

Supporting Information for

**Fluoro-germanium(IV) cations with neutral co-ligands – synthesis, properties and comparison with neutral GeF<sub>4</sub> adducts**

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William Levason<sup>a</sup> and Gillian Reid<sup>a\*</sup>

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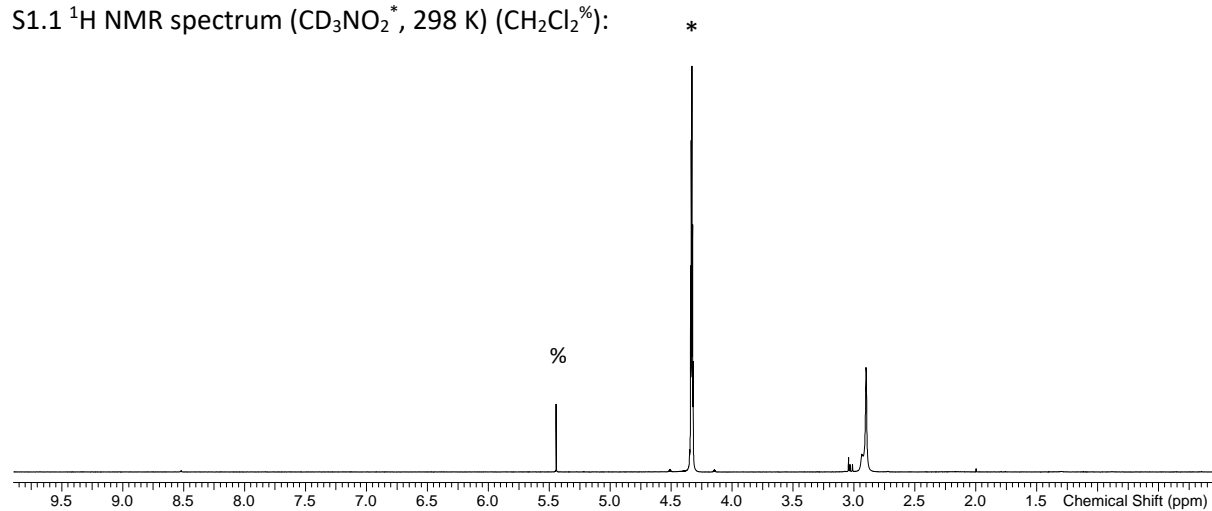
<sup>b</sup> GE Healthcare, Pollards Wood, Nightingales Lane, Chalfont St Giles, Bucks, HP8 4SP, UK.

Containing spectra for the complexes as follows:

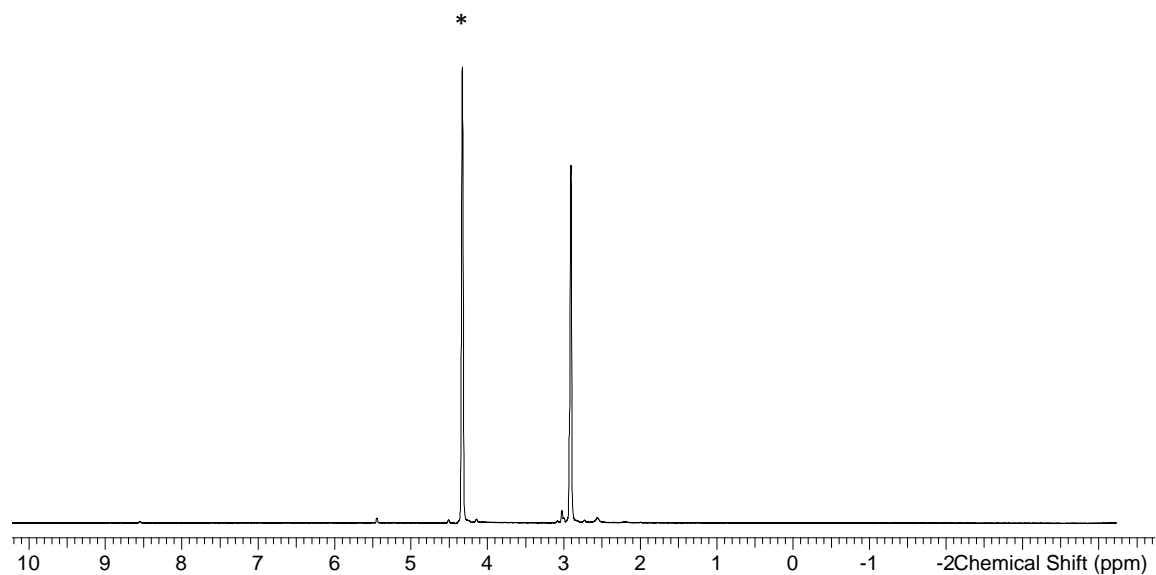
Figure S1 [GeF<sub>4</sub>(dmsO)<sub>2</sub>]  
Figure S2. [GeF<sub>4</sub>(dmf)<sub>2</sub>]  
Figure S3. [GeF<sub>4</sub>(pyNO)<sub>2</sub>]  
Figure S4. [GeF<sub>3</sub>(dmsO)<sub>3</sub>][OTf]  
Figure S5. [GeF<sub>3</sub>(dmf)<sub>3</sub>][OTf]  
Figure S6. [GeF<sub>3</sub>(py)<sub>3</sub>][OTf]  
Figure S7. [GeF<sub>3</sub>(pyNO)<sub>3</sub>][OTf]  
Figure S8. [GeF<sub>3</sub>(OPPh<sub>3</sub>)<sub>3</sub>][OTf]  
Figure S9. [GeF<sub>3</sub>(OPMe<sub>3</sub>)<sub>3</sub>][OTf]  
Figure S10. [GeF<sub>3</sub>(OAsPh<sub>3</sub>)<sub>3</sub>][OTf] and [GeF<sub>2</sub>(OAsPh<sub>3</sub>)<sub>4</sub>][OTf]<sub>2</sub>  
Figure S11. [GeF<sub>3</sub>(terpy)][OTf]  
Figure S12. [GeF<sub>3</sub>(Me<sub>3</sub>tacn)][OTf]  
Figure S13. [GeF<sub>2</sub>(Me<sub>4</sub>-cyclen)][OTf]<sub>2</sub>  
Figure S14. [GeF<sub>2</sub>(Me<sub>4</sub>-cyclam)][OTf]<sub>2</sub>  
Table S1 X-ray crystallographic data  
Figure S15. Frontier orbitals of *cis/trans*-[GeF<sub>4</sub>(OPMe<sub>3</sub>)<sub>2</sub>]  
Figure S16. Frontier orbitals of *fac/mer*-[GeF<sub>3</sub>(OPMe<sub>3</sub>)<sub>3</sub>]<sup>+</sup>  
Figure S17. Frontier orbitals of *cis/trans*-[GeF<sub>2</sub>(OPMe<sub>3</sub>)<sub>4</sub>]<sup>2+</sup>  
Table S2. xyz coordinates from DFT calculations

Figure S1 [GeF<sub>4</sub>(dmsO)<sub>2</sub>]

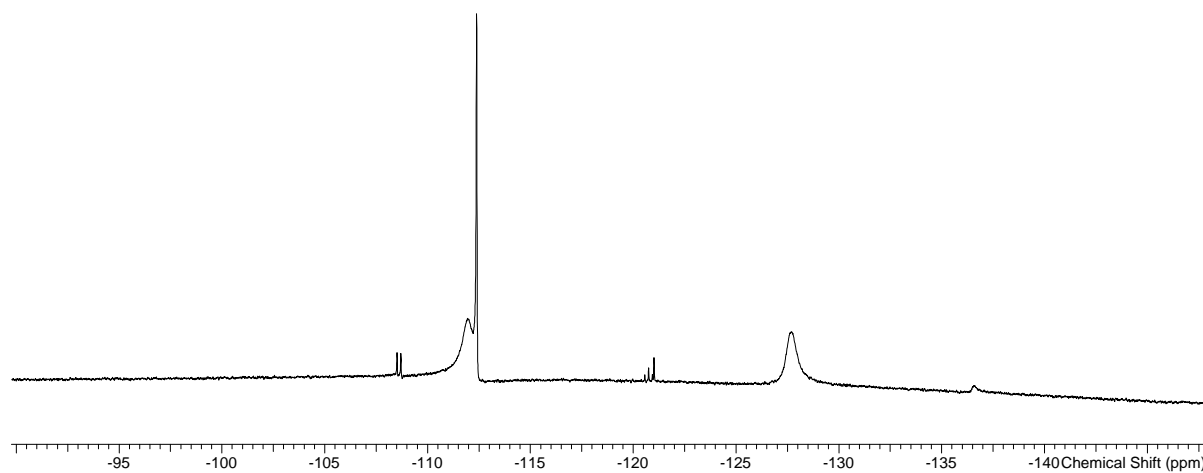
S1.1 <sup>1</sup>H NMR spectrum (CD<sub>3</sub>NO<sub>2</sub><sup>\*</sup>, 298 K) (CH<sub>2</sub>Cl<sub>2</sub><sup>%</sup>):



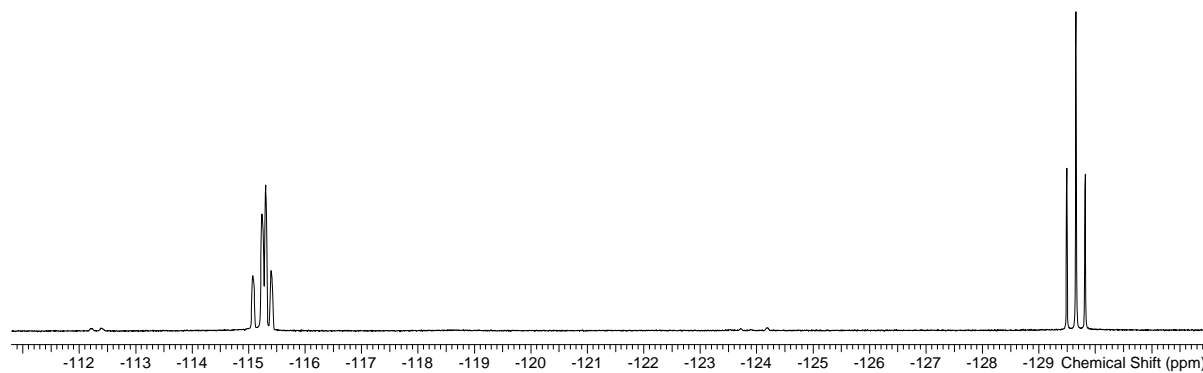
S1.2 <sup>1</sup>H NMR spectrum (CD<sub>3</sub>NO<sub>2</sub><sup>\*</sup>, 253 K):



S1.3  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K):



S1.4  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 253 K):



S1.5 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):

