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Supporting Information

Isolation and Structure of Germylene-Germyliumylidenes Stabilized by N-Heterocyclic Imine

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Contents

1.) Experimental Details

General considerations: All experiments and manipulations were conducted under dry oxygen-free nitrogen using standard Schlenk techniques or in an MBraun glovebox workstation containing an atmosphere of purified nitrogen. Solvents were dried by standard methods. NMR solvents were degassed by multiple freeze-pump-thaw cycles and stored over molecular sieves (3 Å). Reagents were purchased from commercial suppliers and processed as received if not stated otherwise. The starting material amino(imino)germylene **1** was prepared according to the reported procedure.[S1] ^{1}H-, ^{11}B-, ^{13}C{^{1}H}-, and ^{19}F- spectra were recorded on a Bruker Avance II 200 MHz or 400 MHz spectrometer and referenced to residual solvent signals as internal standards (^{1}H and ^{13}C) or an external standard ($Et_2O{\bullet}BF_3$ for ^{11}B, and $CFCl_3$ for ^{19}F). Values for the chemical shift (δ) are given in parts per million. Abbreviations: s = singlet; d = doublet; t = triplet; sept = septet; br = broad; n.r. = not resolved; n.o. = not observed; Dip = 2,6-diisopropylphenyl; Ar^F = 3,5-$(CF_3)_2$-C_6H_3; OR^F = $OC(CF_3)_3$. Elemental analyses and ESI-HRMS were carried out by the microanalytical laboratory and the MS-Service of the Institut für Chemie, Technische Universität Berlin, Germany, respectively.

Synthetic Procedure and Analytical Data for 3[BF_4]

To a stirring mixture of amino(imino)germylene **1** (1.17 g, 1.84 mmol) in toluene (10 ml) was added BF_3•Et_2O (0.46 ml, 3.72 mmol) via syringe at −78 ºC. The reaction mixture was stirred for 12 h while allowed to slowly warm to room temperature. The solvent was removed under vacuum and the residue washed with Et_2O (5 ml) to give a yellow solid. Recrystallization from THF (3 ml) afforded **3**[BF_4] in the form of colorless crystals (854 mg, 87%). The batch contained single crystals suitable for X-ray diffraction analysis.
^{1}H NMR (200.1 MHz, THF-d_8): δ = 1.12 (d, $^3J_{HH}$ = 7 Hz, 24H, CH(CH_3)$_2$), 1.16 (d, $^3J_{HH}$ = 7 Hz, 24H, CH(CH_3)$_2$), 2.56 (sept, $^3J_{HH}$ = 7 Hz, 8H, *C*H(CH$_3$)$_2$), 7.13 (s, 4H, NC*H*), 7.24 (d, $^3J_{HH}$ = 8 Hz, 8H, Ar-H), 7.48 (t, $^3J_{HH}$ = 8 Hz, 4H, Ar-H). ^{13}C{^{1}H} NMR (100.6 MHz, THF-d_8): δ = 23.1 (CH(*C*H$_3$)$_2$), 25.1 (CH(*C*H$_3$)$_2$), 29.8 (*C*H(CH$_3$)$_2$), 119.6 (N*C*H), 126.5 (Ar-C), 132.4 (Ar-C), 132.7 (Ar-C), 147.4 (Ar-C), 151.4 (N*C*N). ^{11}B NMR (64.2 MHz, THF-d_8): δ = −2.9 (n. r.). ^{19}F NMR (188.3 MHz, THF-d_8): δ = −153.9 (n. r., B*F*$_4$), −63.1 (Ge*F*). ESI-HRMS: *m/z* (positive ion mode): 969.4253 (calc. 969.4230 for [M − BF_4]$^+$). ESI-HRMS: *m/z* (negative ion mode): 87.0033 (calc. 87.0024 for [BF_4]$^-$). M.p. at 291-294 °C (dec.).

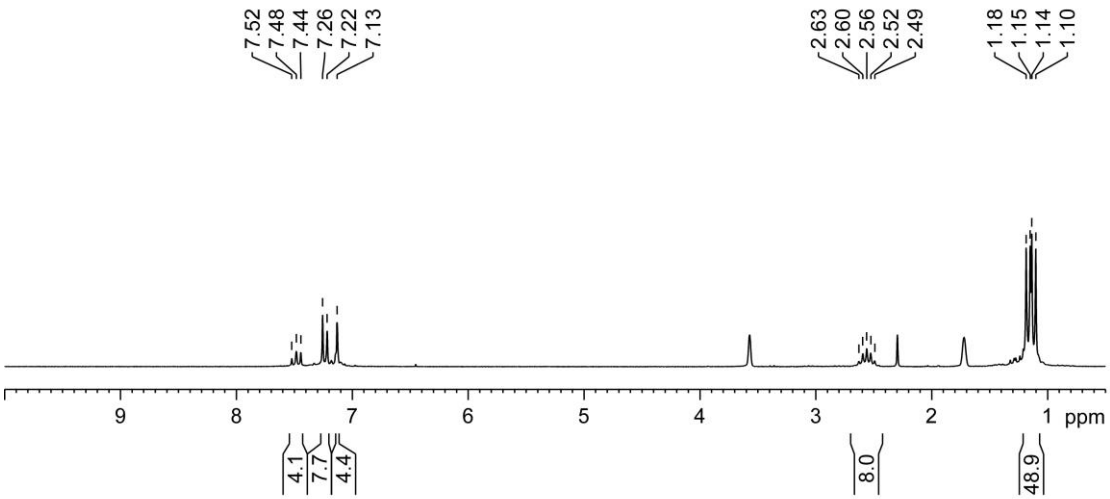


Figure S1. ^{1}H NMR spectrum (200.1 MHz, THF-d_8) of **3**[BF_4].

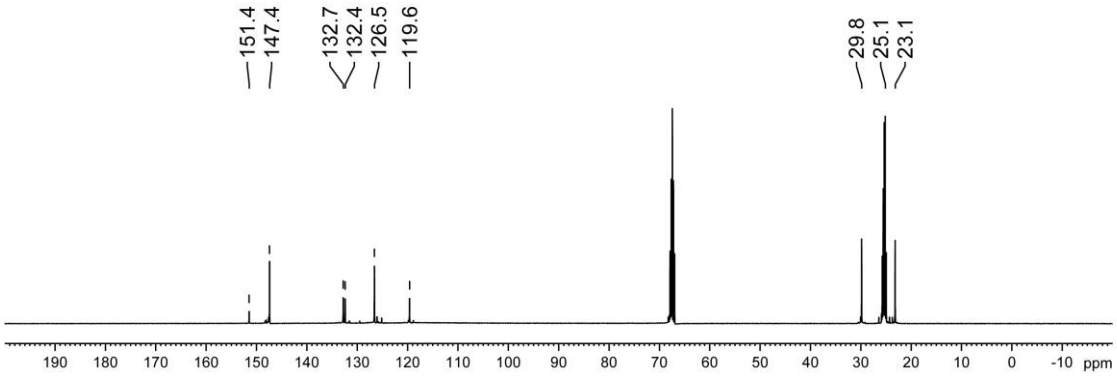


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, THF-d_8) of **3**[BF_4].

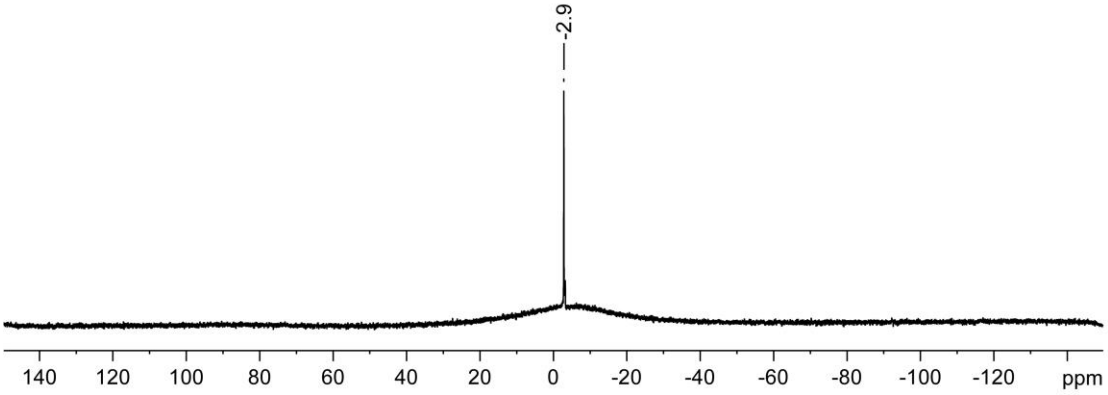


Figure S3. ^{11}B NMR spectrum (64.2 MHz, THF-d_8) of **3**[BF_4].

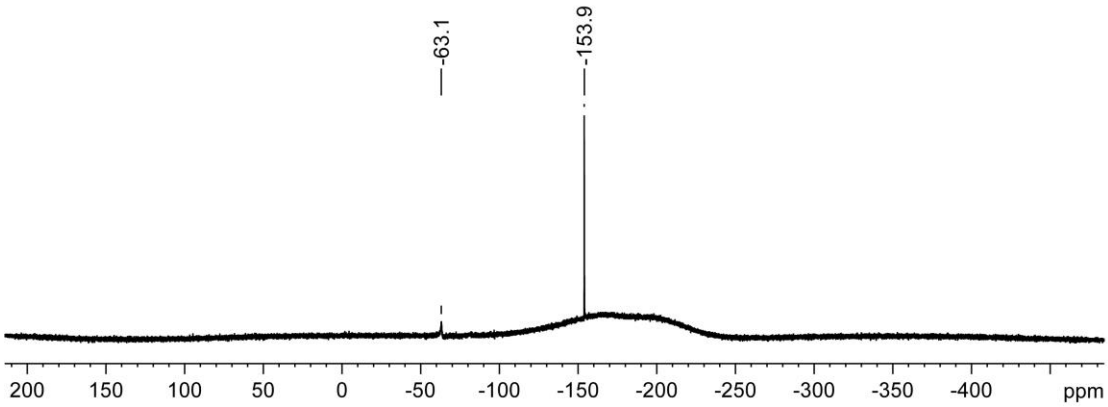


Figure S4. ^{19}F NMR spectrum (188.3 MHz, THF-d_8) of **3**[BF_4].

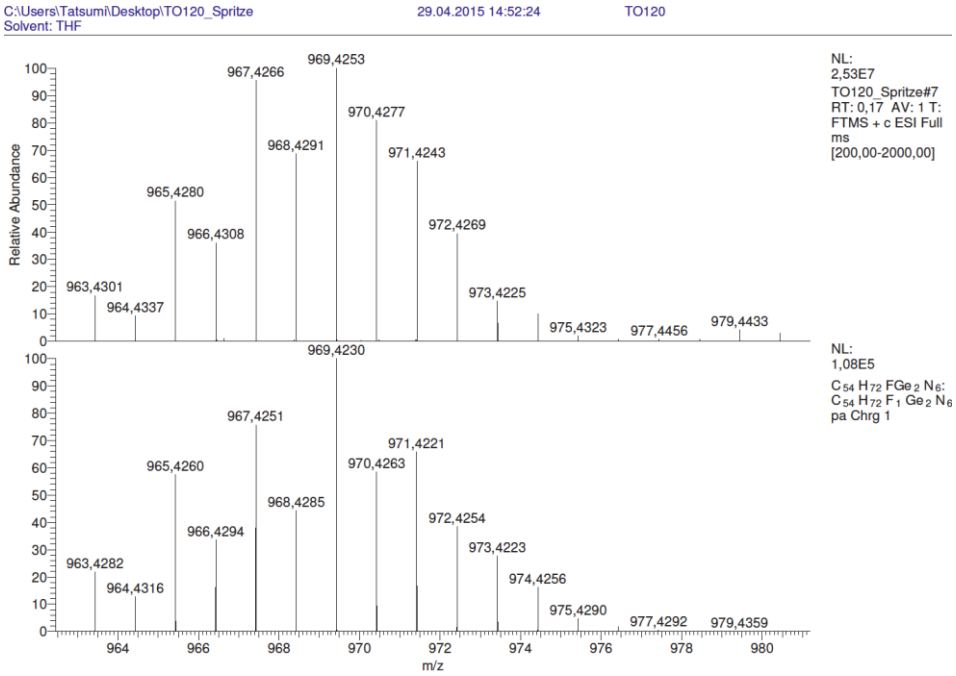


Figure S5. Signal of $[M - BF_4]^+$ as observed in the ESI-HRMS (positive ion mode) analysis of **3**$[BF_4]$. Top (expt.), bottom (calc.).

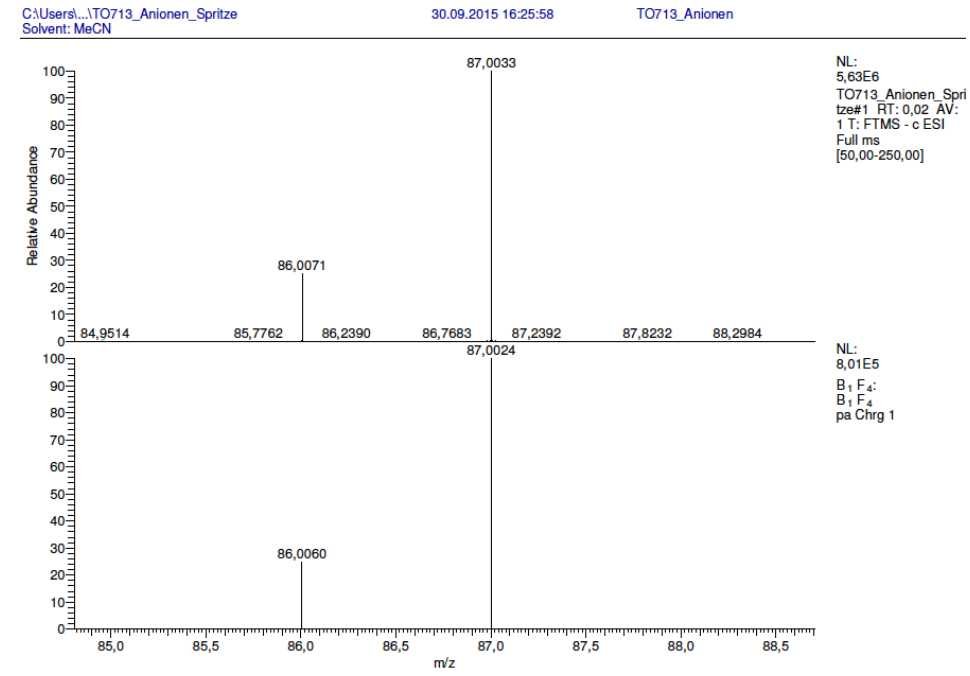


Figure S6. Signal of $[BF_4]^-$ as observed in the ESI-HRMS (negative ion mode) analysis of **3**$[BF_4]$. Top (expt.), bottom (calc.).

Synthetic Procedure and Analytical Data for 3[BAr$^F_4$]

A Schlenk tube equipped with a PTFE-coated magnetic stirring bar was charged with **3**[BF_4] (239 mg, 0.226 mmol) and Na[BAr$^F_4$] (401 mg, 0.452 mmol). CH_3CN (10 ml) was transferred to the reaction vessel by cannula at −30 ºC and the resulting mixture was stirred for 12 h while allowed to slowly warm to room temperature. The volatiles were removed under reduced pressure and the residue was recrystallized from CH_3CN (5 ml) at −30 ºC to afford **3**[BAr$^F_4$] as colorless crystals (211 mg, 51%). The batch contained crystals suitable for single crystal X-ray diffraction analysis.

