Synthesis, Structure and Bonding Nature of Heavy Dipnictene Radical Anions

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Content

Experimental Details

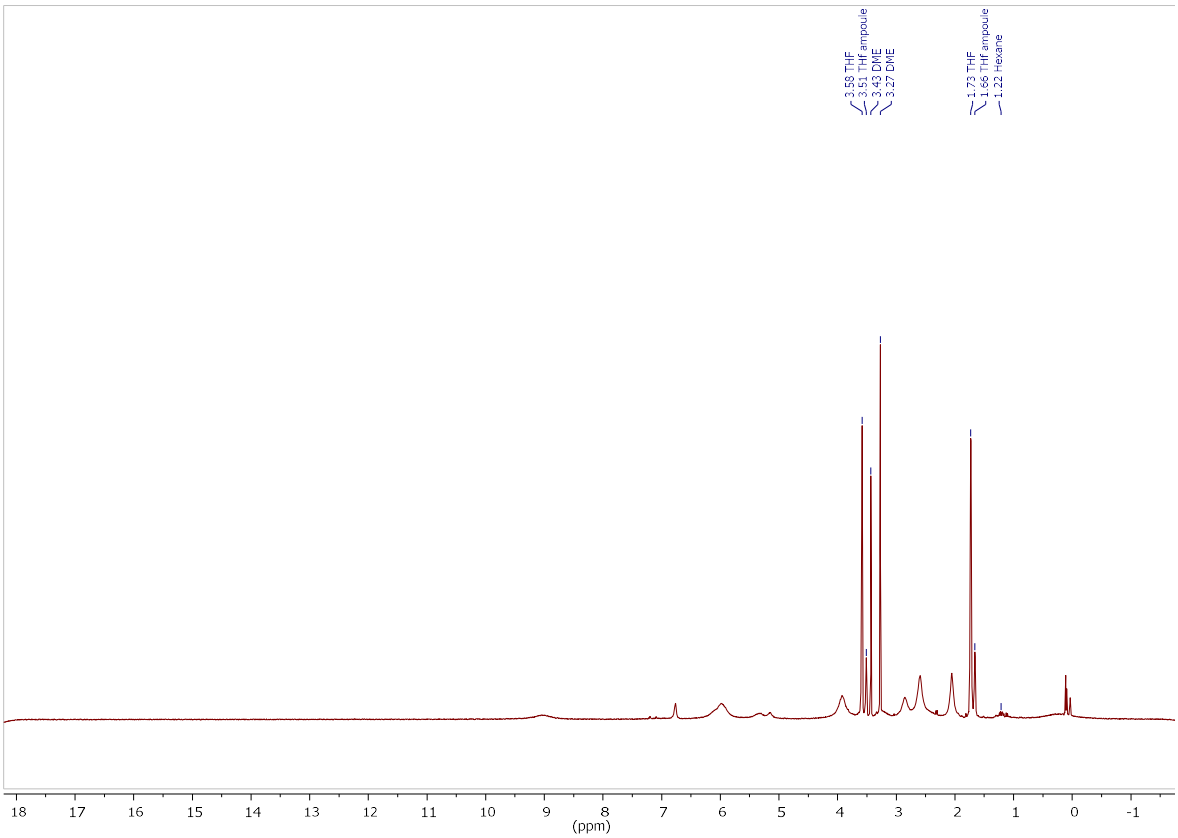

Fig. S1. ^{1}H NMR (300 MHz thf-d_8, 25 °C) of (DME)[K(B-18-C-6)][L(Me_2N)GaSb]$_2$ **3** for Evans' method.

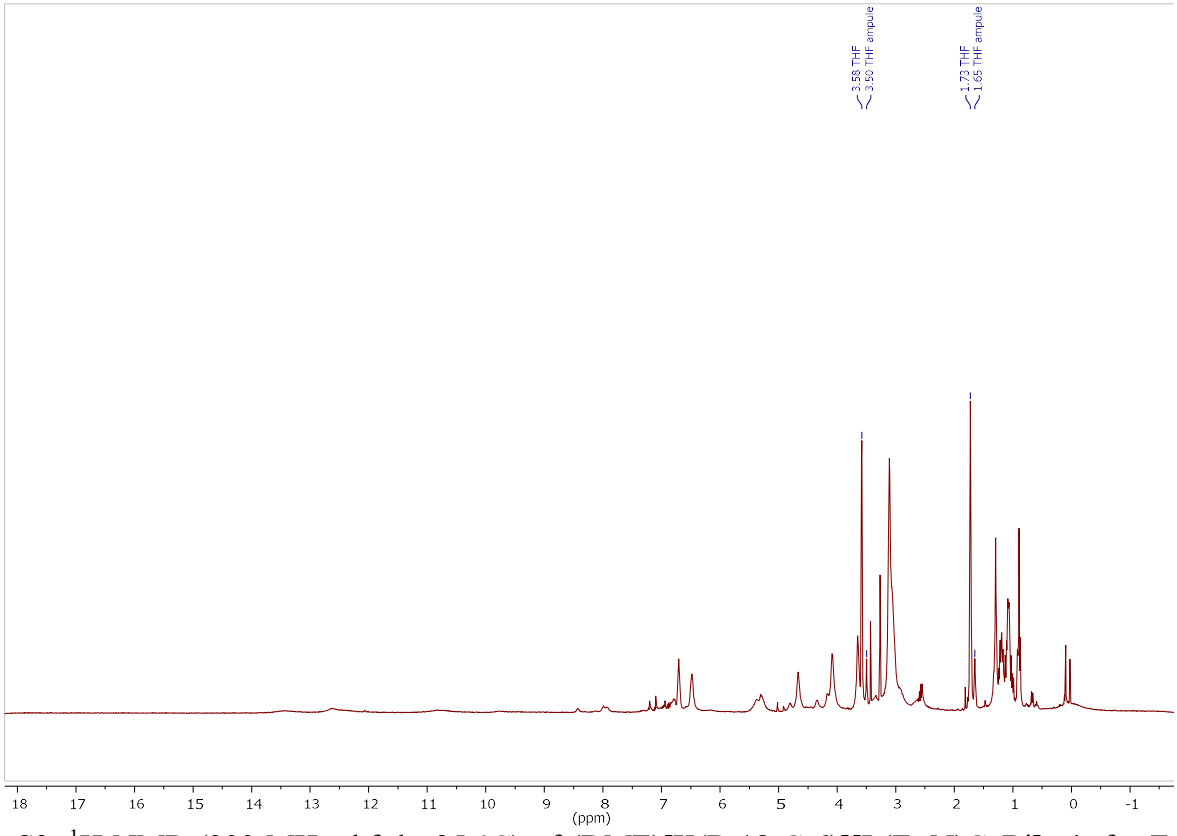

Fig. S2. ^{1}H NMR (300 MHz thf-d_8, 25 °C) of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ **4** for Evans' method.

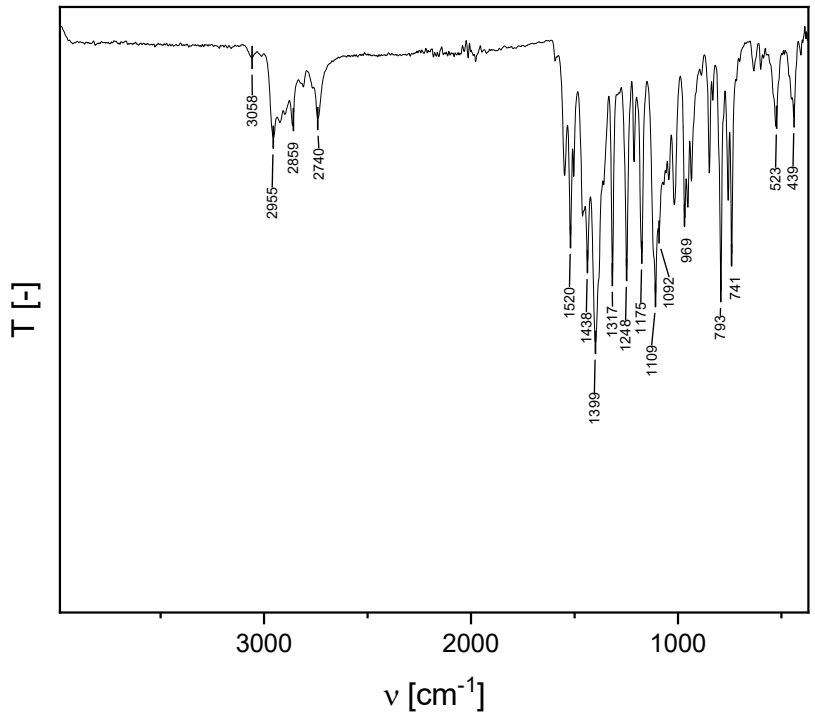

Fig. S3. ATR-IR spectrum of (DME)[K(B-18-C-6)][L(Me_2N)GaSb]$_2$ **3**.

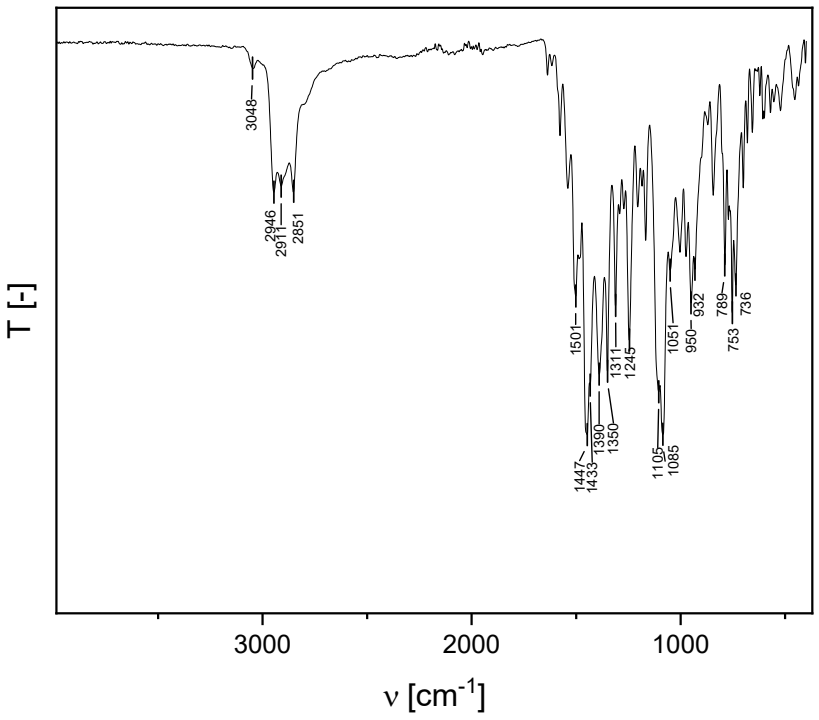

Fig. S4. ATR-IR spectrum of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ **4.**

Fig. S5. Reduction reaction of 10 mg of the dipnictenes **1**, **2** and **3**, **4** with 1 eq. of KC_8 in DME. The pictures were taken shortly after the preparation.

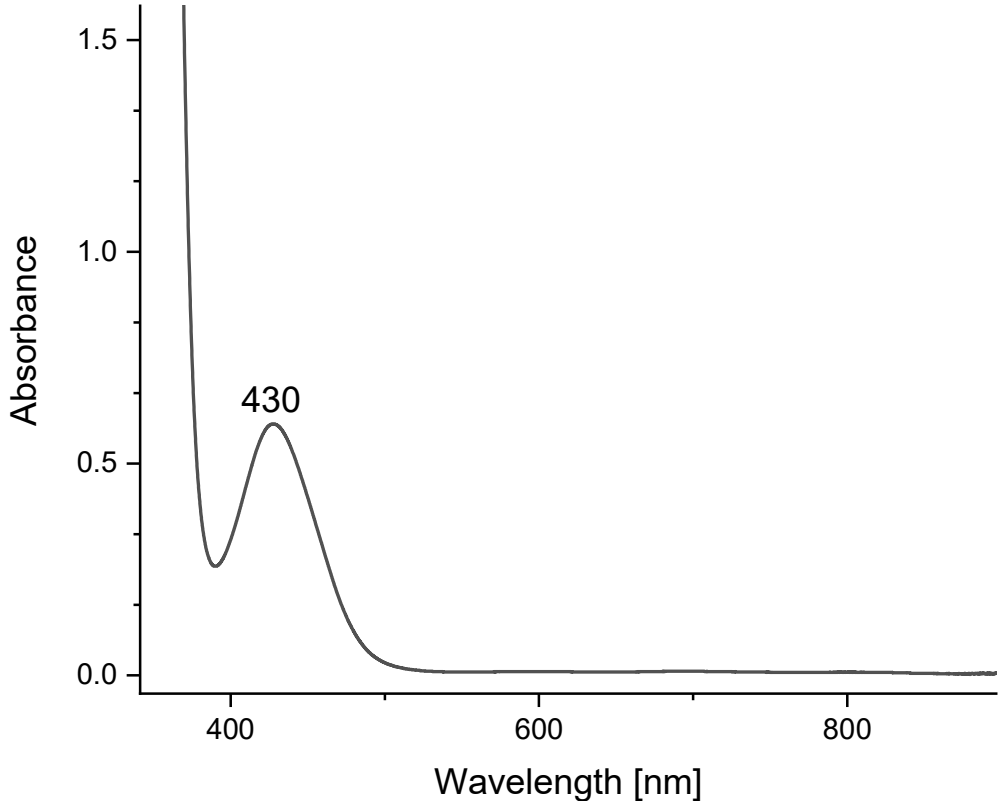

Fig. S6. UV-Vis spectrum of **1** in benzene solution.