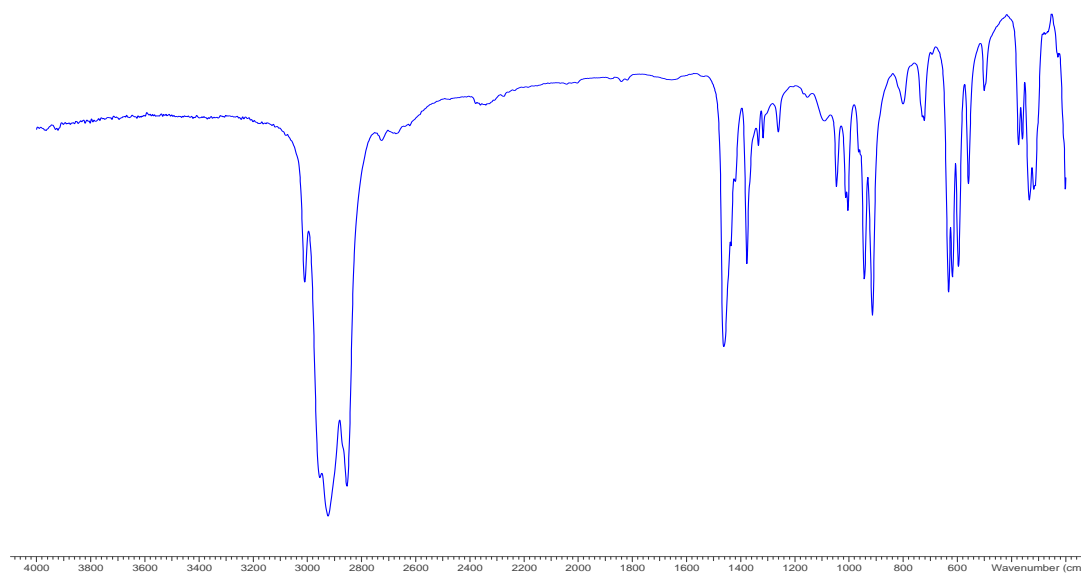
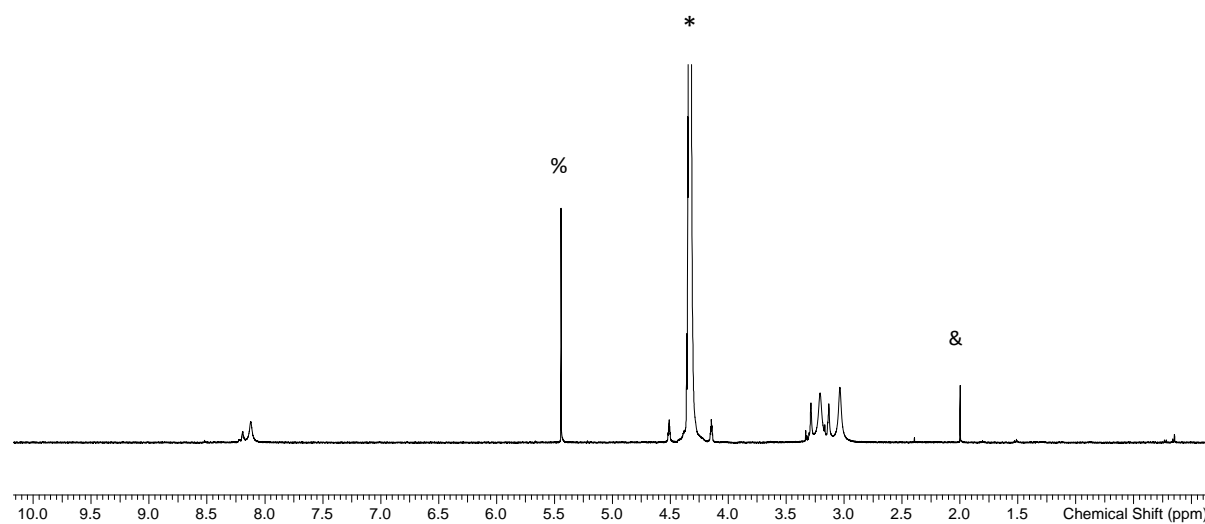
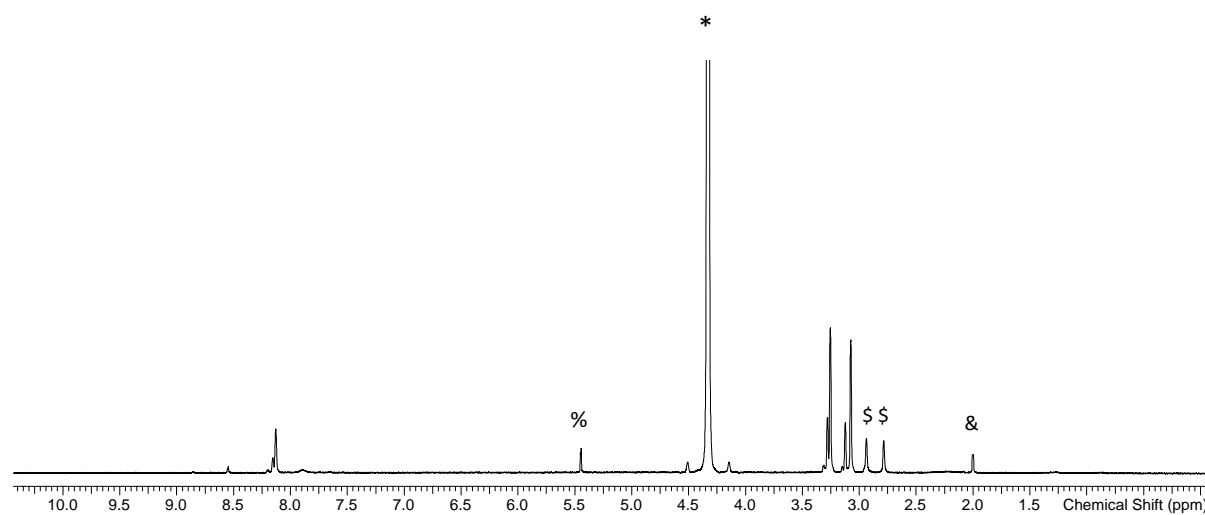


Figure S2.  $[\text{GeF}_4(\text{dmf})_2]$

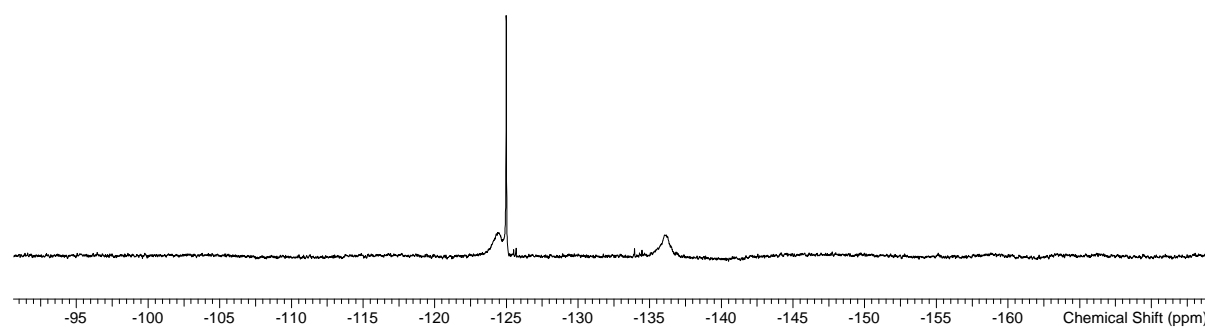
S2.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^\%$ ,  $\text{H}_2\text{O}^\&$ ):



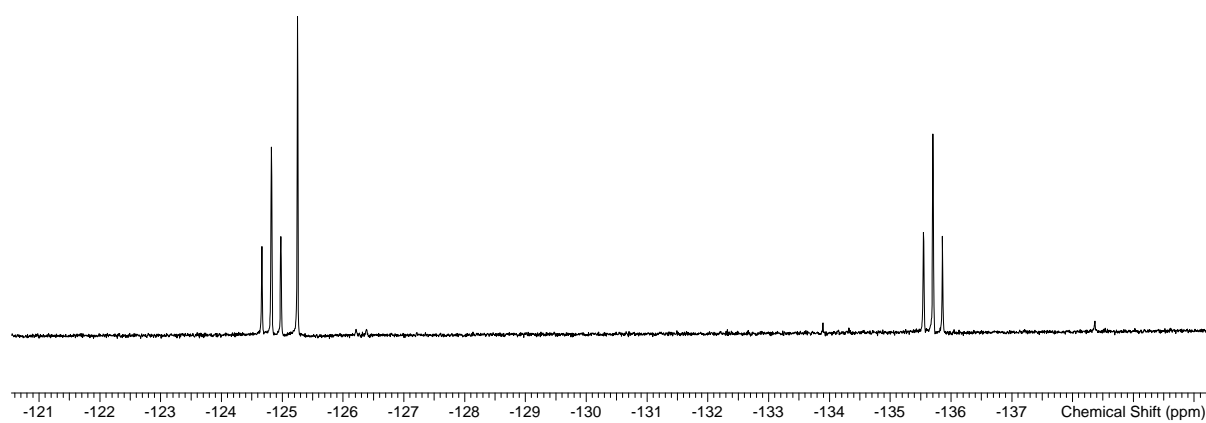
S2.2  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 253 K) ( $\text{CH}_2\text{Cl}_2^\%$ ,  $\text{H}_2\text{O}^\&$ , uncoordinated  $\text{DMF}^\$$ ):



S2.3  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K):



S2.4  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 253 K):



S2.5 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):

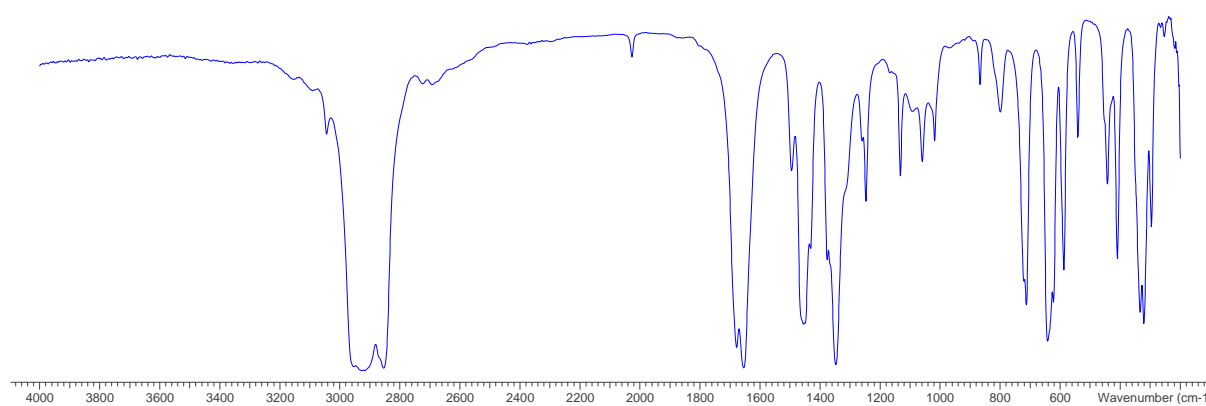
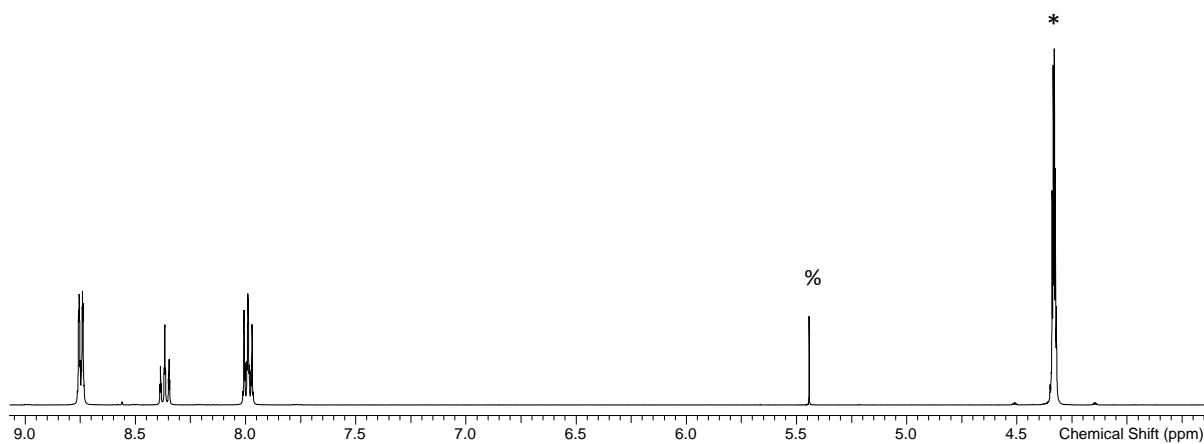
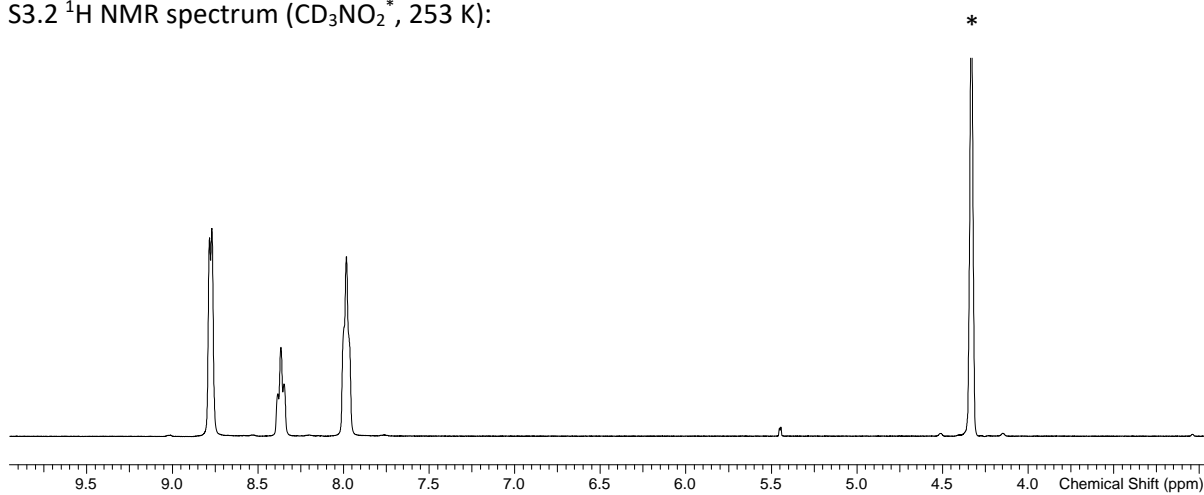