^{1}H NMR (400.1 MHz, CD_3CN): δ = 1.09 (d, $^3J_{HH}$ = 6 Hz, 24H, CH(CH_3)$_2$), 1.13 (d, $^3J_{HH}$ = 6 Hz, 24H, CH(CH_3)$_2$), 2.49 (sept, $^3J_{HH}$ = 6 Hz, 8H, *CH*(CH$_3$)$_2$), 6.94 (s, 4H, NC*H*), 7.21 (d, $^3J_{HH}$ = 8 Hz, 8H, Ar-H), 7.43 (t, $^3J_{HH}$ = 8 Hz, 4H, Ar-H), 7.67 (br, 4H, Ar^F-H$_{para}$), 7.70 (br, 8H, Ar^F-H$_{ortho}$). ^{13}C{^{1}H} NMR (100.6 MHz, CD_3CN): δ = 22.9 (CH(*C*H$_3$)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 29.8 (*C*H(CH$_3$)$_2$), 118.7 (m, Ar^F-C$_{para}$), 119.3 (N*C*H), 125.5 (q, $^1J_{CF}$ = 273 Hz, *C*F$_3$), 126.7 (Ar-C), 129.8 (q, $^2J_{CF}$ = 31 Hz, Ar^F-C$_{meta}$), 132.1 (Ar-C), 132.8 (Ar-C), 135.7 (br, Ar^F-C$_{ortho}$), 147.6 (Ar-C), 151.6 (N*C*N), 162.6 (q, $^1J_{CB}$ = 49 Hz, Ar^F-C$_{ipso}$). ^{11}B NMR (64.2 MHz, CD_3CN): δ = −6.7. ^{19}F NMR (188.3 MHz, CD_3CN): δ = −63.3 (C*F*$_3$), −62.8 (Ge*F*). Elemental analysis calc. (%) for $C_{86}H_{84}BF_{25}Ge_2N_6$: C 56.36, H 4.62, N 4.59; found: C 56.67, H 4.92, N 4.51. M.p. at 274-276 °C (dec.).

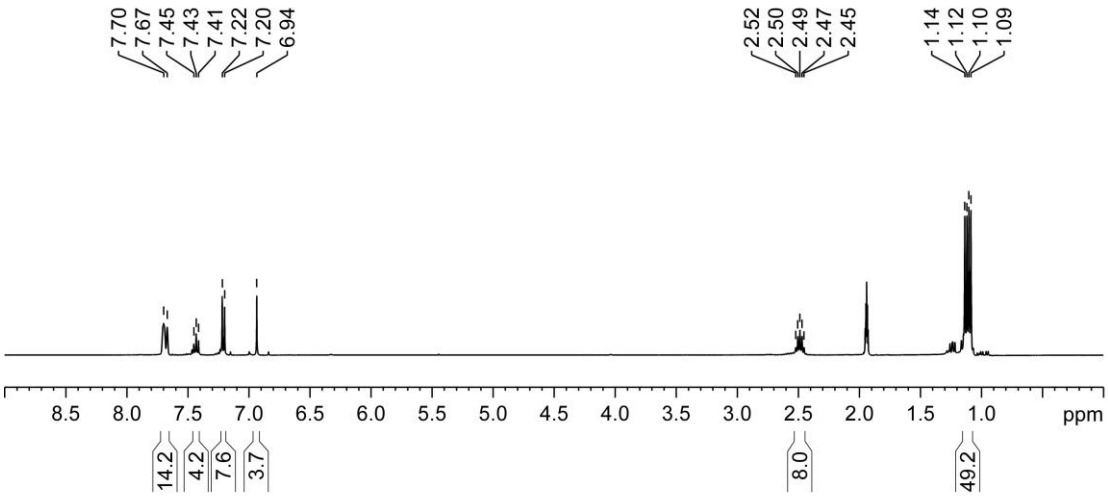


Figure S7. ^{1}H NMR spectrum (400.1 MHz, CD_3CN) of **3**[BAr$^F_4$].

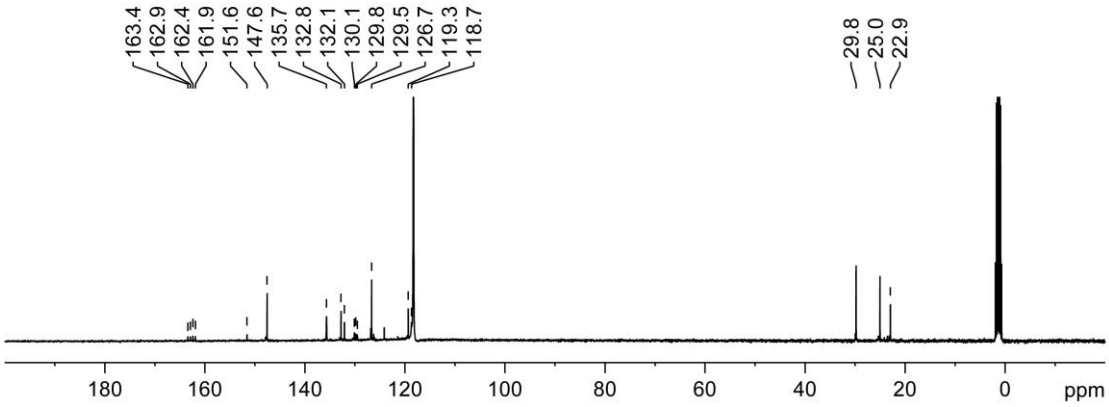


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, CD_3CN) of **3**[BAr^F_4].

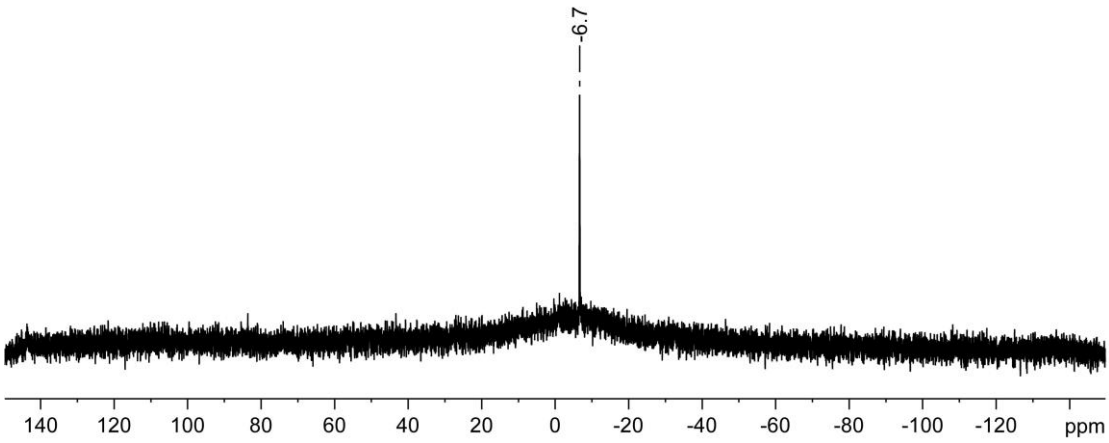


Figure S9. ^{11}B NMR spectrum (64.2 MHz, CD_3CN) of **3**[BAr^F_4].

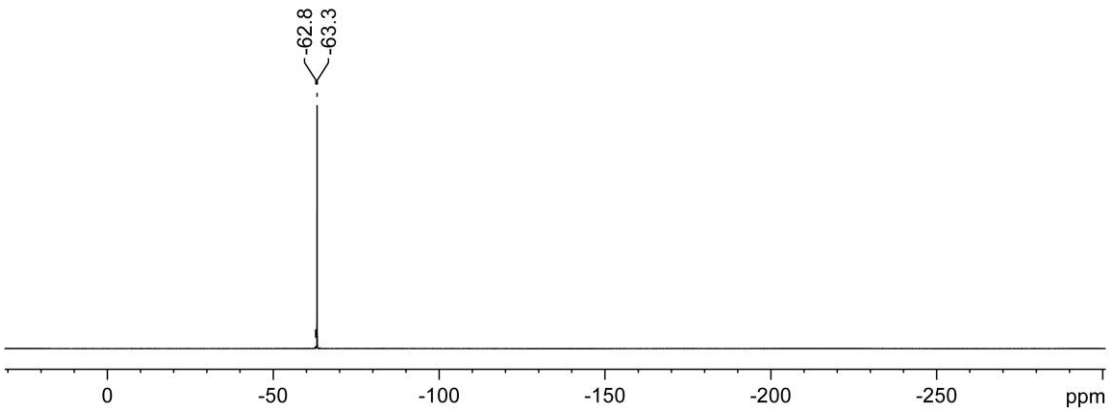


Figure S10. ^{19}F NMR spectrum (188.3 MHz, CD_3CN) of **3**[BAr^F_4].

Synthetic Procedure and Analytical Data for 4[OTf]

Me_3SiOTf (0.2 ml, 1.1 mmol) was added to a stirring mixture of **3**[BF_4] (525 mg, 0.497 mmol) in CH_2Cl_2 (10 ml) via syringe at −30 ºC. The reaction mixture was stirred for 12 h while allowed to slowly warm to room temperature. The solvent was removed under vacuum. The residue was recrystallized from CH_2Cl_2 (5 ml) at −30 ºC to give **4**[OTf] as colorless crystals (409 mg, 66%). The batch contained single crystals suitable for X-ray diffraction analysis.

^{1}H NMR (200.1 MHz, CD_3CN): δ = 1.08 (d, $^3J_{HH}$ = 8 Hz, 24H, CH(CH_3)$_2$), 1.19 (d, $^3J_{HH}$ = 8 Hz, 24H, CH(CH_3)$_2$), 2.58 (sept, $^3J_{HH}$ = 8 Hz, 8H, CH(CH$_3$)$_2$), 7.02 (s, 4H, NCH), 7.24 (d, $^3J_{HH}$ = 8 Hz, 8H, Ar-H), 7.46 (t, $^3J_{HH}$ = 8 Hz, 4H, Ar-H). ^{13}C{^{1}H} NMR (100.6 MHz, CD_3CN): δ = 22.8 (CH(*C*H$_3$)$_2$), 25.9 (CH(*C*H$_3$)$_2$), 29.6 (*C*H(CH$_3$)$_2$), 119.9 (N*C*H), 126.9 (Ar-C), 132.0 (Ar-C), 133.5 (Ar-C), 147.8 (Ar-C), 151.3 (N*C*N). ^{19}F NMR (188.3 MHz, CD_3CN): δ = −79.2. ESI-HRMS: *m/z* (positive ion mode): 1099.3773 (calc. 1099.3766 for [M − OTf]$^+$). ESI-HRMS: *m/z* (negative ion mode): 148.9519 (calc. 148.9515 for [OTf]$^-$). M.p. at 225-228 ºC (dec.).

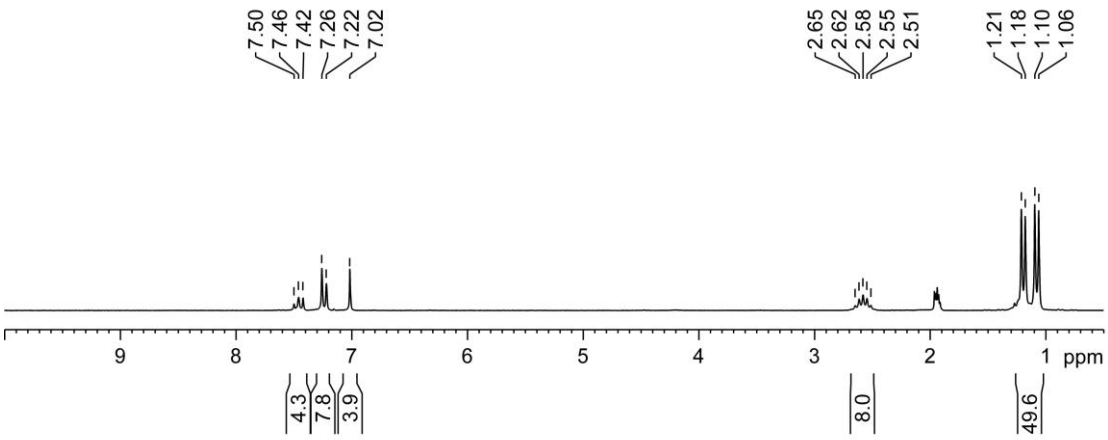


Figure S11. ^{1}H NMR spectrum (200.1 MHz, CD_3CN) of **4**[OTf].

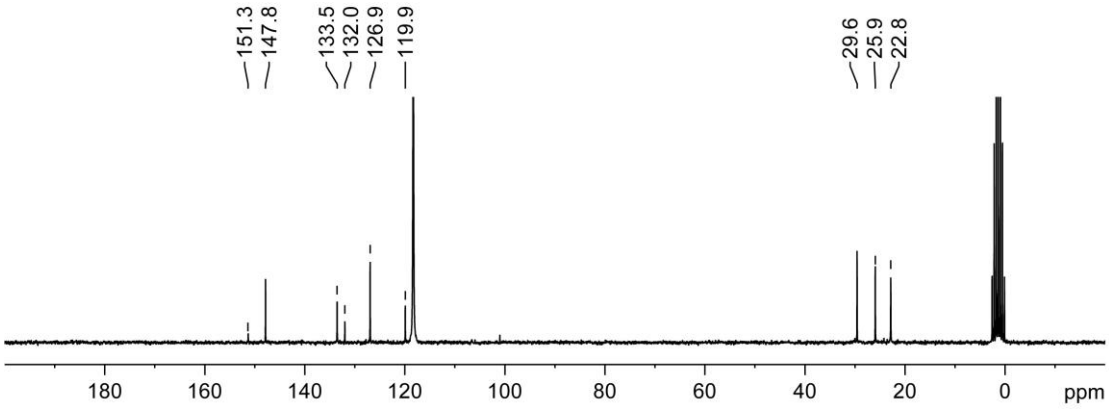


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, CD_3CN) of **4**[OTf]

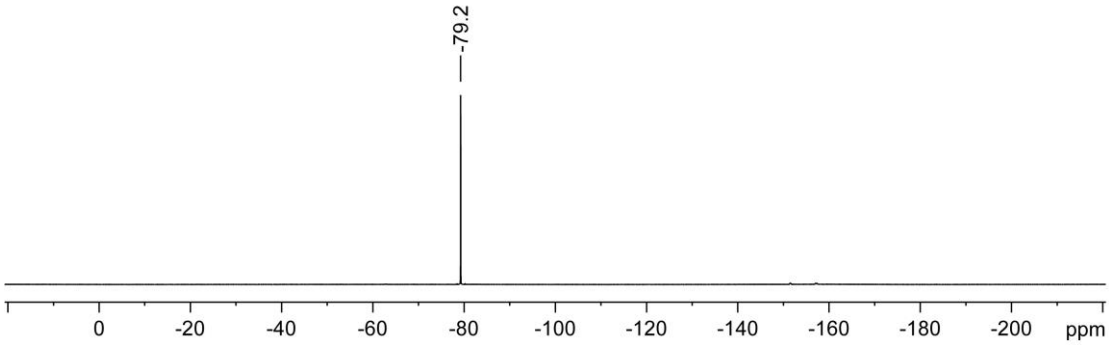


Figure S13. ^{19}F NMR spectrum (188.3 MHz, CD_3CN) of **4**[OTf].

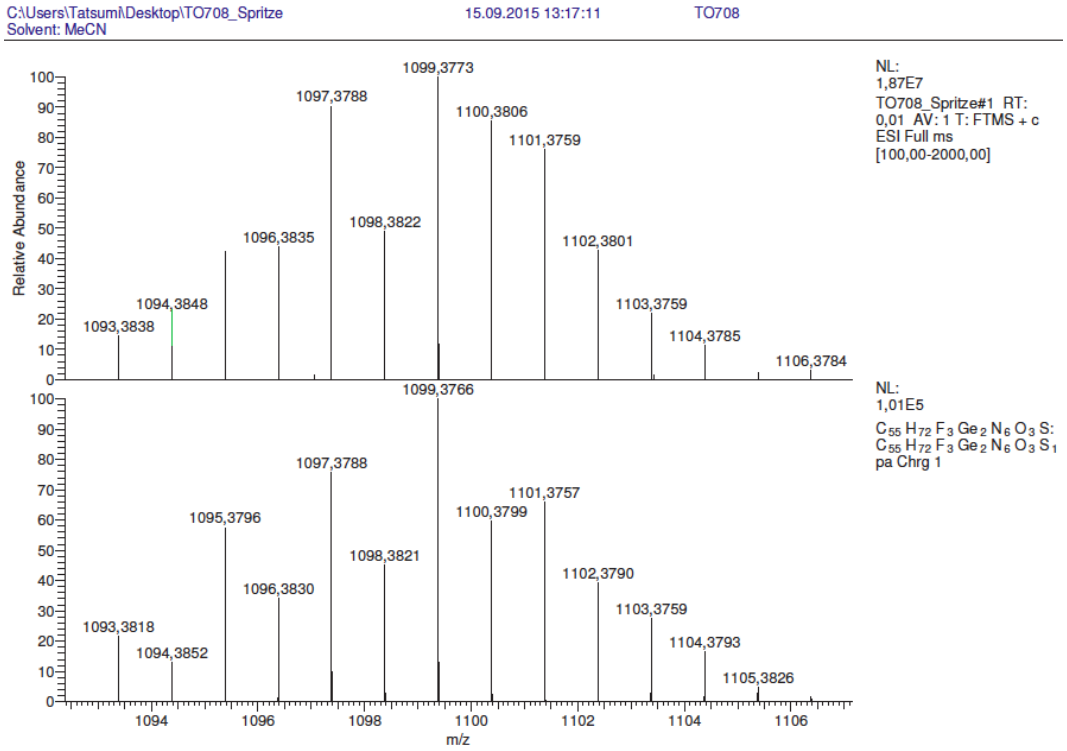


Figure S14. Signal of $[M - OTf]^+$ as observed in the ESI-HRMS (positive ion mode) analysis of **4**[OTf]. Top (expt.), bottom (calc.).

