H	0.65596099693677	11.56109780087131	5.73517886316801
H	5.04262626252064	11.35706351751334	-2.03401023895298
C	5.40003316570456	10.77760547194131	0.04951262694848
H	5.27468502963298	11.79226820491233	0.44852934713748
C	5.82348099302730	10.89126233865732	-1.41336705903828
H	6.05125279644231	9.90753031311515	-1.85318286598282
H	6.73332356056763	11.50520148547118	-1.49971735732577
C	6.48885764690551	10.10174943060851	0.88374437271920
H	6.67189869599570	9.07101153637591	0.53902865157498
H	7.43653798823266	10.65804751682903	0.81504459189105
H	6.19809288112109	10.05908793920913	1.94247890528694

TableS 22. Cartesian coordinates of [L(Me_2N)Ga]SbSb[N(Ph)Ga(NMe_2)L] (**5**) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7358.65076302 E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.54393203 E_h
Enthalphy (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

Sb	3.62971731815856	23.46636438542158	7.83175894299146
Sb	1.55861151087495	24.73029951250967	6.75655325842390
Ga	3.53830615006852	20.37905880974398	7.98758156529777
Ga	3.15578731072583	26.57989126828297	5.88135961648900
N	4.96355710865099	19.50931445878630	9.02284437482003
N	2.49042042784445	18.77100915215630	7.69089398377862
N	2.07153301053216	28.23225369688553	5.54648589874501
N	4.44795958680398	27.57753547563255	7.04980790488430
N	3.95001269780010	21.45746396261961	6.42783938649810
N	4.13742656304107	26.23917673454259	4.30996735215322
N	2.76449996112884	21.84415995904685	8.83933377351010
C	4.70372642363799	18.39569117117204	9.70079293148613
C	3.53704707937108	17.62666109177645	9.53319179999785
H	3.44559984664022	16.76411437263904	10.19178488901184
C	2.54325406084802	17.75683248257922	8.55550030036704
C	5.67147951205650	17.89014534326435	10.73348652771932
H	5.76247481624411	16.79777257424036	10.66990644446872

H	5.27597472695579	18.12781215398244	11.73270578599555
H	6.66342538476396	18.34679724572452	10.64141432496449
C	1.48163587012895	16.69729840804731	8.49875846341320
H	1.29636853615782	16.36485044019961	7.46847433324135
H	0.53292297479626	17.11604115369298	8.86850907629431
H	1.74945203274421	15.83443128326633	9.11932692525143
C	6.19430551445581	20.21783086312118	9.19717122009041
C	7.22016201208299	20.01128320571408	8.24510770086460
C	8.39404478642977	20.75792130143021	8.36716616034387
H	9.19788346439088	20.62087051159971	7.64251596441058
C	8.55571904892607	21.67899547487986	9.39825490153773
H	9.47910834368471	22.25816420742171	9.47310206350732
C	7.54573045287159	21.85415557733959	10.33318702424016
H	7.68183999372062	22.56869623497424	11.14779388728404
C	6.34894850205002	21.13268236626932	10.26026518091226
C	7.06124919432183	18.98525830616633	7.13495889227624
H	6.00618731689416	19.02045206287097	6.81618987546475
C	7.32514896753124	17.56091502226458	7.63020124721954
H	7.24266624750791	16.84539963670930	6.79699447052180
H	6.61016546899128	17.24836674379840	8.40100674909105
H	8.33963504189723	17.47611654280538	8.05062131751557
C	7.92783744180495	19.26850755963406	5.91178918012882
H	7.63570429626255	18.60562667467583	5.08312500350207
H	8.99274159891905	19.07559934608368	6.11630363107536
H	7.83467273116161	20.30705124586621	5.56429110585400
C	5.30159926351389	21.33045126253933	11.33988559891616
H	4.41545367455609	20.74073110688733	11.06742968324861
C	5.80431047325757	20.83750817242304	12.70014352093474
H	6.17249366467719	19.80308871210937	12.66844344968905
H	4.99447738614323	20.89220919865628	13.44400589524621
H	6.63191975412696	21.46750412285092	13.06346229497042
C	4.85055927302338	22.78302953950452	11.46571107428425
H	4.59500017897883	23.21614350543019	10.48974158459829
H	5.63965585093313	23.41016154341949	11.90903787310341
H	3.96076964065280	22.84910787439504	12.10891847304651
C	1.60354716995790	18.70358361815658	6.57283799388481
C	2.12163375144979	18.19521957663911	5.36004507251131
C	1.26795042478834	18.12439821496779	4.25822504041808
H	1.64075483648902	17.73383586615693	3.30971686009989
C	-0.04940138031228	18.56777134622833	4.34398430252837
H	-0.70133901388293	18.51202321384108	3.46911004742571
C	-0.52744285028194	19.09862261549374	5.53446423122654
H	-1.55460401080921	19.46725795933387	5.58687838792276
C	0.28338278961843	19.17910170383028	6.67267347855421
C	3.57748787108357	17.77105070690194	5.25452100553795
H	4.14103491585627	18.41683073531297	5.94922021174807
C	3.79969177788357	16.32729234376201	5.71001197937910
H	3.20048195547188	15.63126326669917	5.10165516718342
H	3.53074644429206	16.17769033474883	6.76396553055297
H	4.85939097145664	16.04814135982086	5.59944793341343