Figure S3.  $[\text{GeF}_4(\text{pyNO})_2]$

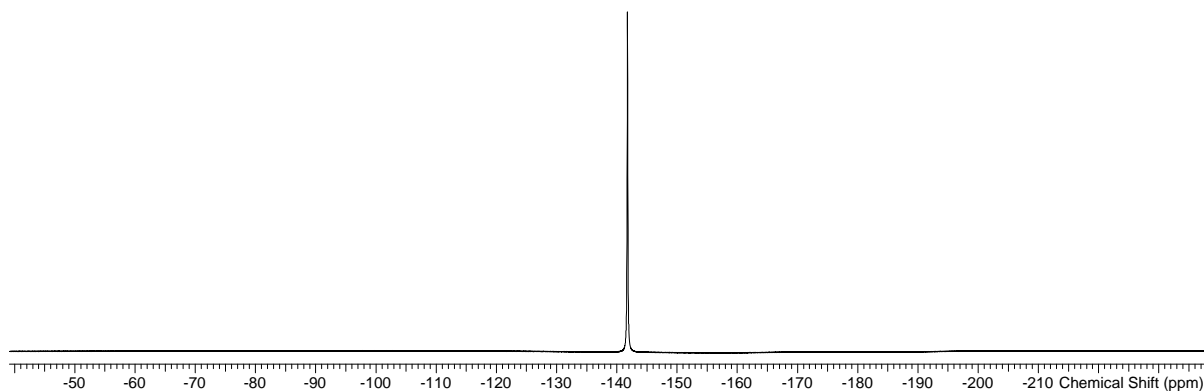
S3.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^{\%}$ ):



S3.2  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 253 K):



S3.3  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K):



S3.5 IR spectrum (Nujol/cm<sup>-1</sup>):

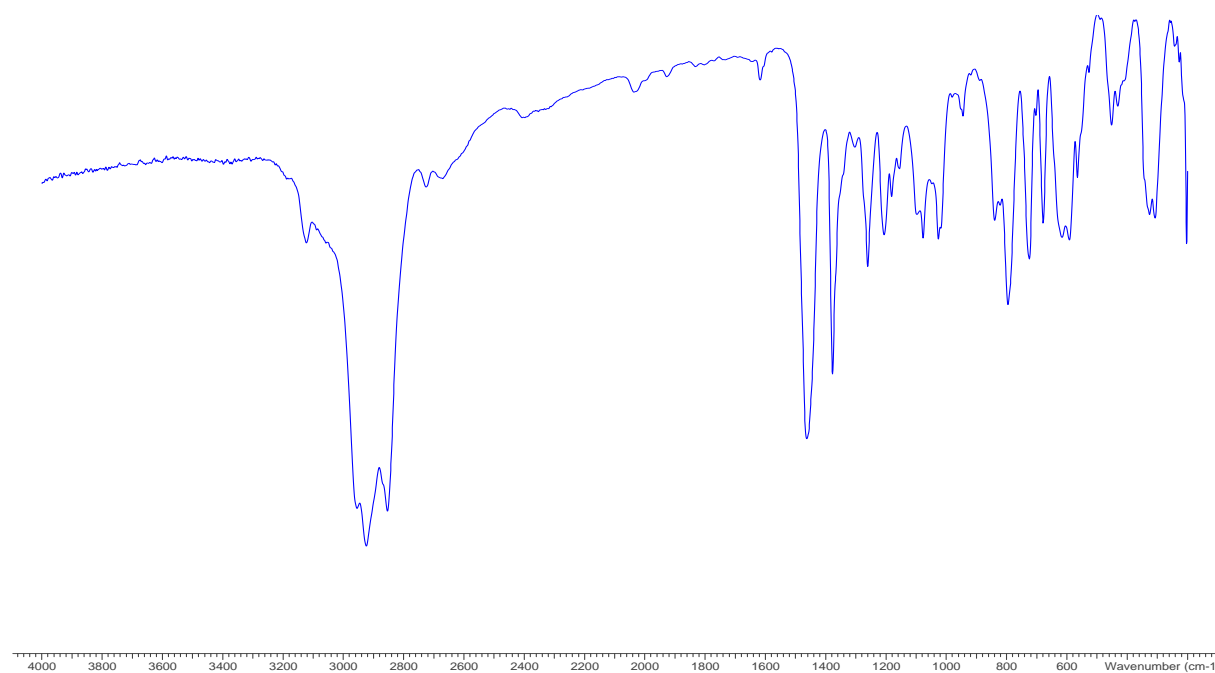
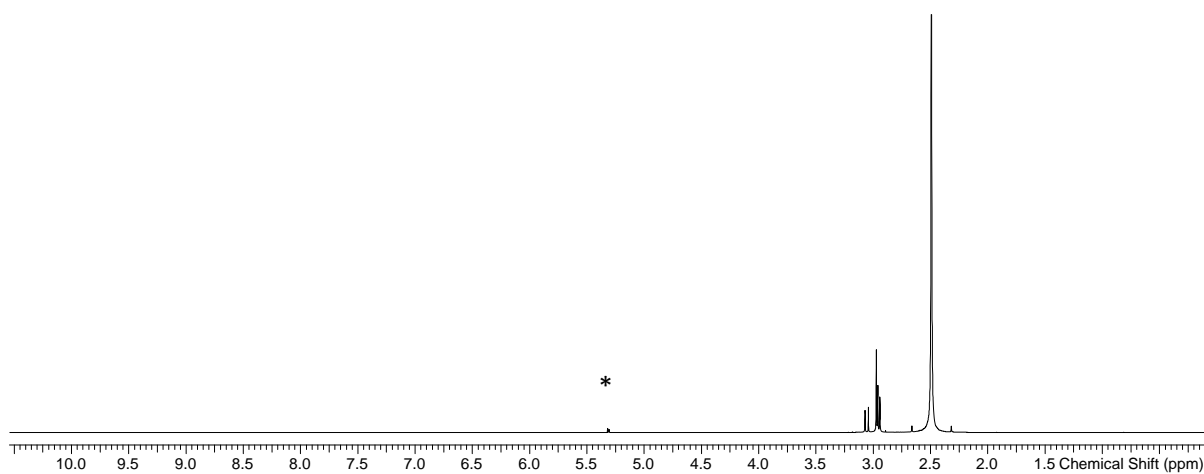
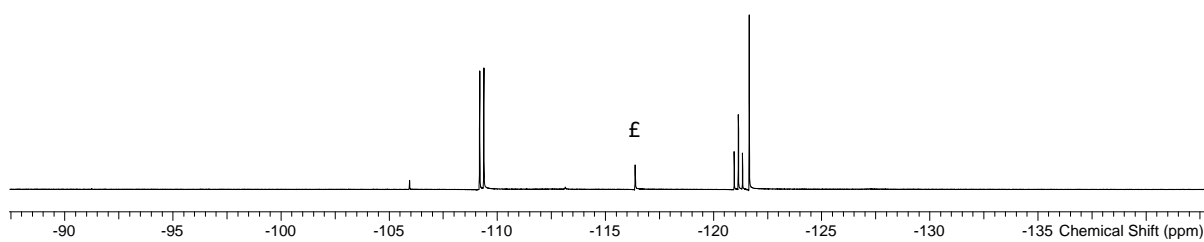


Figure S4.  $[\text{GeF}_3(\text{dmsO})_3][\text{OTf}]$   
S4.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2^*$ , 298 K):



S4.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 298 K) (unidentified impurity<sup>f</sup>). OTf resonance omitted for clarity:



S4.3 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):

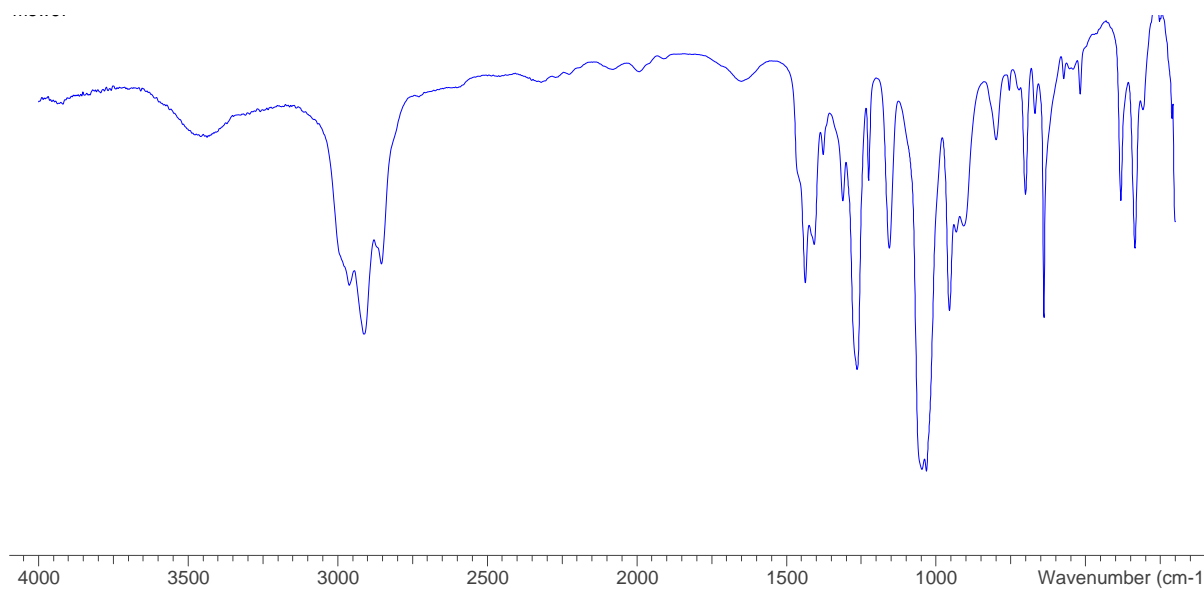
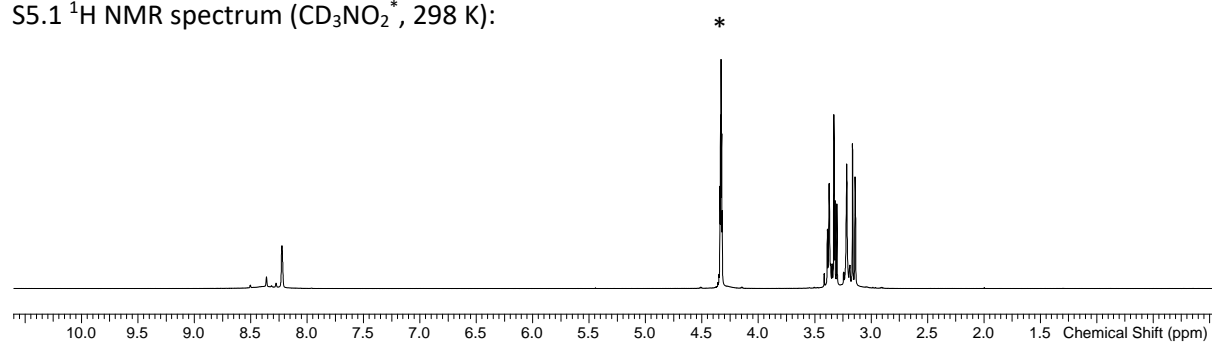


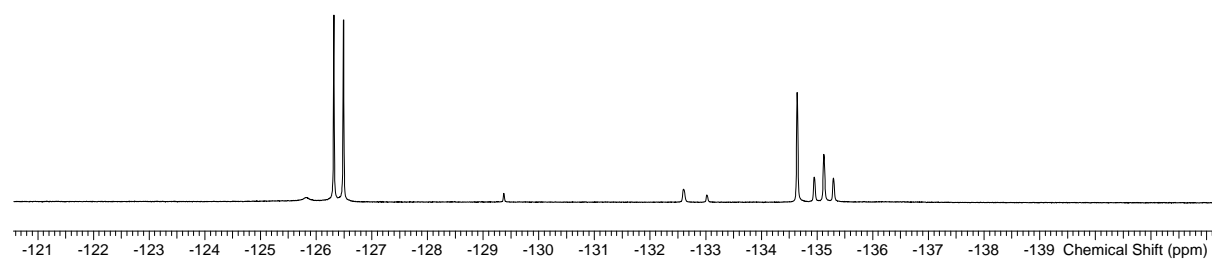


Figure S5.  $[\text{GeF}_3(\text{dmf})_3][\text{OTf}]$

S5.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K):



S5.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K). OTf resonance omitted for clarity:



S5.3 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):