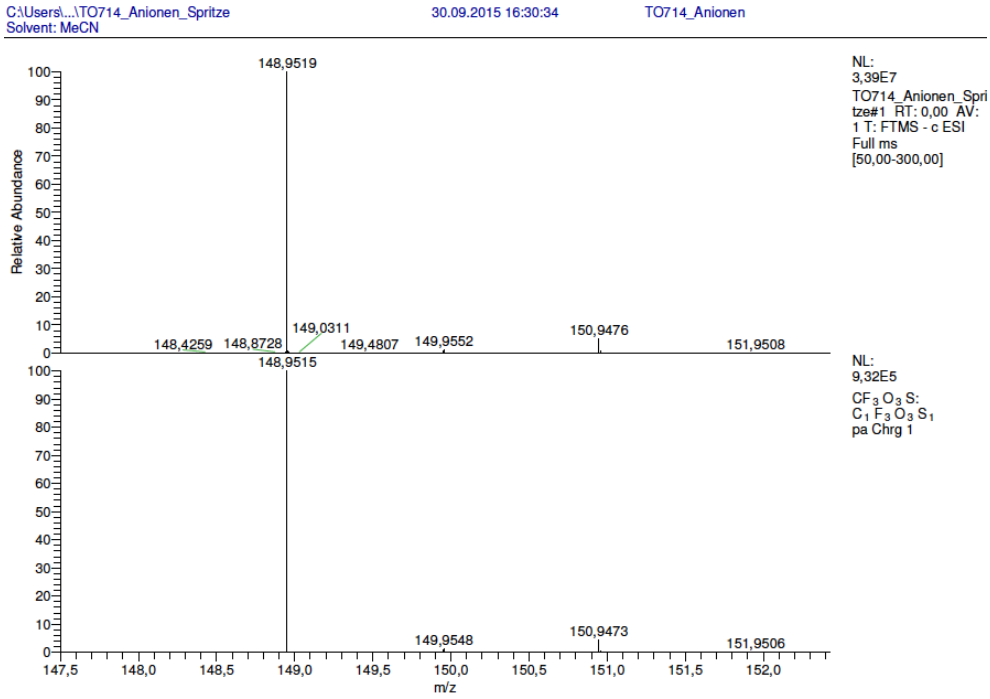


Figure S15. Signal of $[OTf]^-$ as observed in the ESI-HRMS (negative ion mode) analysis of **4**[OTf]. Top (expt.), bottom (calc.).

Synthetic Procedure and Analytical Data for 4[BAr$^F_4$]

A Schlenk tube equipped with a PTFE-coated magnetic stirring bar was charged with **4**[OTf] (222 mg, 0.178 mmol) and Na[BAr$^F_4$] (315 mg, 0.355 mmol). CH_3CN (10 ml) was transferred to the reaction vessel by cannula at −30 ºC and the resulting mixture was stirred for 12 h while allowed to slowly warm to room temperature. The volatiles were removed under reduced pressure and recrystallization of the residue from CH_2Cl_2 at −30 ºC afforded **4**[BAr$^F_4$] as colorless crystals (146 mg, 42%). Colorless crystals of **4**[BAr$^F_4$] of suitable quality for X-ray crystallography were obtained from CH_3CN at −30 ºC.

^{1}H NMR (200.1 MHz, CD_2Cl_2): δ = 1.08 (d, $^3J_{HH}$ = 7 Hz, 24H, CH(C*H*$_3$)$_2$), 1.20 (d, $^3J_{HH}$ = 7 Hz, 24H, CH(C*H*$_3$)$_2$), 2.62 (sept, $^3J_{HH}$ = 8 Hz, 8H, C*H*(CH$_3$)$_2$), 6.70 (s, 4H, NC*H*), 7.18 (d, $^3J_{HH}$ = 8 Hz, 8H, Ar-H), 7.39 (t, $^3J_{HH}$ = 8 Hz, 4H, Ar-H), 7.56 (br, 4H, Ar^F-H$_{para}$), 7.72 (br, 8H, Ar^F-H$_{ortho}$). ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 22.6 (CH(*C*H$_3$)$_2$), 26.0 (CH(*C*H$_3$)$_2$), 29.0 (*C*H(CH$_3$)$_2$), 117.9 (n.r., Ar^F-C$_{para}$), 118.7 (N*C*H), 125.0 (q, $^1J_{CF}$ = 273 Hz, *C*F$_3$), 126.2 (Ar-C), 129.9 (q, $^2J_{CF}$ = 31 Hz, Ar^F-C$_{meta}$), 131.3 (Ar-C), 132.7 (Ar-C), 135.2 (br, Ar^F-C$_{ortho}$), 147.4 (Ar-C), 150.9 (N*C*N), 162.2 (q, $^1J_{CB}$ = 50 Hz, Ar^F-C$_{ipso}$). ^{11}B NMR (64.2 MHz, CD_2Cl_2): δ = −6.6. ^{19}F NMR (188.3 MHz, CD_2Cl_2): δ =, −79.1 (SO_3CF_3), −62.8 (Ar-C*F*$_3$). ESI-HRMS: *m/z* (positive ion mode): 1099.3754 (calc. 1099.3766 for [M − BAr$^F_4$]$^+$). ESI-HRMS: *m/z* (negative ion mode): 863.0640 (calc. 863.0643 for [BAr$^F_4$]$^-$). Elemental analysis calc. (%) for $C_{87}H_{84}BF_{27}Ge_2N_6O_3S$•2$CH_2Cl_2$: C 50.13, H 4.16, N 3.94, S 1.50; found: C 50.73, H 4.25, N 3.62, S 1.11. M.p. at 214-216 °C (dec.).

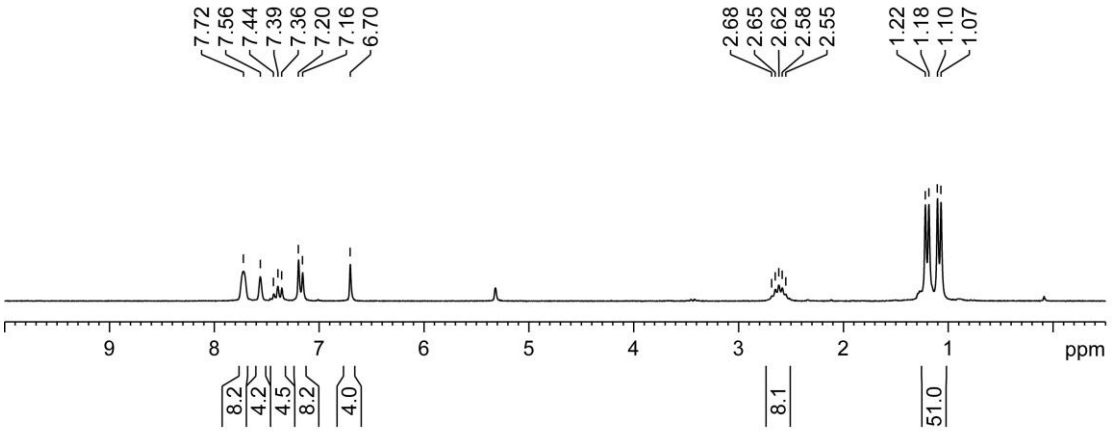


Figure S16. ^{1}H NMR spectrum (200.1 MHz, CD_2Cl_2) of **4**[BAr$^F_4$].

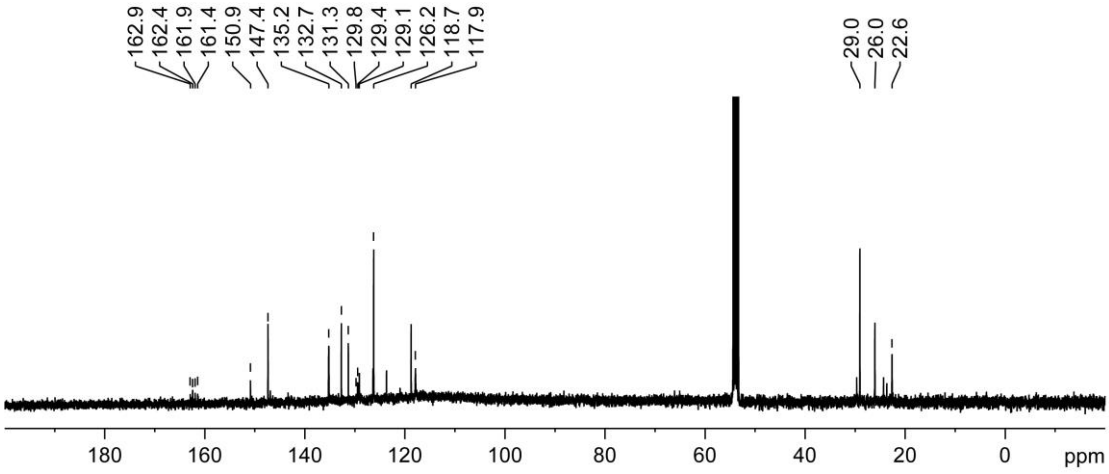


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, CD_2Cl_2) of **4**[BAr^F_4].

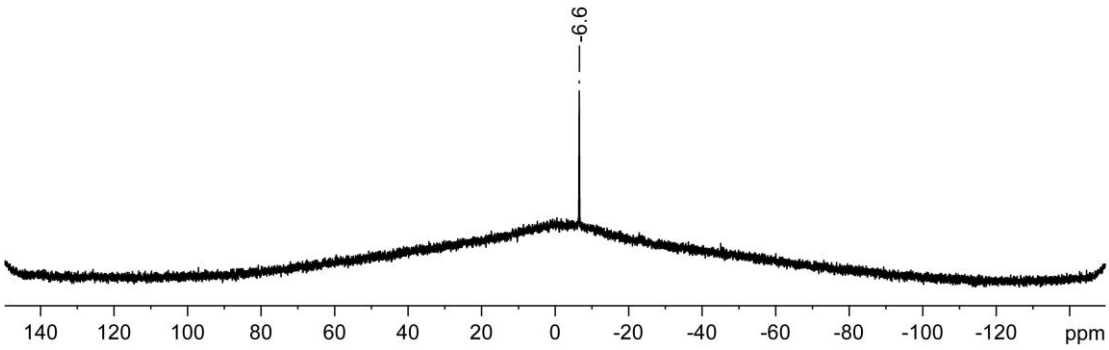


Figure S18. ^{11}B NMR spectrum (64.2 MHz, CD_2Cl_2) of **4**[BAr^F_4].

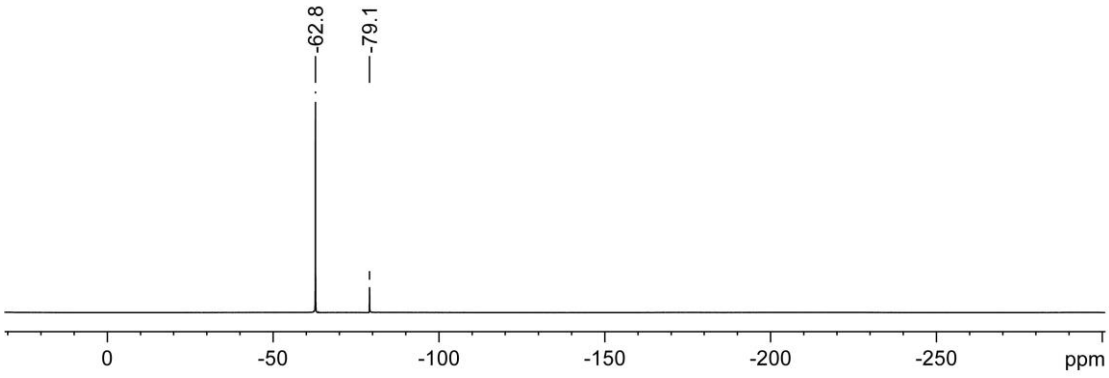


Figure S19. ^{19}F NMR spectrum (188.3 MHz, CD_2Cl_2) of **4**[BAr^F_4].

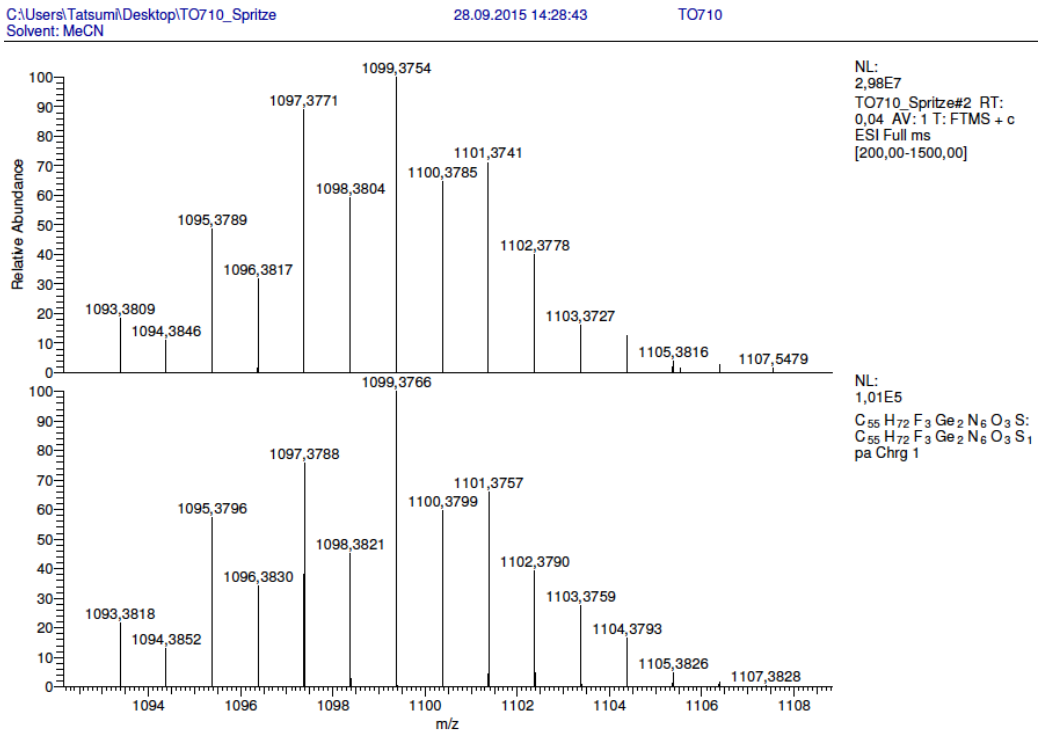


Figure S20. Signal of $[M - BAr^{F}_{4}]^{+}$ as observed in the ESI-HRMS (positive ion mode) analysis of **4**$[BAr^{F}_{4}]$. Top (expt.), bottom (calc.).