C	4.16937802051485	17.97926429290752	3.86358367585953
H	3.75935566343336	17.26671528216983	3.13081179688328
H	5.25844290336265	17.82069193529936	3.89140333502063
H	3.98506576341597	18.99564551848451	3.48511915427323
C	-0.26359315118139	19.79832070493908	7.94361261964193
H	0.49923250747838	19.69293661533066	8.72878778175183
C	-1.52997325356624	19.09499880526893	8.43253429912879
H	-2.37219056215096	19.24958271294005	7.73961289488731
H	-1.82931795662757	19.49874656279684	9.41164955130063
H	-1.38865432787311	18.00833317866655	8.53979644046761
C	-0.51404766845293	21.29581314213996	7.76624459958971
H	0.40356745748764	21.82927390523383	7.48142033536231
H	-0.86136766925589	21.73858553642263	8.71144065713998
H	-1.27529397757382	21.48867625159003	6.99360192669882
C	2.63612582684524	29.43333547121990	5.50857621527816
C	3.91099398435881	29.70390374376806	6.03463732344929
H	4.27511233719092	30.72198663302727	5.90619817607148
C	4.70323086249816	28.86540163608620	6.84008034887203
C	1.89205724652173	30.57782357553889	4.87686284475972
H	1.77509650317009	30.38646579904013	3.79903884765078
H	2.42625746632728	31.52546788166883	5.01303790402975
H	0.87664271534049	30.67298079238114	5.28351501202539
C	5.90134160615777	29.49377963772683	7.49864796183609
H	6.82685414965188	29.09023125832056	7.06204343557899
H	5.93378636141544	29.25760658752026	8.57133184795891
H	5.89689765318595	30.58231742020269	7.36854027021082
C	0.67227368062438	28.10494999853585	5.31150927755585
C	0.18409805889611	27.69255102046032	4.05545489474774
C	-1.20008848901058	27.61824825248001	3.86933263503989
H	-1.58951377668268	27.31092736837050	2.89541497926462
C	-2.08573765949677	27.92154975357505	4.89475120332148
H	-3.16375112354326	27.86170373912927	4.72719754142769
C	-1.59023099945670	28.28194593260662	6.14244896700078
H	-2.28696606875048	28.49429096629818	6.95719684559498
C	-0.21667895977496	28.36917591139652	6.37961596123378
C	1.10443977892625	27.31290350892886	2.91252715427035
H	2.13759765956930	27.36787590069304	3.28540821896093
C	0.85620087667927	25.86703424343024	2.48238504660510
H	-0.16695001901409	25.72941734243356	2.09768451853477
H	0.99371729019543	25.17686262072870	3.32876460254821
H	1.55423019313917	25.57434613180206	1.68334550265362
C	0.97349760142655	28.26967063685953	1.72776735861693
H	1.68749847657895	28.00117807008114	0.93326120499299
H	1.17253843649688	29.31150130188842	2.02097894334434
H	-0.03845099314414	28.23753751457257	1.29252220865715
C	0.27653692829388	28.73655019208433	7.76737083065330
H	1.36731062646055	28.59864817221040	7.77273997772299
C	-0.30725254063681	27.80909622861392	8.83171036867249
H	-1.40340213060133	27.89572320741755	8.89331898334627
H	0.09603323160764	28.06465294690408	9.82357052534619