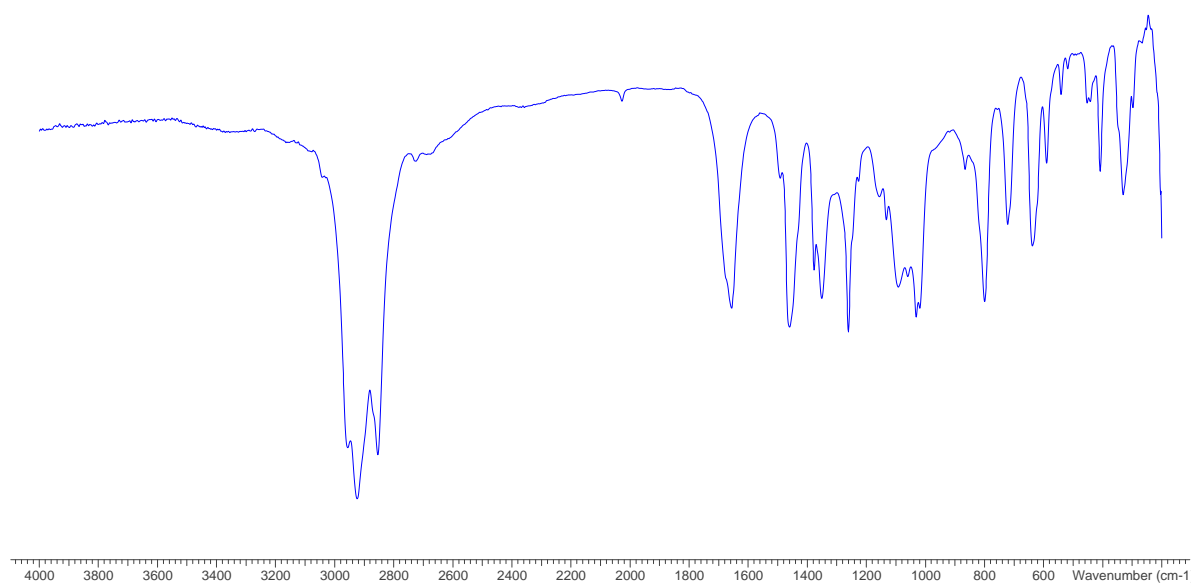
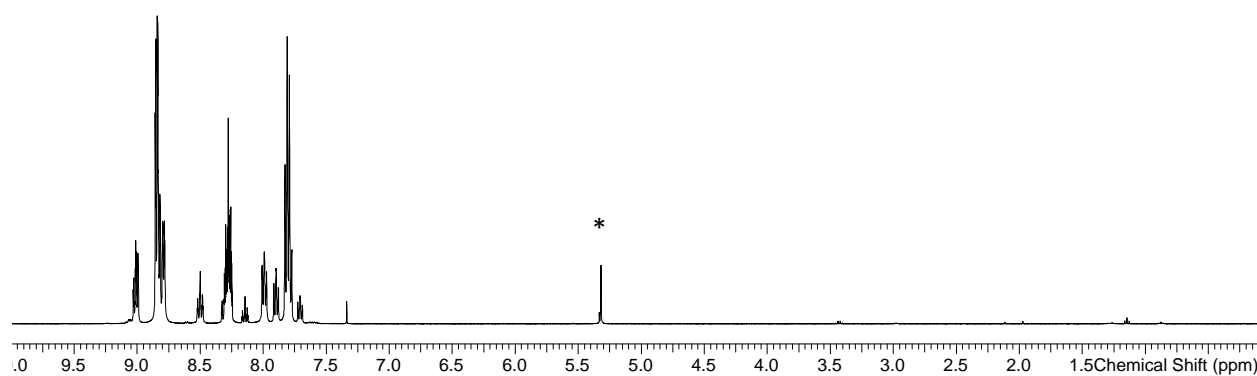
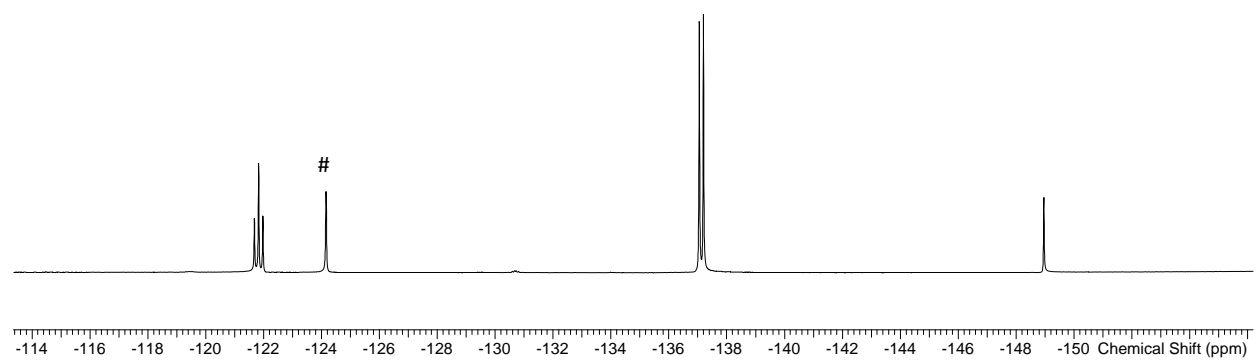


Figure S6.  $[\text{GeF}_3(\text{py})_3][\text{OTf}]$   
S6.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2^*$ , 298 K):



S6.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 298 K) ( $\text{F}^-$  degradation product<sup>#</sup>). OTf resonance omitted for clarity:



S6.3 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):

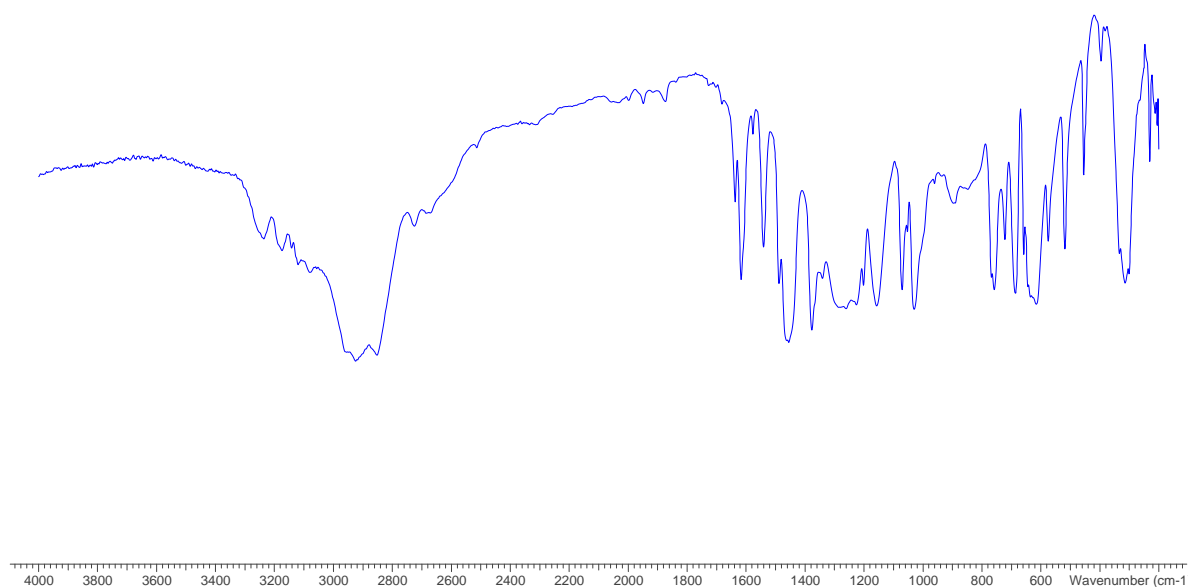
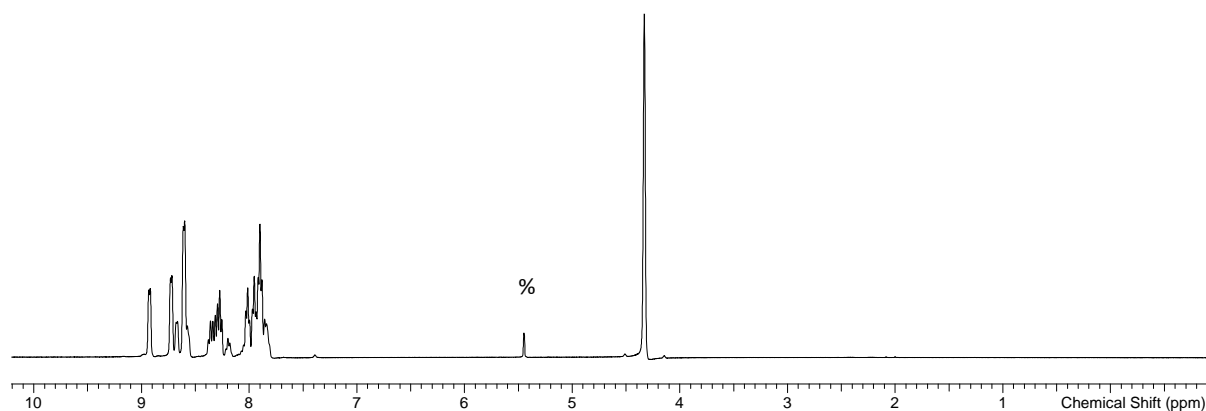
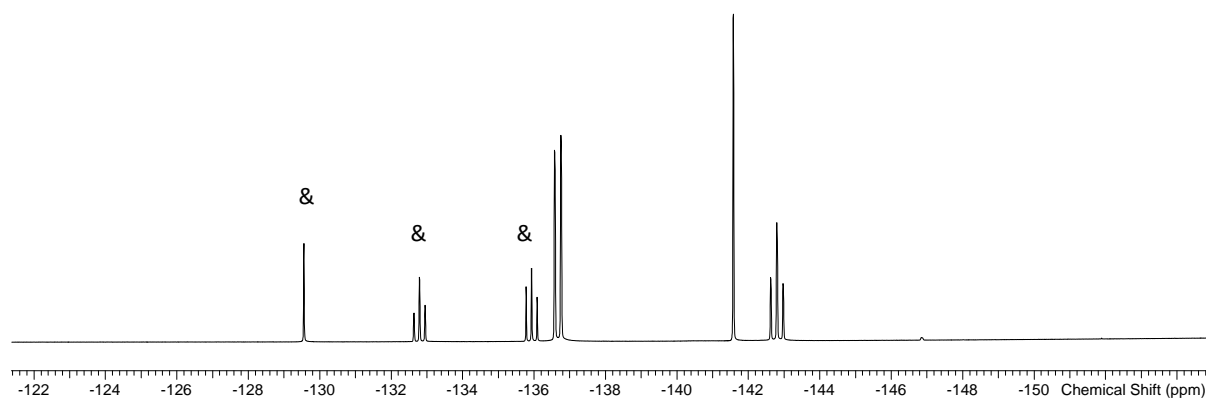


Figure S7.  $[\text{GeF}_3(\text{pyNO})_3][\text{OTf}]$

S7.1:  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^\%$ ): \*



S7.2:  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K) ( $[\text{GeF}_4(\text{pyNO})_2]^\&$  impurity). OTf resonance omitted for clarity:



S7.3 IR spectrum (Nujol/cm<sup>-1</sup>):

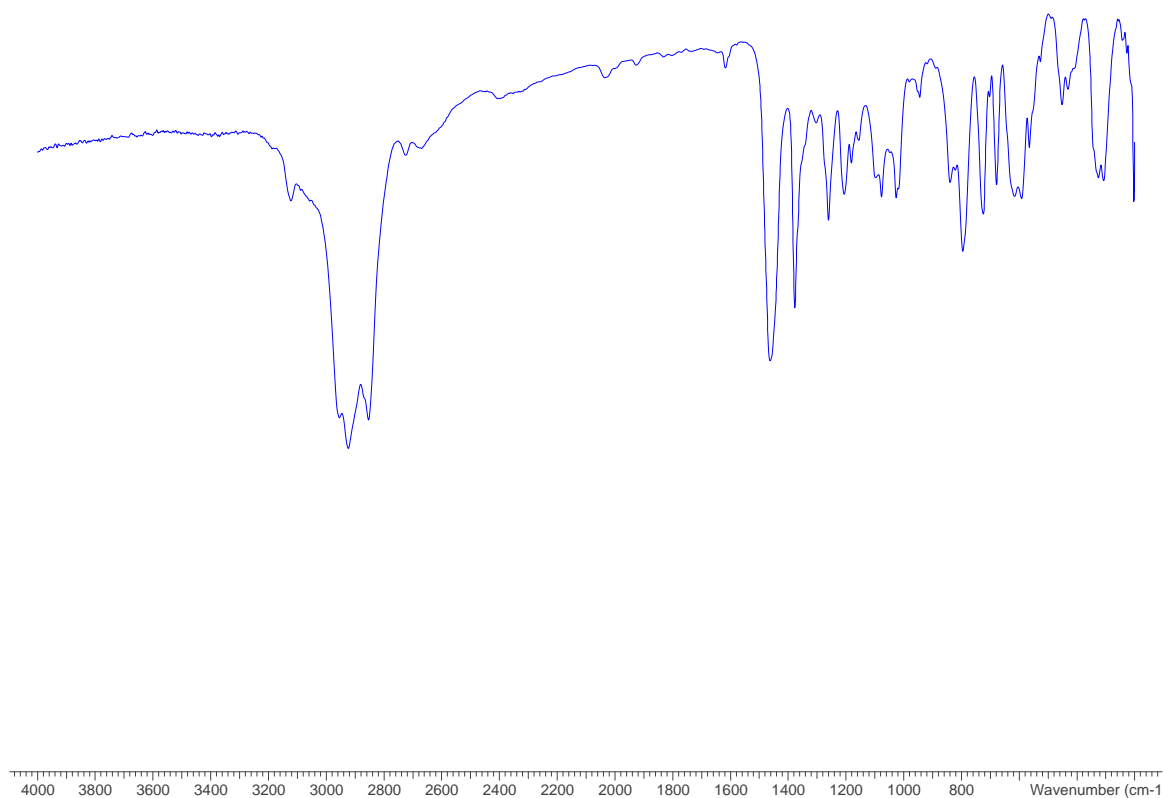
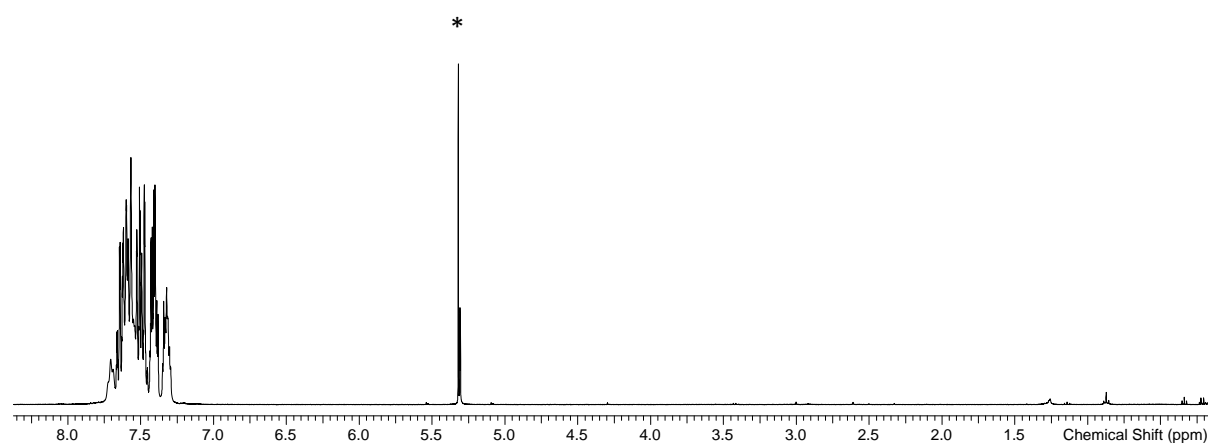
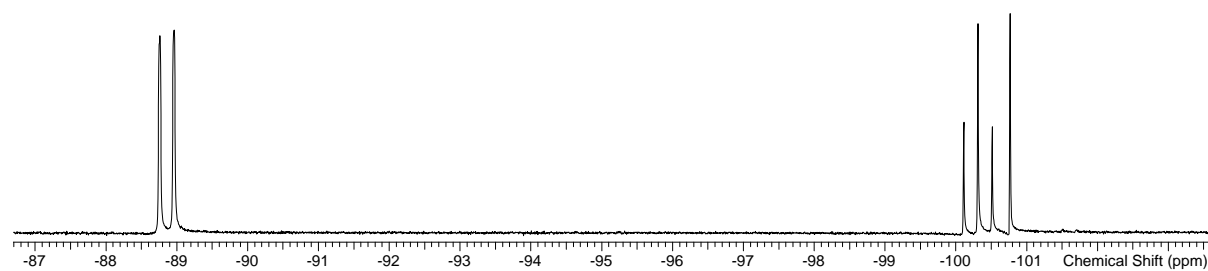