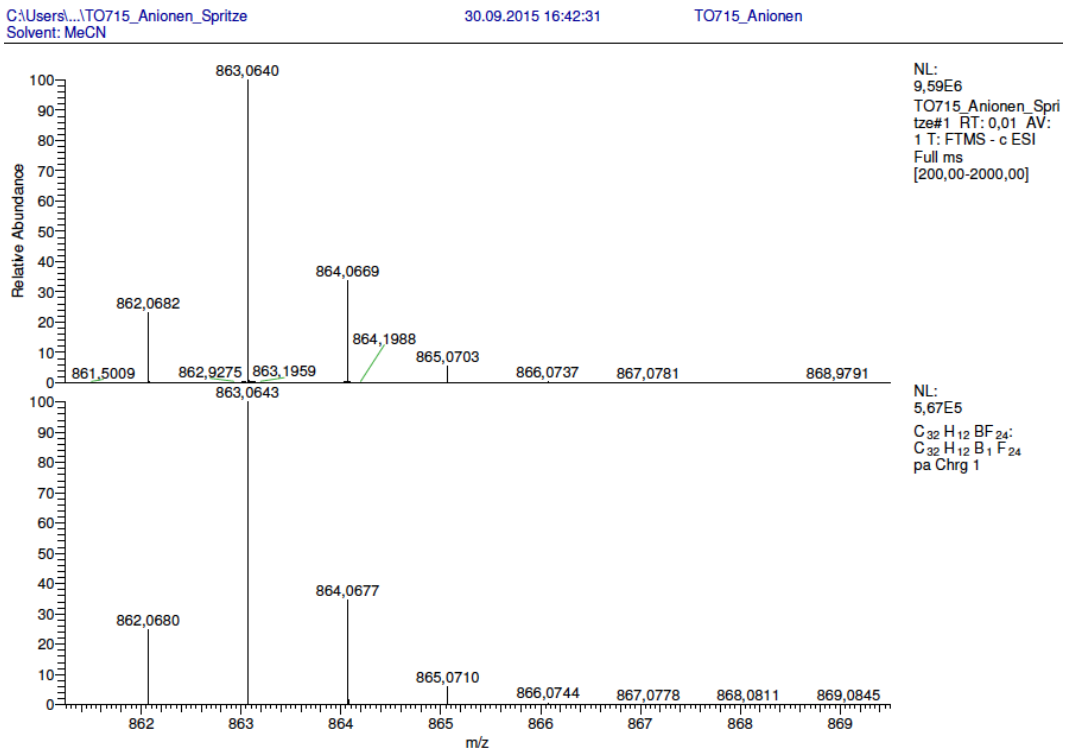


Figure S21. Signal of $[BAr^{F}_{4}]^{-}$ as observed in the ESI-HRMS (negative ion mode)

analysis of **4**[BAr^F_4]. Top (expt.), bottom (calc.).

Synthetic Procedure and Analytical Data for 4[Al(OR^F)$_4$]

A Schlenk tube equipped with a PTFE-coated magnetic stirring bar was charged with **4**[OTf] (213 mg, 0.170 mmol) and Ag[Al(OR^F)$_4$] (368 mg, 0.342 mmol). CH_2Cl_2 (10 ml) was transferred to the reaction vessel by cannula at −30 °C and the resulting mixture was stirred for 12 h while allowed to slowly warm to room temperature. The volatiles were removed under reduced pressure and recrystallization of the residue from CH_2Cl_2 at −30 °C afforded **4**[Al(OR^F)$_4$] as colorless crystals (130 mg, 37%).

^{1}H NMR (200.1 MHz, CD_2Cl_2): δ = 1.28 (t, $^3J_{HH}$ = 7 Hz, 48H, CH(CH_3)$_2$), 2.55 (sept, $^3J_{HH}$ = 7 Hz, 8H, CH(CH$_3$)$_2$), 7.04 (s, 4H, NCH), 7.47 (d, $^3J_{HH}$ = 8 Hz, 8H, Ar-H), 7.68 (t, $^3J_{HH}$ = 8 Hz, 4H, Ar-H). ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 23.7 (CH(CH$_3$)$_2$), 24.2 (CH(CH$_3$)$_2$), 29.7 (CH(CH$_3$)$_2$), 119.3 (NCH), 121.7 (q, $^1J_{CF}$ = 290 Hz, SO$_3$$CF_3$), 126.0 (Ar-C), 126.9 (Ar-C), 133.5 (Ar-C), 146.9 (Ar-C), 149.1 (NCN), n.o. (CCF$_3$), n.o. (CCF$_3$). ^{19}F NMR (188.3 MHz, CD_2Cl_2): δ = −78.0 (SO$_3$CF_3), −75.7 (CCF_3). ESI-HRMS: *m/z* (positive ion mode): 1115.3232 (calc. 1115.3715 for [M +OH −H −Al(OR^F)$_4$]$^+$). 967.4222 (calc. 967.4273 for [M +OH −OTf –Al(OR^F)$_4$]$^+$). ESI-HRMS: *m/z* (negative ion mode): 966.9036 (calc. 966.9032 for [Al(OR^F)$_4$]$^-$). M.p. at 206-208 °C (dec.).

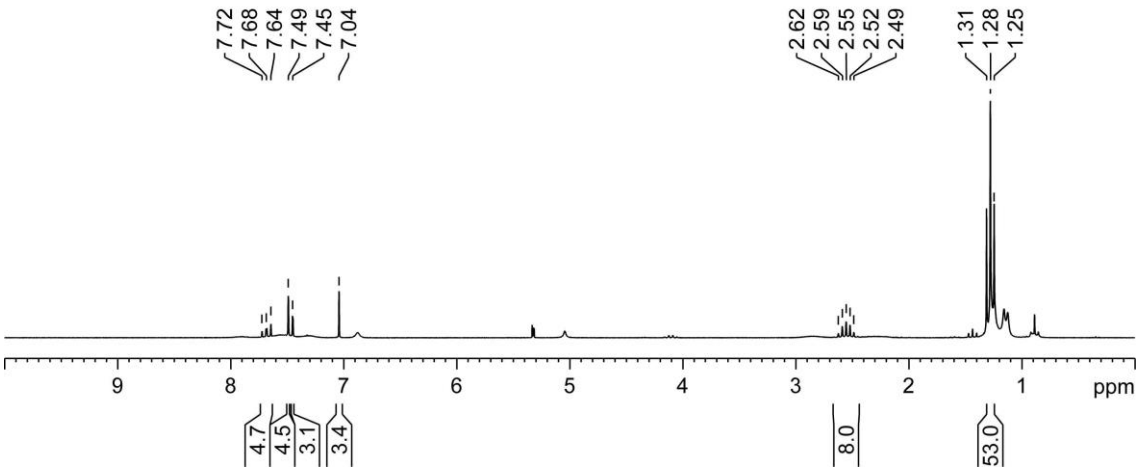


Figure S22. ^{1}H NMR spectrum (200.1 MHz, CD_2Cl_2) of **4**[Al(OR^F)$_4$]. Mind the presence of hexane

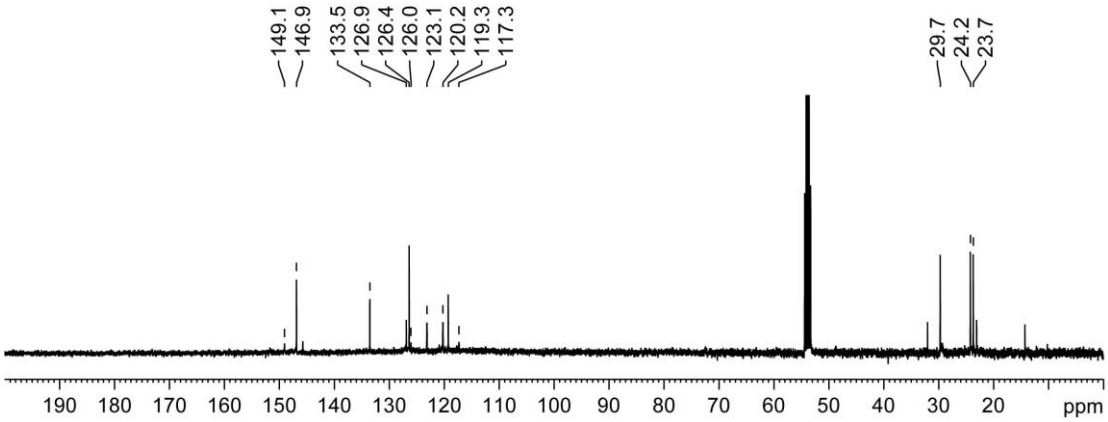


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum (100.6 MHz, CD_2Cl_2) of **4**[$Al(OR^F)_4$]. Mind the presence of hexane

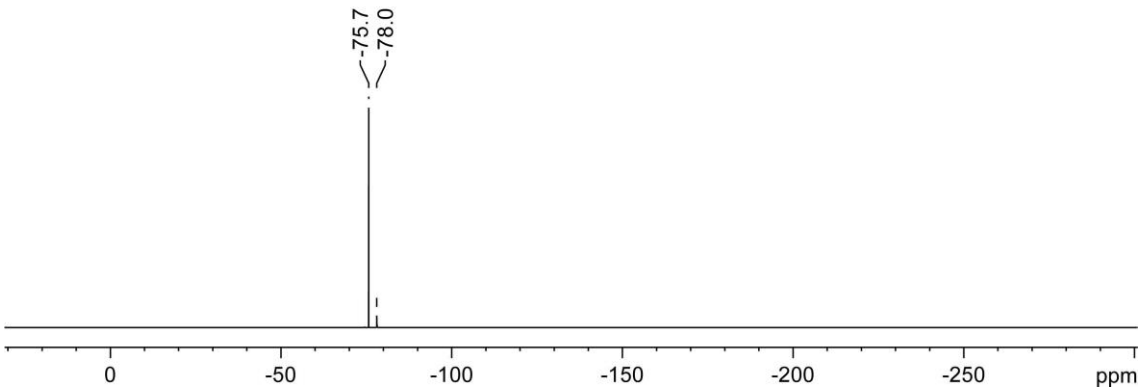


Figure S24. ^{19}F NMR spectrum (188.3 MHz, CD_2Cl_2) of **4**[$Al(OR^F)_4$].

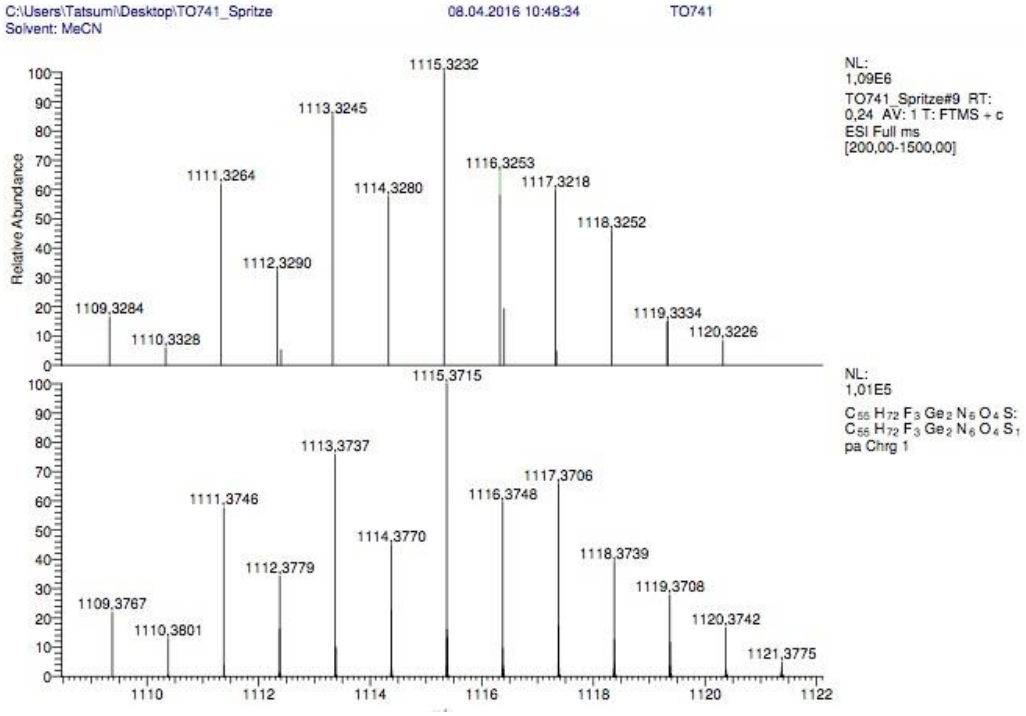


Figure S25. Signal of [M +OH −H −Al(OR^F)$_4$]$^+$ as observed in the ESI-HRMS (positive ion mode) analysis of **4**[Al(OR^F)$_4$]. Top (expt.), bottom (calc.).

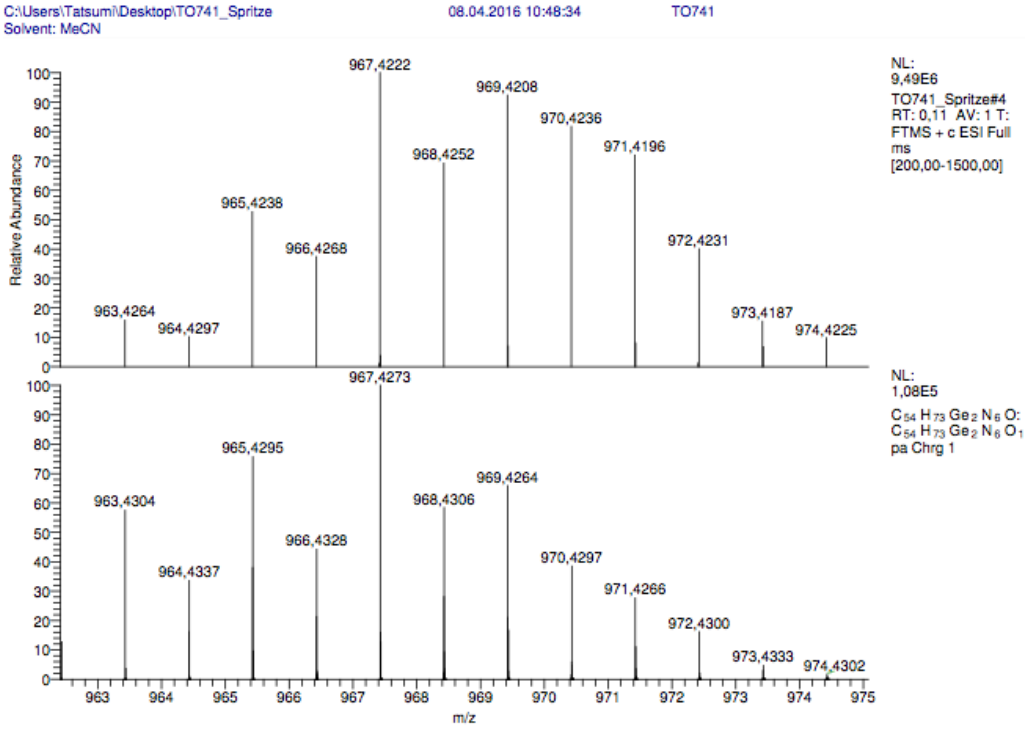


Figure S26. Signal of [M +OH −OTf −Al(OR^F)$_4$]$^+$ as observed in the ESI-HRMS (positive ion mode) analysis of **4**[Al(OR^F)$_4$]. Top (expt.), bottom (calc.).

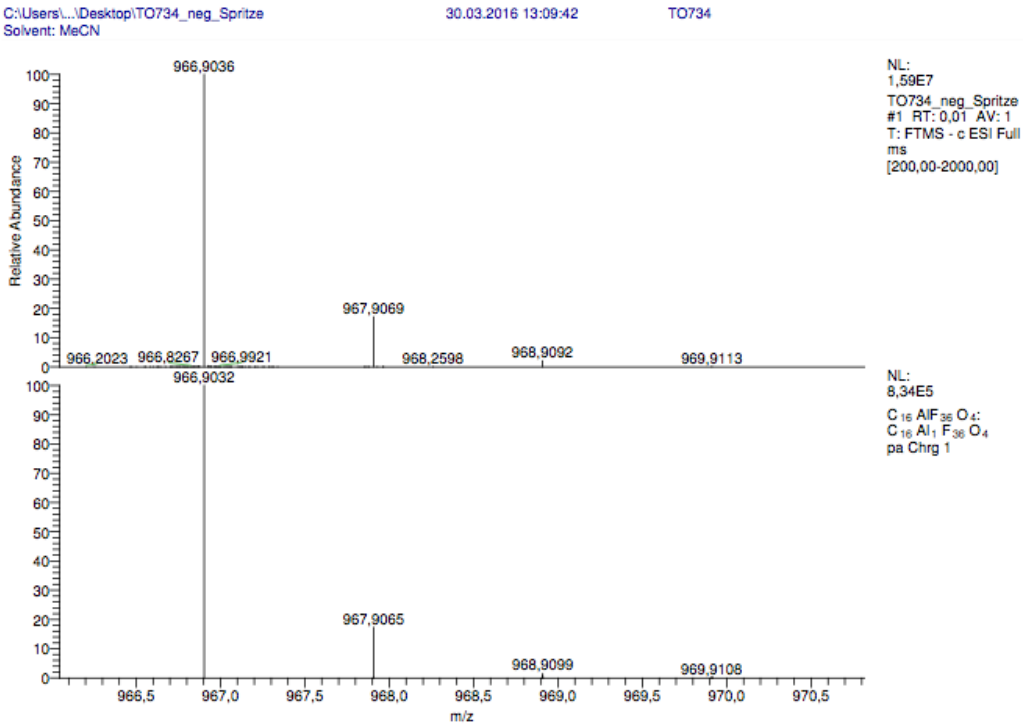


Figure S27. Signal of $[Al(OR^F)_4]^-$ as observed in the ESI-HRMS (negative ion mode) analysis of **4**$[Al(OR^F)_4]$. Top (expt.), bottom (calc.).