H	-0.05834388252010	26.75805001445713	8.61938356815476
C	-0.00802115290309	30.20002760415824	8.10886994374228
H	0.46730177420922	30.88940371864578	7.39642125449900
H	0.37429983857365	30.44388395943325	9.11255569323644
H	-1.09056551845250	30.40629295595107	8.10382725456994
C	5.20815691242775	26.86558570736814	8.02415187153472
C	6.44862872185162	26.28466935811365	7.68874505783195
C	7.16987051758106	25.62207760346878	8.68790436378587
H	8.12847267825148	25.16121991696827	8.43751451021346
C	6.68981188512194	25.53892695103715	9.98511916822814
H	7.27314970766420	25.02981089620573	10.75506384972017
C	5.44974344545597	26.08542420730301	10.29659011812398
H	5.06437017196451	25.98672780856490	11.31181335070737
C	4.68033060474833	26.74000131773993	9.33219179394604
C	7.01361431645112	26.31942303273077	6.28349855679464
H	6.36193214841121	26.96319160351153	5.67865511776025
C	6.96252830749705	24.92432653566505	5.66468036148752
H	7.32761173671792	24.94231453867087	4.62574672477939
H	5.92985740892087	24.55179230501983	5.65460873584771
H	7.58004040022020	24.21073666000788	6.23425990031695
C	8.43259820076617	26.88487009197228	6.22956469480742
H	8.76671426778727	26.97859260701186	5.18449062048614
H	9.15217944964427	26.23035235825820	6.74645448568776
H	8.50082492200675	27.87907982779096	6.69666419078817
C	3.31283095694676	27.29490855681225	9.68796196160056
H	2.67039297701120	27.10566894509362	8.81070213518591
C	3.33633666981082	28.80404452396360	9.94138048677777
H	3.60580305267380	29.37700359846532	9.04433480174469
H	4.05104253132757	29.05616490921622	10.74162330302715
H	2.34143392931611	29.15104514853266	10.26115036062421
C	2.67782081078976	26.57661080458730	10.87351198473564
H	1.62294444960608	26.87061434272871	10.97092417356298
H	3.17416668705425	26.83034981386273	11.82396741469673
H	2.70997244397937	25.48446212733674	10.75443198742325
C	2.90616608408119	21.44664081533863	5.41394755564849
H	2.93153872502025	22.37897382835664	4.82453635135318
H	1.90951967908231	21.38962419743013	5.87139340810449
H	3.01472626145544	20.59404283208811	4.72409249308706
C	5.25898400246136	21.52714101866823	5.80767393698219
H	5.47459602112694	20.63139246212681	5.19768823910065
H	6.04612007638088	21.63862522647858	6.56621759380737
H	5.31448146243578	22.39972333734446	5.13439321486264
C	4.84700114918367	27.25958857524029	3.59894716475821
H	4.36259005146635	27.52855235377587	2.63169206242751
H	5.88374547375334	26.94932220216516	3.34111462441380
H	4.92030142331133	28.18703170899056	4.18570728076049
C	4.07446996887098	25.01045181957211	3.58254015128719
H	3.63253201879975	25.13213137040996	2.57055242241261
H	3.45721294893308	24.27530873338301	4.12164147702886
H	5.07768652105428	24.55578819997779	3.42480422413470

C	2.00196502479890	21.85561481436170	9.97946989564936
C	1.33523779274355	23.01504441016322	10.43542983921321
H	1.41065026744632	23.92786858278717	9.84126391689967
C	0.56780774924899	23.00214919964257	11.59425303194266
H	0.07112608904663	23.92477657831736	11.90776010512834
C	0.41744458180572	21.83704342558011	12.34881340655540
H	-0.18799130151577	21.83186453613561	13.25744846865397
C	1.05764775052949	20.67753341991493	11.91001516460704
H	0.95795560513497	19.74802769812656	12.47789603632399
C	1.83433009873664	20.68281220198687	10.75593108963444
H	2.33174441643295	19.75786033883190	10.44809591688215

Table S23. Cartesian coordinates of [L(Me_2N)Ga]SbSb[N($SiMe_3$)Ga(NMe_2)L] (**4**) [Å] for the optimized geometry.
Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7536.27671217 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

Sb	7.14999785461191	11.45254977245778	5.93201680926219
Sb	5.87062029324592	9.44283805155226	4.77397184371137
Ga	7.81586330454746	10.95993159585531	8.87459651095009
Ga	6.91662033568180	10.19670487691733	2.52591422903813
Si	4.78803565618545	12.15189080632225	8.21361129768302
N	8.65354902228815	12.32948001280590	10.02648825331427
N	7.56901998792504	9.62460675899353	10.29163024835168
N	6.15604323650077	9.03576510494803	1.08366860978726
N	6.30016274495626	11.87410412542476	1.60125948011098
N	6.35477946401301	11.48717991335248	7.85546806356637
N	8.86744678578923	10.37779263601182	7.35138705123067
N	8.78420956114083	10.25006738114927	2.28063433856365
C	8.20673385660465	12.41517865493010	11.27999937960998
C	7.47558248960803	11.40215458092243	11.92254942755269
H	7.13018884765515	11.64165408213554	12.92748267664631
C	7.30836763433696	10.06643382367522	11.52480477861663
C	8.46514014983930	13.64847349705129	12.10255525104297
H	9.16486238907184	14.34098333272256	11.62247836991401
H	8.84071032867996	13.38279307544325	13.09953986607301
H	7.50474485543997	14.16783254849585	12.24921255067629
C	6.86090552711590	9.09697534485875	12.58489849076350
H	6.13537906380683	8.37293633375930	12.19736109279222
H	6.42662010162203	9.63448869622182	13.43652343823695
H	7.71600863289918	8.50955516504122	12.94915139229267
C	9.69169972653183	13.20673677593916	9.57251478195575
C	11.02117324367052	12.96077095905651	9.98847333536606
C	12.03347756980919	13.81064619082977	9.53396955720841
H	13.06226950173848	13.63410298097344	9.85582055188126
C	11.75938799667710	14.86761351545762	8.67781367933103
H	12.56479144159439	15.51781671801792	8.32873929496903
C	10.45218426972344	15.08946386611435	8.26595663023373
H	10.23716878349271	15.91953892043161	7.59152253528792
C	9.39910919566610	14.27780735939906	8.69926720028414