Figure S8.  $[\text{GeF}_3(\text{OPPh}_3)_3][\text{OTf}]$

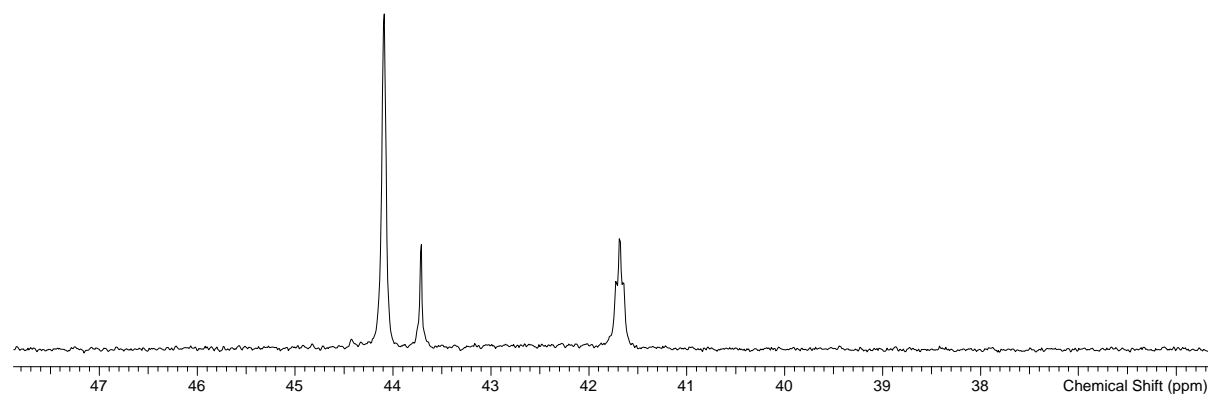
S8.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2^*$ , 298 K):



S8.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 298 K). OTf resonance omitted for clarity:



S8.3  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 298 K):



S8.4 IR spectrum (Nujol/cm<sup>-1</sup>):

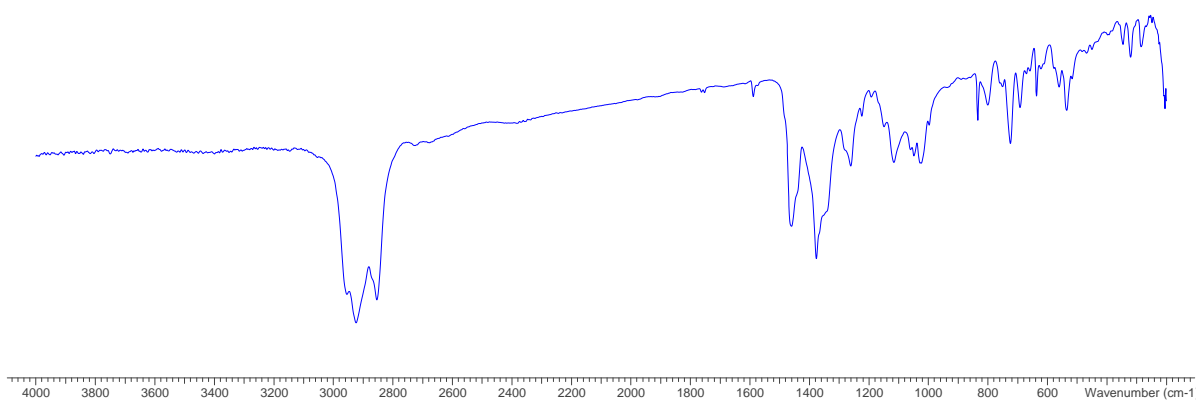
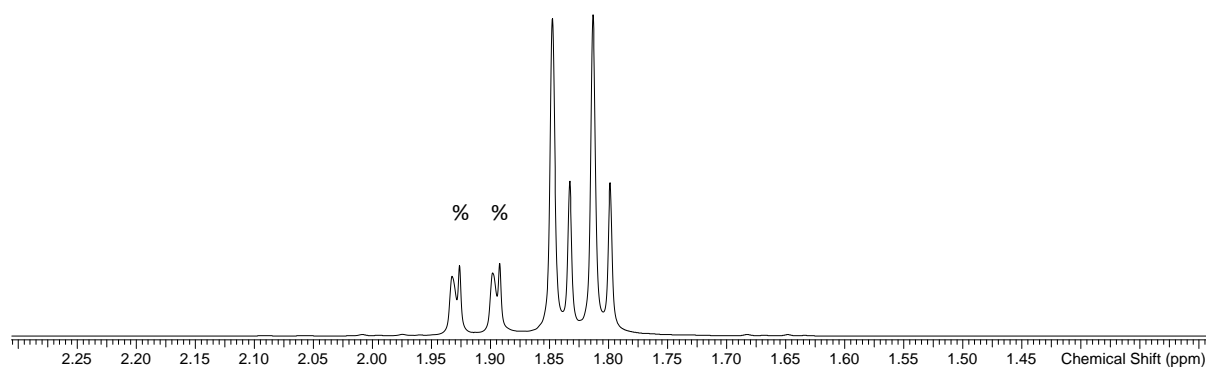
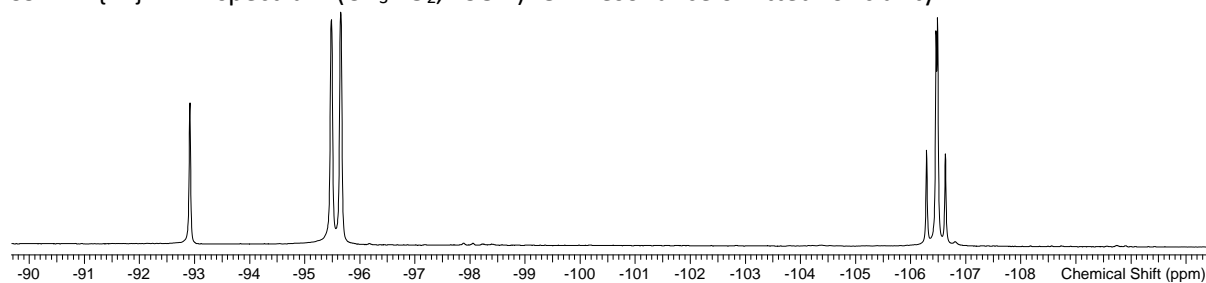


Figure S9.  $[\text{GeF}_3(\text{OPMe}_3)_3][\text{OTf}]$

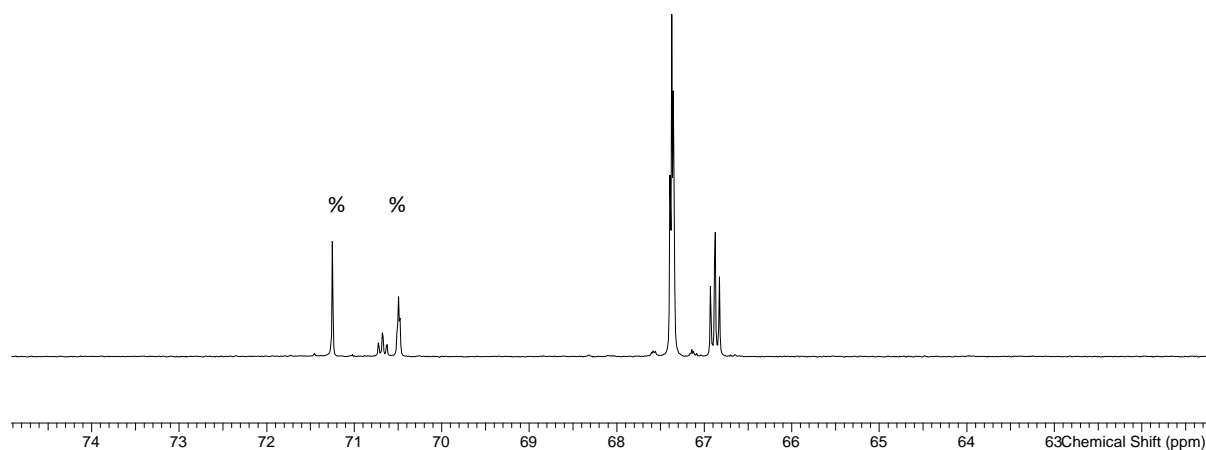
S9.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K) (unidentified species%):



S9.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K). OTf resonance omitted for clarity:



S9.3  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K) (unidentified species%,  $[\text{Me}_3\text{POH}]^+$  impurity%):



S9.4 IR spectrum (Nujol/cm<sup>-1</sup>)