2.) Crystallographic Data for **3**[BF_4], **3**[BAr^F_4], **4**[BAr^F_4] and **4**[$Al(OR^F)_4$]

General Considerations: Data for the single crystal structure determinations of **3**[BF_4], **3**[BAr^F_4], **4**[BAr^F_4] and **4**[$Al(OR^F)_4$] were collected on an Agilent SuperNova diffractometer, equipped with a CCD area Atlas detector and a mirror monochromator utilizing CuK_α radiation (λ = 1.54184 Å). The crystal structures were solved by Direct Methods and refined on F^2 using full-matrix least squares with SHELXL-97[S2]. The positions of the H atoms at the carbon atoms were calculated by standard methods. CCDC deposition numbers: 1448465 for **3**[BF_4], 1448464 for **3**[BAr^F_4], 1448466 for **4**[BAr^F_4] and 1484307 for **4**[$Al(OR^F)_4$].

Table S1. Crystal data and structure refinement for **3**[BF_4].

Empirical formula	$C_{128}H_{176}B_2F_{10}Ge_4N_{12}O_5$	
Formula weight	2464.79	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 12.8884(4) Å	α = 80.538(2)°.
	b = 13.0569(4) Å	β = 81.533(2)°.
	c = 20.9504(6) Å	γ = 68.424(3)°.
Volume	3219.44(17) $Å^3$	
Z	1	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	1.648 mm^{-1}	
F(000)	1296	
Crystal size	0.35 x 0.30 x 0.23 mm^3	
Theta range for data collection	3.67 to 67.50°.	
Index ranges	-15<=h<=13, -15<=k<=14, -23<=l<=25	
Reflections collected	23900	
Independent reflections	11605 [R(int) = 0.0293]	
Completeness to theta = 67.50°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7071 and 0.5963	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11605 / 219 / 800	
Goodness-of-fit on F2	1.052	

Final R indices [I>2sigma(I)]	R1 = 0.0791, wR2 = 0.1874
R indices (all data)	R1 = 0.0905, wR2 = 0.1987
Largest diff. peak and hole	1.069 and -0.919 e.Å^{-3}

Table S2. Crystal data and structure refinement for **3**[BAr$^{F}_{4}$].

Empirical formula	$C_{86}H_{84}BF_{25}Ge_2N_6$
Formula weight	1832.58
Temperature	150.00(10) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	*P*212121
Unit cell dimensions	a = 19.34590(10) Å α = 90°.
	b = 20.75270(10) Å β = 90°.
	c = 21.57030(10) Å γ = 90°.
Volume	8660.04(7) Å^3
Z	4
Density (calculated)	1.406 Mg/m^3
Absorption coefficient	1.741 mm^{-1}
F(000)	3744
Crystal size	0.41 x 0.30 x 0.14 mm^3
Theta range for data collection	2.95 to 67.50°.
Index ranges	-22<=h<=23, -14<=k<=24, -25<=l<=25
Reflections collected	33598
Independent reflections	15403 [R(int) = 0.0389]
Completeness to theta = 67.50°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7926 and 0.5383
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15403 / 446 / 1291
Goodness-of-fit on F2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0519, wR2 = 0.1332
R indices (all data)	R1 = 0.0547, wR2 = 0.1364
Absolute structure parameter	-0.016(17)
Largest diff. peak and hole	0.842 and -0.710 e.Å^{-3}

Table S3. Crystal data and structure refinement for **4**[BAr$^{F}_{4}$].

Empirical formula	$C_{89}H_{87}BF_{27}Ge_2N_7O_3S$
Formula weight	2003.71
Temperature	150.00(10) K
Wavelength	1.54184 Å
Crystal system	Triclinic

Space group	*P*-1	
Unit cell dimensions	a = 12.9054(4) Å	α = 89.046(2)°.
	b = 16.9468(4) Å	β = 73.524(2)°.
	c = 22.4045(4) Å	γ = 88.226(2)°.
Volume	4696.4(2) $Å^3$	
Z	2	
Density (calculated)	1.417 Mg/m^3	
Absorption coefficient	1.917 mm^{-1}	
F(000)	2044	
Crystal size	0.31 x 0.20 x 0.07 mm^3	
Theta range for data collection	2.61 to 67.50°.	
Index ranges	-15<=h<=15, -20<=k<=20, -26<=l<=19	
Reflections collected	32602	
Independent reflections	16923 [R(int) = 0.0308]	
Completeness to theta = 67.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8839 and 0.5897	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16923 / 102 / 1226	
Goodness-of-fit on F2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1235	
R indices (all data)	R1 = 0.0612, wR2 = 0.1343	
Largest diff. peak and hole	1.287 and -0.684 e.$Å^{-3}$	

Table S4. Crystal data and structure refinement for **4**[$Al(OR^F)_4$]

Empirical formula	$C_{284}H_{288}Al_4F_{156}Ge_8N_{24}O_{28}S_4$	
Formula weight	8266.26	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	*P*212121	
Unit cell dimensions	a = 23.0848(3) Å	α = 90°.
	b = 26.6977(3) Å	β = 90°.
	c = 27.5856(4) Å	γ = 90°.
Volume	17001.3(4) $Å^3$	
Z	2	
Density (calculated)	1.615 Mg/m^3	
Absorption coefficient	2.475 mm^{-1}	
F(000)	8320	
Crystal size	0.27 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.50 to 67.49°.	
Index ranges	-26<=h<=27, -31<=k<=31, -33<=l<=33	

Reflections collected	67376
Independent reflections	30534 [R(int) = 0.0740]
Completeness to theta = 67.49°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7864 and 0.5525
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	30534 / 314 / 2326
Goodness-of-fit on F2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0707, wR2 = 0.1770
R indices (all data)	R1 = 0.1169, wR2 = 0.1969
Absolute structure parameter	0.37(7)
Largest diff. peak and hole	1.350 and -0.794 e.$Å^{-3}$

2.1.) Molecular Structure of **3**[BF_4] in the Solid State

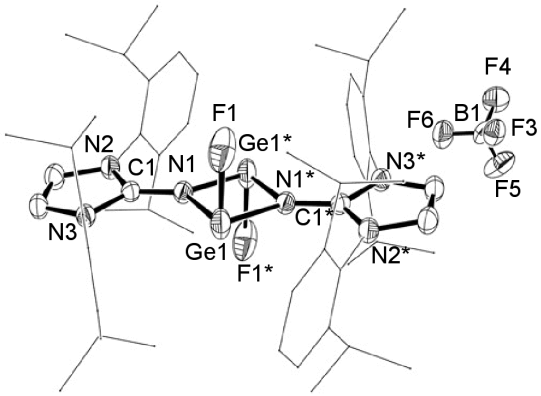


Figure S28. ORTEP representation of the molecular structure of **3**[BF_4] in the solid state. Thermal ellipsoids are at the 40% probability level. Fluorine atoms have 50% occupancies for the F1 or F1* positions. Dip groups are depicted as stick models. Hydrogen atoms and solvent molecules are omitted for clarity. Selected bond lengths (Å) and bond angles (deg): Ge1–F1, 1.894(8); Ge1–N1, 1.965(3); Ge1–N1*, 1.961(3); N1–C1, 1.320(5); N2–C1, 1.363(5); N3–C1, 1.360(5); F1-Ge1-N1, 92.0(2); F1-Ge1-N1*, 93.3(2); N1*-Ge1-N1, 79.39(14); Ge1*-N1-Ge1, 100.62(14)

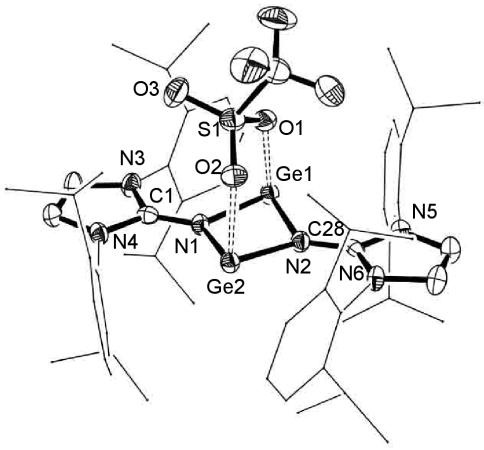
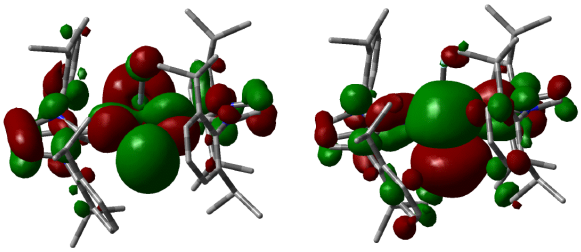


Figure S29. ORTEP representation of the molecular structure of the cation in **4**[$Al(OR^F)_4$] in the solid state. Thermal ellipsoids are at the 40% probability level. Dip groups are depicted as stick models. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and bond angles (deg): Ge1-N1, 1.961(6); Ge1-N2, 1.961(6); Ge1-O1, 2.284(6); Ge2-N2, 1.958(6); Ge2-N1, 1.964(6); Ge2-O2, 2.244(5); N1-C1, 1.327(10); N3-C1, 1.377(10); N4-C1, 1.378(9); N2-C28, 1.333(10); N5-C28, 1.351(10); N6-C28, 1.380(10); N1-Ge1-N2, 78.5(3); N1-Ge1-O1, 88.3(2); N2-Ge1-O1, 88.0(2); N1-Ge2-N2, 78.5(2); N2-Ge2-O2, 88.7(2); N1-Ge2-O2, 90.4(2); C1-N1-Ge1, 128.3(5); C1-N1-Ge2, 130.4(5); Ge1-N1-Ge2, 100.6(3); C28-N2-Ge2, 129.6(5); C28-N2-Ge1, 128.2(5); Ge2-N2-Ge1 100.8(3).

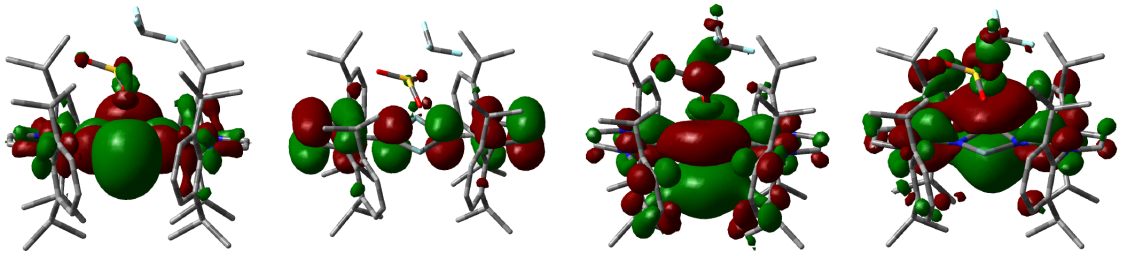
3.) Details to the DFT Calculations

DFT calculations for electronic structure analysis were performed at the B3LYP/6-31G* level of theory while energy differences were calculated at B97-D/6-31G* level.[S3,S4,S5] Stationary points on the potential energy surface (PES) were characterized by harmonic vibrational frequency calculations. We calculated the electronic structure analysis part at B97-D/6-31G* level, as well and found generally negligible difference compared to B3LYP/6-31G* supporting that our results are independent from the chosen method. All calculations were carried out using GAUSSIAN 09 program.[S6]



HOMO LUMO

Figure S30. Kohn-Sham depictions of HOMO and LUMO of germyliumylidene **3**$^{+}$.



HOMO-1 HOMO LUMO LUMO+1

Figure S31. Kohn-Sham depictions of molecular orbitals (HOMO−1, HOMO, LUMO, LUMO+1) of Ge(II) cation **4**$^{+}$.

Table S5. Selected values for the MBOs in **3**$^+$, **4**$^+$, **E** and **F**.

	Ge-N	Ge-F	Ge-O	C=N_{imino}
[FGe(NIPr)$_2$Ge]$^+$ (**3**$^+$) Ge(F)-N_{imino}/Ge-N_{imino}:	0.55/0.89	0.79	–	1.32
[(OTf)Ge$_2$(NIPr)$_2$]$^+$ (**4**$^+$)	0.74	–	0.32	1.29
amino(imino)Ge(II)$^+$ (**E**) Ge-N_{imino}/Ge-N_{amino}:	0.68/1.11	–	–	1.24
Ge(NIPr)$_2$ (**F**)	1.12	–	–	1.55

Table S6. Selected values for the NPA Charges of **3**$^+$, **4**$^+$, **E** and **F**.

	Ge(F)	Ge	F	N_{imino}	N_{amino}	$O_{triflate}$
[FGe(NIPr)$_2$Ge]$^+$ (**3**$^+$)	+1.23	+1.10	−0.72	−1.16	–	–
[(OTf)Ge$_2$(NIPr)$_2$]$^+$ (**4**$^+$)	–	+1.20	–	−1.20	–	−0.95
amino(imino)Ge(II)$^+$ (**E**)	–	+1.15	–	−1.60	−1.69	–
Ge(NIPr)$_2$ (**F**)	–	+0.94	–	−0.99	–	–

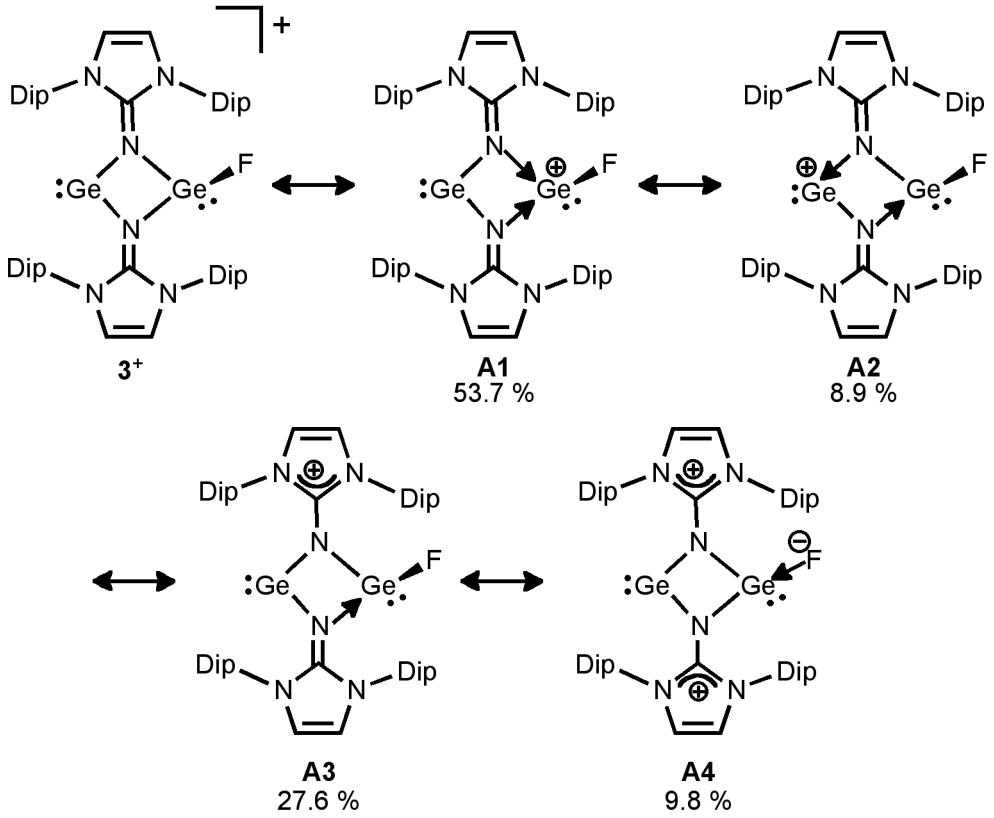


Figure S32. NRT-analysis of $[FGe(NIPr)_2Ge]^+$ (**3**$^+$).