C	11.40124486583358	11.82069353058159	10.91581753356941
H	10.52151962960167	11.17062178149239	11.02838411446478
C	11.78699853480423	12.32973264647120	12.30641118552621
H	12.69293552346190	12.95472164565316	12.25782410229418
H	11.99735547544676	11.48637764099388	12.98273122505404
H	10.99236971783988	12.93695796278191	12.75904842013400
C	12.53616931475366	10.97599155491833	10.33862707507721
H	12.28026016214516	10.56831007444030	9.35029236161705
H	12.76646094805152	10.13415533457485	11.00793453277495
H	13.46159521658547	11.56105171476185	10.22777237843132
C	7.98680993604108	14.61307267326659	8.26526450800023
H	7.39071524707772	13.68841896052392	8.31600612469432
C	7.36171943602958	15.62843528862662	9.22489171736312
H	7.95057628221697	16.55971634913533	9.24466785188768
H	7.30813802740477	15.24467235029479	10.25233084991605
H	6.33834039905509	15.88361192810460	8.90994832295264
C	7.91647972539108	15.12260176754451	6.82837175416820
H	8.44776865786846	14.45655763964514	6.13367619981237
H	8.33452727468408	16.13706835141989	6.72743223417139
H	6.87253266180318	15.16761462966451	6.49115729087726
C	7.60402590615115	8.20681439727881	10.08797579986434
C	8.80428263987293	7.51382752961417	10.36187285559335
C	8.78931294185375	6.11770376427248	10.31103152319970
H	9.70138233794083	5.56172871346674	10.53371119598916
C	7.63773893484419	5.42305552637991	9.96254460394794
H	7.64250492849199	4.33097731707397	9.93519969895918
C	6.49522888491358	6.12485345001811	9.60462483092650
H	5.61069994685733	5.57619287595575	9.27797901301687
C	6.45418298951679	7.52307310619681	9.64201172960677
C	10.10833476705337	8.24164016114685	10.64835586166575
H	10.03393080967057	9.22615218990321	10.15697052160897
C	10.34619906701216	8.49278442642991	12.13935732360495
H	10.26258112717077	7.55544090905294	12.71224034283419
H	9.63624312976241	9.21869539099139	12.55756231622078
H	11.35683913839487	8.89551717824951	12.30624585717695
C	11.30840543498232	7.51512565548490	10.04104004399266
H	11.13779171746216	7.25779389848559	8.98507546241836
H	11.53875082037444	6.58336280821343	10.58013088468110
H	12.20521525401437	8.14739819457214	10.09626971364224
C	5.19531832873832	8.24346790393505	9.19251514031019
H	5.49499737613303	9.24981542828283	8.85522018940413
C	4.18389664605512	8.40601003997371	10.33030528193298
H	3.23404512000924	8.80818953669929	9.94718082541222
H	4.53539655096586	9.09610964397177	11.10940500105542
H	3.96593985676902	7.43500823272670	10.80396717400682
C	4.54211037425293	7.54612777273984	8.00048102521892
H	3.75834009161034	8.18569864696422	7.57201120873272
H	4.06634328737829	6.59521617753799	8.28786472338263
H	5.26824495686058	7.34311377482743	7.19997384651599
C	6.09868159365493	9.44620157096121	-0.17944717565900