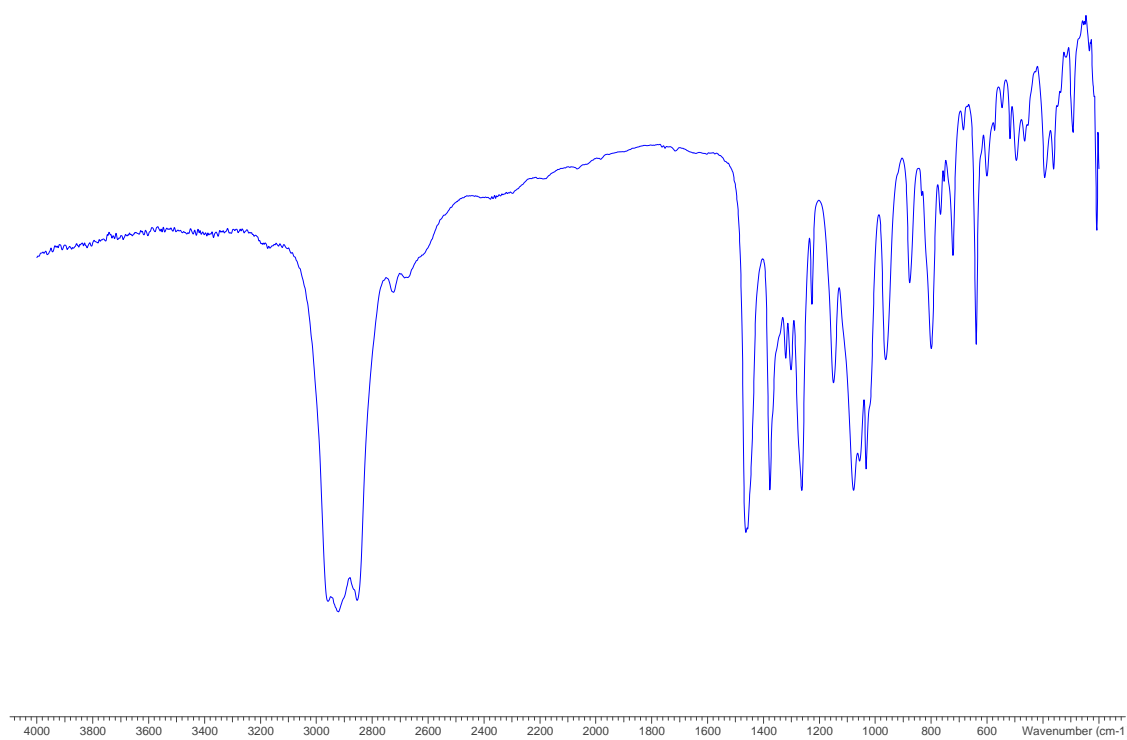
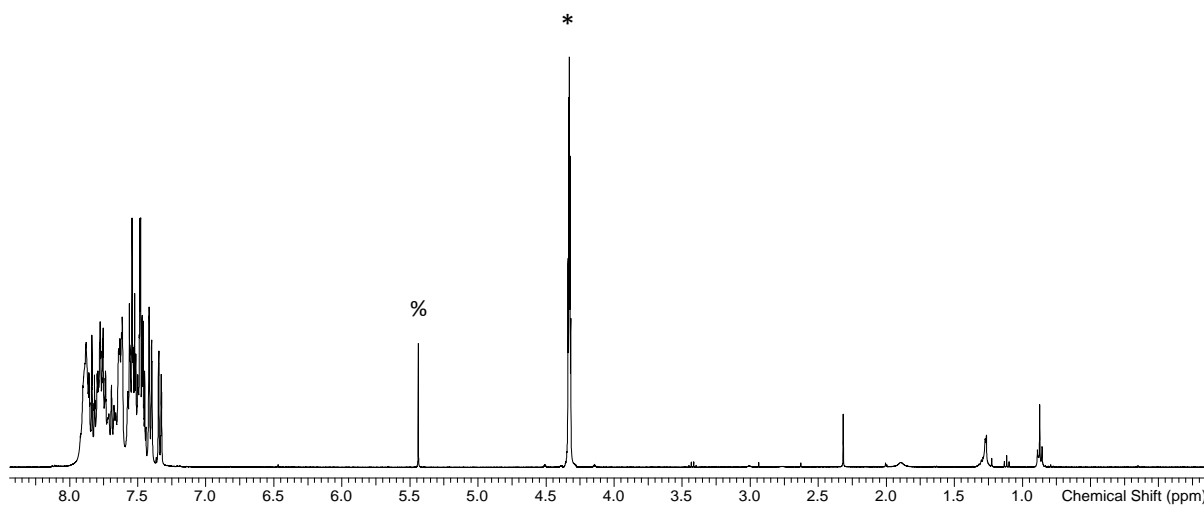
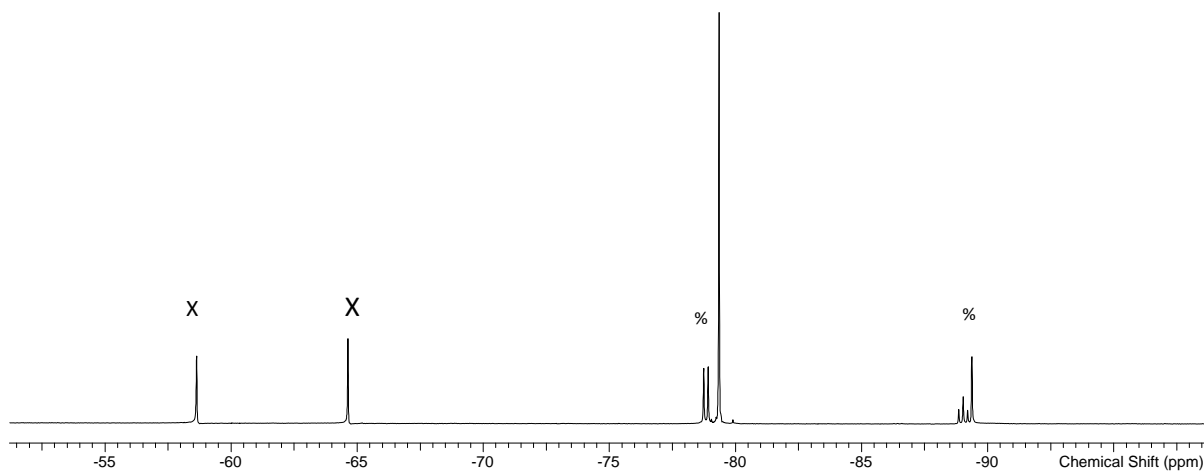




Figure S10.  $[\text{GeF}_3(\text{OAsPh}_3)_3][\text{OTf}]$  and  $[\text{GeF}_2(\text{OAsPh}_3)_4][\text{OTf}]_2$   
 S10.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^\%$ ):



S10.2  $^9\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K) ( $[\text{GeF}_2(\text{OAsPh}_3)_4][\text{OTf}]_2^X$ ,  $[\text{GeF}_3(\text{OAsPh}_3)_3][\text{OTf}]^\%$ )



S10.3 IR spectrum ( $\text{Nujol}/\text{cm}^{-1}$ )

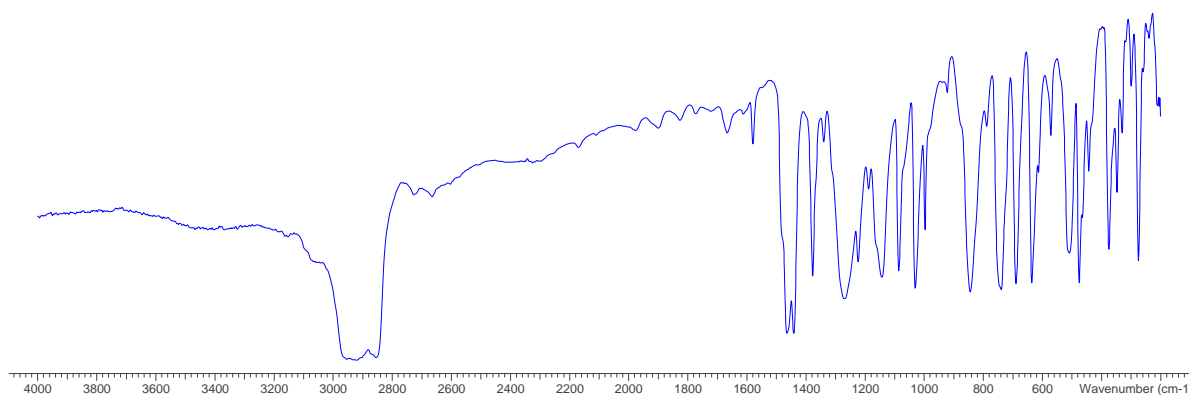
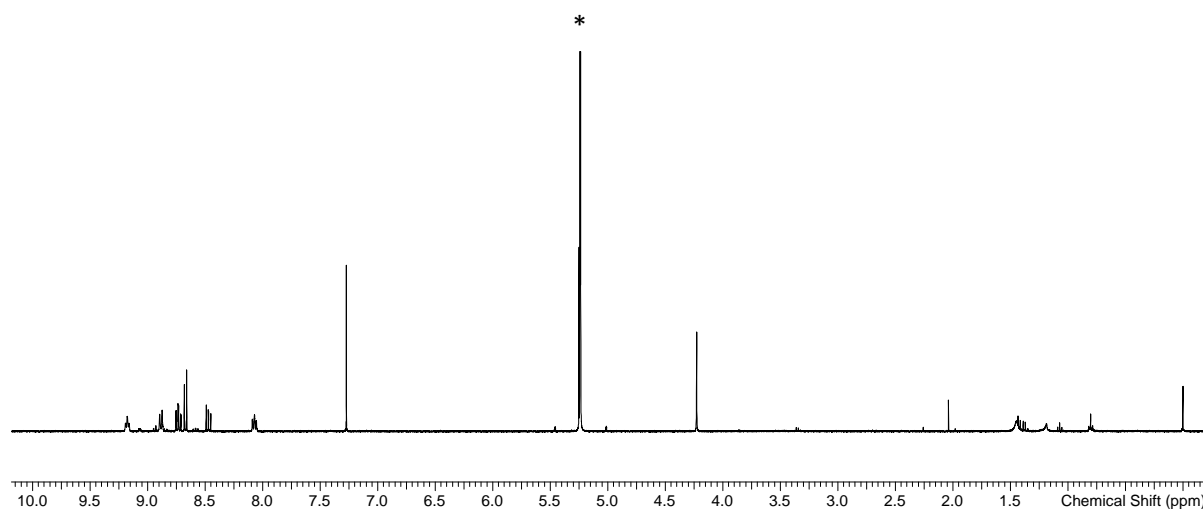
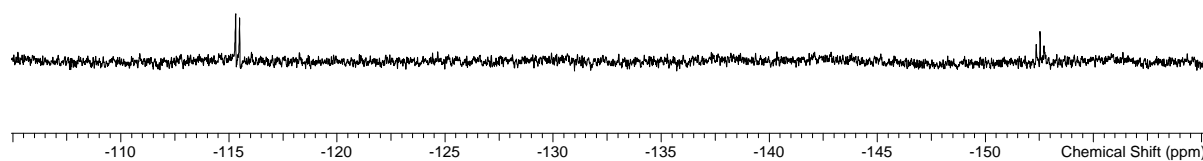


Figure S11.  $[\text{GeF}_3(\text{terpy})][\text{OTf}]$  (complex poorly soluble)  
S11.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2^*$ , 298 K):



S11.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 298 K). OTf resonance omitted for clarity:



S11.3 IR spectrum (Nujol/ $\text{cm}^{-1}$ )

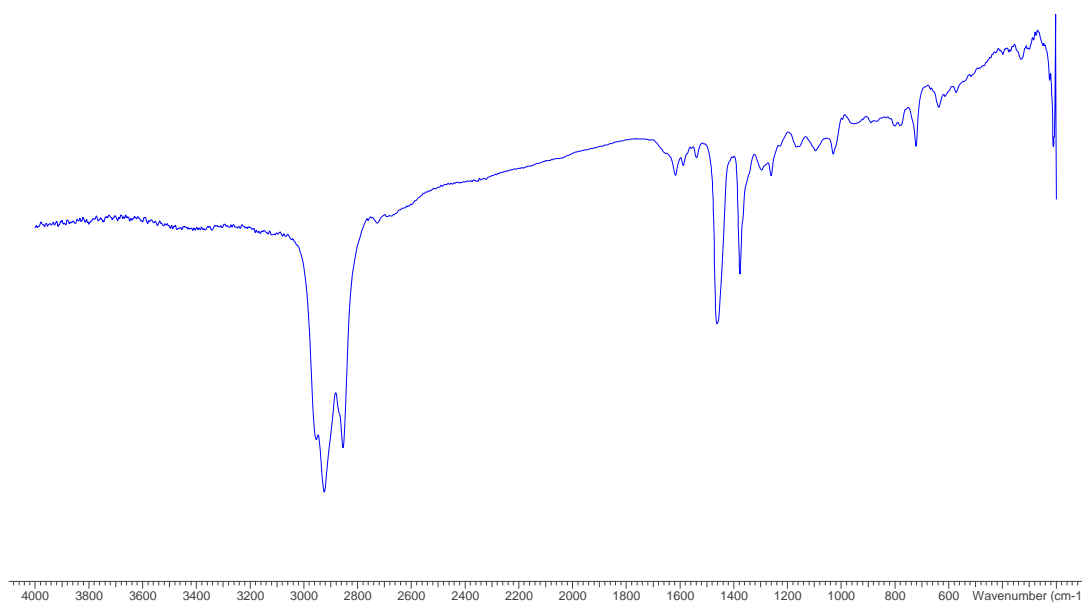
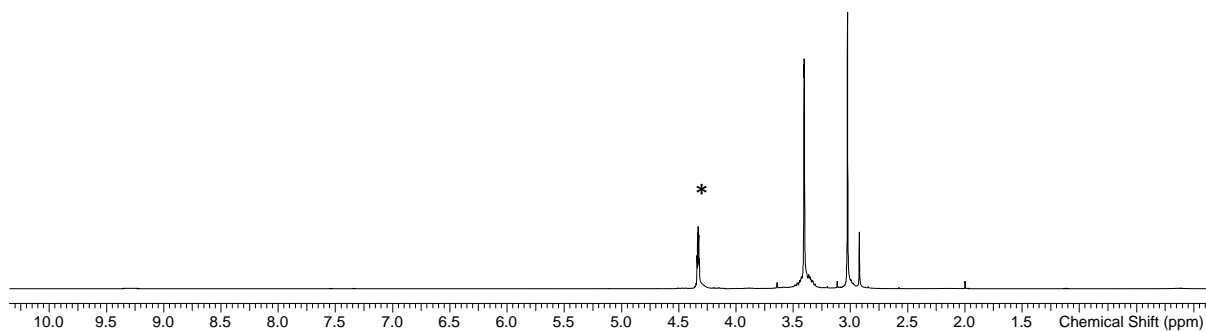
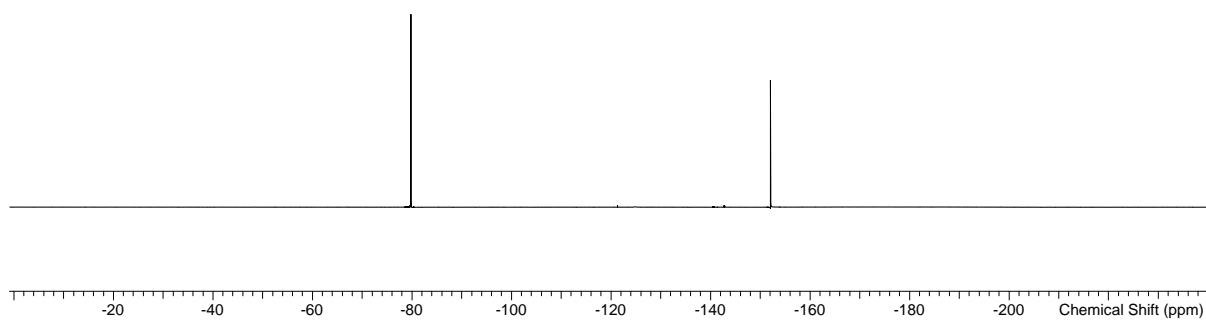


