Supporting Information

Experimental:

General Considerations

All air- and moisture-sensitive manipulations were carried out using standard vacuum line Schlenk techniques or in an MBraun Labmaster inert atmosphere dry-box containing an atmosphere of purified nitrogen. CD_3CN was purchased from Sigma Aldrich and stored over 3 Å molecular sieves without further purification. All glassware was stored in a 170°C oven for several hours and was degassed prior to use. Solvents were distilled over the appropriate drying agent. Anhydrous grade acetonitrile was obtained from Sigma-Aldrich and used without distillation but stored over 3 Å molecular sieves. TMSOTf (99%) was distilled before use $BIMEt_3$[S1] was synthesized following literature procedures other chemicals were purchased from Sigma Aldrich and were used without further purification.

NMR tubes fitted with J-Young valves were charged and sealed inside the glovebox. ^1H NMR spectra were recorded on Bruker spectrometers operating at 300 MHz, ^{13}C NMR at 76 MHz, ^{19}F NMR at 282.5 MHz and ^{11}B NMR at 115.6 MHz. All ^1H and ^{13}C NMR chemical shifts are reported relative to $SiMe_4$ using the ^1H (residual) and ^{13}C chemical shifts of the solvent as a secondary standard. Elemental analysis was performed at the University of Windsor Mass Spectrometry Service Laboratory using a Perkin Elmer 2400 combustion CHN analyser. All quantum chemical calculations were carried out using Gaussian 16.[S2]

Crystals for investigation were covered in Paratone®, mounted onto a goniometer head, and then rapidly cooled under a stream of cold N_2 of the low-temperature apparatus (Oxford Cryostream) attached to the diffractometer. The data were then collected using the APEXII (Bruker AXS) software suite on a Bruker Photon 100 CMOS diffractometer using a graphite monochromator with MoK_α (λ = 0.71073 Å). Data were collected at low temperature 100 K. APEXII software was used for data reductions and SADABS (Bruker AXS) was used for absorption corrections (multi-scan; semi-empirical from equivalents). XPREP was used to determine the space group and the structures were solved and refined using the SHELX[S3] software suite as implemented in the WinGX[S4] or OLEX2[S5] program suites. Validation of the structures was conducted using PLATON.[S6]

Synthesis and characterization of $[(BIMEt_3)Ge][OTf]_2$: $GeCl_2$•diox (0.5 mmol, 115 mg) and $BIMEt_3$ (0.5 mmol, 250 mg) were combined in 4 mL of MeCN, TMSOTf (1.5 mmol, 300 µL) was added to yield a clear orange solution. The solution was left to stir for 2 hours. The mixture was then filtered through a glass filter and the clear solution was layered with 4 mL of diethyl ether and placed in the freezer at -35 °C for 72 hours. Colourless blocks were isolated from the solution yielding 280 mg of crystalline material. The mother liquor was concentrated proceeded as before to yield another 82 mg. Combined yield: 362 mg (84 %) of the composition $C_{32}H_{33}F_6GeN_7O_6S_2$, **MW** = 862.4 g/mol, **MP** = 226 °C (dec.). **EA [calc.]:** C, 44.57; H, 3.86; N, 11.37; **EA [found.]:** C, 44.42; H, 3.73; N, 11.96; **^1H NMR** (300 MHz, CD_3CN) δ = 8.12 – 8.01 (m, 3H, CH_{arom}), 7.74 – 7.61 (m, 3H, CH_{arom}), 7.55 – 7.40 (m, 6H, CH_{arom}), 5.0 (s, 6H, CH_2), 4.28 (q, $^3J_{HH}$ = 7.32 Hz, 6H, CH_2), 1.39 (t, $^3J_{HH}$ = 7.32 Hz, 9H, CH_3). **$^{19}F\{^1H\}$ NMR** (283 MHz, CD_3CN): δ = -79.3. **$^{13}C\{^1H\}$ NMR** (75.5 MHz, CD_3CN): δ = 152.3 (s), 136.3 (s), 134.6 (s), 125.2 (s), 125.0 (s), 116.2 (s), 112.0 (s), 54.9 (s), 40.2(s), 13.6 (s)

Synthesis and characterization of $[(BIMEt_3)GeF_2][OTf]_2$: $[(BIMEt_3)Ge][OTf]_2$ (0.1 mmol, 91 mg) was dissolved in 3 mL of MeCN, XeF_2 (0.1 mmol, 17 mg) was added as a solid yielding vigorous evolution of gas. The clear colourless

solution was left to stir for 2 hours. The mixture was then filtered through a glass filter and was layered with 4 mL of diethyl ether and placed in the freezer at -35 °C for 72 hours. Colourless blocks were isolated from the solution. Yield: 76 mg (83 %) of the composition $C_{32}H_{33}F_8GeN_7O_6S_2 \bullet MeCN_{0.5}$, **MW** = 920.9 g/mol, **MP** = 238 °C (dec.). **EA [calc.]:** C, 43.04; H, 3.78; N, 11.41. **EA [found.]:** C, 43.39; H, 3.79; N, 11.35. **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.61 (dd, *J* = 2.9, 8.4 Hz, 1H, CH_{arom}), 8.15 – 8.02 (m, 2H, CH_{arom}), 7.83 – 7.73 (m, 2H, CH_{arom}), 7.70 – 7.45 (m, 7H, CH_{arom}), 5.74 (d, *J* = 16.8 Hz, CH_2, 2H), 5.32 (d, *J* = 16.8 Hz, CH_2, 2H), 5.16 (s, CH_2, 2H), 4.41 (m, 4H), 4.02 (q, *J* = 7.4 Hz, 2H), 1.51 (t, *J* = 7.3 Hz, 6H), 1.29 (t, *J* = 7.4 Hz, 3H). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.3 (OTf), -109.13 (d, J_{FF} = 43.6 Hz), -133.75 (d, J_{FF} = 43.6 Hz). **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 149.40 (d, *J* = 4.5 Hz), 148.4 (s) 135.8 (s), 135.6 (s), 133.5 (s) 133.17 (d, $J_{C,F}$ = 2.7 Hz), 127.6 (s), 127.5 (s), 127.3 (s), 127.2 (s), 117.32 (d, $J_{C,F}$ = 10.2 Hz), 116.57 (d, $J_{C,F}$ = 4.3 Hz), 113.9 (s), 113.4 (s).

Synthesis and characterization of [(BIMEt$_3$)GeF][OTf]$_3$: $[Ge(BIMEt_3)][OTf]_2$ (0.2 mmol, 180 mg) was dissolved in 6 mL of MeCN, XeF_2 (0.2 mmol, 34 mg) was added as a solid yielding vigorous evolution of gas. The clear colourless solution was left to stir for 2 hours at room temperature. Then TMSOTf (80 µL, 0.2 mmol) was added and the reaction was left to stir for another 2 hours at room temperature. The mixture was then filtered through a glass filter, concentrated to 4 mL and was layered with 8 mL of diethyl ether and placed in the freezer at -35 °C for 72 hours. Colourless crystals precipitated out of the reaction mixture and were isolated by decanting the supernatant. The product was identified by X ray crystallography as $[(BIMEt_3)GeF][OTf]_3$. Yield: 135 mg (63 %) of the composition $C_{33}H_{33}F_8GeN_7O_9S_3 \bullet MeCN_1$, **MW** = 1071.5 g/mol, **MP** = 226 °C (dec.). **EA [calc.]:** C, 39.23; H, 3.39; N, 10.46; **EA [found.]:** C, 39.52; H, 3.29; N, 10.80. **^{1}H NMR** (300 MHz, CD_3CN) δ = 8.21 – 8.36 (m, 3H, CH_{arom}), 7.71 – 7.84 (m, 3H, CH_{arom}), 7.46 – 7.71 (m, 6H, CH_{arom}), 5.57 (s, 6H, CH_2), 4.35 (q, $^3J_{HH}$ = 7.35 Hz, 6H, CH_2), 1.45 (t, $^3J_{HH}$ = 7.35 Hz, 9H, CH_3). **^{19}F{^{1}H} NMR** (283 MHz, CD_3CN): δ = -79.00 (OTf), -125.17 (GeF). **^{13}C{^{1}H} NMR** (75.5 MHz, CD_3CN): δ = 148.4 (s), 135.7 (s), 132.9 (s), 128.2 (s), 127.9 (s), 116.8 (d, $J_{C,F}$ = 6.5 Hz), 114.0 (s), 59.5 (s), 42.2 (s), 14.3 (s)