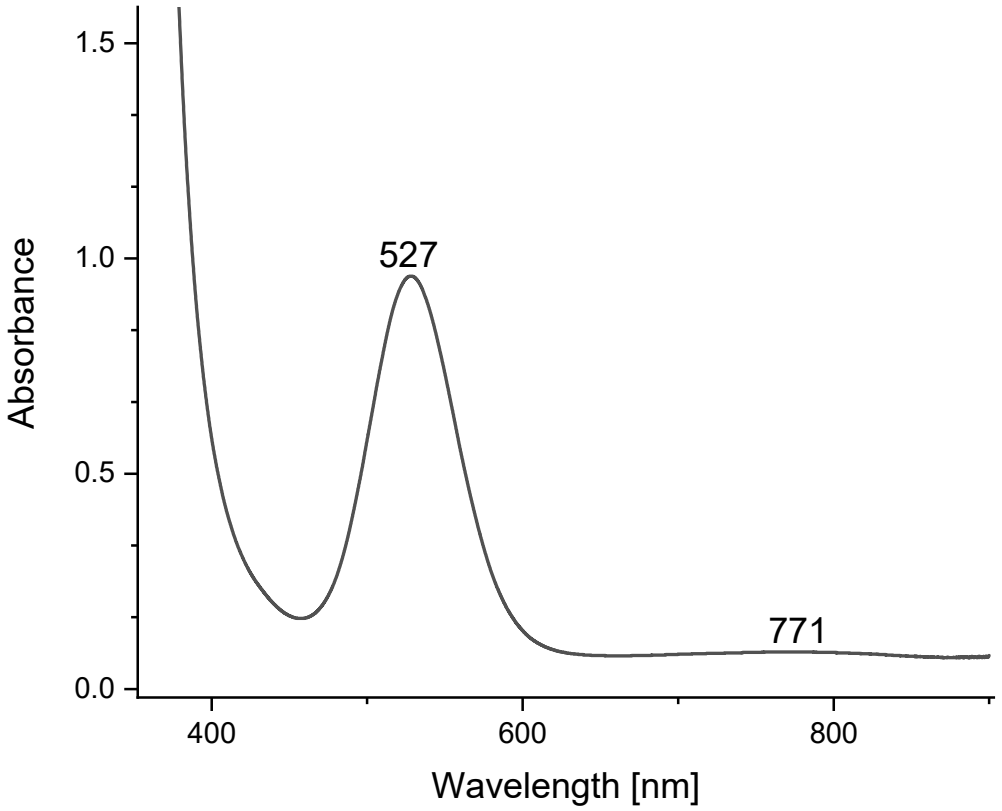

Fig. S7. UV-Vis spectrum of **2** in benzene solution.

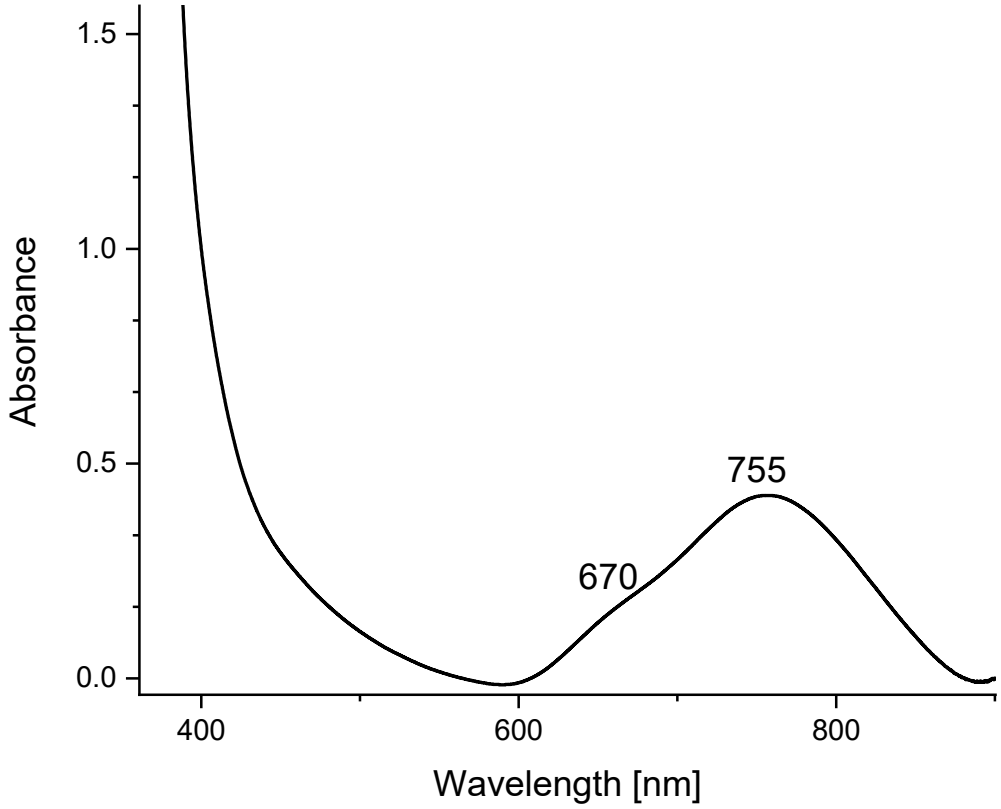

Fig. S8. UV-Vis spectrum of **3** in THF solution.

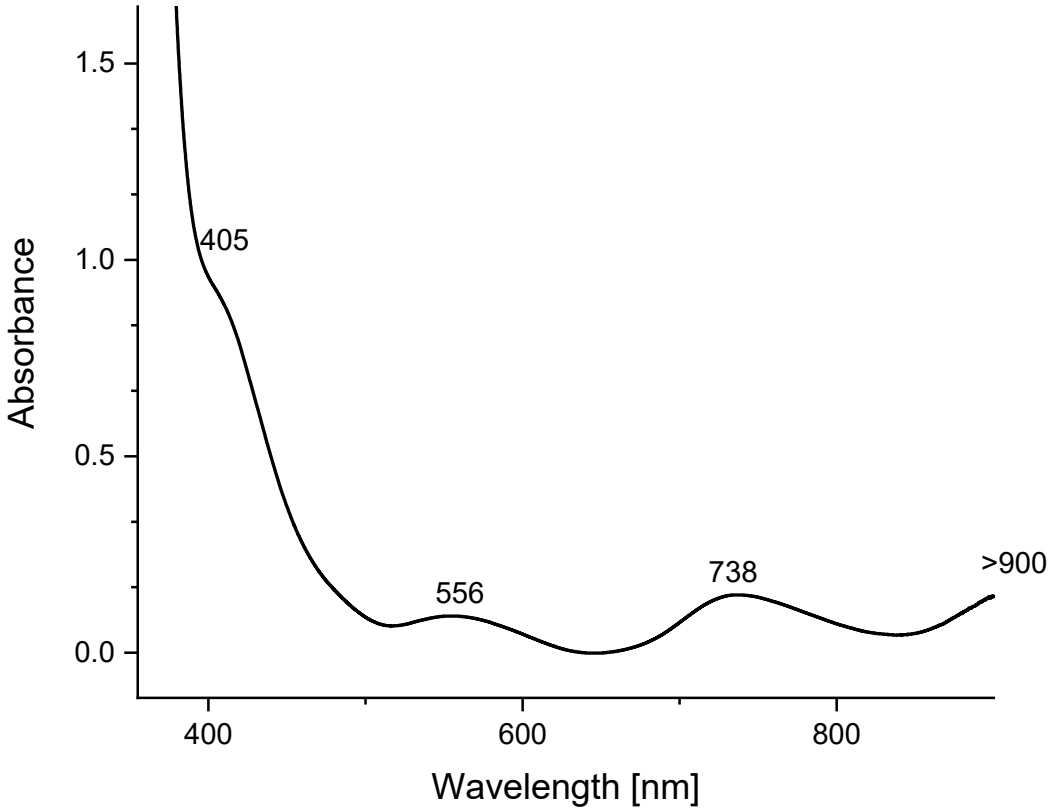

Fig. S9. UV-Vis spectrum of **4** in THF solution.

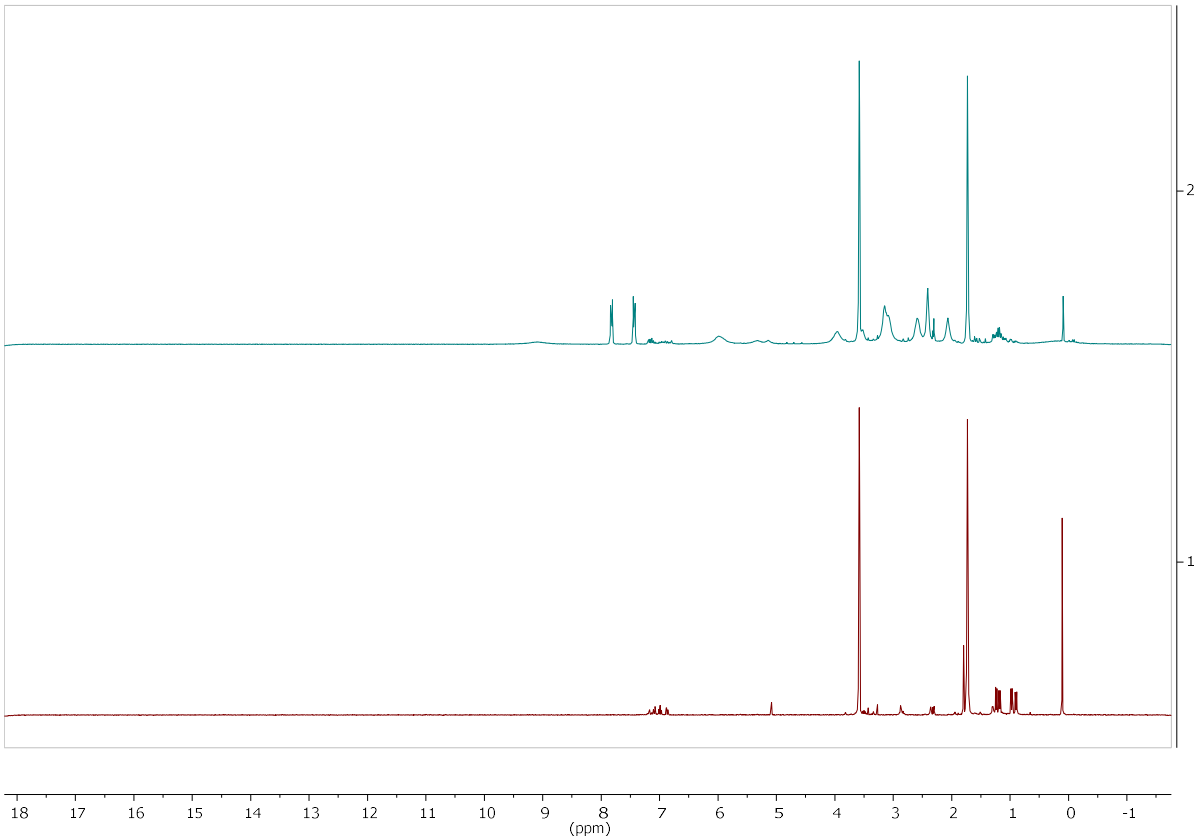

Fig. S10. ^{1}H NMR spectrum (300 MHz, thf-d_8, 25 °C) of the reaction of $[L(Me_2N)GaSb]_2$ **1** and [K cryp-2,2,2]$^{+}$[$C_{10}H_8$]$^{-}$ at ambient temperature. Bottom: before the addition of the reducing agent.