C	6.18803631699744	10.79513594794980	-0.55729328769705
H	6.14937770417837	10.99584485540648	-1.62690864062633
C	6.17126923488063	11.92731236137870	0.28114470047858
C	5.92919957221814	8.42880437933288	-1.27480172104905
H	5.80540720007487	8.91016538891354	-2.25206851015994
H	5.07241774702212	7.76885037252814	-1.08565608775389
H	6.81710705468845	7.77855971520890	-1.30751007949521
C	5.99999909322458	13.26239969326720	-0.39172861793115
H	6.95246302782041	13.81285360803209	-0.37724621305909
H	5.26881969635324	13.88711539519245	0.13916118034767
H	5.68422093570077	13.14038278969733	-1.43457300175673
C	5.69295062522676	7.73198017312576	1.41906830772890
C	6.59893917268000	6.67617236630218	1.64272563396045
C	6.08704423331134	5.40633507648838	1.92802352382597
H	6.78104160866458	4.57752932086676	2.08958494146597
C	4.71985156490690	5.17965064673102	2.01402786650003
H	4.34007183824286	4.17853316075778	2.23178014127183
C	3.83840963514024	6.24111195468571	1.84408763687770
H	2.76374695486189	6.06901531211837	1.94330740153755
C	4.29992550800667	7.52839412649487	1.56041902837431
C	8.10080473495811	6.87631067459947	1.60429415857722
H	8.28953601759201	7.94680132346876	1.43646130974828
C	8.75535100465035	6.09557215314472	0.46516204875036
H	8.32951050998253	6.36963077563595	-0.51197794790646
H	8.62163733728099	5.00882096721235	0.59045715753345
H	9.83755715819726	6.29727592079132	0.42955289029790
C	8.72238607144369	6.51403202609145	2.95363963823724
H	8.56580168968849	5.45141653873042	3.19891208610603
H	8.27801804737167	7.11597403334249	3.76168195537583
H	9.80763160510017	6.69716801786193	2.94360550296210
C	3.30224569170228	8.66542291203674	1.42865983114777
H	3.87901023103146	9.60045876632462	1.38065058575530
C	2.47524120192826	8.56531886101575	0.14604662954856
H	3.10622341535312	8.58165892235355	-0.75385211221599
H	1.77228387710439	9.41016437871101	0.07364266049866
H	1.88482617186869	7.63491731186448	0.12559914987101
C	2.39159184094715	8.75129782980000	2.65235753910117
H	1.71212739708204	9.61279419714943	2.56346669380250
H	2.97906417020096	8.87099580196593	3.57547554592734
H	1.76482316740479	7.85215385270140	2.75985579621933
C	6.11586924281669	13.05610116995180	2.37720650576029
C	7.17522764653858	13.96717669511717	2.57489156144862
C	6.92700675264843	15.12766600196447	3.31561652856061
H	7.73993790275540	15.84035498303696	3.47550795568561
C	5.67389834596272	15.38847757576215	3.85040740402783
H	5.49622673246344	16.30517530343655	4.41781525198090
C	4.64772996539280	14.46541230722856	3.67760143625107
H	3.67075215582393	14.66492587252586	4.11968248497541
C	4.84634233865197	13.28438077970436	2.95876651726261
C	8.57158895218270	13.72771599653094	2.03571045401358

H	8.53614964860327	12.81826848040712	1.42223234259184
C	9.06990288693113	14.87977736911555	1.16245673078311
H	10.04356822802430	14.62677031724667	0.71445906365546
H	9.20866730185248	15.80206856765195	1.74862989135269
H	8.37199035982955	15.11541466620081	0.34497156339176
C	9.55240288869768	13.46081334422464	3.17671991478558
H	10.54796741342716	13.20524469304353	2.78119713956313
H	9.20738029040642	12.62520628120574	3.80033109200998
H	9.66323650065064	14.34663578356746	3.82324862503859
C	3.71840664336134	12.28250829679886	2.79782165536481
H	4.19282230759863	11.28698108926210	2.78862957761856
C	2.96946321666649	12.45965690732649	1.47558860651827
H	3.61350037228627	12.27744838683262	0.60454878862217
H	2.55564224360445	13.47764316240041	1.39077474418026
H	2.12968899306734	11.74988482462409	1.41395031319068
C	2.74651242361989	12.29714233817234	3.97164434454282
H	2.13764258587910	13.21515872589679	3.99786109248512
H	3.27924688455876	12.20546947596644	4.92825589391288
H	2.05157168048895	11.44875985242463	3.89620977642982
C	4.66279781727929	12.48457851755044	10.06615370122414
H	5.42016865009574	13.21587518005861	10.38955732993761
H	4.80879259284307	11.56710933432735	10.65642325290434
H	3.66954942341963	12.89208535198180	10.31493226938177
C	3.36279559412813	11.03134934690338	7.70073152471795
H	3.53004281160134	10.63626239184398	6.68638731499143
H	2.41634989891795	11.59561777750473	7.70044770729583
H	3.24450082270471	10.17788415476903	8.38111105669920
C	4.50560596187670	13.78198042409264	7.30620083274654
H	4.75676370198833	13.69682280603295	6.23732478882289
H	5.11112035037662	14.59624293821872	7.72806242151542
H	3.44642410182906	14.07753857903389	7.37501075832706
C	8.87802033274607	8.94183773313082	7.13364523316322
H	7.87854471423928	8.51284966430037	7.29234103155812
H	9.58533503857634	8.42893494811902	7.80809728542985
H	9.16189601599368	8.70434400455235	6.09402438203954
C	10.16251244120422	10.96767457516914	7.06108057063042
H	10.46934513206288	10.73264235474350	6.02755002890995
H	10.95059584816902	10.58797391163153	7.73662189714407
H	10.12996141077660	12.06143893917991	7.16105325256175
C	9.73217879844301	9.85382995585764	3.27246180587185
H	10.29444317927515	8.93697698715568	2.99126244806432
H	9.22345685512557	9.64404274439583	4.22570010829077
H	10.49856559672902	10.63639575773278	3.46678453230445
C	9.38380181945192	10.42395115684577	0.99175271116663
H	8.65327923429464	10.77539654168658	0.24843416303360
H	9.82470659137999	9.48244492987064	0.58897844875266
H	10.21470744724797	11.16268733281626	1.01240194596873