[(BIMEt$_3$)Ge][OTf]$_2$

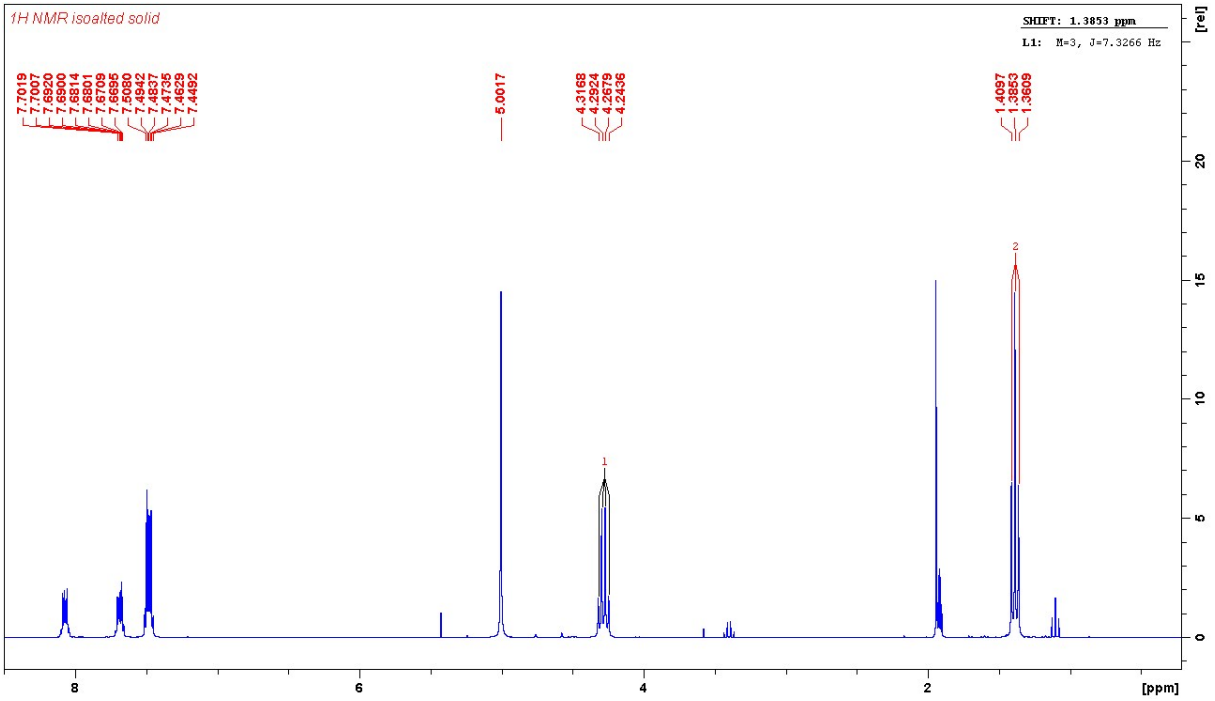


Figure S1: ^{1}H NMR (300 MHz, CD_3CN) spectrum of [(BIMEt$_3$)Ge][OTf]$_2$ the quartet (3.42 ppm) and triplet (1.12 ppm) resonances belong to diethyl ether, an impurity present in the NMR solvent.

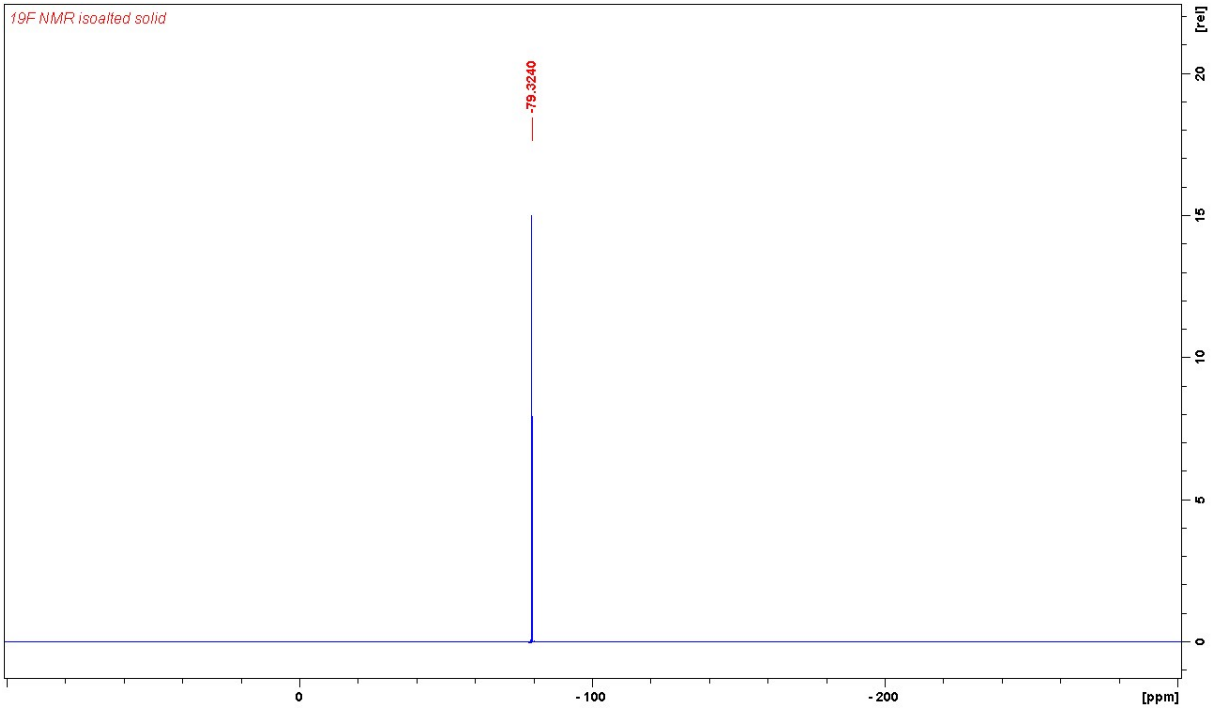


Figure S2: ^{19}F{^{1}H} NMR (283 MHz, CD_3CN) spectrum of [(BIMEt$_3$)Ge][OTf]$_2$