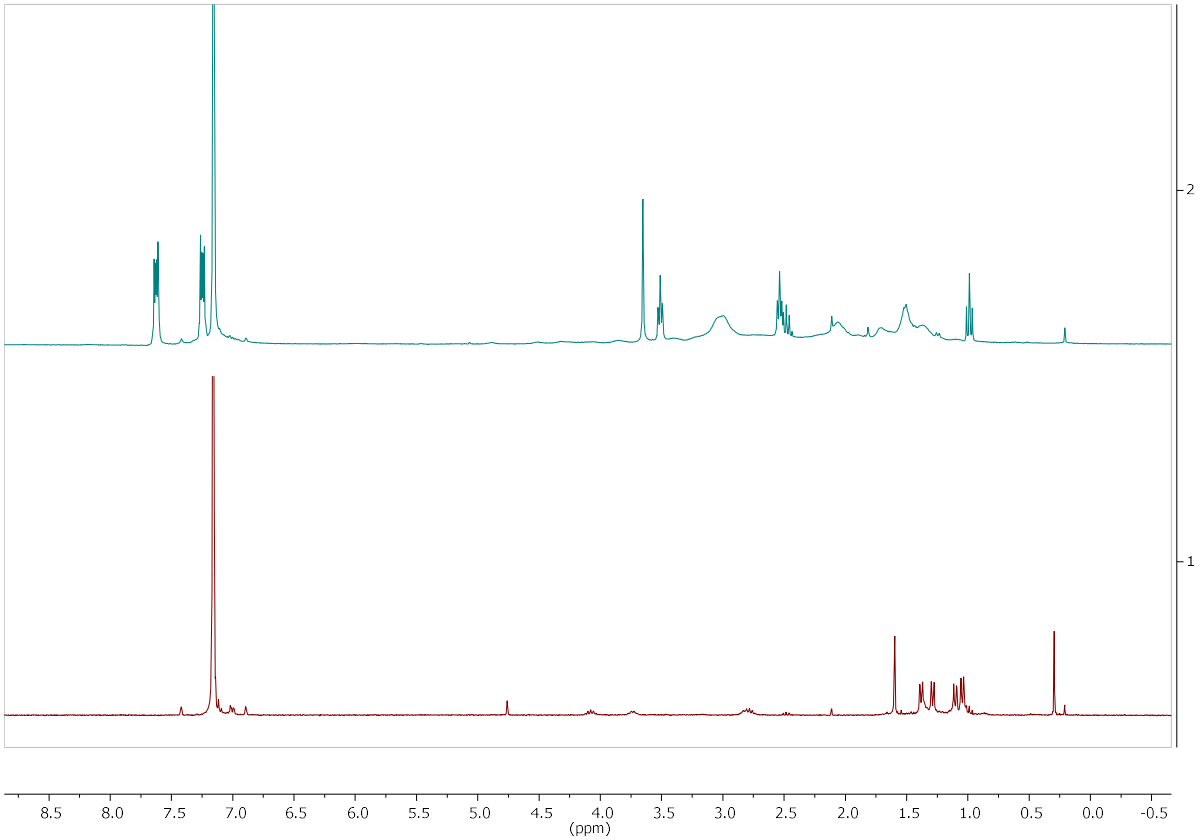

Fig. S11. ^{1}H NMR spectrum (300 MHz, C_6D_6) of the reaction of $[L(Et_2N)GaBi]_2$ **2** and [K cryp-2,2,2]$^{+}$[$C_{10}H_8$]$^{-}$ at ambient temperature in C_6D_6. Bottom: before the addition of the reducing agent.

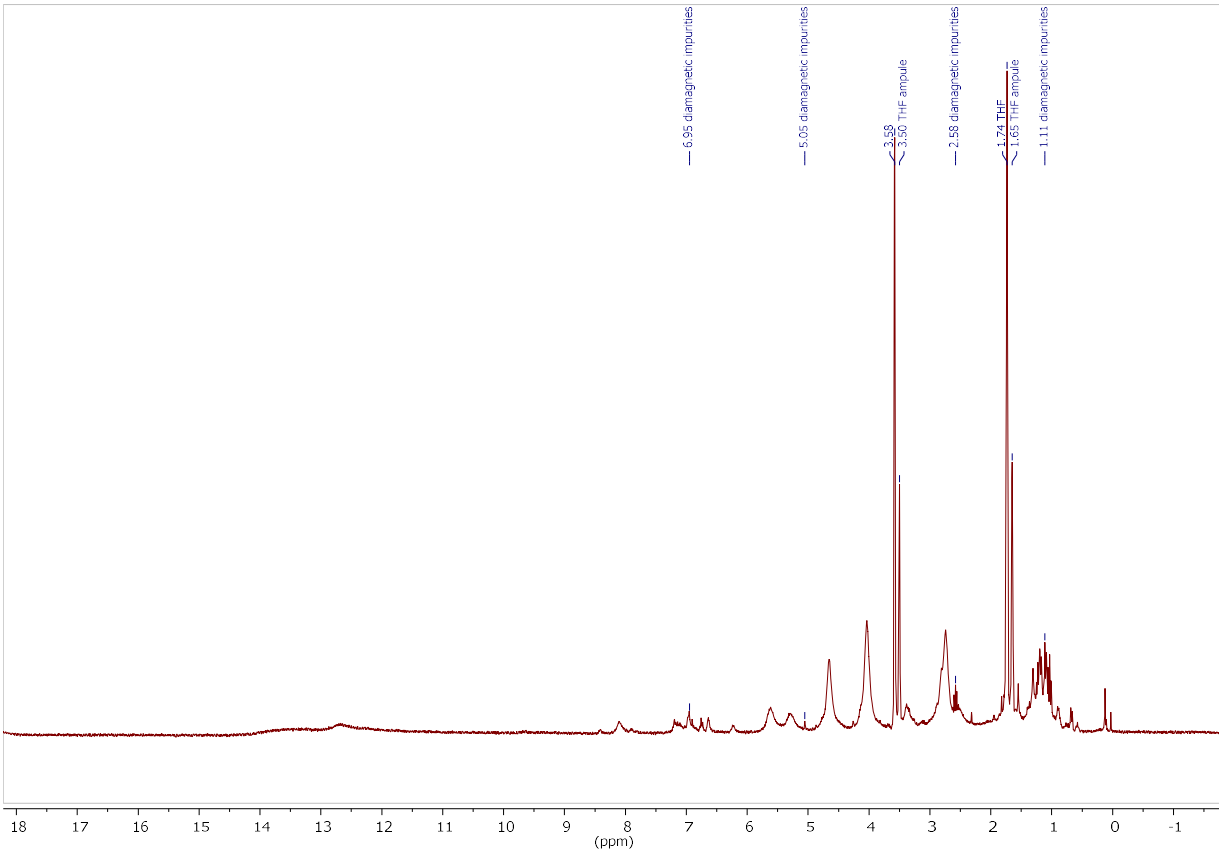

Fig. S12. ^{1}H NMR (300 MHz thf-d_8, 25 °C) of a freshly prepared $[K(B\text{-}18\text{-}C\text{-}6)][L(Et_2N)GaBi]_2$ **4** solution for Evans' method.

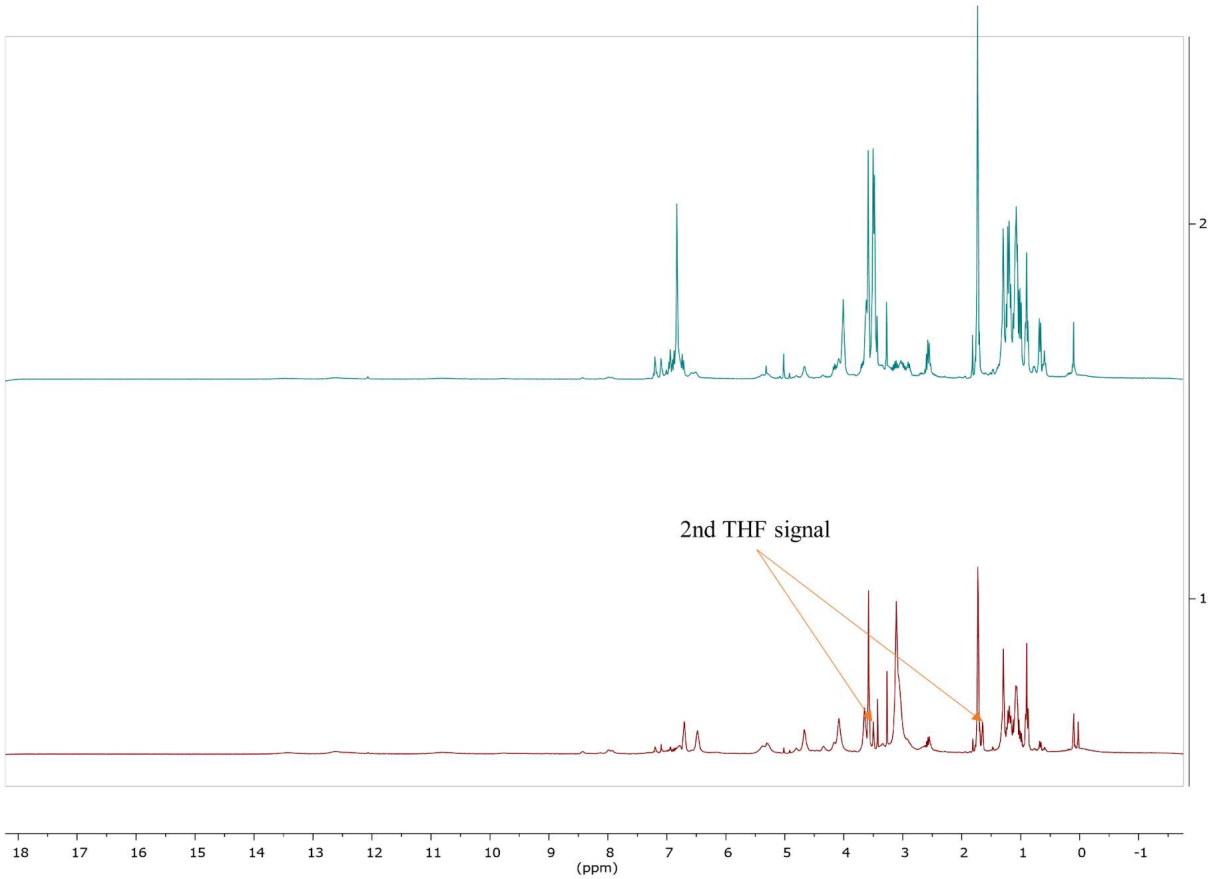

Fig. S13. ^{1}H NMR (300 MHz thf-d_8, 25 °C) of [K(B-18-C-6)][L(Et_2N)GaBi]$_2$ **4** for Evans' method. Bottom, measured after 20 min. Top, after 5 h.

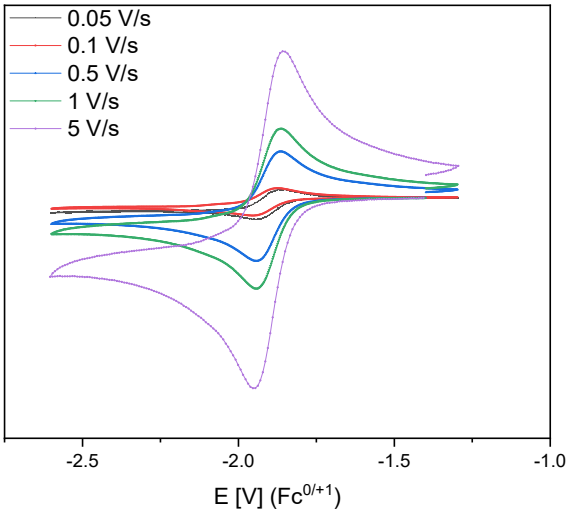

Fig. S14. Cyclic voltammograms of [L(Me_2N)GaSb]$_2$ **1** in THF solution (1 mM) at 45 °C containing [n-Bu_4N][PF_6] (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

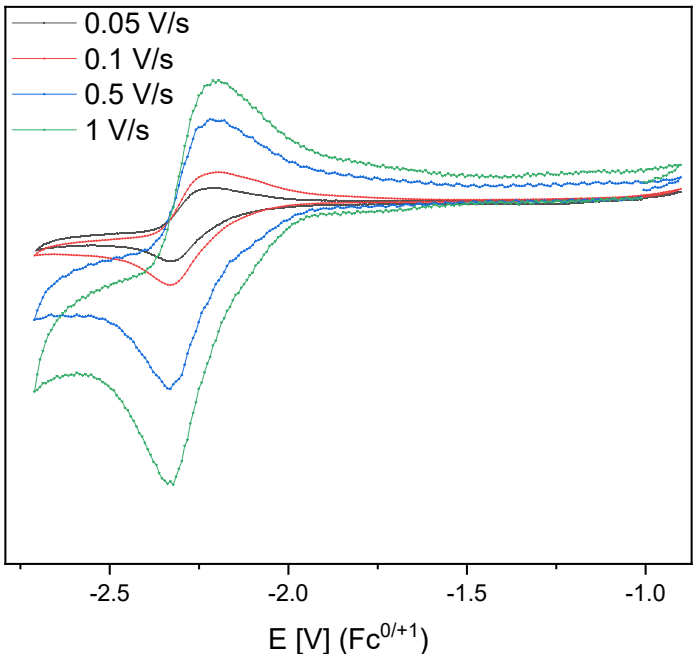

Fig. S15. Cyclic voltammograms of $[L(Et_2N)GaBi]_2$ **2** in THF solution (1 mM) at 45 °C containing $[n\text{-}Bu_4N][PF_6]$ (100 mM) as electrolyte at varying scan rate showing the reversible reduction event.

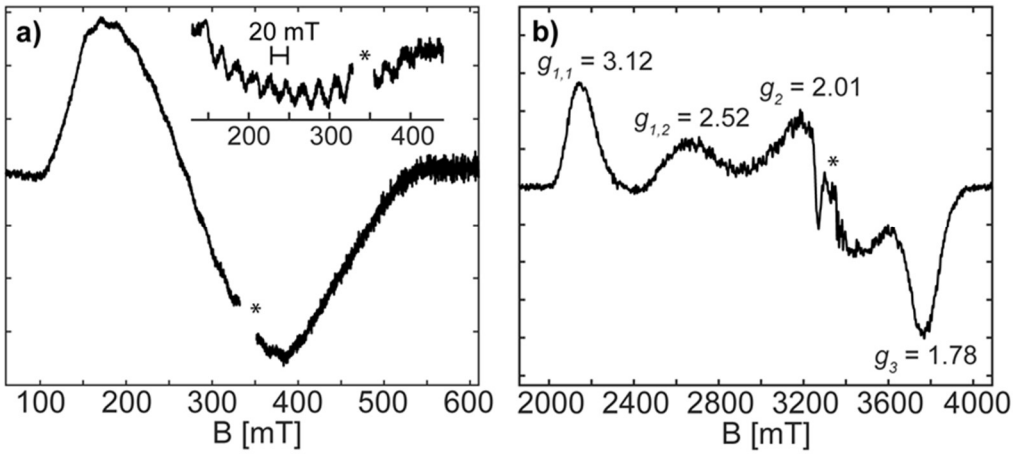

Figure S16. a) EPR spectra of frozen solutions of **4** as collected CW X-band derivative spectrum (~9.64 GHz, 6 K), insert: Bi hyperfine in the second derivative exhibiting a multiline pattern with approximately equal splitting of 20 mT (~500 MHz). **b)** First derivative of pulsed W-band EPR absorption spectrum (94.01 GHz, 7 K, smoothed over 20 points). The asterisks indicate small impurities originating from organic radicals in the sample (X-band) and transition metal contaminations in the resonator (W-band). Spectrometer conditions are described in the Experimental Section.