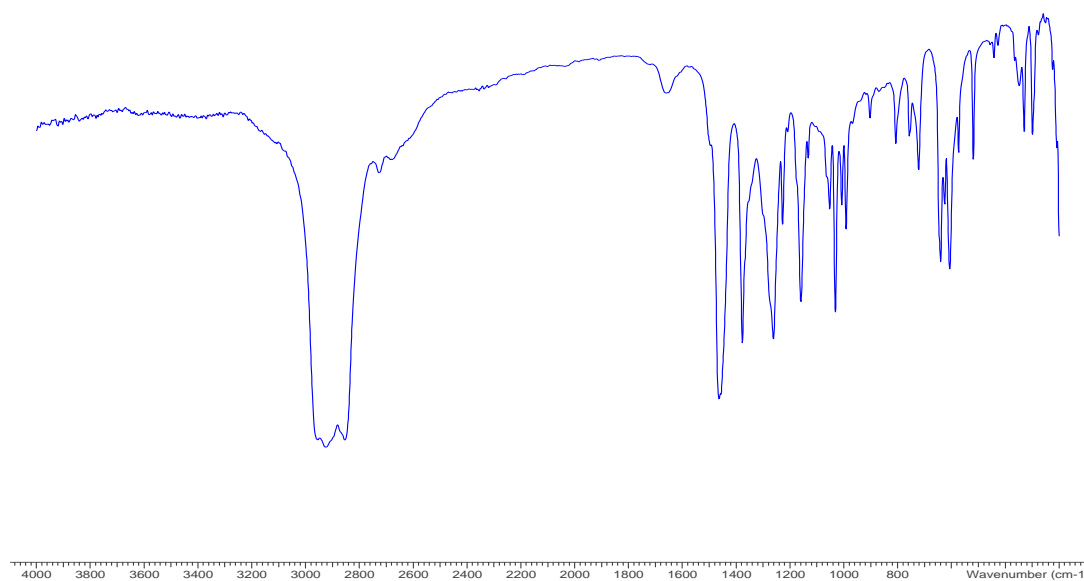
Figure S12.  $[\text{GeF}_3(\text{Me}_3\text{-tacn})][\text{OTf}]$   
S12.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K):



S12.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K):



S12.3 IR spectrum (Nujol/ $\text{cm}^{-1}$ ):



S12.4: LRMS (ESI<sup>+</sup>) (LHS: actual spectrum, RHS: simulated spectrum)

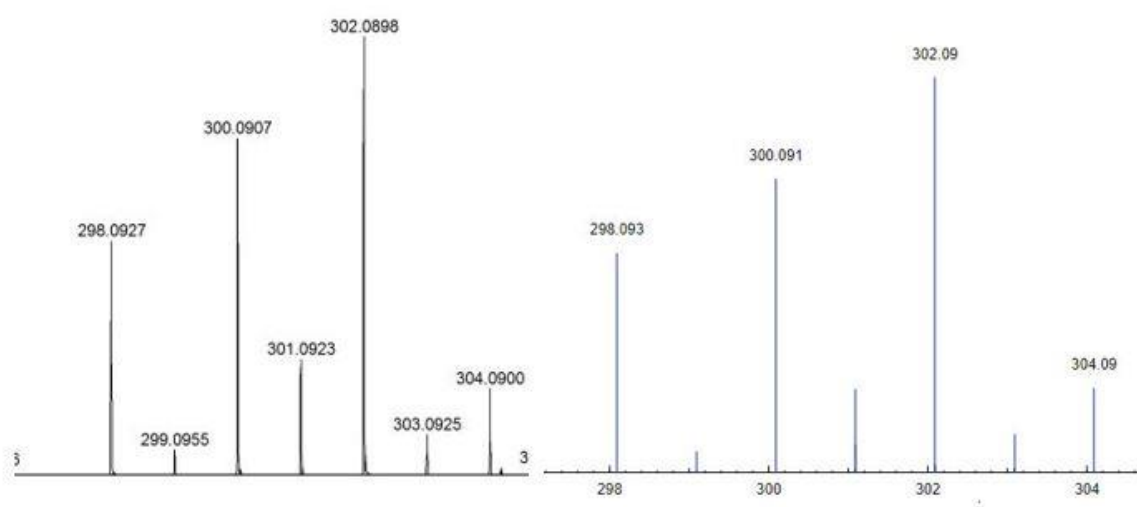
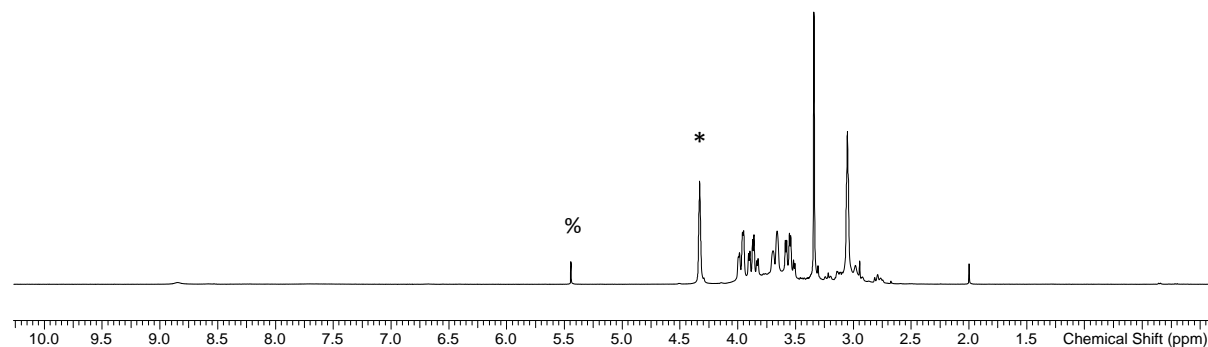
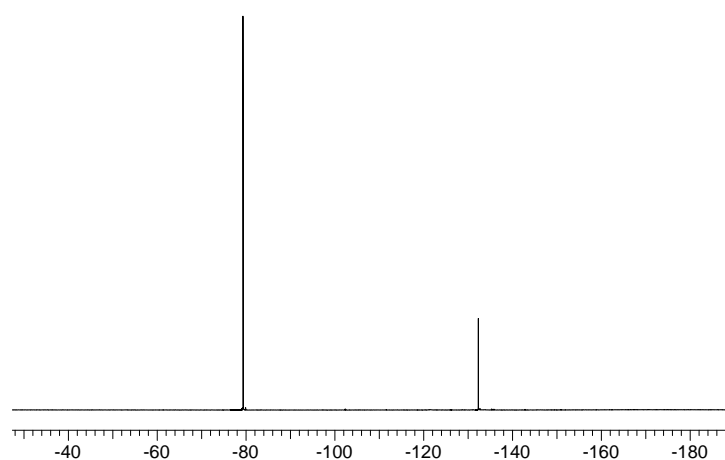


Figure S13.  $[\text{GeF}_2(\text{Me}_4\text{-cyclen})][\text{OTf}]_2$

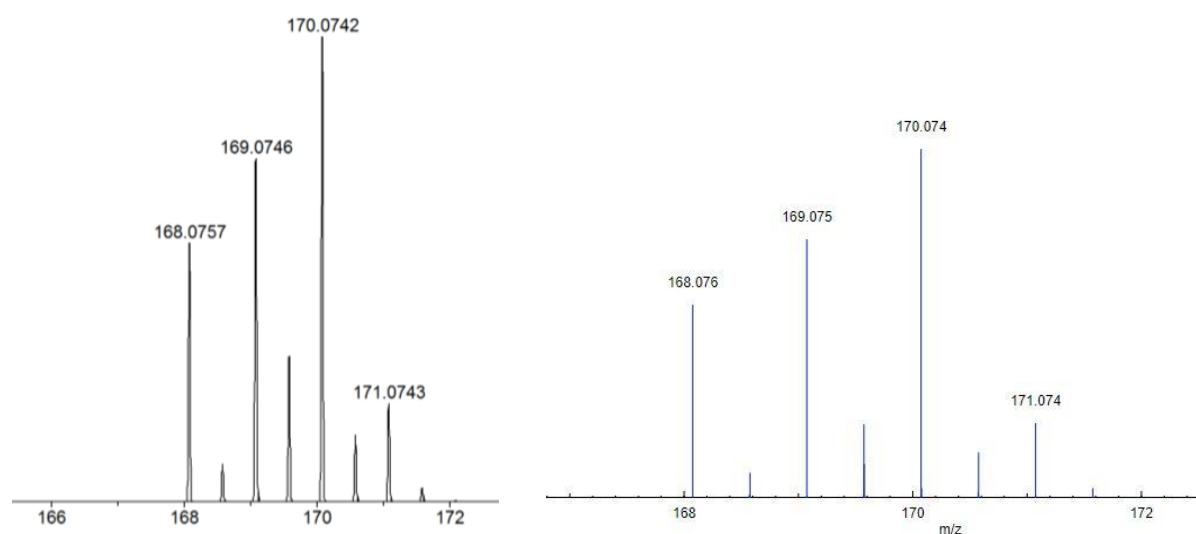
S13.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^{\%}$ ):



S13.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K):



S13.3 LRMS ( $\text{ESI}^+$ ,  $\text{CH}_3\text{NO}_2$ ) (LHS: actual spectrum, RHS: simulated spectrum)



S13.4 IR spectrum (Nujol/cm<sup>-1</sup>):

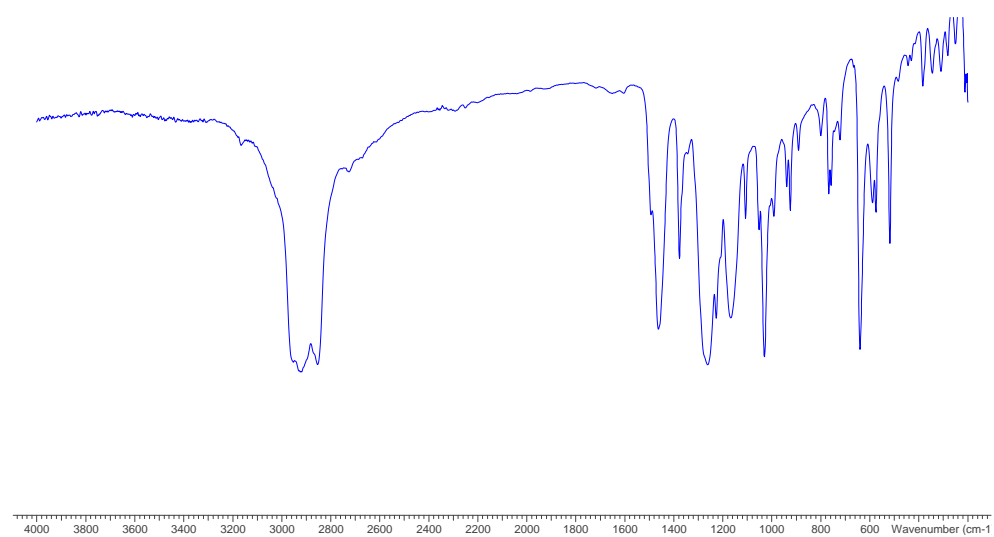
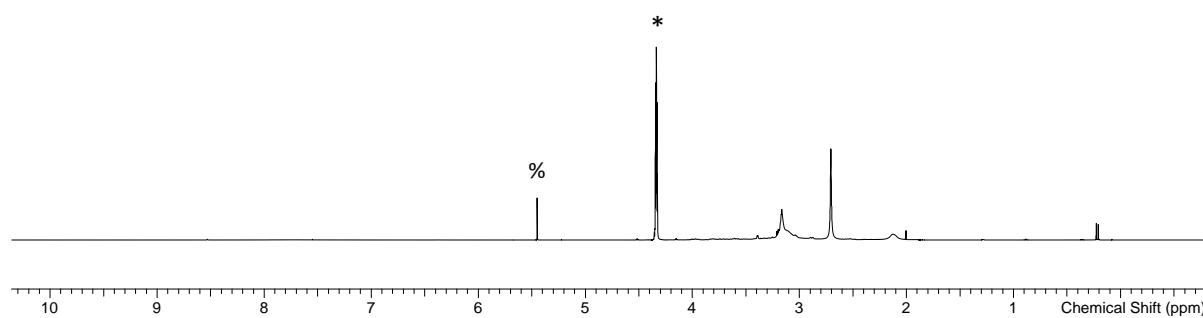
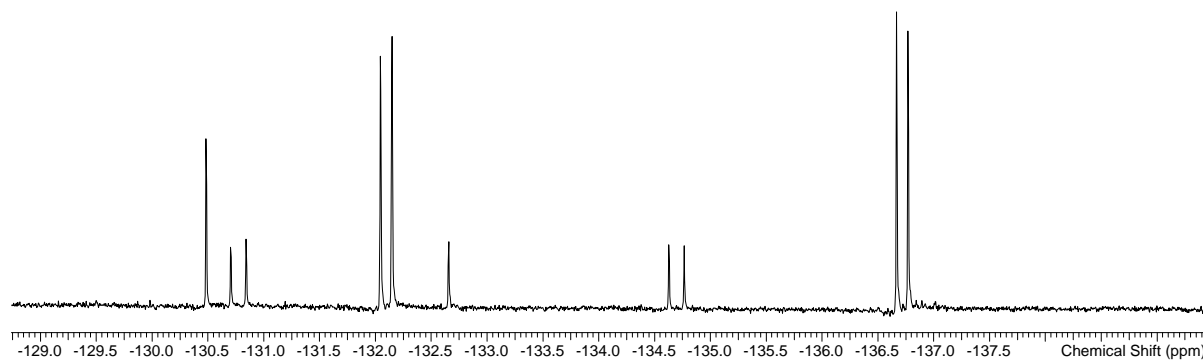