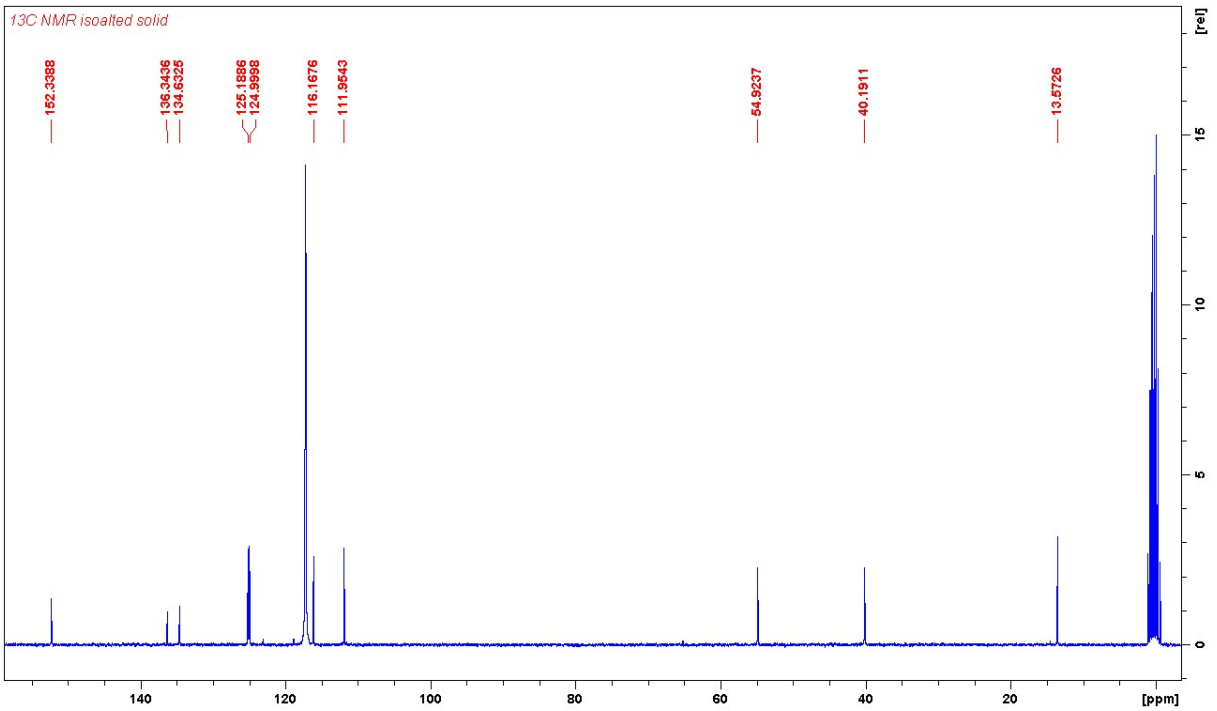


Figure S3: $^{13}C\{^{1}H\}$ NMR (75.5 MHz, CD_3CN) spectrum of $[(BIMEt_3)Ge][OTf]_2$

$[(BIMEt_3)GeF_2][OTf]_2$

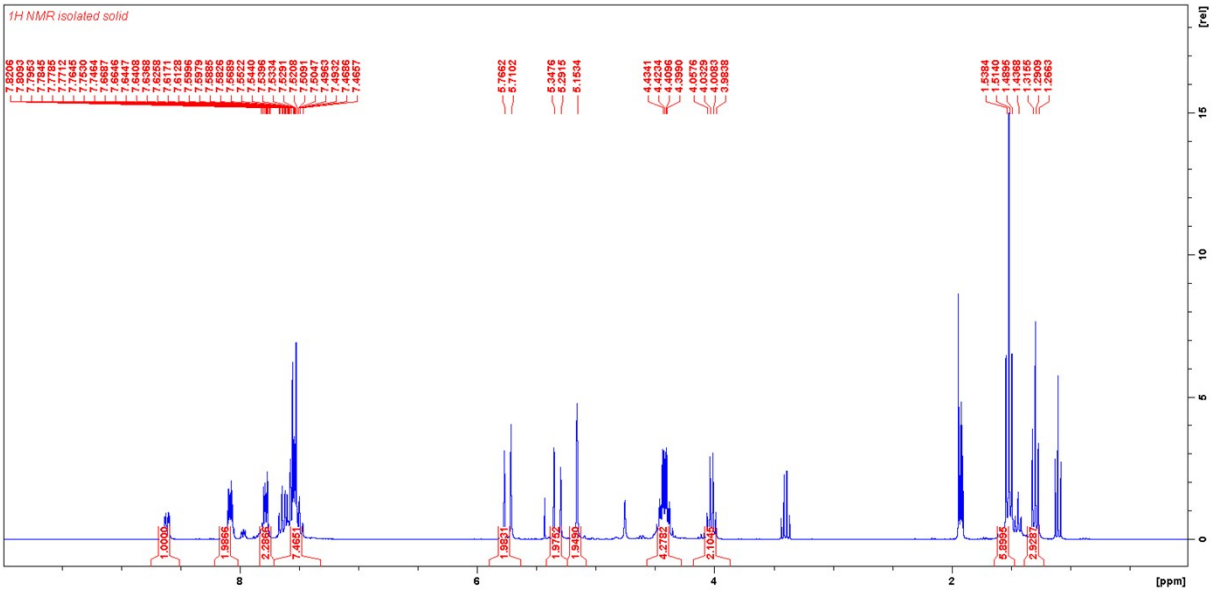


Figure S4: ^{1}H NMR (300 MHz, CD_3CN) spectrum of $[(BIMEt_3)GeF_2][OTf]_2$ the quartet (3.42 ppm) and triplet (1.12 ppm) resonances belong to diethyl ether, an impurity present in the NMR solvent.

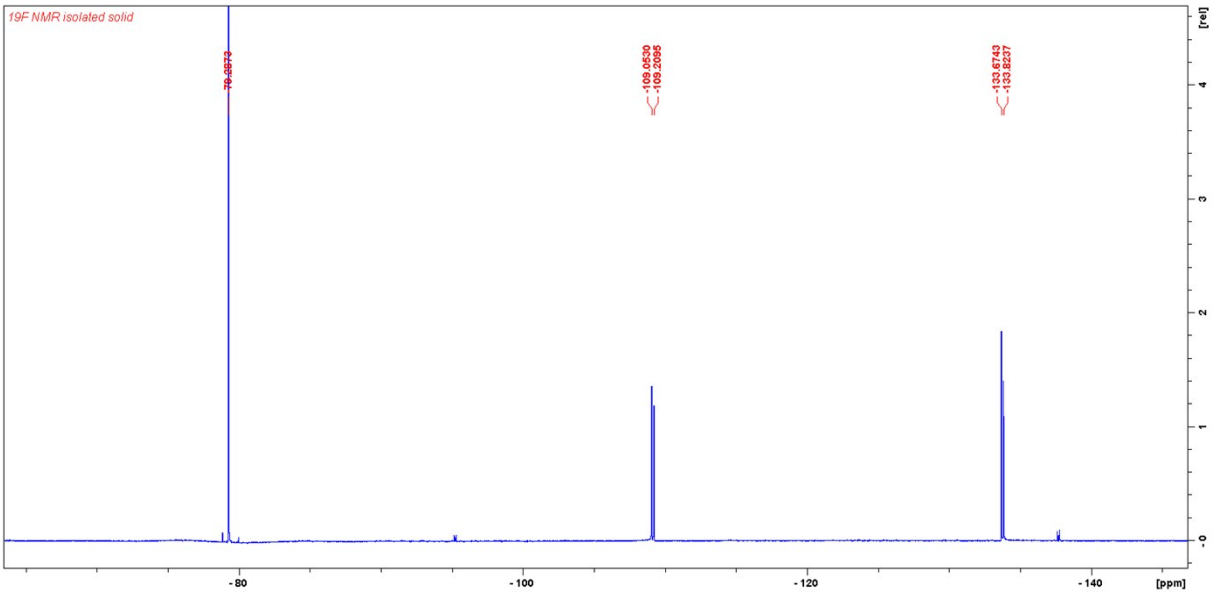


Figure S5: $^{19}F\{^{1}H\}$ NMR (283 MHz, CD_3CN) spectrum of $[(BIMEt_3)GeF_2][OTf]_2$