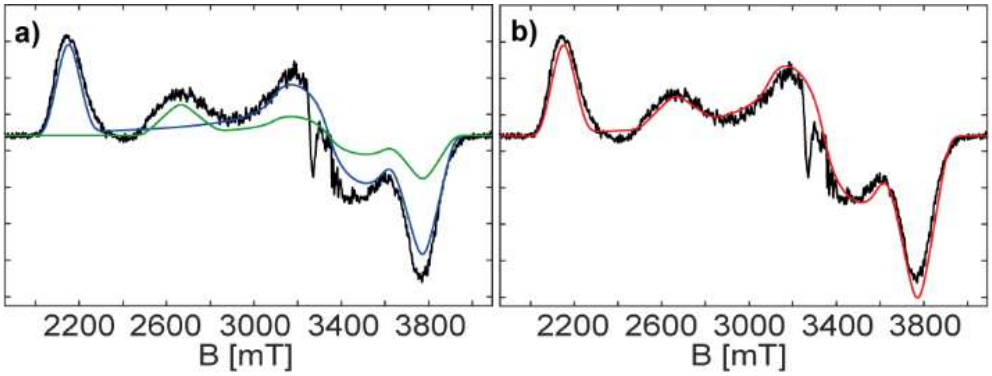

Figure S17. First derivative of pulsed W-band EPR absorption spectrum of **4** (94.01 GHz, 7 K, smoothed over 20 points) in black with **a)** the simulation of the two individual components (component **4-1** in blue, component **4-2** in green) and **b)** the sum of the individual simulations. EPR simulation parameters for component **4-1**: **g** = [3.12 2.01 1.78], 2 x **A**(^{209}Bi) = [450 700 350] MHz, lw (linewidth, peak-to-peak) = 50 mT, weighted to 75 % of the total spin concentration. EPR simulation parameters for component **4-2**: **g** = [2.52 2.01 1.78], 2 x **A**(^{209}Bi) = [600 700 350] MHz, lw (linewidth, peak-to-peak) = 50 mT, weighted to 25 % of the total spin concentration. Spectrometer conditions are described in the Experimental Section.

Crystallographic Details.

The crystals were mounted on nylon loops in inert oil. Data of **3**, and **4** were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated Mo_{Ka} radiation, l = 0.71073 Å) 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-2014)[2,3]. Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups.

In **3** the dimethoxy ethane shows rather large displacement ellipsoids. Reducing the occupancy to 50% yields ellipsoids of realistic size but significantly increases the R-values. No residual electron density maxima giving an alternate orientation could be found, thus the model with partial occupancy was discarded. The structure contains highly disordered solvent – possibly n-hexane or dimethoxy ethane. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.[4] Since the nature and amount of the solvent is not clear it was not included in the sum formula. In **4** two ethyl groups are disordered over two positions. Their corresponding bond lengths and angle were restrained to be equal (SADI) and RIGU restraints were applied to their anisotropic displacement parameters. Due to their proximity, C65 and C65' were refined with common displacement parameters (EADP). The dimethoxy ethane ligand is disordered over two positions. All corresponding bond length and angle were restrained to be equal (SADI). The anisotropic displacement parameters of its atoms were refined with RIGU restraints. In addition, two highly disordered solvent molecules (either n-hexane or dimethoxy ethane or a mixture of both, exact occupancy unknown) could not be modelled sufficiently. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. Since the nature and exact amount of the solvent is not clear it was not included in the sum formula.

CCDC-2077932 (**3**), and -2080779 (**4**) 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 S1. Crystallographic data of (DME)[K(B-18-C-6][L(Me_2N)GaSb]$_2$ (**3**) and (DME)[K(B-18-C-6][L(Et_2N)GaBi]$_2$ (**4**).

	3	**4**
Empirical formula	$C_{89}H_{145}Ga_2KN_6O_{10}Sb_2$	$C_{89}H_{143}Bi_2Ga_2KN_6O_8$
M	1881.14	2021.59
Crystal size [mm]	0.348 × 0.076 × 0.070	0.376 × 0.104 × 0.070
T [K]	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a [Å]	19.3507(10)	19.493(2)
b [Å]	17.6402(10)	17.962(2)
c [Å]	31.0106(17)	30.744(4)
α [°]	90	90
β [°]	100.619(3)	101.573(5)
γ [°]	90	90
V [Å^3]	10404.2(10)	10546(2)
Z	4	4
Dcalc [g·cm-3]	1.201	1.273
μ(MoK$_\alpha$) [mm^{-1}]	1.117	3.920
Transmissions	0.75/0.65	0.75/0.49
F(000)	3936	4120
Index ranges	$-27 \le h \le 27$	$-27 \le h \le 27$
	$-25 \le k \le 25$	$-25 \le k \le 25$
	$-44 \le l \le 44$	$-43 \le l \le 43$
θ_{max} [°]	30.589	30.508
Reflections collected	320168	338181
Independ. reflections	31900	32182
R_{int}	0.0746	0.1112
Refined parameters	1020	1091
R_1 [I > 2σ(I)]	0.0438	0.0433
wR_2 [all data]	0.1102	0.0985
GooF	1.079	1.023
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.804/-0.886	4.127/-1.746

Computational details

The ORCA quantum chemistry package version (4.2.1)[5-7] was used for the DFT calculations. The geometric parameters of the species were optimized in the gas phase employing the PBE0 density functional[8] with ultrafine grid and Def2-SVP[8] basis set on H, C, N and Def2-TZVP[9] on Bi, Ga, Sb, utilizing atom-pairwise dispersion correction with Becke-Johnson damping scheme (D3BJ).[10,11] A small and medium effective core potential was employed on Sb and Bi respectively.[12] For **3** and **4** the respective minimally augmented Karlsruhe basis sets were used on Bi, N, Ga and Sb.[13] To accelerate the calculations the RIJCOSX approximation with ultrafine grid was utilized with the def-2J auxiliary basis sets,[14] as well as the AutoAux generation procedure for the diffuse basis sets.[15] Frequency calculations were carried out for all optimized structures. The electron densities and frontier molecular orbitals were calculated with Def2-TZVP[9] basis set on H, C, and Def2-QZVPP[9] on Bi, Ga, Sb, for **3** and **4** the respective minimally augmented Karlsruhe basis were used on Bi, N, Ga and Sb.[13] Electronic excitations were calculated analogous using the time-dependent DFT (TD-DFT) formalism utilizing ORCA quantum chemistry package version (5.0.0)[5-7] taking solvent effects (only thf for comparability) into account utilizing the conductor-like polarized continuum model (CPCM).[16] Natural bond orbital analysis was performed using the NBO 6.0 program.[17]

Atoms in molecules (AIM)[18-20] and electron localization function (ELF)[21,22] computations were performed with the Multiwfn program 3.7[23] replacing the inner-core density by a pseudo-potential.[24] The high-quality rectangular grid with a mesh size of 0.06 Bohr with basin boundary refinement was employed. 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 and used to plot grid-data.[25]

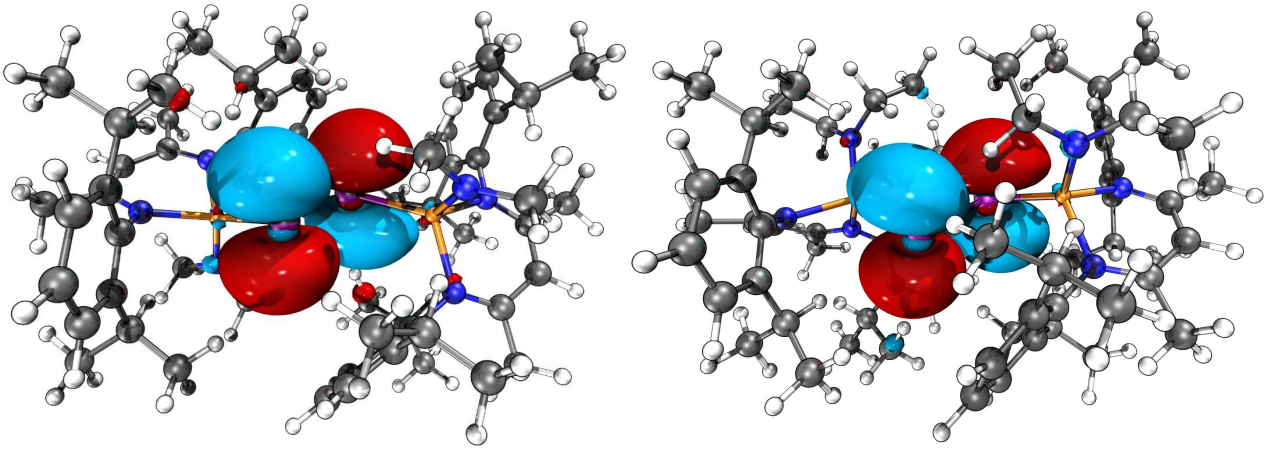

Fig. S18. Biorthogonalized SOMO of (DME)[K(B-18-C-6)][L(Me$_2$N)GaSb]$_2$ **3** (left) and (DME)[K(B-18-C-6)][L(Et$_2$N)GaBi]$_2$ **4** (right), isovalue 0.03.

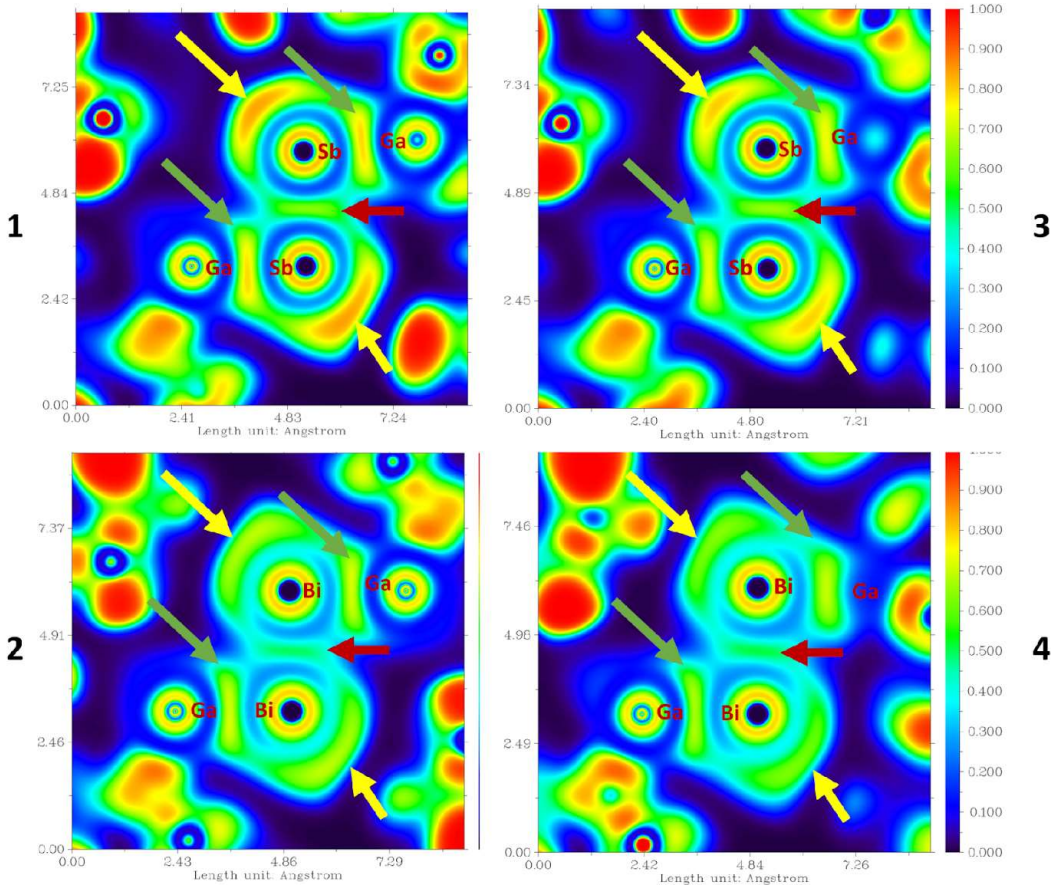

Fig. S19. ELF distribution in [(L(Me$_2$N)GaSb]$_2$ **1,** (DME)[K(B-18-C-6)][L(Me$_2$N)GaSb]$_2$ **3** and [(L(Et$_2$N)GaBi]$_2$ **2,** (DME)[K(B-18-C-6)][L(Et$_2$N)GaBi]$_2$ **4** in the M–E–E(-M) plane, V(M,E), V(E), and V(E,E) basins are indicated by green, yellow, and red arrows, respectively.