Table S24. Cartesian coordinates of [L(Me_2N)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

Enthalpy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.54538584 E_h

Gibbs free energy (PBE0/D3BJ/def2-S(TZ)VP) = -7518.75505712 E_h

Sb	7.03461884703783	11.46526160314096	5.97027273829124
Sb	5.88663793235097	9.43882944427222	4.70172576373251
Ga	7.77570212424760	10.92729526750987	8.91502310524010
Ga	6.95123538660020	10.19827714454319	2.47237188824818
Si	4.66014901465613	12.34681421202372	8.40713190044964
N	8.65326730979616	12.33018436615076	9.99496997443190
N	7.60331534125892	9.60653252321315	10.38791750405665
N	6.22534267870681	9.04067855150138	1.00847820362925
N	6.30035379249443	11.87278675921126	1.56474983655676
C	6.09663061842225	11.24191936335396	7.93371033468520
N	8.82453838036140	10.34867178125892	7.38027144192964
N	8.81790905098786	10.28872677015962	2.24947859302999
C	8.22583984685453	12.45051989312475	11.25441814393945
C	7.50590294752536	11.45835873322900	11.93660216442293
H	7.17367512147920	11.73171342742575	12.93736073966388
C	7.33907331968461	10.10412405989859	11.59408364054488
C	8.49090162108513	13.71066637847478	12.03353845227408
H	9.21186552646636	14.37221378122542	11.54145567796989
H	8.83918555231021	13.48150419291026	13.04898273054216
H	7.53558755422002	14.25042881804466	12.13563536865957
C	6.83992296391234	9.19242156734887	12.67932348534424
H	5.80078833771685	8.90129638686673	12.46798384969389
H	6.87255932932277	9.68756265141363	13.65646534506954
H	7.42089034339456	8.26153990249332	12.72182574123215
C	9.70810776015329	13.17410429230368	9.52002040273813
C	11.03301762309891	12.90889942031307	9.93916980575258
C	12.05998557267497	13.73813678494258	9.47998593968971
H	13.08495369552901	13.54814472429123	9.80600070309326
C	11.80592700080729	14.79027637798136	8.61171473500869
H	12.62258541800826	15.42447460872036	8.25946744630818
C	10.50479645988084	15.02527932341282	8.18866359850329
H	10.30665381626119	15.84809179465357	7.50045594870952
C	9.43821944573359	14.23523598242720	8.62860639553832
C	11.39090986169381	11.76499230709027	10.87049838173402
H	10.50624524737521	11.11800989011922	10.96190376521953
C	11.74981639536976	12.26618080052875	12.27093815693122
H	12.65154251797428	12.89856827425113	12.24156542615407
H	11.95533172247018	11.41933368286144	12.94427070079464
H	10.94295463380340	12.86291827735205	12.71541985129394
C	12.53438379273128	10.91924221309167	10.31200587826206
H	12.30076015876464	10.52660081974093	9.31210775892948
H	12.74084848069289	10.06738231675529	10.97611632659964
H	13.46719194493607	11.49771452641546	10.23356756425793
C	8.03496901705965	14.58411853733616	8.17649223730974
H	7.42168837552315	13.67088285119423	8.25156258717738
C	7.41974781415003	15.63621425864718	9.10223018592676
H	8.01118067307347	16.56523460090901	9.07312289838700
H	7.38373420250277	15.29727459125050	10.14555753403937