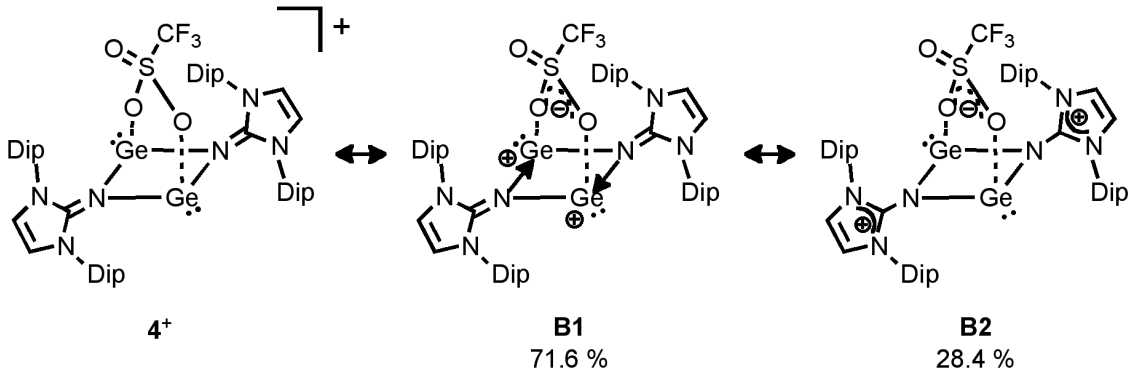
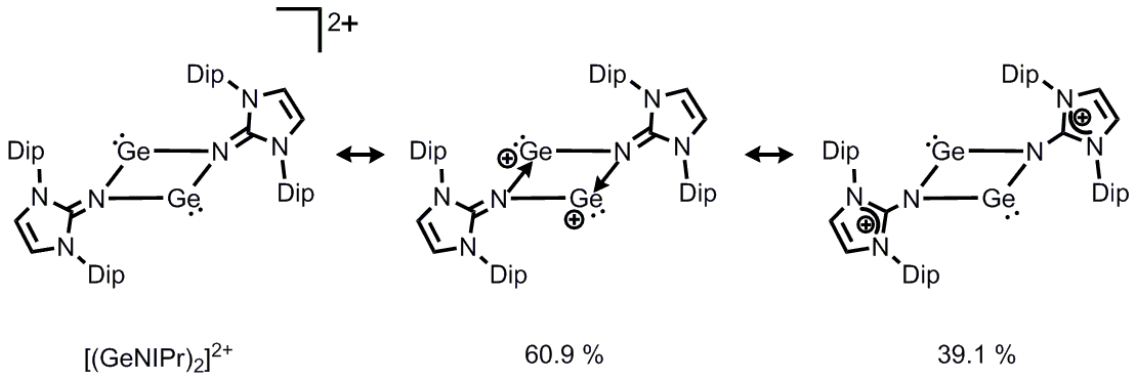


Figure S33. NRT-analysis of $[(OTf)Ge_2(NIPr)_2]^+$ (**4**$^+$).



$[(GeNIPr)_2]^{2+}$ 60.9 % 39.1 %

Figure S34. NRT-analysis of dicationic model compound $[(GeNIPr)_2]^{2+}$.

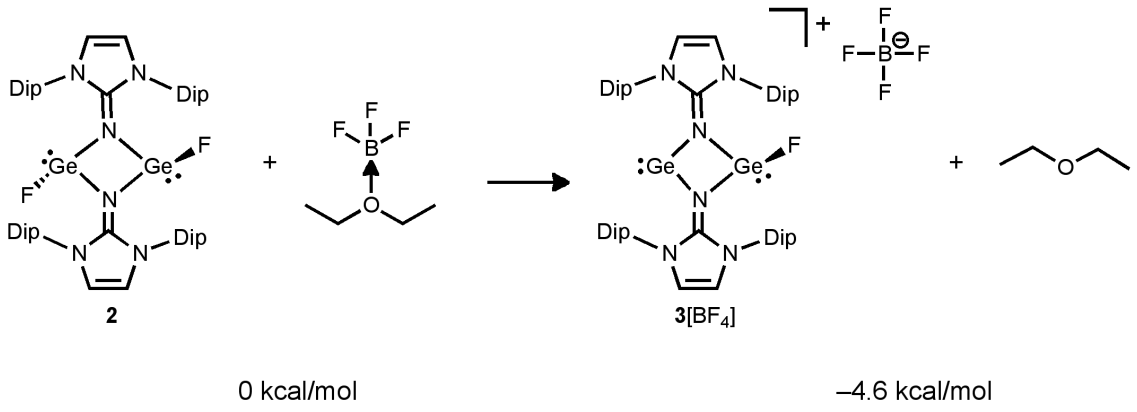


Figure S35. Calculated mechanism of the formation of **3**[BF_4] from germylene fluoride dimer **2**.

Calculation of the reaction free energy occurred at B97-D/6-31G* level of theory. In this case dispersion correction is mandatory to describe the system accurately. Ion-pairs were calculated together and the position of the BF_4^- anion was carefully optimized.

Table S7. Cartesian geometry of **2** at B97-D/6-31G* level in Angstrom [Å].

C	-1.817833	3.119603	1.852795
C	-2.67224	2.645463	0.826823
C	-2.96042	3.390675	-0.337915
C	-2.415882	4.685507	-0.432714
C	-1.593339	5.192031	0.578101
C	-1.291662	4.413497	1.704661
N	-3.204945	1.317397	0.935695
C	-2.503152	0.160727	0.601249
N	-3.41337	-0.876312	0.831219
C	-4.647779	-0.350088	1.235436
C	-4.519083	1.000292	1.300932
N	-1.276074	0.06059	0.171757
Ge	0.002656	1.495796	-0.501855
F	-0.208718	1.014921	-2.293918
C	-3.235884	-2.197536	0.290893
C	-2.774446	-3.231348	1.139571
C	-2.574963	-4.499002	0.56535

C	-2.790509	-4.712725	-0.802629
C	-3.239877	-3.668365	-1.619537
C	-3.48356	-2.388944	-1.086893
C	-2.49575	-2.963495	2.617806
C	-1.353686	-3.83068	3.186125
C	-4.004986	-1.274394	-1.989843
C	-5.371409	-1.660784	-2.602021
C	-3.805612	2.826678	-1.476967
C	-3.097925	2.963235	-2.844286
C	-1.452171	2.222931	3.035906
C	-2.603147	2.175597	4.069725
N	1.264405	-0.069433	-0.184122
Ge	-0.015705	-1.518169	0.464159
F	0.209303	-1.068548	2.260871
C	2.496216	-0.153207	-0.602369
N	3.402971	0.894403	-0.798707
C	4.643823	0.382858	-1.203388
C	4.52278	-0.966252	-1.301268
N	3.207117	-1.298073	-0.955497
C	3.226071	2.199693	-0.218472
C	2.770694	3.260494	-1.036637
C	2.594169	4.516512	-0.42989
C	2.825671	4.693827	0.9407
C	3.260934	3.621731	1.728536
C	3.48094	2.352036	1.162868
C	2.471878	3.033954	-2.517751
C	3.755408	3.220013	-3.361641
C	3.98462	1.20745	2.037442
C	5.366855	1.547192	2.641548
C	2.679342	-2.630744	-0.883888
C	2.966904	-3.405878	0.261283
C	2.430508	-4.706204	0.31848

C	1.617745	-5.191008	-0.710593
C	1.317411	-4.384155	-1.817404
C	1.834584	-3.082832	-1.927602
C	3.804473	-2.86936	1.419023
C	3.085066	-3.034307	2.776982
C	1.47142	-2.159501	-3.090745
C	2.629936	-2.077338	-4.113976
C	5.195419	-3.544454	1.441359
C	0.163319	-2.562043	-3.799288
C	2.967584	0.848122	3.142319
C	1.335045	3.932147	-3.047741
C	-3.787795	-3.149048	3.449157
C	-2.985302	-0.911806	-3.090764
C	-5.1983	3.498054	-1.502857
C	-0.134755	2.630997	3.723603
H	-5.4909	-1.001743	1.428088
H	-3.409782	-3.838675	-2.684406
H	-2.604257	-5.699344	-1.233483
H	-4.167508	-0.374562	-1.381392
H	-3.385133	-0.094906	-3.71404
H	-2.033678	-0.578599	-2.655546
H	-2.79387	-1.778445	-3.744204
H	-5.2747	-2.549168	-3.247602
H	-6.111285	-1.886995	-1.816814
H	-5.755032	-0.830833	-3.218349
H	1.054681	3.603243	-4.06016
H	-4.158794	-4.184055	3.358662
H	-3.587215	-2.944295	4.513975
H	-4.58263	-2.46598	3.110582
H	-3.726003	2.507396	-3.627746
H	-0.126363	-1.765641	-4.501044
H	-0.653509	-2.697389	-3.075639

H	5.22689	-1.733303	-1.599408
H	-2.209031	-5.315914	1.187356
H	2.137375	1.992763	-2.635462
H	-0.454305	-3.749188	2.558698
H	-1.648714	-4.891568	3.258897
H	2.637338	-5.328506	1.190872
H	1.196824	-6.196926	-0.643449
H	0.650507	-4.764226	-2.590637
H	3.958983	-1.792853	1.263353
H	5.095007	-4.632501	1.589869
H	5.803599	-3.137916	2.266588
H	5.734988	-3.37771	0.494678
H	2.925419	-4.098957	3.015231
H	2.112429	-2.521316	2.77373
H	1.305239	-1.1528	-2.679789
H	0.286081	-3.496912	-4.373328
H	3.559075	-1.718717	-3.645971
H	2.363213	-1.381401	-4.92655
H	2.821339	-3.069995	-4.556044
H	-5.216842	1.777686	1.58683
H	2.235013	5.353796	-1.028369
H	-2.178337	-1.914723	2.712557
H	0.448065	3.859296	-2.400855
H	1.649309	4.988283	-3.108255
H	-2.62305	5.286106	-1.320052
H	-1.164993	6.192283	0.480591
H	-0.614655	4.808352	2.461525
H	-3.955818	1.75332	-1.296087
H	-5.101069	4.582915	-1.675017
H	-5.811786	3.072946	-2.314692
H	-5.730384	3.350139	-0.548857
H	-2.946583	4.022674	-3.109562

H	-2.122149	2.456207	-2.83697
H	-1.298688	1.205011	2.647827
H	-0.242284	3.585238	4.267912
H	-3.538664	1.813466	3.617425
H	-2.336077	1.497786	4.8974
H	-2.782918	3.180423	4.488514
H	5.48538	1.042915	-1.373038
H	3.438054	3.762825	2.796454
H	2.660111	5.672756	1.396861
H	4.118113	0.31644	1.410066
H	3.354758	0.010658	3.745884
H	2.004262	0.544488	2.71094
H	2.802869	1.706851	3.813304
H	5.299743	2.423513	3.307104
H	6.103039	1.771751	1.852421
H	5.736934	0.694937	3.235339
H	-1.101805	-3.479409	4.198622
H	3.709074	-2.601081	3.576436
H	0.148372	1.854402	4.4499
H	0.679744	2.732202	2.991834
H	3.536845	3.046727	-4.428471
H	4.145231	4.245907	-3.249325
H	4.542413	2.514537	-3.052021

Table S8. Cartesian geometry of **3**$^{+}$ at B97-D/6-31G* level in Angstrom [Å].

C	-2.384404	-4.793429	-1.22454
C	-2.46152	-3.805282	-2.215813
C	-2.821066	-2.484703	-1.896788
C	-3.102443	-2.209479	-0.536543
C	-2.999103	-3.173202	0.492564
C	-2.647216	-4.481393	0.114565
C	-2.894672	-1.385283	-2.957179

C	-4.363408	-1.138776	-3.384254
N	-3.47931	-0.867586	-0.168203
C	-2.589095	0.157214	0.073098
N	-3.369777	1.239231	0.43955
C	-4.717818	0.873438	0.452484
C	-4.783106	-0.434688	0.082928
N	-1.270462	0.095307	-0.011798
Ge	-0.037815	-1.596984	0.075232
F	0.170925	-1.733895	-1.731053
C	-2.806965	2.477936	0.897639
C	-2.739115	3.566796	-0.005704
C	-2.044505	4.710632	0.426281
C	-1.446626	4.759027	1.693959
C	-1.551868	3.672998	2.570956
C	-2.240336	2.504152	2.193285
C	-3.351556	3.475307	-1.405822
C	-2.377852	2.780394	-2.390631
C	-2.35451	1.332583	3.166906
C	-3.146875	1.755651	4.426677
C	-3.250482	-2.825372	1.957475
C	-4.642527	-3.333206	2.400401
N	1.255183	0.047866	0.075144
C	2.562265	0.006107	-0.123761
N	3.37883	1.008442	-0.609959
C	4.697834	0.556822	-0.691998
C	4.710009	-0.728292	-0.244213
N	3.400361	-1.068966	0.100661
C	2.884826	2.307897	-0.96657
C	2.94411	3.336604	0.00487
C	2.330656	4.559969	-0.319604
C	1.694839	4.743136	-1.554749
C	1.670319	3.711611	-2.50113

C	2.261683	2.462867	-2.228018
C	2.970045	-2.330992	0.647134
C	2.67322	-2.387919	2.031818
C	2.224596	-3.617858	2.542518
C	2.076196	-4.734255	1.707671
C	2.37136	-4.642981	0.343965
C	2.818888	-3.434929	-0.225257
C	3.5817	3.11835	1.377882
C	2.492267	2.862833	2.446763
C	2.838544	-1.160488	2.928126
C	1.965278	-1.207947	4.197545
C	3.129588	-3.345414	-1.71832
C	2.144011	-4.157432	-2.589483
C	2.210544	1.346649	-3.267411
C	3.032705	1.742233	-4.516823
Ge	0.028456	1.531751	0.013393
C	4.579685	-3.817238	-1.991491
C	0.755141	0.995573	-3.655766
C	4.327528	-0.962211	3.300885
C	-2.145988	-3.37967	2.886801
C	-0.967925	0.773976	3.558323
C	4.487189	4.296888	1.798847
C	-3.785114	4.845727	-1.96603
C	-2.027725	-1.670395	-4.199101
H	2.960688	2.712819	3.433166
H	1.801451	3.719816	2.50872
H	1.903126	1.96509	2.204913
H	5.000933	4.049521	2.740999
H	5.247685	4.511323	1.031986
H	3.902036	5.214244	1.969718
H	3.022811	0.918943	-5.248608
H	2.604867	2.635461	-4.999472

H	4.078799	1.964006	-4.251956
H	0.758123	0.200047	-4.416432
H	0.187749	0.619098	-2.792311
H	0.236404	1.872375	-4.074866
H	4.806705	-3.736852	-3.066681
H	5.32289	-3.223404	-1.437013
H	4.6977	-4.871495	-1.692109
H	2.337281	-3.936591	-3.65095
H	2.286153	-5.241151	-2.447578
H	1.104222	-3.892972	-2.357242
H	4.444814	-0.057198	3.91987
H	4.697052	-1.826212	3.876125
H	4.952118	-0.850191	2.401276
H	2.015563	-0.234628	4.709406
H	0.914837	-1.420072	3.946979
H	2.320447	-1.974806	4.904251
H	-2.305664	-3.005418	3.910955
H	-2.173721	-4.480102	2.926455
H	-1.147046	-3.072911	2.540733
H	-4.827216	-3.071361	3.454782
H	-5.444136	-2.892853	1.786244
H	-4.698818	-4.428938	2.299558
H	-4.406102	-0.32869	-4.130597
H	-4.783448	-2.049637	-3.840451
H	-4.997775	-0.854751	-2.531559
H	-2.030226	-0.782245	-4.850276
H	-0.99286	-1.900493	-3.912618
H	-2.436081	-2.510247	-4.784745
H	-2.833344	2.725934	-3.392914
H	-1.434003	3.344301	-2.464381
H	-2.138752	1.755289	-2.072188
H	-4.344115	4.697488	-2.902617

H	-4.428003	5.38855	-1.255899
H	-2.913677	5.478343	-2.199067
H	-3.252395	0.899	5.111416
H	-2.621739	2.561603	4.963094
H	-4.151463	2.119254	4.160107
H	-1.089266	-0.062359	4.264295
H	-0.42482	0.400257	2.676198
H	-0.351735	1.54565	4.046857
H	2.517636	-0.275738	2.361047
H	1.975144	-3.702744	3.599825
H	1.718016	-5.678013	2.123693
H	2.239243	-5.514947	-0.296177
H	3.041961	-2.290776	-2.023009
H	4.210775	2.217643	1.335082
H	2.345943	5.374029	0.406245
H	1.221764	5.700217	-1.782967
H	1.187352	3.870178	-3.46664
H	2.66598	0.441769	-2.839695
H	-3.246109	-1.728504	2.060805
H	-2.563693	-5.253518	0.880252
H	-2.103286	-5.812423	-1.497886
H	-2.222429	-4.060334	-3.247358
H	-2.509484	-0.461347	-2.498958
H	-2.91088	0.517437	2.681837
H	-4.251638	2.844722	-1.341712
H	-1.967819	5.572933	-0.235866
H	-0.906977	5.656176	2.003264
H	-1.102511	3.725859	3.563884
H	-5.486321	1.584423	0.730572
H	-5.622388	-1.10746	-0.039705
H	5.514978	-1.44231	-0.134677
H	5.486826	1.199157	-1.063936

Table S9. Cartesian geometry of **4**$^{+}$ at B97-D/6-31G* level in Angstrom [Å].