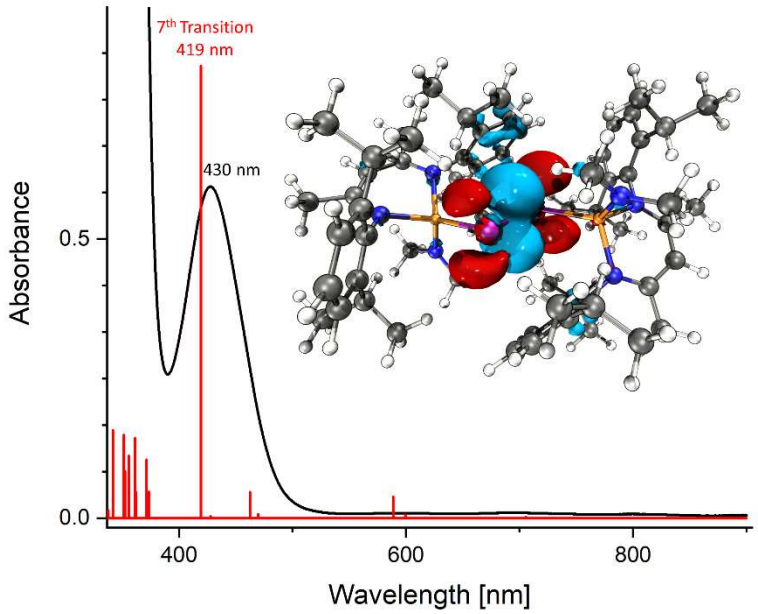

Fig. S20. UV-Vis spectrum of **1** (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transition.

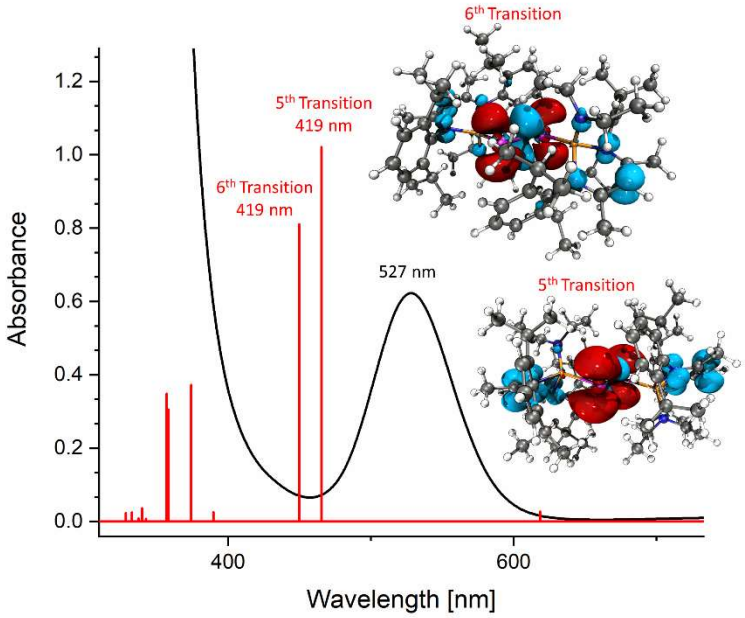

Fig. S21. UV-Vis spectrum of **2** (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions.

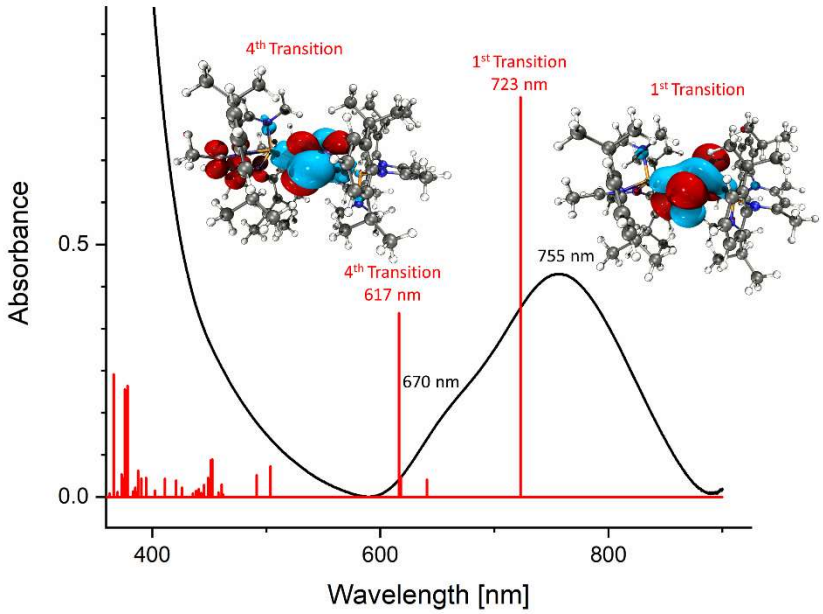

Fig. S22. UV-Vis spectrum of **3** (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions.

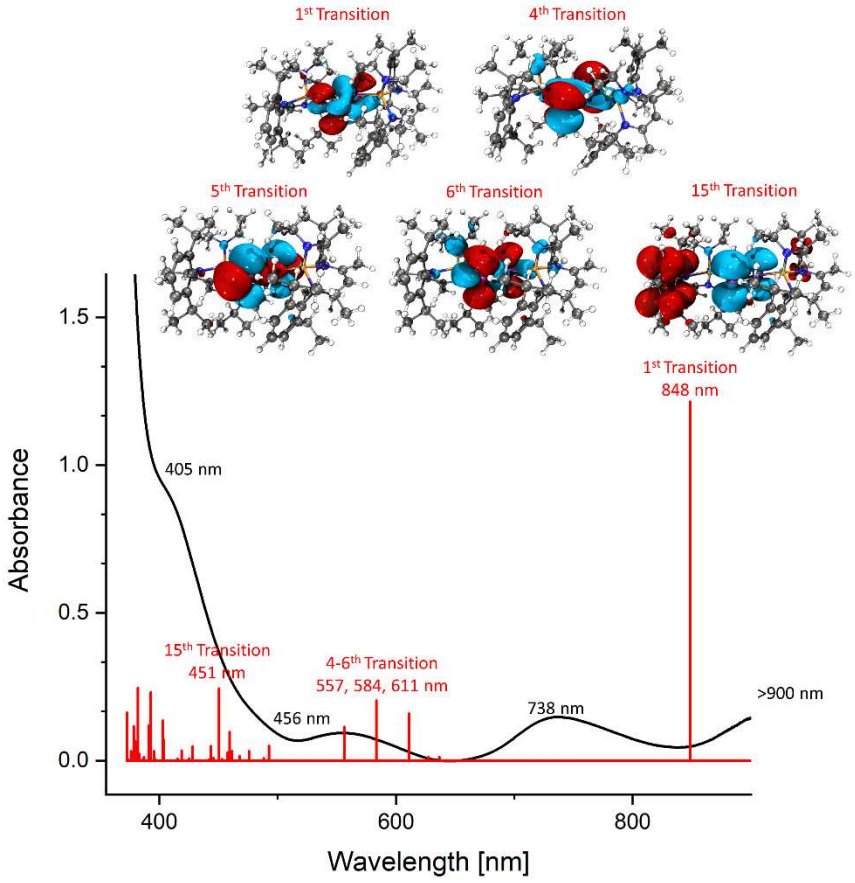

Fig. S23. UV-Vis spectrum of **4** (black), calculated transition maxima (red) and depiction of the electron difference density of the ground and excited state for the dominant transitions.

Table S2. Calculated X–Y bond lengths (r, Å) (exp.), 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, populations of V(X,Y) ELF basins ($\bar{N}$[V(X,Y)], e), and AIM parameters at the bond critical points ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|$/ $G(r_b)$, $H(r_b)$, atomic units) for the Ga_2Sb_2 skeleton of $[L(NMe_2)GaSb]_2$ **1**.

X-Y	r(X-Y)	q(X)	q(Y)	WBI	ON[a]	$\bar{N}[V(X,Y)]$[b]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert/G(r_b)$	$H(r_b)$
Ga2-Sb1	2.60 (2.62)	1.36 (1.37)	-0.16 (-0.16)	0.97	1.96 0.392/0.608	2.259 0.975/1.264	0.069	-0.030	2.384	-0.027
Ga85-Sb84	2.60 (2.62)	1.38 (1.34)	-0.16 (-0.16)	0.96	1.96 0.390/0.601	2.297 0.997/1.280	0.069	-0.031	2.406	-0.027
Sb1–Sb84	2.62 (2.65)			1.82	σ 1.95 0.502/0.498 π 1.91 0.501/0.499	1.438 0.660/0.764 1.410 0.728/0.671	0.076	-0.011	2.009	-0.030
Sb1 lone- Sb84 pair					1.94 1.93	2.720/2.691 2.619/2.584				

[a]: Squared polarization coefficients c_X ($|c_X|^2$) of the σXY bond NBOs. [b]: Contributions of X_1-X_2 electrons into the basins ($\underline{N}[V(X_1, X_2)|X_1/X_2]$, e) are given.

Table S3. Calculated X–Y bond lengths (r, Å) (exp.), 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, populations of V(X,Y) ELF basins ($\bar{N}$[V(X,Y)], e), and AIM parameters at the bond critical points ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|$/ $G(r_b)$, $H(r_b)$, atomic units) for the Ga_2Bi_2 skeleton of $[L(Et_2N)GaBi]_2$ **2**.

X-Y	r(X-Y)	q(X)	q(Y)	WBI	ON[a]	$\bar{N}[V(X,Y)]$[b]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert/G(r_b)$	$H(r_b)$
Ga2-Bi1	2.67 (2.71)	1.33 (1.33)	-0.10 (-0.11)	0.98	1.96 0.411/0.589	2.216 1.031/1.161	0.065	-0.0154	2.199	-0.023
Ga91-Bi90	2.67 (2.71)	1.33 (1.36)	-0.10 (-0.20)	0.98	1.96 0.412/0.588	2.216 1.031/1.161	0.065	-0.0154	2.199	-0.023
Bi1–Bi90	2.77 (2.81)			1.81	σ 1.94 0.499/0.501 π 1.90 0.500/0.500	1.323 0.693/0.617 1.324 0.617/0.6930	0.066	- 0.0429	1.655	-0.020
Bi1 lone- Bi90 pair					1.95 1.95	2.860/2.830 2.860/2.831				

[a]: Squared polarization coefficients c_X ($|c_X|^2$) of the σXY bond NBOs. [b]: Contributions of X_1-X_2 electrons into the basins ($\underline{N}[V(X_1, X_2)|X_1/X_2]$, e) are given.

Table S4. Calculated X–Y bond lengths (r, Å) (exp.), X and Y NPA (AIM) atomic charges (q, |e|), Natural (Becks/AIM) spin density (ρ_s, |e|), Wiberg bond indices (WBI), occupation numbers (ON, |e|) of the σXY bonds according to NBO analysis for α and β spin orbitals, populations of V(X,Y) ELF basins ($\bar{N}$V(X,Y)], e), and AIM parameters at the bond critical points ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|$/ $G(r_b)$, $H(r_b)$, atomic units) for the Ga_2Sb_2 skeleton of (DME)[K(B-18-C-6)][L(Me_2N)GaSb]$_2$ **3**.

X-Y	r(X-Y)	q(X)	q(Y)	ρ_s(X)	ρ_s(Y)	WBI	ON(α)[a]	ON(β)[a]	$\bar{N}[V(X,Y)]$[b]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert$ /$G(r_b)$	$H(r_b)$
Ga2-Sb1	2.56 (2.60)	1.35 (1.27)	-0.49 (-0.39)	0.01 (0.02/ 0.01)	0.47 (0.44/ 0.43)	1.08	0.95 0.376/0.624	0.95 0.386/0.614	2.215 1.149/1,043	0.07 1	-0.0270	2.317	-0.028
Ga85-Sb84	2.56 (2.58)	1.37 (1.24)	-0.51 (-0.39)	0.02 (0.03/ 0.01)	0.45 (0.43/ 0.42)	1.08	0.95 0.377/0.623	0.95 0.383/0.617	2.232 1.173/1.037	0.07 2	-0.0273	2.318	-0.028
Sb1–Sb84	2.73 (2.73)					1.37	σ 0.97 0.500/0.500	σ 0.97 0.499/0.501 π 0.93 0.494/0.506	0.912 0.683/0.637 0.785 0.396/0.387	0.06 5	- 0.0013	2.015	-0.022
Sb1 lone-Sb84 pair							0.96/0.92 0.96/0.92	0.96 0.95	3,747/3.687 3.740/3.671				

[a]: Squared polarization coefficients c_X ($|c_X|^2$) of the σXY bond NBOs. [b]: Contributions of X_1-X_2 electrons into the basins ($\underline{N}[V(X_1, X_2)|X_1/X_2]$, e) are given.