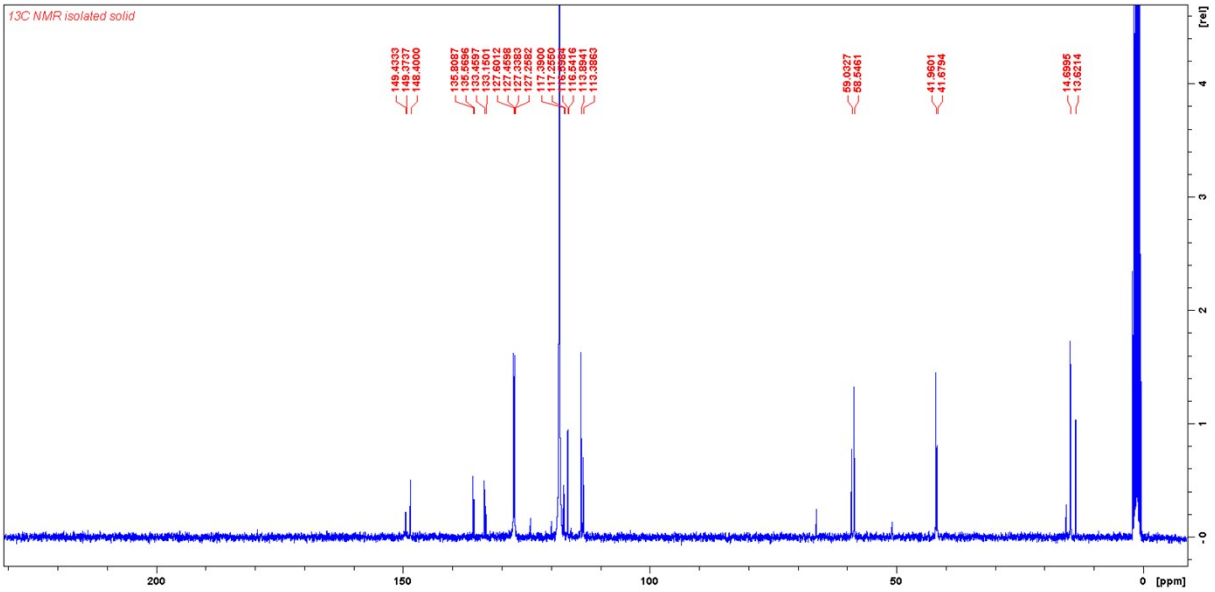


Figure S6: $^{13}C\{^{1}H\}$ NMR (75.5 MHz, CD_3CN) spectrum of $[(BIMEt_3)GeF_2][OTf]_2$

[(BIMEt$_3$)GeF][OTf]$_3$

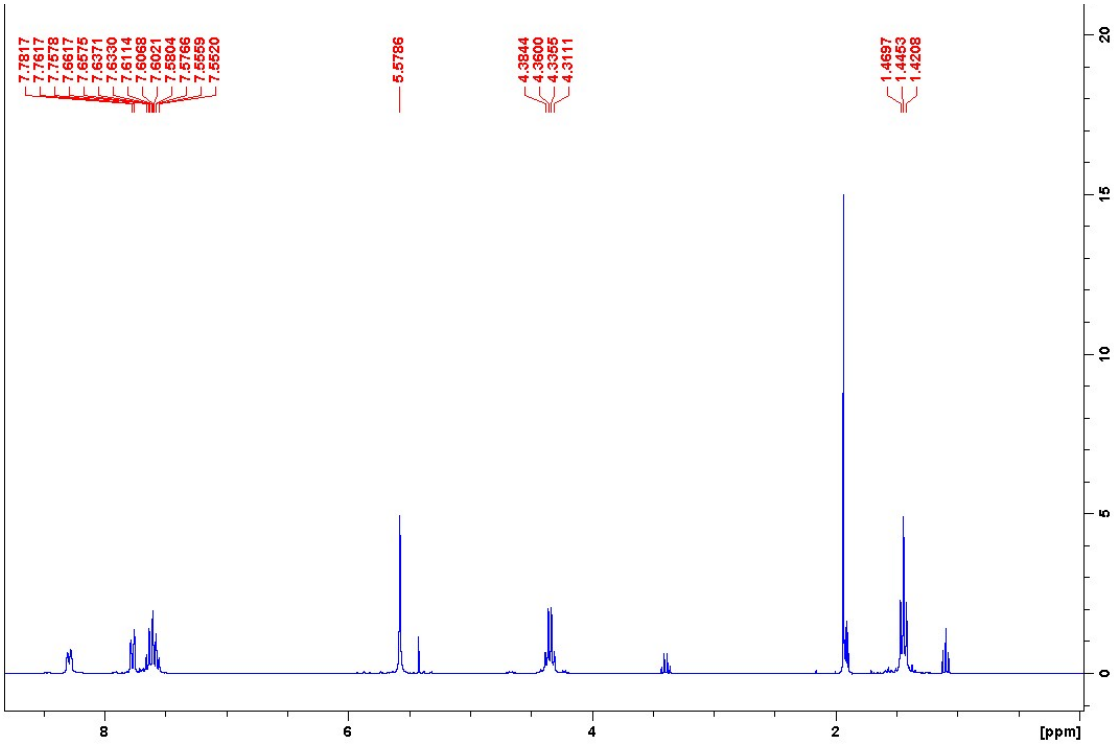


Figure S7: ^{1}H NMR (300 MHz, CD_3CN) spectrum of [(BIMEt$_3$)GeF][OTf]$_3$ the quartet (3.42 ppm) and triplet (1.12 ppm) resonances belong to diethyl ether, an impurity present in the NMR solvent.