H	6.39194960933052	15.87803914759349	8.79178298809721
C	7.98829197637501	15.05991959940852	6.72730529767683
H	8.52182215610072	14.37341455375520	6.05624839407836
H	8.41968067084932	16.06711513777623	6.61477313807302
H	6.95158728239677	15.11051796255064	6.36902383920247
C	7.57713594274718	8.18589876934220	10.20610857065234
C	8.79369652516305	7.47338256223535	10.32025121265504
C	8.76752632039196	6.08234143887803	10.20681316485032
H	9.69663291226475	5.51823458924287	10.29808192201184
C	7.57896934606213	5.39984869071516	9.97297977215811
H	7.57790400329598	4.31067711302046	9.88984094891920
C	6.40031401339921	6.11372068950302	9.82440969233019
H	5.47153743863190	5.57908429171063	9.61266042491553
C	6.37100758878587	7.50944682175395	9.92805666030470
C	10.10909148797039	8.18757127831521	10.57314124608411
H	10.03546426868955	9.17349346576484	10.08438016273445
C	10.33985276837432	8.43012974229389	12.06710827977733
H	10.30030582628540	7.48041862657336	12.62383868203087
H	9.59209298777523	9.10978549536182	12.49771754326419
H	11.32950494583111	8.87920672414435	12.24088551139251
C	11.30345340179242	7.45759316718070	9.96376568170267
H	11.13279704999626	7.20774969075931	8.90589594507030
H	11.52937644475013	6.52220733626377	10.49880651891245
H	12.20348813920958	8.08483829414304	10.02219707425411
C	5.05012692339335	8.21356036602110	9.68325507661884
H	5.21829321199859	9.29598045097663	9.79640846709005
C	3.95974467614214	7.79980006661040	10.67292507495002
H	3.03960114319138	8.37529531347166	10.48737416355408
H	4.25297458393871	7.96367566470940	11.72012711933691
H	3.70666651518764	6.73340567839808	10.56666786231348
C	4.57774688666300	7.95001083635219	8.25139161623622
H	3.68289578475350	8.54317737768264	8.01557407108964
H	4.32144928900246	6.88876125085614	8.10897270634431
H	5.34594020637534	8.19745322337278	7.50386989622936
C	6.17212806873276	9.46633153430380	-0.24987119089225
C	6.23449285446793	10.82176672367007	-0.60900439865088
H	6.20196470173823	11.03598187412142	-1.67622114330812
C	6.18180205825408	11.94163785902136	0.24455385179000
C	6.03809646697540	8.45992143477649	-1.36024836471691
H	5.90989493241444	8.95098608032523	-2.33212805496252
H	5.19757755557874	7.77503407181580	-1.18753824648230
H	6.94330321096959	7.83388680170618	-1.39372204588923
C	5.98390592119470	13.28147403984762	-0.41146232576527
H	6.92114279586519	13.85666123503492	-0.37681184403538
H	5.23039218641692	13.87929741429346	0.11922601371583
H	5.68411236289270	13.16657797093254	-1.45984573177552
C	5.78255315832583	7.72493225538727	1.32298710832530
C	6.70489254069358	6.68443858139938	1.55205561968851
C	6.21303991234892	5.40244903918136	1.81746774901111
H	6.92026865015147	4.58576217986565	1.98323486416999

C	4.84929784682831	5.14830290724847	1.87762649693523
H	4.48555446839330	4.13801794536406	2.07981963169311
C	3.95037744771554	6.19390318484136	1.70135042005889
H	2.87766611245521	5.99995689051845	1.77951092778225
C	4.39149627485655	7.49255831171462	1.43770146773903
C	8.20311663237104	6.91252637659226	1.53603969375769
H	8.37450970909454	7.98818773196569	1.38311945903640
C	8.88512783284543	6.15752818435784	0.39559021335890
H	8.46531107066232	6.43539288443051	-0.58309451344584
H	8.76998377735228	5.06707211968472	0.50654350590686
H	9.96374363570691	6.37950798157999	0.37495741259802
C	8.81514427264286	6.54516346742546	2.88831804001079
H	8.67465315802864	5.47713518690985	3.11951713863699
H	8.35155900495259	7.12980420365190	3.69816061934994
H	9.89699898123925	6.74738623565812	2.89294006411918
C	3.37339433479582	8.61068676211436	1.29963367902886
H	3.93173364519134	9.55730819296751	1.26077853174469
C	2.56046429592413	8.49945529674494	0.00904041102439
H	3.19959850271578	8.52856876771181	-0.88478892865669
H	1.84391233877412	9.33242942098695	-0.06798265071280
H	1.98611916621592	7.55925033826613	-0.01927857882582
C	2.44999058371127	8.67290243275107	2.51516835557562
H	1.75146989218357	9.51854506440062	2.42207326874295
H	3.02606748704252	8.80384549464488	3.44391655587315
H	1.84369251189097	7.75894322451869	2.61478141205760
C	6.08322105910863	13.03966746999206	2.35456432680134
C	7.12141868023586	13.97042250787591	2.57077171547942
C	6.84207131917504	15.11957296712475	3.31776502641326
H	7.63843928869107	15.84789292197046	3.49018838446680
C	5.57919274632844	15.34873548273126	3.84430651475707
H	5.37638451385594	16.25684090224962	4.41720797055621
C	4.57544249750607	14.40433783499284	3.65649631413689
H	3.59016766041404	14.57960922994459	4.09077719485134
C	4.80544479730913	13.23376502497207	2.93007946543834
C	8.52890210513810	13.75742254449809	2.05023104493954
H	8.51655265169552	12.85260541594930	1.42917163881040
C	9.02527699664658	14.92298366009195	1.19446506165536
H	10.01194805564637	14.68899848144727	0.76495570107544
H	9.13663810905211	15.84400192490879	1.78854182575867
H	8.34050242395517	15.15162413735446	0.36396606457348
C	9.49408926211465	13.49425330595328	3.20561197498869
H	10.49436468807056	13.23512233760504	2.82468963869772
H	9.13998205232716	12.66245060829643	3.82957537704675
H	9.59823453547956	14.38420637768153	3.84738314935235
C	3.69983777791059	12.21036983269336	2.74998125125930
H	4.19743918896234	11.22809257812906	2.69620320736291
C	2.92985904005695	12.41901522392515	1.44471848751819
H	3.57177783893580	12.29614751941798	0.56148124625581
H	2.48301876470993	13.42581682724450	1.40662659819307
H	2.11306158812408	11.68518696088068	1.35945253321265