C	3.617331	-1.423102	-0.359411
C	3.459787	-1.936474	-1.674389
C	3.462189	-3.333425	-1.822222
C	3.623574	-4.177742	-0.714804
C	3.792978	-3.641142	0.56451
C	3.792869	-2.248276	0.77644
C	3.29682	-1.008444	-2.879589
C	2.615027	-1.685133	-4.085322
C	4.026192	-1.678803	2.171853
C	3.303968	-2.478461	3.278839
N	3.585955	0.008622	-0.179792
C	2.45397	0.795354	-0.240398
N	2.902036	2.098097	-0.128457
C	4.295421	2.111441	-0.012759
C	4.716851	0.820394	-0.035452
C	2.076781	3.240409	-0.42979
C	1.539291	4.007936	0.632629
C	0.651121	5.0429	0.285674
C	0.309304	5.288118	-1.050484
C	0.877381	4.525817	-2.078367
C	1.788182	3.492855	-1.792492
N	1.194679	0.394676	-0.399201
Ge	0.464573	-1.462282	-0.279334
N	-1.21018	-0.365928	-0.442312
C	-2.476649	-0.765456	-0.400109
N	-3.611184	0.022133	-0.332568
C	-4.752894	-0.781373	-0.424783
C	-4.337969	-2.072724	-0.503394
N	-2.940186	-2.065522	-0.462406
C	-3.59976	1.462073	-0.38587
C	-3.608826	2.194093	0.829043

C	-3.492235	3.592372	0.731108
C	-3.382485	4.226315	-0.514277
C	-3.40807	3.477081	-1.694527
C	-3.521548	2.075011	-1.65731
C	1.928111	3.742677	2.083302
C	0.806013	4.06816	3.091697
C	2.425799	2.700662	-2.932587
C	3.225173	3.635811	-3.870046
C	-3.769576	1.494079	2.177004
C	-3.211371	2.30404	3.364098
C	-3.539775	1.282605	-2.961308
C	-4.734896	1.702907	-3.847426
C	-2.092035	-3.20135	-0.711879
C	-1.711586	-3.455379	-2.049328
C	-0.809603	-4.511835	-2.274019
C	-0.323011	-5.279107	-1.209703
C	-0.730714	-5.010676	0.104282
C	-1.621753	-3.960303	0.388829
C	-2.240245	-2.639734	-3.226402
C	-1.089414	-1.977631	-4.013386
C	-2.067329	-3.645936	1.815997
C	-3.444184	-4.294888	2.104702
Ge	-0.481126	1.476285	-0.233031
C	-5.263177	1.171254	2.437922
C	-2.204054	1.445793	-3.7169
C	-3.103679	-3.524753	-4.155509
C	5.546002	-1.629837	2.471061
C	1.369519	1.901473	-3.724941
C	3.203217	4.548194	2.439292
C	-1.051001	-4.08861	2.888924
C	4.660568	-0.41879	-3.315552
O	-0.426514	1.094492	2.04954

S	0.38171	0.047371	2.721294
C	-0.65204	-0.397387	4.246392
F	-0.783808	0.682399	5.036251
O	0.39276	-1.234284	1.960814
O	1.660417	0.476481	3.233761
F	-1.88308	-0.823556	3.877664
F	-0.042419	-1.379207	4.933475
H	-1.365782	-3.698295	3.867548
H	-1.00929	-5.187289	2.966986
H	-0.042246	-3.70978	2.672499
H	-3.765332	-4.050905	3.12997
H	-4.218383	-3.940107	1.408683
H	-3.373846	-5.391096	2.015395
H	-2.182671	-2.554261	1.895707
H	-0.336996	-5.613151	0.921974
H	0.381268	-6.090569	-1.40247
H	-0.493158	-4.731741	-3.294846
H	-1.494227	-1.375143	-4.841288
H	-0.495494	-1.318061	-3.362366
H	-0.418131	-2.737263	-4.442367
H	-3.506106	-2.921583	-4.985188
H	-2.501579	-4.341549	-4.584498
H	-3.946319	-3.972754	-3.605805
H	-2.884168	-1.835357	-2.843844
H	-4.886156	-3.002357	-0.58673
H	-5.741546	-0.34105	-0.427291
H	-2.229	0.888116	-4.666254
H	-2.007276	2.50556	-3.942859
H	-1.368543	1.063281	-3.113666
H	-4.759016	1.088708	-4.761745
H	-5.689293	1.57476	-3.312997
H	-4.650355	2.759254	-4.147803

H	-3.662527	0.215	-2.728779
H	-3.338628	3.978292	-2.661217
H	-3.285227	5.312559	-0.561348
H	-3.481187	4.192485	1.640019
H	-3.218009	0.543577	2.127346
H	-3.246581	1.686026	4.272477
H	-2.170866	2.610113	3.191481
H	-3.820827	3.20318	3.551384
H	-5.368594	0.65776	3.406913
H	-5.851995	2.102103	2.473803
H	-5.688444	0.522556	1.658939
H	1.851972	1.350554	-4.547801
H	0.863582	1.174077	-3.072721
H	0.609073	2.569834	-4.157386
H	3.713448	3.044169	-4.660886
H	2.562564	4.371445	-4.352578
H	4.0005	4.185464	-3.313908
H	3.139827	1.979842	-2.511624
H	0.625209	4.737409	-3.11889
H	-0.397063	6.084659	-1.292124
H	0.211582	5.651932	1.075206
H	3.49879	4.340225	3.47982
H	4.047074	4.286731	1.782529
H	3.013606	5.629481	2.339999
H	1.097524	3.69711	4.085668
H	0.642395	5.15532	3.174406
H	-0.141097	3.588555	2.807579
H	2.163738	2.674862	2.182515
H	4.837204	3.044632	0.070487
H	5.703933	0.383812	0.038655
H	2.36895	-0.924102	-4.841207
H	3.282671	-2.422665	-4.558993

H	1.687905	-2.195283	-3.788181
H	4.516892	0.26375	-4.169207
H	5.14217	0.144866	-2.503787
H	5.340678	-1.226488	-3.63033
H	2.652429	-0.172765	-2.574186
H	5.716937	-1.194057	3.46827
H	5.971366	-2.646651	2.459091
H	6.093081	-1.025056	1.731028
H	3.373515	-1.925046	4.226955
H	2.242134	-2.623309	3.038148
H	3.771869	-3.464916	3.430163
H	3.637317	-0.652634	2.199115
H	3.334116	-3.769385	-2.812198
H	3.62054	-5.260652	-0.854324
H	3.923729	-4.305921	1.418434

Table S10. Cartesian geometry of **E** at B97-D/6-31G* level in Angstrom [Å].

C	-3.715511	0.294399	0.993749
C	-2.967739	-0.223952	-0.09323
C	-3.271117	0.052442	-1.450716
C	-4.352663	0.916537	-1.698917
C	-5.0938	1.47145	-0.646247
C	-4.781111	1.159962	0.681552
N	-1.901182	-1.154723	0.196024
C	-0.548921	-0.936125	0.075791
N	0.054434	-2.115195	0.452671
C	-0.912942	-3.05311	0.815516
C	-2.123518	-2.45976	0.653181
N	0.096042	0.163096	-0.313343
Ge	2.082033	0.446435	-0.706108
N	1.521575	2.209149	-0.435242
Si	2.511772	3.674157	-0.374362

C	1.476454	-2.28851	0.572233
C	2.156019	-2.979749	-0.459401
C	3.557242	-3.051031	-0.360652
C	4.238203	-2.455477	0.711004
C	3.532684	-1.791932	1.722762
C	2.127578	-1.695613	1.681937
C	1.399882	-3.563047	-1.654789
C	2.094841	-4.791615	-2.278131
C	1.370606	-1.000836	2.811641
C	1.911194	0.420152	3.090042
C	-2.474861	-0.585872	-2.593272
C	-2.637934	0.136987	-3.946699
C	-3.474434	-0.122242	2.447028
C	-3.522117	1.048177	3.456623
C	1.172862	-2.472801	-2.731864
C	1.424573	-1.867899	4.09306
C	-2.854815	-2.078678	-2.765671
C	-4.535401	-1.17614	2.860527
H	0.610188	-2.893156	-3.580781
H	0.601904	-1.621247	-2.330905
H	2.139415	-2.099064	-3.106479
H	1.434312	-5.237028	-3.037278
H	3.033988	-4.510249	-2.780376
H	2.321798	-5.555912	-1.518814
H	0.40717	-3.888138	-1.305927
H	4.123606	-3.573883	-1.130673
H	5.326625	-2.518067	0.761216
H	4.071435	-1.351875	2.56288
H	0.855484	-1.381916	4.90141
H	0.997601	-2.867316	3.914273
H	2.465115	-1.994602	4.431451
H	1.312245	0.896675	3.882284

H	2.956361	0.387346	3.436097
H	1.864278	1.056507	2.192541
H	0.312909	-0.902459	2.525712
H	-0.630882	-4.044633	1.147224
H	-3.129874	-2.827351	0.797006
H	-1.932961	-0.294611	-4.673369
H	-3.654122	0.001607	-4.350232
H	-2.438803	1.21539	-3.863221
H	-2.259545	-2.520579	-3.580855
H	-2.673083	-2.663385	-1.852775
H	-3.920421	-2.16972	-3.029929
H	-1.407978	-0.534986	-2.326636
H	-4.331293	-1.538597	3.880497
H	-5.538169	-0.72039	2.849835
H	-4.557009	-2.041101	2.180606
H	-3.319863	0.658421	4.466584
H	-2.778766	1.823689	3.229575
H	-4.518169	1.516629	3.479317
H	-2.478772	-0.586471	2.523306
H	-4.617775	1.162816	-2.726054
H	-5.926502	2.142227	-0.865159
H	-5.377647	1.582115	1.490474
C	1.640971	5.042992	-1.331608
C	2.718013	4.164699	1.434772
C	4.18122	3.245725	-1.136675
H	2.256243	5.958692	-1.354494
H	1.442687	4.748316	-2.375572
H	0.676172	5.313547	-0.868693
H	4.873	4.103519	-1.084549
H	4.668685	2.407423	-0.607478
H	4.087245	2.962657	-2.199134
H	3.318951	5.084997	1.533602

H	1.744867	4.352008	1.919776
H	3.227516	3.370797	2.007204
Si	-0.194309	1.924231	-0.258146
C	-0.928732	2.501832	1.359613
C	-1.127113	2.627224	-1.716272
H	-2.215145	2.501676	-1.6246
H	-0.911824	3.706738	-1.788639
H	-0.797068	2.161127	-2.657872
H	-2.025269	2.421023	1.326433
H	-0.555229	1.928743	2.222278
H	-0.676947	3.563298	1.527399

Table S11. Cartesian geometry of **F** at B97-D/6-31G* level in Angstrom [Å].

C	-0.265544	-3.519296	-0.455496
C	-1.263682	-2.97837	-1.298962
C	-1.16758	-3.014025	-2.710743
C	-0.055421	-3.662391	-3.276924
C	0.935418	-4.227858	-2.463613
C	0.835497	-4.1456	-1.068266
N	-2.401788	-2.355192	-0.699279
C	-2.362712	-1.063006	-0.130077
N	-3.634139	-0.93294	0.455798
C	-4.383217	-2.103434	0.28349
C	-3.621416	-2.982132	-0.421329
N	-1.391324	-0.222012	-0.071341
Ge	-0.021455	0.150295	-1.270377
N	1.357541	0.281389	-0.032594
C	2.343058	1.092685	0.10966
N	3.575349	0.811186	0.72465
C	4.356385	1.968708	0.817888
C	3.658145	2.988131	0.248517
N	2.442885	2.46609	-0.205973

C	3.891175	-0.458597	1.304404
C	3.741342	-0.623243	2.701261
C	4.096893	-1.868459	3.250911
C	4.569519	-2.905526	2.436765
C	4.674343	-2.72622	1.050532
C	4.331089	-1.499766	0.454114
C	3.128987	0.485375	3.557736
C	1.58475	0.365334	3.538346
C	4.446629	-1.270301	-1.052359
C	5.756087	-0.517601	-1.386714
C	1.376495	3.183077	-0.829618
C	0.232611	3.491156	-0.055483
C	-0.842886	4.119062	-0.708568
C	-0.776678	4.423314	-2.073428
C	0.375942	4.123958	-2.813689
C	1.477608	3.493058	-2.20869
C	0.189619	3.217032	1.445706
C	0.638891	4.487142	2.208592
C	2.728723	3.112149	-3.004872
C	2.973731	4.015669	-4.231392
C	-4.053299	0.221796	1.18902
C	-4.584452	1.322099	0.481578
C	-4.963476	2.458025	1.220738
C	-4.825671	2.48818	2.613259
C	-4.299071	1.380946	3.29325
C	-3.896862	0.227684	2.596276
C	-4.721254	1.316514	-1.038266
C	-3.71092	2.301523	-1.668717
C	-3.239978	-0.948974	3.320029
C	-3.830858	-1.209026	4.721876
C	-2.2378	-2.384748	-3.598145
C	-3.123846	-3.482445	-4.232444

C	-0.365032	-3.45534	1.065939
C	0.911764	-2.856998	1.692874
C	-1.18453	2.726958	1.941847
C	2.671489	1.62613	-3.433477
C	4.343992	-2.566878	-1.878614
C	3.650981	0.505564	5.009854
C	-6.166441	1.634486	-1.482257
C	-1.710505	-0.72371	3.403984
C	-1.629254	-1.463584	-4.67793
C	-0.669439	-4.85855	1.640355
H	-3.767614	2.255538	-2.769539
H	-3.925889	3.336523	-1.354244
H	-2.686752	2.053349	-1.357767
H	-6.247907	1.575034	-2.580212
H	-6.882996	0.92437	-1.038309
H	-6.460947	2.651958	-1.176011
H	-4.472315	0.3099	-1.404853
H	-5.372255	3.322395	0.69386
H	-5.124089	3.378175	3.172303
H	-4.185377	1.420107	4.377401
H	-1.221212	-1.605491	3.850269
H	-1.280402	-0.540517	2.409582
H	-1.490878	0.151626	4.03711
H	-3.419387	-2.146925	5.128442
H	-3.567797	-0.400979	5.424122
H	-4.929298	-1.29201	4.688325
H	-3.407001	-1.85661	2.720212
H	-5.391036	-2.181443	0.674023
H	-3.824017	-3.989476	-0.765539
H	0.783405	-2.773349	2.78375
H	1.78929	-3.495933	1.509046
H	1.120365	-1.859631	1.280281

H	-0.769019	-4.805454	2.737722
H	-1.605736	-5.265293	1.223644
H	0.147568	-5.55997	1.401958
H	-1.201411	-2.797493	1.335724
H	1.623174	-4.564486	-0.439835
H	1.797991	-4.719768	-2.918694
H	0.039562	-3.708885	-4.36322
H	-2.883327	-1.76521	-2.959085
H	-2.436345	-0.976812	-5.250094
H	-1.002802	-0.687078	-4.212008
H	-1.00714	-2.031224	-5.389476
H	-3.903302	-3.028694	-4.86705
H	-2.515857	-4.156815	-4.857998
H	-3.61607	-4.088758	-3.454462
H	1.134125	1.219517	4.071149
H	1.195905	0.338856	2.510348
H	1.269726	-0.561459	4.044521
H	3.261263	1.396397	5.528349
H	3.30832	-0.379279	5.57112
H	4.752287	0.531823	5.045291
H	3.385208	1.454291	3.103533
H	3.994598	-2.029562	4.324685
H	4.842136	-3.864906	2.882924
H	5.025215	-3.549171	0.426973
H	5.815478	-0.324739	-2.47126
H	5.804571	0.447209	-0.860185
H	6.630639	-1.12293	-1.093977
H	4.297458	-2.315343	-2.95024
H	5.221703	-3.217265	-1.724705
H	3.43474	-3.126055	-1.614542
H	3.602593	-0.634463	-1.354416
H	5.334534	1.945549	1.283445

H	3.903913	4.034954	0.114252
H	-1.116194	2.490267	3.015835
H	-1.966744	3.493027	1.823377
H	-1.491829	1.818058	1.406635
H	0.634049	4.297621	3.295407
H	1.656052	4.791664	1.91136
H	-0.04678	5.325725	1.999463
H	0.909099	2.42167	1.673084
H	3.953213	3.775882	-4.675131
H	2.209346	3.853556	-5.008995
H	2.96413	5.08264	-3.956037
H	3.590043	1.355527	-3.981853
H	2.574906	0.965606	-2.560465
H	1.803166	1.445577	-4.08764
H	3.599319	3.220289	-2.33968
H	-1.742387	4.359774	-0.141905
H	-1.629164	4.897658	-2.564794
H	0.413036	4.374194	-3.874437

Table S12. Cartesian geometry of $[(GeNIPr)_2]^{2+}$ at B97-D/6-31G* level in Angstrom [Å].