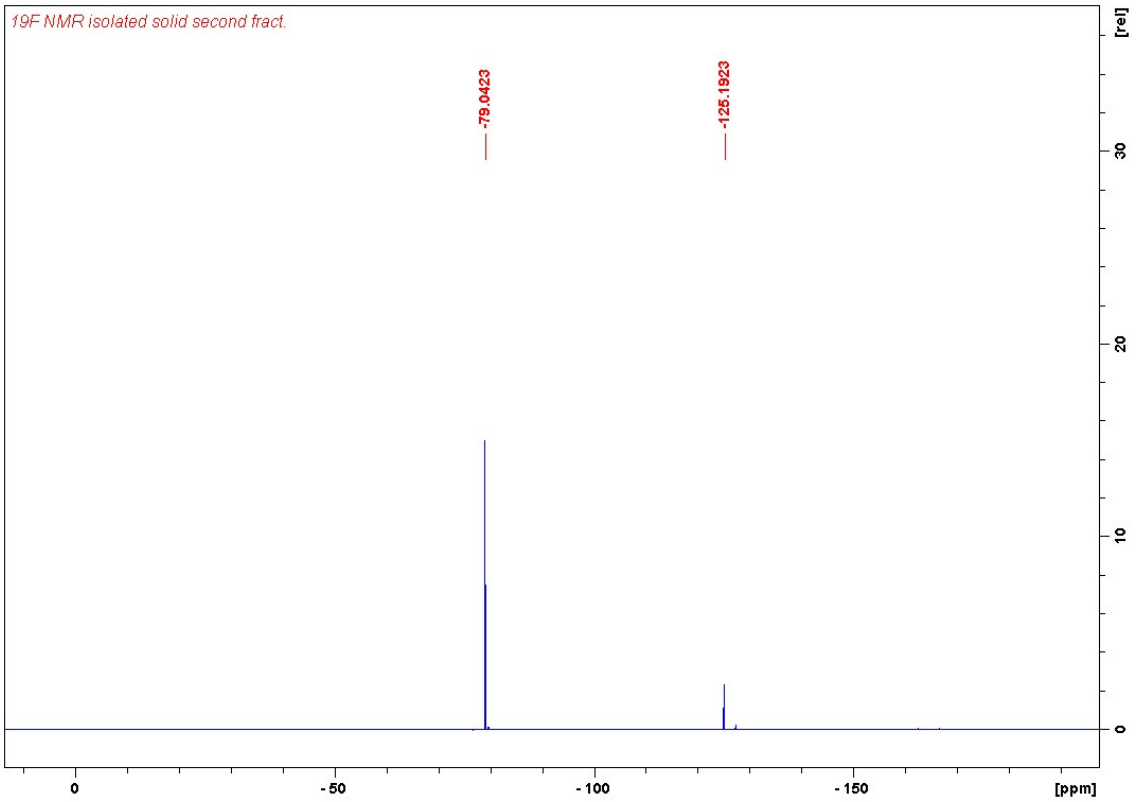


Figure S8: ^{19}F{^{1}H} NMR (283 MHz, CD_3CN) spectrum of [(BIMEt$_3$)GeF][OTf]$_3$

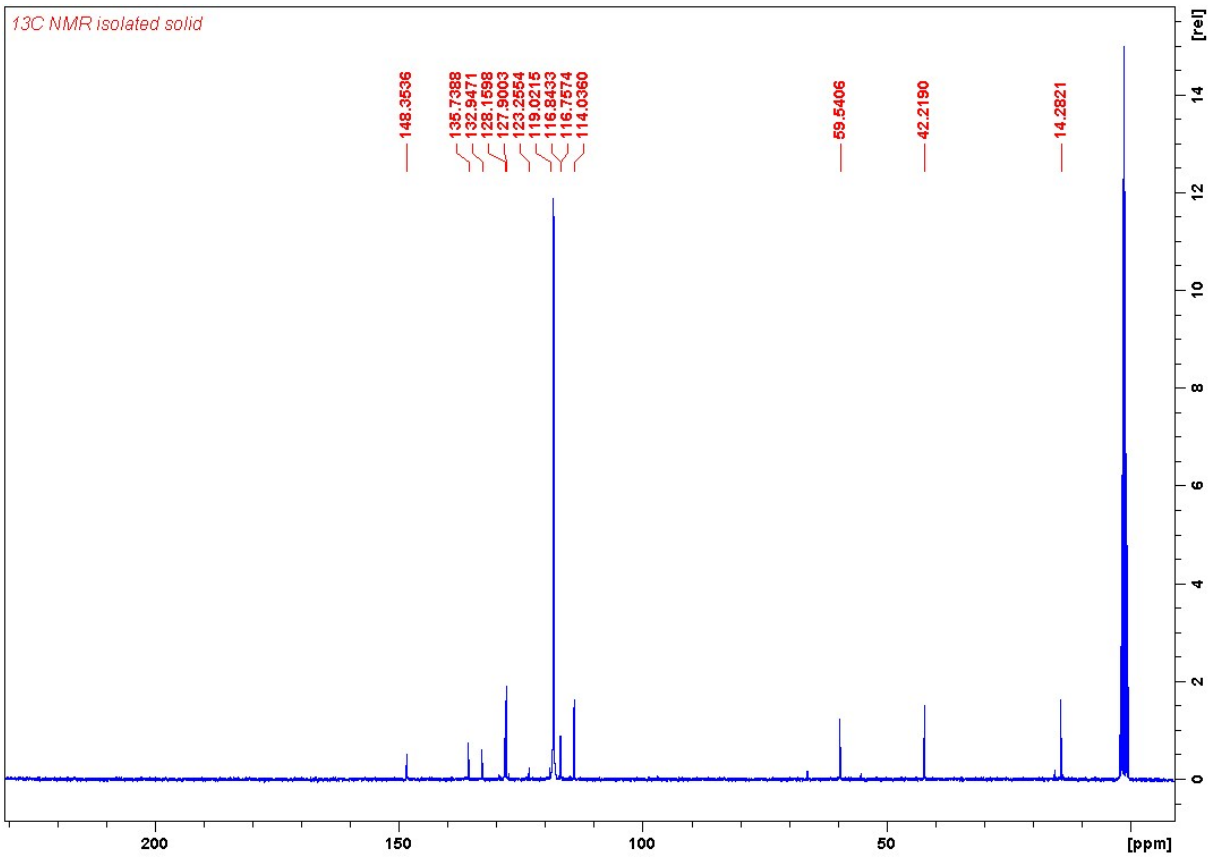


Figure S9: $^{13}C\{^{1}H\}$ NMR (75.5 MHz, CD_3CN) spectrum of $[(BIMEt_3)GeF][OTf]_3$

Fluorination reaction With Selectfluor®

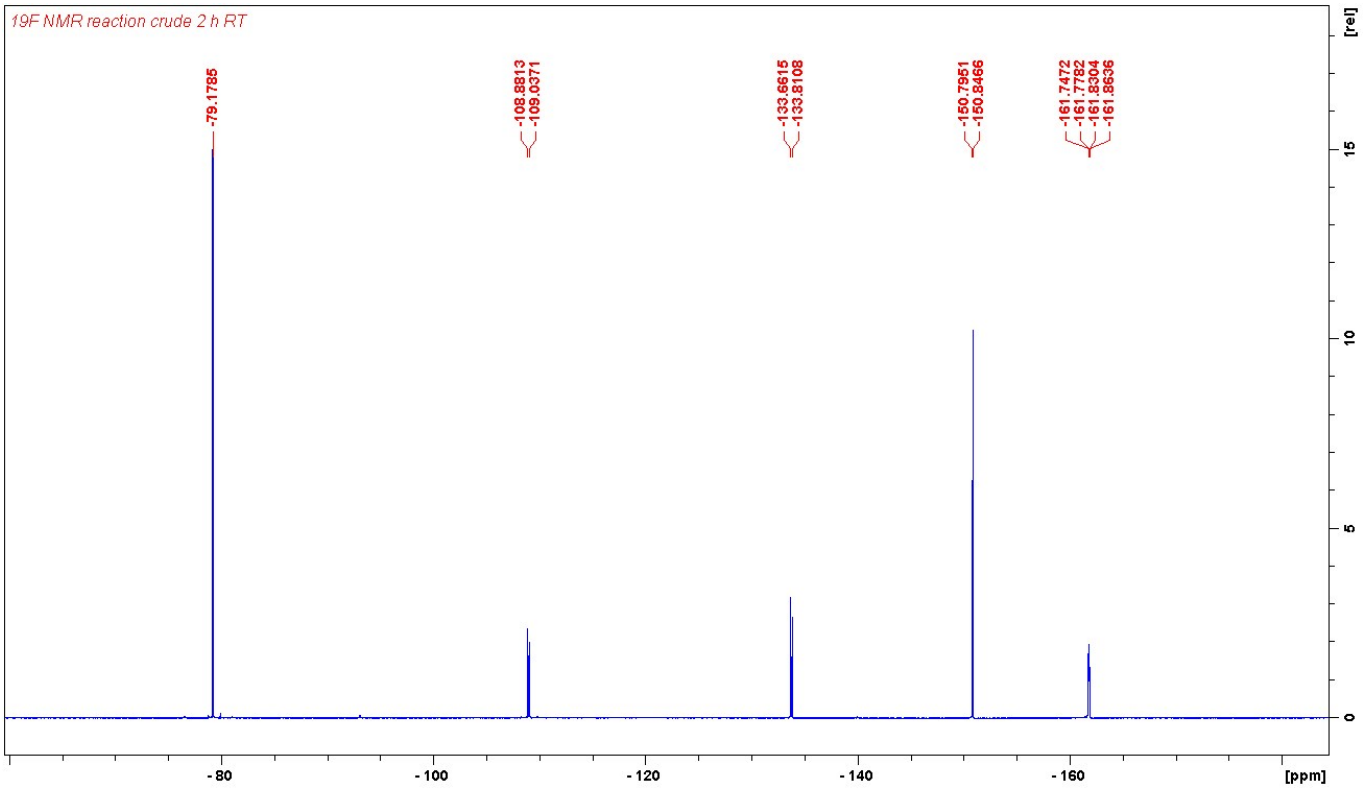


Figure S10: $^{19}F\{^{1}H\}$ NMR (283 MHz, CD_3CN) spectrum of the equimolar reaction of $[(BIMEt_3)Ge][OTf]_2$ with selectfluor®