C	2.74782214042598	12.15513015947652	3.93913269016061
H	2.13964920580234	13.06886716012493	4.03336728613457
H	3.30163065753770	12.00188912667667	4.87698938638374
H	2.05140361259160	11.31229815296242	3.82506533208538
C	4.79868967061985	12.97633532656927	10.18424590496005
H	5.68840104128714	13.61209558549572	10.30864466515970
H	4.88431500891918	12.14340853783299	10.89915146611790
H	3.91461452500947	13.57563415030593	10.45633061379874
C	3.05960967427876	11.35459135051646	8.27206051635831
H	2.96509834773402	10.90677379956188	7.26964840938675
H	2.18357096608470	12.00081119225401	8.44214215538387
H	3.02443718901801	10.54066908892265	9.01309013352151
C	4.46280934643851	13.84710884332839	7.28431854554488
H	4.46109228283060	13.55722677244256	6.22291800124954
H	5.26629549658760	14.58280694616163	7.42183170323218
H	3.50680564391946	14.35094393945936	7.50011903178264
C	8.78249248744254	8.91823444581904	7.14828979301460
H	7.79226864587829	8.50550148024472	7.39122319161973
H	9.53188680493052	8.37975544910957	7.75508952669732
H	8.96508934552321	8.68147675068570	6.08483184314689
C	10.12676988053000	10.89897866131517	7.06036370130984
H	10.40292638869605	10.65616572294955	6.01995133676059
H	10.92135197741455	10.49593370380738	7.71653772842091
H	10.13023307958519	11.99286787883659	7.16053380611946
C	9.75516884923537	9.90257890192754	3.25576030615638
H	10.33779419047338	8.99717498467644	2.97897017508811
H	9.23388333031605	9.67930142551164	4.19916851761796
H	10.50443379609999	10.69686955248178	3.46780206355154
C	9.43313727678331	10.48690276312290	0.97199558979303
H	8.70596038514130	10.82920048384398	0.22087940642451
H	9.90065353477637	9.55902676988580	0.56737668263435
H	10.24713907855861	11.24369835657114	1.01124092689821
H	5.65762123918458	10.23428850432017	7.87565377935811

TableS 25. Cartesian coordinates of $[L(Me_2N)GaN(Ph)Sb]_2$ (**10**) [Å] for the optimized geometry.

Energy (PBE0/D3BJ/def2-S(TZ)VP) = -7644.53075775 E_h
Zero-point correction (PBE0/D3BJ/def2-S(TZ)VP) = 1.63905760 E_h
Enthalphy (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

Sb	1.99261000860432	5.65620834074922	6.32732580839768
Ga	1.71357695919904	4.08963390234678	3.41587751752125
N	0.75265332026892	2.77607646792375	2.29234694082163
N	0.84679469040734	5.66296476246697	2.57879320412835
N	3.52608931194215	4.08785091227173	2.99134009890580
N	1.30847803829523	4.02673806304107	5.25813470641101
C	0.35438022890024	3.10879591168155	1.06608618189895
C	0.29621061480472	4.42870561860157	0.58756092454075
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C	4.56321322757948	7.31715614234207	7.79331517049526
H	5.28319872872753	6.52491337358299	7.57842673368324

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