Table S5. Calculated X–Y bond lengths (r, Å) (exp.), X and Y NPA (AIM) atomic charges (q, |e|), Natural (Becks/AIM) spin density (ρ_s, |e|), Wiberg bond indices (WBI), occupation numbers (ON, |e|) of the σXY bonds according to NBO analysis for α and β spin orbitals, populations of V(X,Y) ELF basins ($\bar{N}$[V(X,Y)], e), and AIM parameters at the bond critical points ($\rho(r_b)$, $\Delta\rho(r_b)$, $|V(r_b)|$/ $G(r_b)$, $H(r_b)$, atomic units) for the Ga_2Bi_2 skeleton of (DME)[K(B-18-C-6)][L(Et_2N)GaBi]$_2$ **4**.

X-Y	r(X-Y)	q(X)	q(Y)	ρ_s(X)	ρ_s(Y)	WBI	ON(α)[a]	ON(β)[a]	$\bar{N}$[V(X,Y)][b]	$\rho(r_b)$	$\Delta\rho(r_b)$	$\lvert V(r_b)\rvert$ /$G(r_b)$	$H(r_b)$
Ga3-Bi1	2.64 (2.70)	1.34 (1.24)	-0.44 (-0.33)	0.01 (0.02/ 0.01)	0.49 (0.47/ 0.45)	1.09	0.95 0.339/0.605	0.94 0.406/0.594	2.195 1.200/0,968	0.066	-0.0065	2.074	-0.024
Ga4-Bi2	2.64 (2.68)	1.34 (1.24)	-0.47 (-0.35)	0.02 (0.02/ 0.01)	0.43 (0.42/ 0.40)	1.09	0.94 0.391/0.609	0.94 0.400/0.600	2.202 1.199/0.974	0.066	-0.0062	2.071	-0.023
Bi1–Bi2	2.89 (2.93)					1.35	σ 0.97 0.503/0.407	σ 0.97 0.501/0.499 π 0.92 0.476/0.524	0.697 0.345/0.350 0.734 0.372/0.360	0.054	0.0311	1.647	-0.014
Bi1 lone-Bi2 pair							0.96/0.92 0.96/0.92	0.96 0.95	3,961/3.897 3.972/3.906				

[a]: Squared polarization coefficients c_X ($|c_X|^2$) of the σXY bond NBOs. [b]: Contributions of X_1-X_2 electrons into the basins ($\underline{N}$[V(X_1, X_2)|X_1/X_2], e) are given.

Table S6. Overview of most intense **c**alculated UV-Vis transition by TD-DFT for **1**-**4**.

	Excited State	Excitation energy E [cm^{-1}]	Wavelength λ [nm]	Oscillator strength f (electric/velocity)	Transition orbital contribution (> 5%)
1	7	23852.4	419.2	0.149/0.200	HOMO-4 → LUMO (7.1) HOMO-3 → LUMO (71.1)
2	5	21485.4	465.4	0.094/0.095	HOMO-4 → LUMO (53.8) HOMO-3 → LUMO (39.2)
	6	22232.8	449.8	0.074/0.168	HOMO-4 → LUMO (43.6) HOMO-3 → LUMO (45.3)
3	1	13829.7	723.1	0.055/0.117	HOMO-1(β) → SOMO (6.4) HOMO (β) → SOMO (88.7)
	4	16219.7	616.5	0.025/0.026	SOMO → LUMO(α)+1 (21.6) HOMO-1(β) → SOMO (68.4)
4	1	11783.3	848.7	0.056/0.231	HOMO (β) → SOMO (96.6)
	4	16365.5	611.0	0.007/0.0165	HOMO-3 (β) → SOMO (16.9) HOMO-2 (β) → SOMO (16.6) HOMO-1 (β) → SOMO (61.0)
	5	17135.6	583.6	0.009/0.0194	SOMO → LUMO(α)+2 (81.7) SOMO → LUMO(α)+15 (11.1)
	6	17970.0	556.5	0.005/0.004	HOMO-4 (β) → SOMO (32.2) HOMO-3 (β) → SOMO (8.3) HOMO-2 (β) → SOMO (28.0) HOMO-1 (β) → SOMO (27.2)
	15	22194.4	450.6	0.011/0.004	SOMO → LUMO(α)+4 (55.0) SOMO → LUMO(α)+5 (27.9)

Table S7. Cartesian coordinates of $[L(Me_2N)GaSb]_2$ **1** [Å] for the optimized geometry.

Sb	-2.88665266	7.222704001	0.019784319	Sb	-1.66968342	4.907113154	-0.171072979
Ga	-2.07422035	7.386233793	2.488356019	Ga	-2.24156069	4.574618883	-2.690562137
N	-3.19319325	8.705441787	3.476035536	N	-1.5356504	2.835866994	-3.345579495
N	-2.52950357	5.904361454	3.766235917	N	-1.00536655	5.647836787	-3.860513821
N	-0.27019253	7.794138561	2.766032219	N	-3.97753918	4.727296312	-3.36930266
C	-3.36394732	8.624357456	4.791494006	C	-1.04058117	2.710743653	-4.574412575
C	-3.09679303	7.460628558	5.529287206	C	-0.66021789	3.800605033	-5.37256607
H	-3.25004043	7.532162828	6.605123238	H	-0.28602596	3.554115641	-6.366060056
C	-2.81266635	6.171257803	5.036540236	C	-0.51968478	5.15053947	-4.987361745
C	-3.85675405	9.828832251	5.545203343	C	-0.87477902	1.334990393	-5.159350603
H	-3.04302636	10.56876593	5.61004173	H	-1.86283691	0.932942067	-5.432686349
H	-4.17013485	9.565761408	6.562476815	H	-0.24760786	1.356827538	-6.058494943
H	-4.68680467	10.32300522	5.023586489	H	-0.44195226	0.63674131	-4.430200436
C	-2.84186413	5.049491732	6.038479066	C	0.25984239	6.020907676	-5.937261377
H	-3.30523081	4.146890279	5.618335109	H	0.28922614	7.068870722	-5.617105957
H	-3.37829236	5.347171837	6.947276869	H	1.29019419	5.648136519	-6.029513179
H	-1.81307753	4.776106932	6.318146308	H	-0.19252589	5.963418584	-6.938492406
C	-3.80718922	9.75210268	2.730205087	C	-1.66890775	1.700044083	-2.493451427
C	-5.15621663	9.590155837	2.335710465	C	-0.60822934	1.393555152	-1.606827362
C	-5.76776643	10.6150852	1.61049079	C	-0.73434005	0.273655124	-0.781158034
H	-6.81252626	10.50766113	1.309847262	H	0.07671201	0.018772946	-0.097667534
C	-5.06861925	11.76298511	1.254402406	C	-1.87717266	-0.518575227	-0.804823471
H	-5.56385166	12.55422499	0.686656401	H	-1.95255797	-1.392848474	-0.153497967
C	-3.73260963	11.88859438	1.610793519	C	-2.92590394	-0.18219778	-1.648836457
H	-3.17786497	12.78212918	1.313196375	H	-3.83354556	-0.790984011	-1.651163957
C	-3.07733013	10.89304492	2.343135477	C	-2.84793101	0.926339701	-2.498613075
C	-5.94408368	8.340081424	2.681519218	C	0.64366033	2.25073053	-1.543756461
H	-5.21800918	7.583639144	3.014501233	H	0.3259362	3.282569803	-1.770378853
C	-6.67698998	7.772915277	1.468016957	C	1.27686254	2.259446802	-0.15627557
H	-7.4609373	8.454779387	1.103674017	H	1.72154104	1.284673113	0.099049195
H	-7.16964942	6.824453431	1.729241657	H	2.08526841	3.002167266	-0.11168768
H	-5.98333638	7.579580969	0.63501446	H	0.53859039	2.519172582	0.616531531
C	-6.91587182	8.58104219	3.83784296	C	1.67504137	1.858815111	-2.603527557
H	-6.39450512	8.899179955	4.751483007	H	1.28877455	1.983460006	-3.624017684
H	-7.47097816	7.659987394	4.075384693	H	2.5738138	2.489511884	-2.513432872
H	-7.65044318	9.361124588	3.580308873	H	1.98534347	0.80865346	-2.4802209
C	-1.61066657	11.06494387	2.679574485	C	-4.04372887	1.277441204	-3.358762254
H	-1.28389898	10.15536116	3.2029857	H	-3.76052992	2.136266686	-3.980882037
C	-0.77699157	11.17722593	1.403567367	C	-5.21254524	1.723430267	-2.480532362
H	-0.92763632	10.30134131	0.755207282	H	-4.91325052	2.551677131	-1.823705727
H	0.29515837	11.24259988	1.64405765	H	-6.05443866	2.070386011	-3.099715569
H	-1.0447178	12.07604876	0.825118161	H	-5.57618559	0.896115855	-1.849812523
C	-1.37032328	12.25977817	3.601715494	C	-4.45948292	0.133026886	-4.282350578
H	-1.64774395	13.20822994	3.114241136	H	-4.81610282	-0.740447758	-3.71376618
H	-0.30665432	12.32657197	3.879308066	H	-5.28062927	0.452413134	-4.94287743
H	-1.95844224	12.18287199	4.528511893	H	-3.6269345	-0.20725347	-4.916580165
C	-2.38630292	4.551357025	3.330870959	C	-0.62844324	6.93166452	-3.363630723
C	-3.47741347	3.930521675	2.673900122	C	0.61460446	7.083662308	-2.708958033
C	-3.31834999	2.62163288	2.209125235	C	0.91621191	8.318151419	-2.124049639
H	-4.13916199	2.13322046	1.6833246	H	1.87292734	8.446453242	-1.612249059
C	-2.12366569	1.931081818	2.384188246	C	0.0182373	9.374204157	-2.16500608
H	-2.01922564	0.915629331	1.996857964	H	0.26438037	10.32567489	-1.6882826
C	-1.06192606	2.555103354	3.021175399	C	-1.20267135	9.21130827	-2.811288113
H	-0.11700897	2.019743373	3.141968096	H	-1.90755839	10.04312182	-2.834580698
C	-1.16291118	3.86889281	3.492812394	C	-1.55022547	8.002889318	-3.421481114
C	-4.78419479	4.667896134	2.455728806	C	1.64484451	5.971987984	-2.626671178
H	-4.50960899	5.707741652	2.2022308	H	1.18736786	5.05559049	-3.029700385
C	-5.59129446	4.118370486	1.28556753	C	2.06416904	5.683399024	-1.186833775
H	-4.97793978	4.042171539	0.375462413	H	1.20125581	5.414929383	-0.558202112

H	-6.43790815	4.783416029	1.063627481	H	2.78378248	4.851263959	-1.157106975
H	-6.00819794	3.122394403	1.5028933	H	2.55064199	6.554638065	-0.722203478
C	-5.64390902	4.712687899	3.721077814	C	2.87810598	6.296800039	-3.473751076
H	-6.60025821	5.218645966	3.516686463	H	3.57822513	5.446461431	-3.482255067
H	-5.15476839	5.258088384	4.539029671	H	2.61445644	6.533777107	-4.513377303
H	-5.87214843	3.694301882	4.074075039	H	3.41560317	7.167148763	-3.064715999
C	0.06336739	4.51704516	4.102991915	C	-2.87869711	7.861442293	-4.141785722
H	-0.22689796	5.517239021	4.452149342	H	-3.23156017	6.835629774	-3.95301987
C	1.14510194	4.705057184	3.039758958	C	-3.95451501	8.814786158	-3.632160882
H	1.5228591	3.734579977	2.680861086	H	-3.7368927	9.863650794	-3.891573047
H	1.99899232	5.267889176	3.448167152	H	-4.92190476	8.564699634	-4.093112036
H	0.7505123	5.256651292	2.176330026	H	-4.0713122	8.747216338	-2.54000286
C	0.61310783	3.730448546	5.293194001	C	-2.70773505	8.023867323	-5.653726299
H	-0.15014068	3.554084862	6.065905716	H	-2.04360907	7.260133877	-6.077836366
H	1.44904494	4.275299842	5.758914086	H	-3.68081646	7.935086707	-6.161870254
H	0.99674411	2.74572384	4.982788273	H	-2.2867641	9.013232224	-5.896951442
C	0.68152549	7.984944222	1.712917182	C	-5.08502856	5.276335311	-2.645782806
H	1.06744957	9.025188293	1.667267054	H	-5.99290506	4.643601162	-2.733043218
H	0.23590859	7.758377367	0.73166851	H	-4.84890126	5.367032912	-1.574837653
H	1.57207102	7.330615824	1.825422444	H	-5.3745711	6.290080479	-2.998919882
C	0.24810302	8.115326642	4.061541997	C	-4.24486815	4.562967146	-4.767691106
H	1.14572653	7.512134932	4.319414252	H	-4.47538435	5.52278992	-5.28285926
H	-0.50002356	7.937667576	4.849912136	H	-3.38419543	4.119770833	-5.292489388
H	0.56330681	9.180291991	4.149027681	H	-5.11864843	3.900455323	-4.948614411

Table S8. Cartesian coordinates of $[L(Et_2N)GaBi]_2$ **2** [Å] for the optimized geometry.