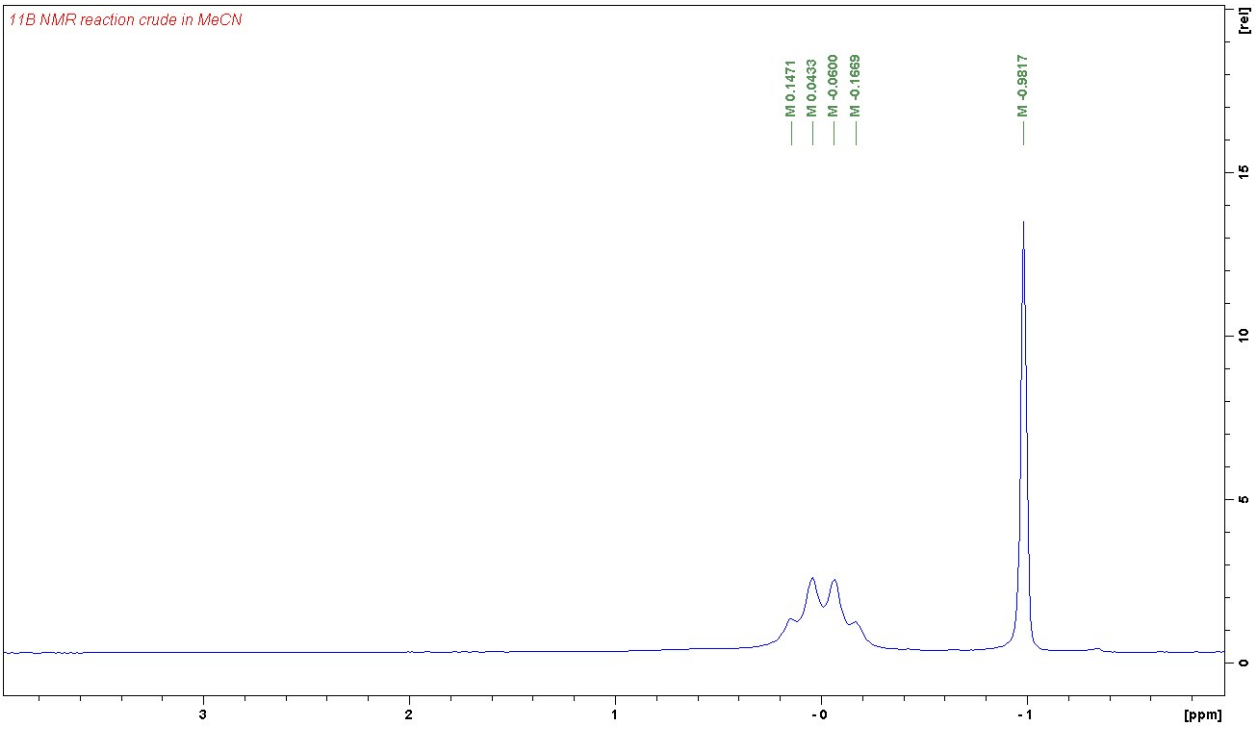


Figure S11: ^{11}B NMR (115.6 MHz, CD_3CN) spectrum of the equimolar reaction of $[(BIMEt_3)Ge][OTf]_2$ with selectfluor®

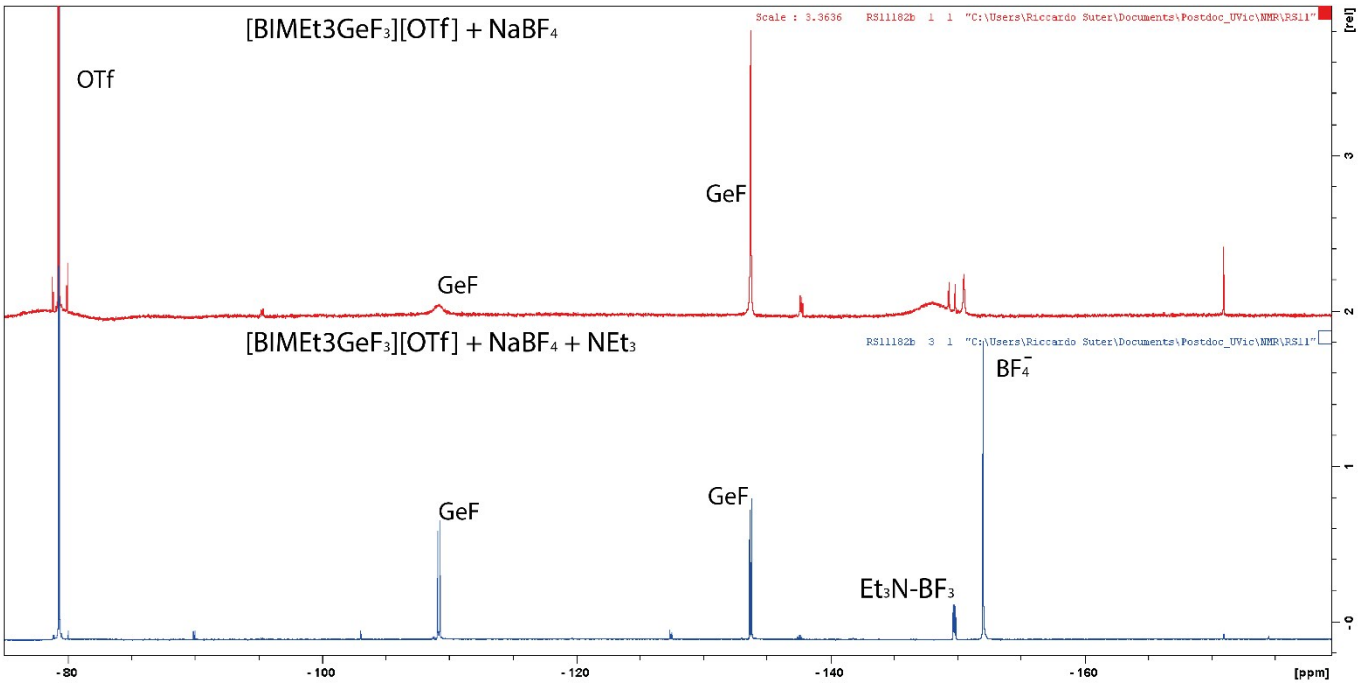
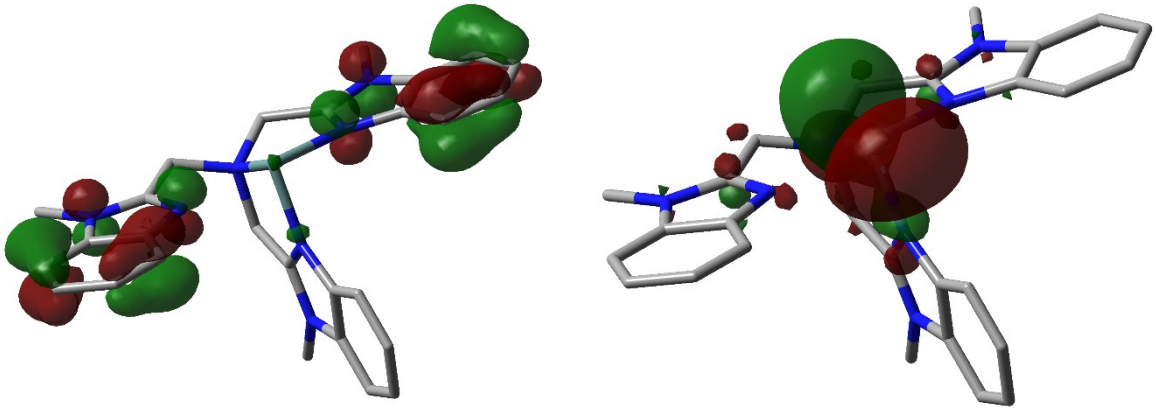