C	2.681733	-2.497593	-1.795727
C	2.406325	-2.921414	-0.473917
C	3.320327	-2.791824	0.600071
C	4.552307	-2.17456	0.313366
C	4.8504	-1.718418	-0.978494
C	3.931203	-1.88653	-2.021685
N	1.083267	-3.415234	-0.187383
C	0.003224	-2.590846	0.000062
N	-1.074848	-3.417751	0.187838
C	-0.665458	-4.75022	0.120763
C	0.677045	-4.748659	-0.119828
N	0.001582	-1.248412	-0.000131

Ge	-1.537598	-0.001911	-0.000213
N	-0.001559	1.248428	-0.000132
Ge	1.537619	0.00193	-0.000261
C	-2.3991	-2.926938	0.473987
C	-3.313115	-2.799627	-0.60027
C	-4.546502	-2.18496	-0.31402
C	-4.845899	-1.729113	0.977646
C	-3.926607	-1.894965	2.021112
C	-2.67577	-2.503426	1.79563
C	-2.957521	-3.257093	-2.015096
C	-2.293749	-2.099963	-2.800655
C	-1.696226	-2.698184	2.949482
C	-1.340723	-1.354112	3.621227
C	2.9661	-3.249916	2.015024
C	2.299216	-2.09441	2.800321
C	1.702339	-2.694678	-2.949294
C	2.28174	-3.688644	-3.984742
C	-0.003244	2.590861	0.000221
N	-1.083319	3.415219	-0.187184
C	-0.677163	4.748655	-0.119467
C	0.665332	4.750248	0.121172
N	1.074783	3.417791	0.188111
C	-2.406331	2.921343	-0.473828
C	-3.320397	2.791648	0.600096
C	-4.552313	2.174316	0.313281
C	-4.850276	1.718167	-0.978611
C	-3.931015	1.886367	-2.021727
C	-2.681617	2.497551	-1.79567
C	-2.966272	3.249676	2.015096
C	-4.180412	3.798469	2.795878
C	-1.70218	2.694794	-2.949179
C	-1.343534	1.351706	-3.621221

C	2.399048	2.926991	0.474202
C	2.675708	2.503324	1.79579
C	3.926568	1.894887	2.021224
C	4.845886	1.729206	0.977754
C	4.546492	2.185208	-0.313861
C	3.313083	2.799849	-0.600057
C	1.696137	2.69791	2.949648
C	1.340688	1.353752	3.621249
C	2.957525	3.257536	-2.014815
C	4.170041	3.810303	-2.795316
C	2.273635	3.692818	3.98525
C	2.293942	2.100479	-2.800639
C	-2.2816	3.688842	-3.984536
C	-2.299261	2.094194	2.800331
C	-4.170003	-3.809586	-2.795836
C	-2.273773	-3.693167	3.98498
C	4.180147	-3.79896	2.795778
C	1.343801	-1.351495	-3.621206
H	-2.044128	2.422149	3.820613
H	-2.985642	1.236222	2.87473
H	-1.370374	1.756333	2.312923
H	-3.835836	4.238121	3.743761
H	-4.710109	4.574396	2.222947
H	-4.896974	2.999244	3.043251
H	-2.229612	4.064387	1.937939
H	-5.288484	2.058149	1.107952
H	-5.813493	1.244782	-1.175975
H	-4.185703	1.559095	-3.030599
H	-0.599319	1.513379	-4.41588
H	-0.918876	0.642607	-2.893101
H	-2.230873	0.884192	-4.074911
H	-1.554003	3.853116	-4.794486

H	-3.207547	3.292955	-4.42993
H	-2.512623	4.659031	-3.518539
H	-0.771043	3.129017	-2.555985
H	-1.386785	5.556132	-0.254009
H	1.372953	5.559411	0.25613
H	2.037958	2.428194	-3.820784
H	2.982797	1.244518	-2.875384
H	1.365991	1.759724	-2.313493
H	3.8242	4.249216	-3.743082
H	4.697309	4.58765	-2.222073
H	4.889052	3.013343	-3.042874
H	2.218447	4.070016	-1.937268
H	5.282663	2.070972	-1.108814
H	5.810226	1.257903	1.174609
H	4.182293	1.56778	3.029887
H	0.763962	3.130249	2.556852
H	0.596136	1.513365	4.416007
H	0.917688	0.643846	2.892945
H	2.229183	0.888233	4.074713
H	1.545901	3.855185	4.795464
H	3.200571	3.298795	4.430239
H	2.502397	4.663694	3.51957
H	0.59964	-1.513035	-4.415942
H	0.919103	-0.642456	-2.893043
H	2.231201	-0.883962	-4.074757
H	1.554147	-3.852835	-4.794711
H	3.2077	-3.292747	-4.430097
H	2.512732	-4.658877	-3.518821
H	0.771166	-3.128896	-2.556177
H	4.185992	-1.559252	-3.030529
H	5.813666	-1.245099	-1.175782
H	5.288423	-2.058463	1.108096

H	3.835485	-4.238683	3.743599
H	4.709759	-4.574888	2.22277
H	4.896815	-2.999869	3.043275
H	2.043974	-2.422412	3.82056
H	2.985698	-1.236531	2.874831
H	1.370396	-1.756425	2.312867
H	2.229329	-4.064517	1.937783
H	1.386641	-5.556152	-0.254404
H	-1.373118	-5.559364	0.255629
H	-2.03773	-2.427512	-3.820845
H	-2.982519	-1.243924	-2.875293
H	-1.365783	-1.759391	-2.313398
H	-3.824079	-4.248463	-3.743586
H	-4.697486	-4.586908	-2.222758
H	-4.888849	-3.012494	-3.043449
H	-2.218539	-4.069673	-1.937629
H	-1.546035	-3.855674	4.795162
H	-3.20067	-3.299127	4.430035
H	-2.502613	-4.663977	3.519199
H	-0.596186	-1.513848	4.415975
H	-0.917685	-0.644149	2.893001
H	-2.229197	-0.888595	4.074737
H	-0.764063	-3.130516	2.55665
H	-5.282652	-2.070589	-1.108971
H	-5.810223	-1.257796	1.174549
H	-4.182346	-1.567962	3.029804

Table S13. Cartesian geometry of **3**[BF_4] at B97-D/6-31G* level in Angstrom [Å].

C	-1.861673	3.914811	-1.547627
C	-0.523309	3.452478	-1.548416
C	0.106842	2.8811	-2.684255
C	-0.659794	2.812339	-3.861134

C	-1.977735	3.289519	-3.902903
C	-2.57072	3.835431	-2.760702
N	0.215794	3.522752	-0.312539
C	0.478001	2.441637	0.496922
N	1.189078	2.942043	1.570944
C	1.334787	4.324021	1.435222
C	0.734112	4.682807	0.267164
N	0.086523	1.194478	0.305453
Ge	0.863191	-0.436133	0.950959
N	-0.858829	-1.136808	0.355305
Ge	-1.703763	0.558648	-0.527166
F	-2.634463	1.110853	0.955061
C	1.651905	2.132849	2.669266
C	3.032748	1.825909	2.739001
C	3.444744	0.969593	3.776956
C	2.519893	0.440094	4.68556
C	1.161883	0.771235	4.593582
C	0.692192	1.631626	3.583756
C	4.009078	2.342489	1.682154
C	5.477611	2.386094	2.150071
C	-0.775715	2.045121	3.513394
C	-1.743698	0.985016	4.072395
C	1.537264	2.334389	-2.626215
C	2.586798	3.464065	-2.48418
C	-2.537205	4.481448	-0.297331
C	-2.559286	6.028295	-0.349582
C	-1.214673	-2.400723	0.193465
N	-2.462031	-2.864649	-0.174183
C	-2.436326	-4.258242	-0.287485
C	-1.181306	-4.672114	0.036495
N	-0.435189	-3.535483	0.351616
C	-3.569886	-2.032624	-0.566308

C	-4.392748	-1.474992	0.442147
C	-5.478205	-0.690524	0.016919
C	-5.727948	-0.480775	-1.346771
C	-4.880291	-1.026498	-2.316994
C	-3.76455	-1.799204	-1.947402
C	-4.081925	-1.708418	1.921566
C	-4.709426	-0.652552	2.852029
C	-2.801068	-2.334649	-3.004964
C	-2.41781	-1.255382	-4.043286
C	0.997262	-3.456119	0.483879
C	1.569555	-3.573266	1.772751
C	2.9389	-3.272623	1.888254
C	3.682317	-2.859169	0.77186
C	3.097083	-2.794199	-0.499397
C	1.736586	-3.119678	-0.675245
C	0.713856	-3.971336	2.977269
C	1.51261	-4.733681	4.054983
C	1.115977	-3.097831	-2.069939
C	0.92747	-1.649637	-2.577526
C	-4.518341	-3.126736	2.363423
C	0.01799	-2.741296	3.608806
C	1.963933	-3.92925	-3.061955
C	-3.391016	-3.581514	-3.704549
C	3.890859	1.488066	0.39871
C	1.91281	1.445562	-3.828475
C	-3.970637	3.938615	-0.0995
C	-0.961045	3.403368	4.233333
H	4.565025	1.853473	-0.386153
H	4.161051	0.440895	0.597369
H	2.869356	1.507502	-0.004474
H	6.083996	2.892689	1.384456
H	5.589642	2.924123	3.105736

H	5.887221	1.370269	2.267963
H	-2.011111	3.730308	4.156089
H	-0.699527	3.315219	5.301002
H	-0.321049	4.180223	3.784136
H	-2.774527	1.292244	3.851362
H	-1.57349	0.009387	3.593653
H	-1.645944	0.870401	5.165206
H	-3.036691	6.432756	0.558059
H	-1.544866	6.449841	-0.426097
H	-3.135045	6.370591	-1.225269
H	-4.359017	4.292044	0.869421
H	-4.649794	4.30841	-0.884751
H	-3.980287	2.840635	-0.098683
H	3.587751	3.011744	-2.417469
H	2.559295	4.120798	-3.369563
H	2.421292	4.080085	-1.588362
H	2.867136	0.939385	-3.627225
H	1.151149	0.673525	-4.011228
H	2.024401	2.049752	-4.74509
H	-1.638734	-1.652874	-4.712153
H	-3.282682	-0.971181	-4.664191
H	-2.030796	-0.351863	-3.54878
H	-2.68025	-3.967786	-4.453187
H	-3.603131	-4.383854	-2.980085
H	-4.332036	-3.325899	-4.218681
H	-4.262411	-3.283651	3.424446
H	-5.609574	-3.240222	2.252244
H	-4.025054	-3.911932	1.772042
H	-4.323208	-0.792968	3.873334
H	-4.454377	0.36075	2.51427
H	-5.806701	-0.757474	2.891755
H	-0.58606	-3.050409	4.478765

H	0.767753	-2.008084	3.945999
H	-0.649505	-2.242256	2.891062
H	0.824551	-5.115678	4.825716
H	2.065008	-5.582705	3.622566
H	2.237411	-4.070269	4.554247
H	1.432555	-3.991709	-4.026167
H	2.937309	-3.454441	-3.241703
H	2.122347	-4.951514	-2.681035
H	0.631474	-1.660779	-3.63869
H	0.128927	-1.144721	-2.012874
H	1.850763	-1.066222	-2.474757
H	1.598265	1.700414	-1.728854
H	-0.22027	2.372738	-4.755253
H	-2.54667	3.225506	-4.833071
H	-3.602332	4.187125	-2.798747
H	-1.95328	4.176826	0.583959
H	3.716715	3.373358	1.424632
H	4.497791	0.705585	3.867087
H	2.860622	-0.233855	5.474772
H	0.456198	0.356803	5.313001
H	-1.057766	2.182922	2.463485
H	-1.871824	-2.64305	-2.503744
H	-5.065562	-0.829836	-3.373483
H	-6.579213	0.131503	-1.652075
H	-6.126651	-0.224866	0.75779
H	-2.989831	-1.630056	2.036878
H	0.119117	-3.566843	-2.021428
H	-0.080859	-4.644898	2.616373
H	3.42506	-3.347064	2.86179
H	4.737613	-2.601068	0.87604
H	3.702451	-2.500466	-1.355829
H	-0.733726	-5.657616	0.075664

H	-3.324717	-4.803916	-0.57828
H	0.641756	5.63967	-0.229098
H	1.869452	4.902964	2.17764
B	5.2021	-0.938258	-2.972739
F	5.744872	-2.075261	-2.294843
F	6.065698	-0.485042	-3.979786
F	3.934431	-1.317747	-3.540002
F	4.965699	0.097678	-2.012926

Table S14. Cartesian geometry of $BF_3{\cdot}OEt_2$ at B97-D/6-31G* level in Angstrom [Å].

B	0.399345	-1.122127	0.053989
F	1.584127	-1.283568	-0.605861
F	0.49538	-0.93452	1.413003
F	-0.618178	-1.948028	-0.350254
O	-0.141964	0.483264	-0.52913
C	-1.585389	0.626603	-0.774924
H	-1.707376	1.580774	-1.311302
H	-1.829971	-0.201	-1.448318
C	-2.417567	0.575782	0.504671
H	-3.48489	0.637091	0.237482
H	-2.24018	-0.368026	1.037853
H	-2.18341	1.417256	1.174002
C	0.438499	1.644009	0.166553
C	1.951917	1.657757	-0.003591
H	-0.019503	2.532391	-0.295652
H	0.148197	1.591242	1.225163
H	2.337884	2.589379	0.441218
H	2.418737	0.804326	0.503297
H	2.22278	1.631227	-1.068893

Table S15. Cartesian geometry of OEt_2 at B97-D/6-31G* level in Angstrom [Å].

C	2.083687	0.613203	-0.166957
C	1.254149	-0.628256	0.202654
O	-0.076429	-0.60209	-0.315432
C	-0.928195	0.315152	0.370235
C	-2.348089	0.132386	-0.164776
H	1.229599	-0.753314	1.306055
H	1.715999	-1.529796	-0.230387
H	3.121936	0.492384	0.184074
H	2.093463	0.749924	-1.259672
H	1.67328	1.524817	0.295112
H	-0.894223	0.117217	1.463222
H	-0.592953	1.360201	0.215426
H	-3.037613	0.826147	0.342625
H	-2.376788	0.333922	-1.246791
H	-2.690579	-0.899696	0.006855

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