Bi	-0.09238185	-0.33990564	1.34046818	Bi	0.09301410	0.33874549	-1.33993510
Ga	2.56392709	-0.10043865	1.52796859	Ga	-2.56326763	0.09920268	-1.52763182
N	3.06136449	-0.99797020	3.24364338	N	-3.06056490	0.99665014	-3.24341698
N	3.74685199	-1.28062775	0.40483184	N	-3.74629638	1.27936749	-0.40464783
N	3.36885424	1.59512973	1.46569858	N	-3.36825657	-1.59635064	-1.46542027
C	4.30110419	-1.45354814	3.39693325	C	-4.30026316	1.45229974	-3.39680625
C	5.16494565	-1.71202479	2.31973138	C	-5.16418001	1.71083204	-2.31967745
H	6.15955420	-2.06760889	2.58777654	H	-6.15875866	2.06644175	-2.58780917
C	4.84939982	-1.78511447	0.94597795	C	-4.84879212	1.78386214	-0.94588911
C	4.81389836	-1.73561229	4.78253193	C	-4.81295522	1.73431988	-4.78245214
H	5.82807681	-2.15133246	4.75685575	H	-5.82705207	2.15024377	-4.75685952
H	4.15197724	-2.43367316	5.31443077	H	-4.15087415	2.43217743	-5.31441496
H	4.82055415	-0.80829262	5.37416352	H	-4.81978692	0.80692715	-5.37396875
C	5.84907410	-2.52465821	0.09570855	C	-5.84871516	2.52317188	-0.09569354
H	5.83222043	-3.59506692	0.34892388	H	-5.83343399	3.59330596	-0.35008258
H	6.86172941	-2.15854160	0.31803376	H	-6.86105993	2.15552961	-0.31692481
H	5.65262187	-2.41868811	-0.97719606	H	-5.65146176	2.41847917	0.97717849
C	2.14668010	-1.04020517	4.33697543	C	-2.14578084	1.03880864	-4.33666860
C	1.97495687	0.07037053	5.18948578	C	-1.97403192	-0.07180491	-5.18912105
C	1.14369161	-0.06315730	6.30723239	C	-1.14262529	0.06162879	-6.30677351
H	1.02468569	0.78672476	6.98403547	H	-1.02360098	-0.78828407	-6.98353150
C	0.46250057	-1.24318462	6.56453909	C	-0.46132209	1.24159808	-6.56404238
H	-0.17386866	-1.33321132	7.44808630	H	0.17516298	1.33154933	-7.44751330
C	0.56269136	-2.29790085	5.66406727	C	-0.56155637	2.29635553	-5.66362626
H	-0.02060581	-3.20298600	5.83859970	H	0.02182110	3.20139526	-5.83812268
C	1.37938251	-2.21475445	4.53374989	C	-1.37838940	2.21330578	-4.53340576
C	2.60660837	1.41859683	4.91239905	C	-2.60581420	-1.41997627	-4.91207268
H	3.14665416	1.34351367	3.95812786	H	-3.14595502	-1.34482911	-3.95786026
C	3.59969457	1.83810398	5.99424517	C	-3.59881183	-1.83943041	-5.99401777
H	4.06172438	2.80497954	5.74160288	H	-4.06094320	-2.80626469	-5.74140782
H	4.41078908	1.10429146	6.11355723	H	-4.40983706	-1.10556027	-6.11343516
H	3.10739568	1.94878882	6.97385062	H	-3.10641088	-1.95017042	-6.97356572
C	1.51921807	2.48001581	4.73174412	C	-1.51852468	-2.48147310	-4.73127950

H	1.96233928	3.44308076	4.43674091	H	-1.96175048	-3.44449085	-4.43628506
H	0.95440029	2.64384802	5.66366741	H	-0.95363365	-2.64538687	-5.66314401
H	0.79926917	2.18387028	3.95376636	H	-0.79862237	-2.18535719	-3.95324951
C	1.39037554	-3.34793102	3.52206618	C	-1.38945658	3.34654435	-3.52179430
H	1.58237798	-2.87934104	2.54155950	H	-1.58157738	2.87801671	-2.54128028
C	2.50737049	-4.36445828	3.76336837	C	-2.50639011	4.36309583	-3.76327484
H	2.44216856	-5.18540581	3.03163421	H	-2.44122431	5.18409036	-3.03159177
H	2.42706447	-4.80465657	4.77050463	H	-2.42596568	4.80322031	-4.77043368
H	3.50477822	-3.91585727	3.66208995	H	-3.50382674	3.91454667	-3.66206020
C	0.03773122	-4.05160192	3.44047025	C	-0.03680304	4.05018406	-3.44008501
H	0.02352875	-4.76145361	2.60283026	H	-0.02266718	4.76005037	-2.60245835
H	-0.78179509	-3.33349583	3.28593661	H	0.78269247	3.33206573	-3.28545669
H	-0.18209085	-4.62878652	4.35186691	H	0.18312136	4.62734257	-4.35147343
C	3.37134408	-1.60711199	-0.93736610	C	-3.37075934	1.60588017	0.93753566
C	3.55082075	-0.66575996	-1.98077734	C	-3.55019159	0.66458132	1.98099809
C	3.11967365	-1.00488578	-3.26655615	C	-3.11897921	1.00377450	3.26673979
H	3.24223075	-0.28537888	-4.07646148	H	-3.24152096	0.28431544	4.07669096
C	2.51877768	-2.22885178	-3.53550114	C	-2.51806812	2.22775409	3.53559464
H	2.17685436	-2.46371433	-4.54605748	H	-2.17611894	2.46267786	4.54612946
C	2.34764292	-3.14139034	-2.50600695	C	-2.34695901	3.14023404	2.50604212
H	1.87043547	-4.10219034	-2.71317705	H	-1.86973834	4.10104332	2.71314090
C	2.76416911	-2.85431613	-1.20140648	C	-2.76353418	2.85308373	1.20147523
C	4.21136860	0.67798078	-1.74059406	C	-4.21078852	-0.67915512	1.74092330
H	3.89188902	1.01388913	-0.74142756	H	-3.89139313	-1.01511182	0.74174574
C	5.73672911	0.55469752	-1.73681486	C	-5.73614338	-0.55581656	1.73725265
H	6.20134601	1.53774952	-1.56347010	H	-6.20081536	-1.53884035	1.56388730
H	6.09977233	0.17177308	-2.70470488	H	-6.09910558	-0.17291957	2.70518414
H	6.09600668	-0.12172441	-0.95085994	H	-6.09542898	0.12067209	0.95136257
C	3.78456915	1.74867965	-2.73938342	C	-3.78395039	-1.74982528	2.73972898
H	2.68904635	1.81404363	-2.82266103	H	-2.68842321	-1.81523485	2.82292615
H	4.19137297	1.56302466	-3.74631460	H	-4.19066920	-1.56410328	3.74668265
H	4.15800051	2.73154608	-2.41724493	H	-4.15744998	-2.73269278	2.41766867
C	2.53279005	-3.90436668	-0.13265990	C	-2.53225764	3.90306801	0.13264400
H	2.86519974	-3.48925656	0.83022134	H	-2.86431466	3.48770875	-0.83024889
C	3.34356438	-5.17351155	-0.40301185	C	-3.34358541	5.17192941	0.40265333
H	4.41336283	-4.95884167	-0.53428253	H	-4.41334884	4.95685229	0.53351620
H	2.99551731	-5.67928882	-1.31764524	H	-2.99605836	5.67784136	1.31741093
H	3.23726056	-5.88532547	0.43075262	H	-3.23723625	5.88376136	-0.43109103
C	1.04859552	-4.23791947	-0.00874434	C	-1.04815935	4.23712556	0.00897393
H	0.88642299	-5.00670889	0.76053330	H	-0.88611081	5.00580006	-0.76044616
H	0.64435648	-4.63086653	-0.95440463	H	-0.64422641	4.63043736	0.95461324
H	0.45804919	-3.34891205	0.25646814	H	-0.45725854	3.34826368	-0.25593939
C	4.80024204	1.78530640	1.45545960	C	-4.79965239	-1.78646194	-1.45521361
H	5.08119345	2.56505278	0.71808143	H	-5.08066592	-2.56616595	-0.71781405
H	5.28312938	0.86429564	1.09292908	H	-5.28251251	-0.86541783	-1.09273247
C	5.42819282	2.14946424	2.79845965	C	-5.42757286	-2.15064721	-2.79821906
H	6.50095132	2.37253347	2.68079245	H	-6.50034774	-2.37365450	-2.68058303
H	5.33531298	1.32068134	3.51556628	H	-5.33461778	-1.32190351	-3.51536089
H	4.95082042	3.03642365	3.24309960	H	-4.95023135	-3.03765295	-3.24279766
C	2.58138975	2.80438065	1.44681773	C	-2.58085036	-2.80563522	-1.44643840
H	2.91945773	3.50958836	2.23458269	H	-2.91893139	-3.51087607	-2.23416703
H	1.54050200	2.55176085	1.71358945	H	-1.53994679	-2.55307789	-1.71320402
C	2.56093731	3.54010169	0.11180495	C	-2.56046484	-3.54128071	-0.11138327
H	2.00379739	4.48690772	0.19043548	H	-2.00338648	-4.48812718	-0.18995074
H	2.07867798	2.92258880	-0.66144709	H	-2.07817994	-2.92375763	0.66184402
H	3.57624061	3.78251426	-0.23792680	H	-3.57578950	-3.78361110	0.23834239

Table S9. Cartesian coordinates of $[L(Me_2N)GaSb]_2^{\bullet-}$ **3**. [Å] for the optimized geometry.

Sb	-3.122680322	7.131654146	0.05273982	Sb	-1.901429282	4.69815312	-0.162183704
Ga	-2.197089361	7.346383863	2.433456398	Ga	-2.210124628	4.577069263	-2.700063905
N	-3.252632516	8.716139897	3.493544151	N	-1.491129792	2.835102213	-3.450912463
N	-2.523328523	5.945853615	3.881585023	N	-0.890209876	5.652008318	-3.851611734
N	-0.382786087	7.811558978	2.699116623	N	-3.870932083	4.796812227	-3.575740666
C	-3.30006832	8.709378847	4.819527094	C	-0.965534781	2.743239517	-4.666733479
C	-2.969212391	7.589388815	5.597701866	C	-0.540497649	3.849439371	-5.417725162
H	-3.030894325	7.719866804	6.677181725	H	-0.14033279	3.629471128	-6.407415846
C	-2.714566917	6.275269851	5.149189047	C	-0.38683577	5.183351132	-4.978145532
C	-3.734642875	9.956407829	5.544995705	C	-0.788088005	1.381577877	-5.287076273
H	-3.01356407	10.76469371	5.34770955	H	-1.769931283	0.921026788	-5.472017131
H	-3.794265795	9.789040182	6.627327921	H	-0.242405504	1.445526111	-6.236294653
H	-4.706899649	10.31585955	5.181531644	H	-0.251508711	0.704998458	-4.606637818
C	-2.674212891	5.202092439	6.206013737	C	0.449449733	6.061617301	-5.876112031
H	-3.277484564	4.333407532	5.907232795	H	0.446565907	7.1101201	-5.556652613
H	-3.036200139	5.582975743	7.168627266	H	1.488988914	5.702053603	-5.889093695
H	-1.645350345	4.836110198	6.335757789	H	0.072013736	5.99523039	-6.907354818
C	-3.951127644	9.722073296	2.774072709	C	-1.677470676	1.661760411	-2.668008261
C	-5.341952378	9.559958786	2.57218568	C	-0.669928771	1.296002028	-1.744035355
C	-6.045846508	10.57106635	1.91475322	C	-0.842478713	0.127138372	-0.998744458
H	-7.122579416	10.45961416	1.763512901	H	-0.073267361	-0.168352657	-0.283576915
C	-5.399457477	11.70404317	1.432446726	C	-1.983655441	-0.656830881	-1.133578758
H	-5.966400602	12.48563886	0.92012224	H	-2.097700099	-1.567605752	-0.539816627
C	-4.022914179	11.81799146	1.578283983	C	-2.988518936	-0.256734139	-2.003261825
H	-3.506997493	12.68900092	1.165425513	H	-3.904035938	-0.849313602	-2.080989294
C	-3.275639248	10.8348612	2.234903903	C	-2.862161107	0.90442476	-2.772447406
C	-6.073836257	8.31056708	3.027537377	C	0.562514403	2.159854409	-1.544801385
H	-5.30760881	7.582585969	3.331117884	H	0.233807376	3.201905604	-1.696987227
C	-6.86686621	7.683223664	1.882804217	C	1.113779878	2.07445968	-0.125706216
H	-7.670292143	8.347840171	1.52634017	H	1.559032263	1.088996796	0.089620906
H	-7.340126155	6.746449529	2.21518993	H	1.902371643	2.826574835	0.016599562
H	-6.203108039	7.450495225	1.035276586	H	0.324934439	2.278433138	0.613596611
C	-6.970822519	8.573364357	4.237700912	C	1.655886097	1.867647802	-2.573381326
H	-6.397465795	8.941269741	5.100936414	H	1.324037846	2.083002585	-3.598577692
H	-7.480493236	7.647125992	4.54770458	H	2.540771489	2.49443833	-2.377631542
H	-7.745680279	9.322073338	4.003243309	H	1.971735186	0.811952131	-2.526513851
C	-1.769858133	10.97797892	2.316271535	C	-4.026141998	1.353464395	-3.630508944
H	-1.379630694	10.07994904	2.817529264	H	-3.697963009	2.236767316	-4.194163474
C	-1.16227983	11.00515551	0.913365603	C	-5.18193954	1.80396988	-2.736973462
H	-1.426046054	10.09259177	0.356441867	H	-4.844267866	2.572294515	-2.027422376
H	-0.064534991	11.06378891	0.968596547	H	-5.995366113	2.234394016	-3.341299356
H	-1.517896262	11.87358832	0.334539115	H	-5.592926277	0.958061147	-2.161434147
C	-1.349888821	12.20112844	3.130238016	C	-4.483234593	0.288034302	-4.625291665
H	-1.688523426	13.13850442	2.658306197	H	-4.881954058	-0.603677481	-4.114718342
H	-0.252592756	12.24800882	3.216826482	H	-5.284864435	0.684519447	-5.268596304
H	-1.768044295	12.17422307	4.148509857	H	-3.661465003	-0.046964165	-5.277276936
C	-2.398324083	4.568465566	3.526337358	C	-0.482847319	6.916992638	-3.334694546
C	-3.5298476	3.89666786	3.010087514	C	0.752656867	7.023592849	-2.659781567
C	-3.408399712	2.545076074	2.680168236	C	1.110623468	8.258426295	-2.110691462
H	-4.267439788	2.017262861	2.264520767	H	2.058770663	8.34792645	-1.574361092
C	-2.201683357	1.870204633	2.823940868	C	0.275815662	9.362098343	-2.211966387
H	-2.123188881	0.820176776	2.531704467	H	0.563136244	10.31386203	-1.758964432
C	-1.087789221	2.554166848	3.290696224	C	-0.94387458	9.239982676	-2.866887016
H	-0.128261556	2.035723165	3.365054752	H	-1.60979162	10.10235458	-2.920527287
C	-1.158997719	3.905489383	3.642857732	C	-1.34947709	8.028878632	-3.43188967
C	-4.840640948	4.627712556	2.790447536	C	1.705007908	5.852548877	-2.501552307
H	-4.569905418	5.65527986	2.491640371	H	1.216658939	4.963519318	-2.927865895
C	-5.655587721	4.047121746	1.640247601	C	1.991303329	5.556481563	-1.031170188
H	-5.034666812	3.963029253	0.734663262	H	1.057776497	5.341201687	-0.487573341