Figure S12: $^{19}F\{^{1}H\}$ NMR (283 MHz, CD_3CN) spectra of the equimolar reaction of $[(BIMEt_3)GeF][OTf]_3$ with $NaBF_4$ (top) and after the addition of a small excess of NEt_3 (bottom)

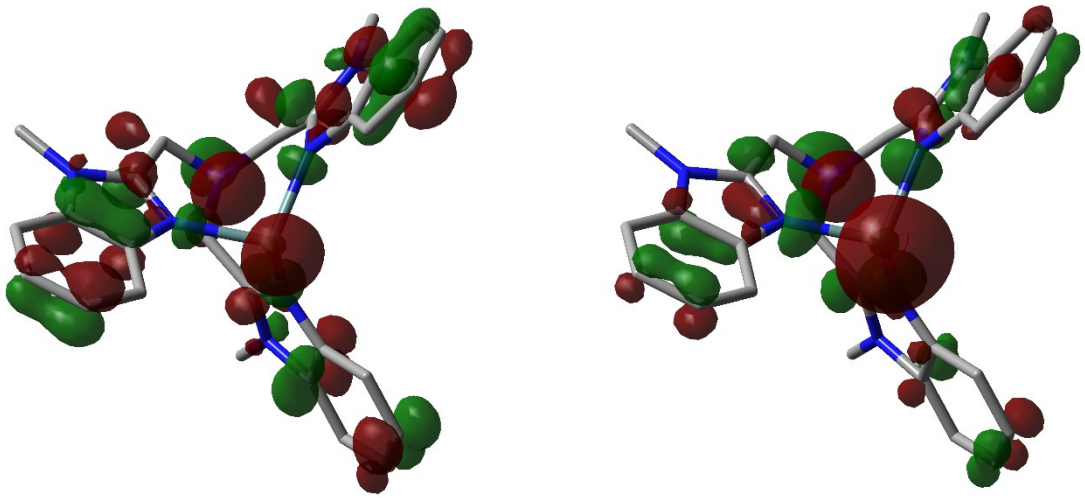
Calculation details

Figure S13: Molecular Orbitals of [**A**]$^{2+}$

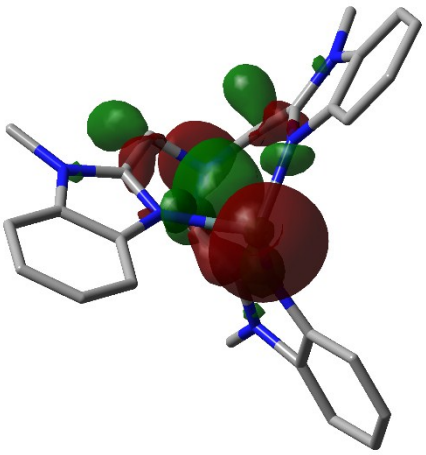


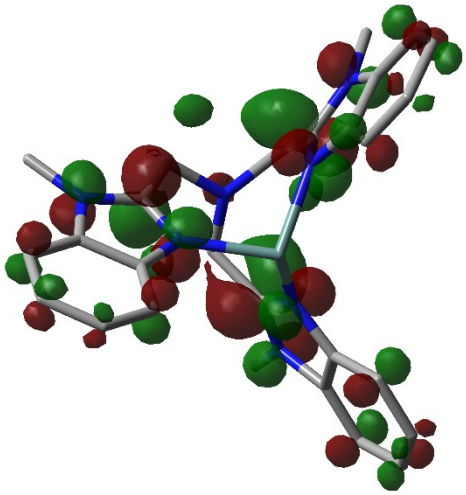
HOMO **LUMO**

Figure S14: Molecular Orbitals of [**B**]$^{2+}$



HOMO-3 **HOMO-6**





HOMO-7

Optimized geometry for [**A**]$^{2+}$on PBEPBE/TZVP

2 1

Ge	-0.00076642	-0.00020004	-0.97661975
N	-0.00164638	0.00014920	2.02730925
N	-3.57262320	-0.55328770	1.30105073
N	-1.85322676	-0.03758844	-0.01879803
N	1.30655620	3.36879452	1.30205750
N	0.89262841	1.62264556	-0.01848510
N	2.26432754	-2.81535198	1.30296444
N	0.95887571	-1.58455400	-0.01806476
C	-1.23760474	-0.71319773	2.30693288
H	-1.66987355	-0.46252585	3.29482193
H	-1.01883241	-1.79435631	2.33014564
C	-0.00166164	1.42725001	2.30672914
H	0.43062205	1.67637702	3.29499550
H	-1.04736077	1.77838048	2.32893234
C	1.23393711	-0.71341117	2.30796128
H	1.23218828	-1.21300238	3.29589599
H	2.06079095	0.01668944	2.33189145
C	-2.22546296	-0.43646399	1.21059836
C	-4.11859242	-0.22140636	0.05648708
C	-5.44207031	-0.17733363	-0.38790482
H	-6.28343547	-0.43297560	0.25675979
C	-5.63715367	0.21276161	-1.71083444
H	-6.65202033	0.26238601	-2.10686708
C	-4.55460282	0.54522023	-2.55127049
H	-4.75684390	0.84625781	-3.57979850
C	-3.23646829	0.50131082	-2.10347121
H	-2.41149484	0.76395688	-2.76643263
C	-3.02769555	0.10535152	-0.77645669
C	0.73301790	2.14424931	1.21096415
C	1.86800123	3.67546267	0.05789373
C	2.56940372	4.79893800	-0.38585353
H	2.76890396	5.65522577	0.25898043
C	3.00594852	4.77246347	-1.70838543
H	3.55755613	5.62603243	-2.10387124
C	2.75228089	3.66901438	-2.54911595
H	3.11509193	3.69333482	-3.57730461
C	2.05359305	2.55014933	-2.10202815
H	1.86826591	1.70462508	-2.76522001
C	1.60512267	2.56770722	-0.77541727
C	1.48924929	-1.70736117	1.21187001
C	2.25153209	-3.45392727	0.05828216
C	2.87605116	-4.62180188	-0.38566587
H	3.51778396	-5.22240613	0.25954163
C	2.63721804	-4.98572032	-1.70887383
H	3.10246985	-5.88917275	-2.10456928
C	1.80853411	-4.21467558	-2.55003852
H	1.65014640	-4.54026414	-3.57877552
C	1.18655728	-3.05151312	-2.10270184
H	0.54708088	-2.46853005	-2.76623494
C	1.42355746	-2.67283450	-0.77538376
C	1.32872503	4.27148671	2.45328069
H	2.36497981	4.55825251	2.67481642
H	0.74074571	5.17254374	2.23193500
H	0.90125866	3.77725330	3.33125663
C	-4.36563715	-0.98557084	2.45210815
H	-5.13077251	-0.23060211	2.67516484
H	-4.85368543	-1.94416282	2.22959025
H	-3.72360155	-1.11114868	3.32951980
C	3.03401039	-3.28594497	2.45483862
H	2.76430431	-4.32686849	2.67594759
H	4.10852234	-3.22694678	2.23449342
H	2.81875258	-2.66881852	3.33271231

Optimized geometry for [**B**]$^{2+}$ on PBEPBE/TZVP

2 1

Ge	0.01259510	-0.42886900	-1.18346253
N	-0.00725533	1.03548838	0.22290610
N	2.16868078	-0.72045382	-0.53393582
N	0.02055223	-1.71643904	0.76699073
N	-2.14086504	-0.75424401	-0.54825219
N	-3.68385152	-2.06560979	0.40626083
N	3.72497833	-2.03428739	0.39598287
N	-0.03071938	1.75585299	2.32323782
C	-4.37729829	-1.13128810	-0.37021531
C	-2.35864209	-1.79322400	0.25304838
C	2.39721939	-1.77131217	0.24897997
C	-3.39281007	-0.30673387	-0.96729423
C	-0.00601975	0.67389076	1.50718751
C	-0.03494313	2.42922620	0.17411157
C	1.24898795	-2.57504713	0.76709621
H	1.05857173	-3.42980792	0.09738356
H	1.43517826	-2.98627311	1.77350816
C	-3.76242184	0.74818152	-1.81136834
H	-3.01913356	1.39337543	-2.28123446
C	-0.04931966	2.89517169	1.50802023
C	3.41605880	-0.25514216	-0.94727048
C	-1.20331701	-2.58110381	0.77969568
H	-1.38505185	-2.98141822	1.79120838
H	-1.00937988	-3.44309288	0.12028886

C	4.40883441	-1.08084465	-0.36563199
C	-5.74423687	-0.94285233	-0.58931985
H	-6.50345625	-1.57899649	-0.13314859
C	3.77487219	0.81742476	-1.77355649
H	3.02500808	1.46414277	-2.23073261
C	-5.12310686	0.93488598	-2.03661643
H	-5.45063108	1.74022356	-2.69510063
C	-0.07687773	4.25615750	1.81977320
H	-0.08761427	4.62040303	2.84748435
C	0.02718328	-0.76110023	1.93695837
H	0.93074821	-0.94705418	2.53985853
H	-0.83964236	-0.98042942	2.58099743
C	-6.09522247	0.10607607	-1.43646241
H	-7.14995972	0.29071267	-1.64356601
C	-0.04818837	3.32264929	-0.90271294
H	-0.03697167	2.97916698	-1.93843214
C	5.77368601	-0.87640706	-0.58338415
H	6.53930521	-1.51326706	-0.13906384
C	5.13348037	1.02017402	-1.99748673
H	5.45279208	1.83976510	-2.64227534
C	-0.08981235	5.13780431	0.74061930
H	-0.11115508	6.21110551	0.93263728
C	-0.07573801	4.68031504	-0.59391104
H	-0.08647663	5.41135253	-1.40316606
C	6.11390697	0.18995632	-1.41297829
H	7.16663171	0.38769204	-1.61822398
C	-0.03339376	1.78127267	3.78546118
H	0.85519872	2.31348412	4.15060180
H	-0.93689826	2.29008001	4.14719487
H	-0.02076011	0.75988946	4.18076224
C	-4.30979181	-3.14882117	1.16145463
H	-4.79158313	-3.85964811	0.47601030
H	-3.55605450	-3.68267621	1.75056581
H	-5.06370420	-2.73674194	1.84500597
C	4.36144183	-3.12423630	1.13246291
H	3.61267165	-3.67613418	1.71121592
H	4.85079358	-3.81782836	0.43484310
H	5.11070273	-2.71680738	1.82388290

X-ray data

Table S1: Crystal data and structure refinement for $[(BIMEt_3)Ge][OTf]_2$

Identification code	1587203
Empirical formula	$C_{32}H_{33}F_6GeN_7O_6S_2$
Formula weight	862.40
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.7605(7)
b/Å	11.2818(5)
c/Å	21.5537(10)
α/°	90
β/°	96.184(2)
γ/°	90
Volume/Å^3	3568.3(3)
Z	4
ρ_{calc}g/cm^3	1.6051
μ/mm^{-1}	1.062
F(000)	1762.7
Crystal size/mm^3	0.26 × 0.21 × 0.18
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.56 to 66.52
Index ranges	-22 ≤ h ≤ 22, -17 ≤ k ≤ 17, -33 ≤ l ≤ 33
Reflections collected	116595
Independent reflections	13707 [R_{int} = 0.0299, R_{sigma} = 0.0187]
Data/restraints/parameters	13707/0/490
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0320, wR_2 = 0.0798
Final R indexes [all data]	R_1 = 0.0430, wR_2 = 0.0864
Largest diff. peak/hole / e Å^{-3}	0.93/-1.07

Table S2: Crystal data and structure refinement for $[(BIMEt_3)GeF_2][OTf]_2$

Identification code	1587202
Empirical formula	$C_{32}H_{33}F_8GeN_7O_6S_2$
Formula weight	900.36
Temperature/K	170.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.2065(6)
b/Å	18.0706(8)
c/Å	14.8299(8)
α/°	90
β/°	106.697(2)
γ/°	90
Volume/Å^3	3646.6(3)
Z	4
ρ_{calc}g/cm^3	1.640
μ/mm^{-1}	1.050
F(000)	1832.0
Crystal size/mm^3	0.155 × 0.12 × 0.068
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.708 to 54.324
Index ranges	-18 ≤ h ≤ 18, -23 ≤ k ≤ 23, -19 ≤ l ≤ 19
Reflections collected	103933
Independent reflections	8058 [R_{int} = 0.0950, R_{sigma} = 0.0359]
Data/restraints/parameters	8058/0/508
Goodness-of-fit on F^2	1.107
Final R indexes [I>=2σ (I)]	R_1 = 0.0422, wR_2 = 0.0954
Final R indexes [all data]	R_1 = 0.0688, wR_2 = 0.1097
Largest diff. peak/hole / e Å^{-3}	0.80/-0.58

Table S3: Crystal data and structure refinement for $[(BIMEt_3)GeF][OTf]_3$

Identification code	1587201
Empirical formula	$C_{35}H_{36}F_{10}GeN_8O_9S_3$
Formula weight	1071.49
Temperature/K	170.0
Crystal system	triclinic
Space group	P-1
a/Å	11.55(3)
b/Å	14.24(3)
c/Å	14.38(3)
α/°	84.79(14)
β/°	80.30(13)
γ/°	88.99(12)
Volume/Å^3	2323(9)
Z	2
ρ_{calc}g/cm^3	1.532
μ/mm^{-1}	0.892
F(000)	1088.0
Crystal size/mm^3	0.39 × 0.35 × 0.3
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.744 to 50.884
Index ranges	-13 ≤ h ≤ 13, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17
Reflections collected	31482
Independent reflections	8328 [R_{int} = 0.0893, R_{sigma} = 0.0814]
Data/restraints/parameters	8328/254/672
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0972, wR_2 = 0.2478
Final R indexes [all data]	R_1 = 0.1631, wR_2 = 0.3124
Largest diff. peak/hole / e Å^{-3}	1.28/-0.79

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