H	-6.501571878	4.71051663	1.408165711	H	2.661487796	4.68735784	-0.938133435
H	-6.071410104	3.054664367	1.88044266	H	2.483523763	6.407937577	-0.535629743
C	-5.672644472	4.706728074	4.071550173	C	3.01198545	6.084249669	-3.263355094
H	-6.63414224	5.207875559	3.877526704	H	3.653442364	5.189368224	-3.21329828
H	-5.160812692	5.274591887	4.861592031	H	2.836732097	6.321195681	-4.322583565
H	-5.891861664	3.698199553	4.460297346	H	3.577763339	6.923839822	-2.827770291
C	0.108678162	4.62277483	4.060585351	C	-2.680850799	7.925486794	-4.151842546
H	-0.169355432	5.64513184	4.34898071	H	-3.050150213	6.901620116	-3.98303165
C	1.061533411	4.737662439	2.871445709	C	-3.737091074	8.884734641	-3.61305097
H	1.438157107	3.747659769	2.567692518	H	-3.504861255	9.936669905	-3.850222684
H	1.926697889	5.36978189	3.126494257	H	-4.713161441	8.658288574	-4.069221399
H	0.550434155	5.181805583	2.006588094	H	-3.839057363	8.788430144	-2.521143603
C	0.806495846	3.958622994	5.247169833	C	-2.508543662	8.11517215	-5.660559142
H	0.141074362	3.852391289	6.118031022	H	-1.859319171	7.345345004	-6.098775853
H	1.680153218	4.553277992	5.558831377	H	-3.483535141	8.055818628	-6.170357612
H	1.17029638	2.950975897	4.988715416	H	-2.066273432	9.100803846	-5.884323107
C	0.515826833	7.991299402	1.600151699	C	-5.025967753	5.295972256	-2.89289917
H	0.862034298	9.044279394	1.497581496	H	-5.925149713	4.669268271	-3.080970738
H	0.032349071	7.709237585	0.652073764	H	-4.856023324	5.319156985	-1.805172356
H	1.434664831	7.374248596	1.702107149	H	-5.297666867	6.330864686	-3.19963864
C	0.178683619	8.196424963	3.95319953	C	-4.050745473	4.696549392	-4.988892182
H	1.119905385	7.646227751	4.18457944	H	-4.288663553	5.67432726	-5.470329531
H	-0.518801963	8.010974892	4.783500533	H	-3.147322171	4.309642201	-5.483779271
H	0.448595373	9.280077285	3.994834551	H	-4.892303129	4.016581719	-5.258243012

Table S10. Cartesian coordinates of $[L(Et_2N)GaBi]_2^{\bullet-}$ **4**. [Å] for the optimized geometry.

Bi	1.98166003	3.85987069	10.17867004	H	2.30052511	3.00036734	5.32354455
Bi	3.10565550	6.51002283	9.92866696	H	5.19570218	8.62805159	13.36900844
Ga	3.88673060	3.21055727	11.88814603	C	3.11471791	8.32961781	13.80916864
Ga	1.86064872	6.77891806	7.61782889	H	6.08907277	5.05339126	12.82930426
N	3.96293196	4.19702321	13.69926284	C	7.07661600	6.22903046	14.33276849
N	3.50479514	1.45193228	12.78955771	C	6.69617325	6.90280592	11.95341572
N	5.72858069	3.09463694	11.43175667	H	1.07538134	7.74065323	14.12968041
N	-0.17696627	6.95737468	7.53097402	H	1.53142355	4.12671682	13.51827466
N	2.11305202	8.69974918	6.96453428	C	1.01932434	4.63212982	15.54029091
N	2.21336728	5.69175648	6.10066952	C	-0.06977453	5.51602938	13.44626372
C	4.35471371	3.56204181	14.78324967	H	2.59685952	-1.85266870	9.70060609
C	3.68849615	5.59608243	13.71777584	C	1.01500434	-1.52080978	11.11480857
C	4.03166630	1.18088277	13.98531261	H	4.80511696	0.96576834	10.73662705
C	2.66310660	0.48575643	12.17599313	C	5.45345368	-1.07289143	10.72909023
C	6.21973549	3.85476219	10.30511948	C	4.26172830	0.12848904	8.86055723
C	6.67772425	2.17758740	12.00221668	H	-0.43459101	-0.89266257	12.57413950
C	-0.75150632	7.79546655	6.68419550	H	1.52234025	1.95939730	14.00084234
C	-0.95770359	6.21054885	8.46372828	C	0.43805968	0.45119935	15.05881184
C	1.25169828	9.23174458	6.10717564	C	-0.46193634	1.91009161	13.21593906
C	3.28368457	9.43092132	7.30973025	H	-2.10122093	3.06051945	9.07157272
C	1.45957755	5.72136507	4.87503030	C	-2.41785105	4.74999782	10.35491753
C	3.32520784	4.77075289	6.11946948	H	0.27520156	4.56598233	6.75455034
C	4.52346240	2.15603544	14.85837771	C	-1.65048955	4.35159442	5.82963539
C	4.62678569	4.30116636	16.07128009	C	-0.47882060	2.62480802	7.20370134
C	4.71844119	6.53252787	13.47816867	H	-2.54611341	6.58942946	11.45603098
C	2.35802182	6.02453944	13.92139150	H	-0.57506896	8.72327883	9.10640719
C	4.09579476	-0.25317149	14.44614054	C	-2.50890267	9.11361681	9.94126181
C	3.09352328	-0.25565873	11.05389590	C	-0.43900777	8.50710478	11.22428470
C	1.36140389	0.28835464	12.69645023	H	6.50779901	9.96455497	6.34875518
H	7.24980730	4.21657118	10.50441649	C	5.48422099	11.06644104	7.88390095
H	5.60779413	4.76506363	10.18872294	H	3.75913137	7.55114454	5.56720705
C	6.19603190	3.12176612	8.96842524	C	5.02066615	8.63213104	4.20974335
H	7.25676027	1.66642462	11.20223902	C	5.78332253	7.17614140	6.11980463

H	6.14352061	1.36916936	12.52840000	H	4.27454132	11.88836938	9.45587311
C	7.66923266	2.80094472	12.98495781	H	1.56058371	9.39745309	9.27577512
C	-0.05067678	8.74360836	5.90731984	C	0.93422964	11.38689124	8.79553424
C	-2.25131902	7.81527228	6.51689159	C	2.38345847	10.70731133	10.73833412
C	-1.19398145	4.83080442	8.25384997	H	2.89025573	9.39845298	13.84585123
C	-1.44412580	6.85052897	9.62459620	H	8.09181443	5.90085908	14.05803573
C	1.65639911	10.44923863	5.31547080	H	6.74734379	5.61786224	15.18327240
C	4.49529203	9.24754669	6.61133629	H	7.14105842	7.27444531	14.67860878
C	3.21796570	10.34612747	8.38768676	H	6.00368949	6.89509180	11.09818645
H	0.46728693	6.15576265	5.06997246	H	7.65138130	6.46445942	11.62526297
H	1.25686092	4.68986592	4.51556869	H	6.89293195	7.95438096	12.22009508
C	2.09246610	6.50317233	3.72347059	H	0.76725904	5.51392774	16.15257218
H	3.93419114	4.98803283	7.01293182	H	1.91804495	4.16930287	15.97054438
C	2.95229619	3.29202649	6.16324176	H	0.19419984	3.90807858	15.63483301
H	3.99683534	4.93916290	5.24934857	H	0.09214753	5.77675768	12.39058160
H	4.95610150	1.78749875	15.78870172	H	-0.48667652	6.39083313	13.97127025
H	5.66630525	4.11836351	16.38341514	H	-0.83214492	4.72512985	13.47779172
H	3.97923867	3.91269657	16.87106445	H	0.38384105	-2.31786807	10.71352725
H	4.46702815	5.38131836	15.97803993	H	5.12413753	-2.07025343	10.39200996
C	4.40672917	7.89421333	13.54807863	H	5.62408486	-1.12548553	11.81488013
C	6.13455231	6.11051899	13.13417060	H	6.42113236	-0.85380187	10.25054188
C	2.09905424	7.39593246	13.97557096	H	3.92301088	-0.81190630	8.39642574
C	1.22724129	5.02644401	14.07782279	H	5.22185598	0.39784926	8.39679729
H	3.09126558	-0.67907196	14.57275079	H	3.53533617	0.91785763	8.61323246
H	4.63752083	-0.33864852	15.39605167	H	-0.31706485	-0.33414971	14.89056862
H	4.59541731	-0.87199843	13.68609673	H	0.03004046	1.15034685	15.80616908
C	2.25945623	-1.26165823	10.55518537	H	1.32532951	-0.02582586	15.50035474
C	4.42370391	-0.00048576	10.37382623	H	-0.20719777	2.50390305	12.32391264
C	0.56628872	-0.72965782	12.16509151	H	-0.88100932	2.58964177	13.97345990
C	0.77156885	1.19189508	13.76406018	H	-1.25292639	1.19508155	12.93811365
H	5.15545386	2.89562611	8.69089207	H	-2.97301663	4.17414049	11.09959978
H	6.75859020	2.17467048	9.00852365	H	-1.75178001	5.41603595	5.58195638
H	6.63310227	3.74292630	8.16878867	H	-2.65619687	3.95942242	6.05757052
H	8.21419438	3.64026484	12.52471498	H	-1.27889077	3.83690663	4.92954401
H	8.41441202	2.06072746	13.32376972	H	-1.42728530	2.07638226	7.32882742
H	7.14276931	3.18452363	13.87142140	H	0.15681848	2.42399400	8.07964188
H	-0.64799142	9.27637482	5.16740259	H	0.02509224	2.20524274	6.32018406
H	-2.50118951	7.79080620	5.44597496	H	-3.09248719	8.97838327	9.01931351
H	-2.65937462	8.75295373	6.92231964	H	-2.30546919	10.18983880	10.06317348
H	-2.74198600	6.97540792	7.02216895	H	-3.14626796	8.79872772	10.78346372
C	-1.92628316	4.12756665	9.21374981	H	0.53879828	8.00045823	11.19015135
C	-0.70057822	4.12063353	7.00726293	H	-1.00381484	8.10080728	12.07735661
C	-2.17641463	6.10150016	10.55059141	H	-0.27330727	9.57722785	11.41980722
C	-1.20138222	8.31944658	9.91520902	H	6.33348508	11.72265140	8.09107640
H	2.53529444	10.22105483	4.69472634	H	5.12859105	7.78735868	3.51154275
H	1.95737299	11.27052970	5.98180278	H	5.96415654	9.20232131	4.19260245
H	0.84019955	10.79300702	4.66849478	H	4.22905858	9.28815304	3.81619730
C	5.57299869	10.09113663	6.90124288	H	5.88977067	6.31363769	5.44479218
C	4.69560024	8.12622930	5.61342210	H	5.53116591	6.79602447	7.12183080
C	4.32045522	11.16622755	8.63887148	H	6.76190888	7.67968747	6.18323585
C	1.99956396	10.40886939	9.29153060	H	1.34425538	12.40677074	8.70501474
H	2.15070858	7.57506161	3.96252508	H	0.08927346	11.42473330	9.50209712
H	1.49686231	6.39491678	2.80113468	H	0.52946659	11.08987797	7.81783231
H	3.11199732	6.14885729	3.50629703	H	3.13998508	9.99384213	11.09806403
H	2.43196033	3.06285516	7.10567815	H	1.50477451	10.61608488	11.39159441
H	3.85632907	2.66302266	6.11626069	H	2.77440890	11.73000791	10.86327078

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