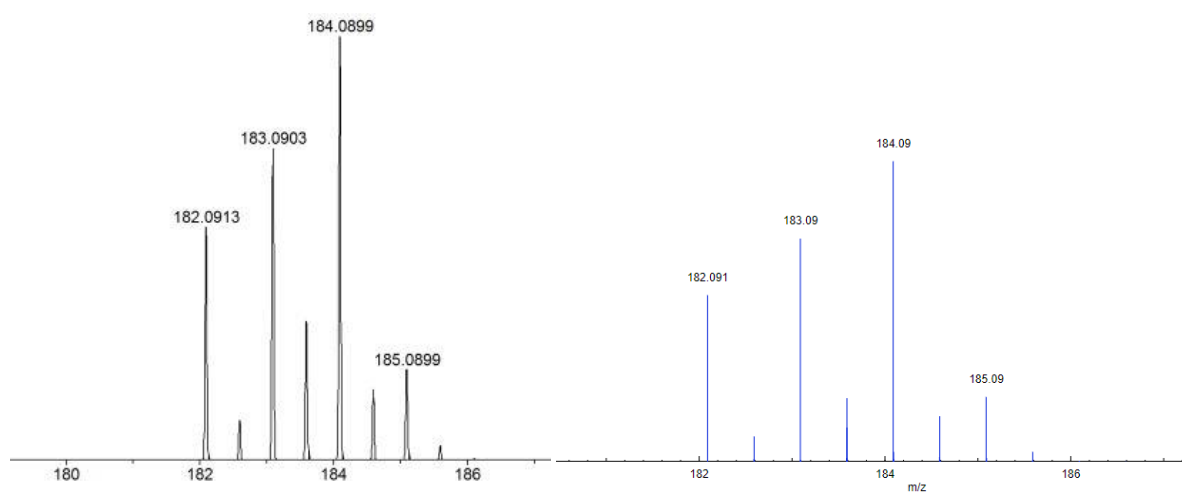
Figure S14.  $[\text{GeF}_2(\text{Me}_4\text{-cyclam})][\text{OTf}]_2$   
 S14.1  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{NO}_2^*$ , 298 K) ( $\text{CH}_2\text{Cl}_2^\%$ ):



S14.2  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum ( $\text{CD}_3\text{NO}_2$ , 298 K). OTf resonance omitted for clarity:



S14.3 LRMS ( $\text{ESI}^+$ ,  $\text{CH}_3\text{NO}_2$ )(LHS: actual spectrum, RHS: simulated spectrum)



S14.4 IR spectrum (Nujol/cm<sup>-1</sup>):

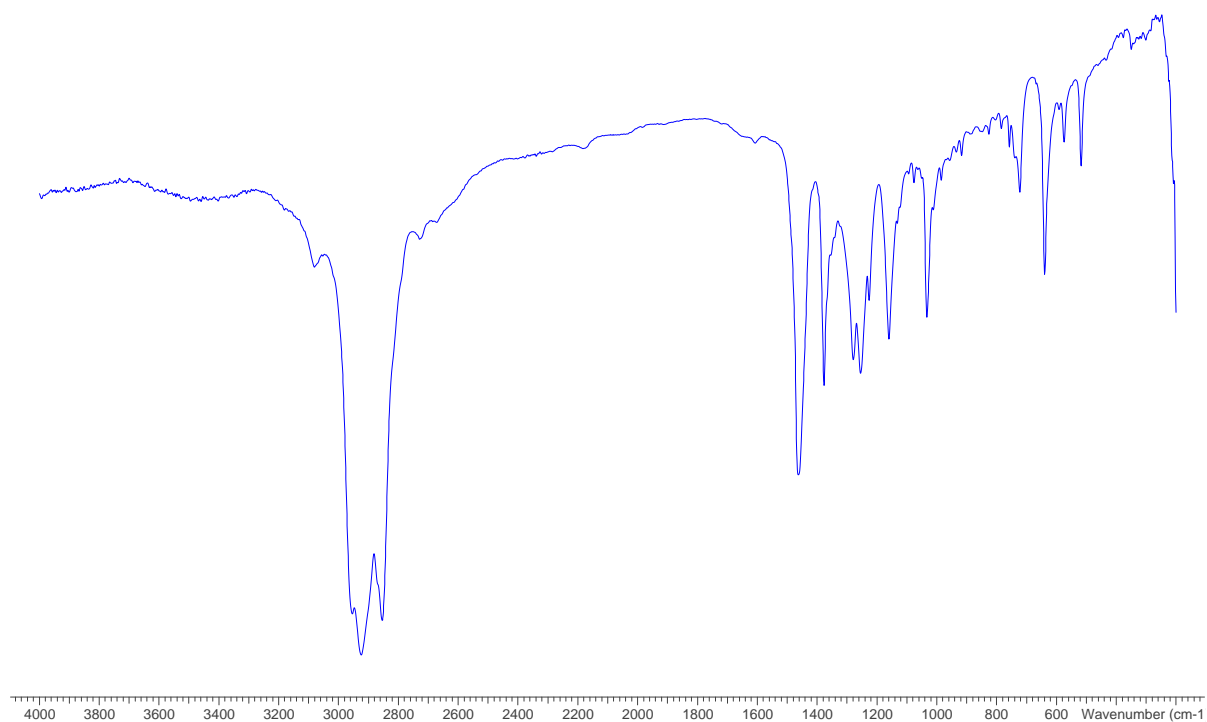


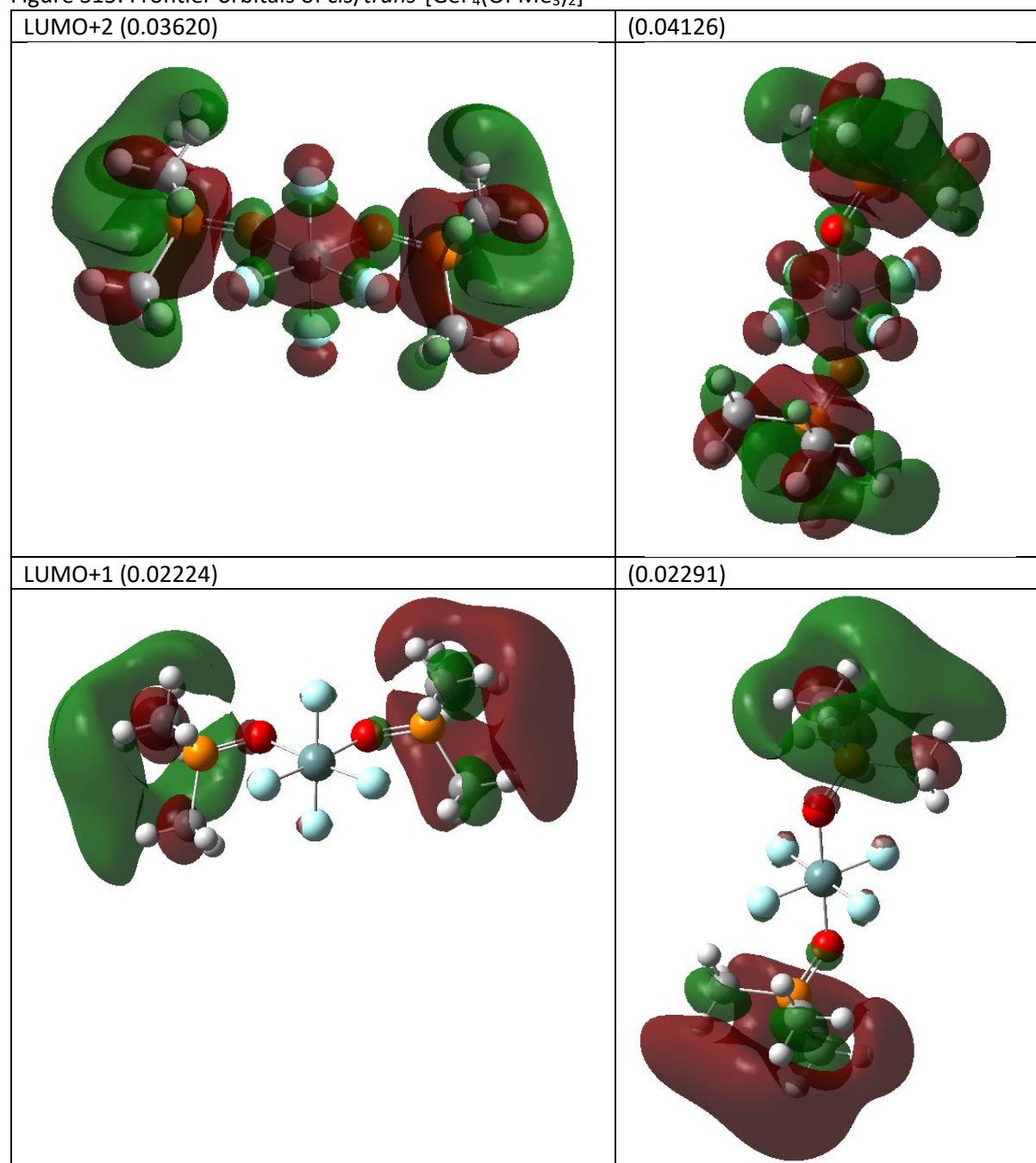


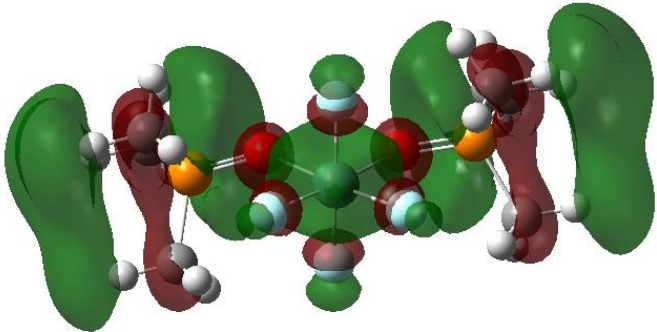
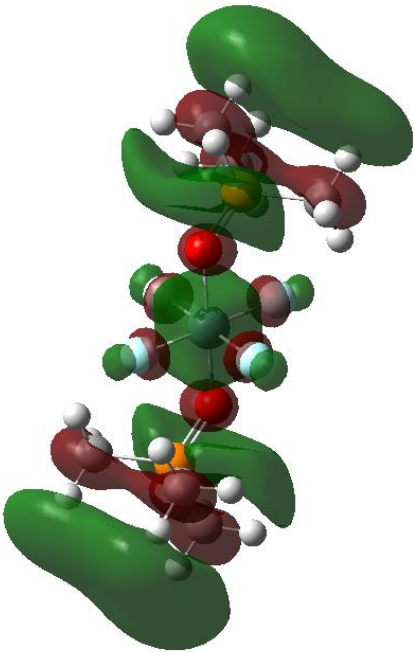
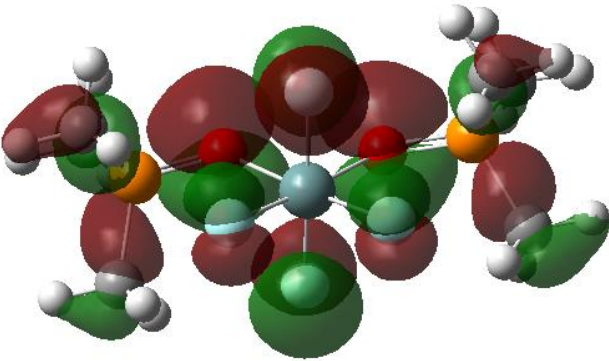
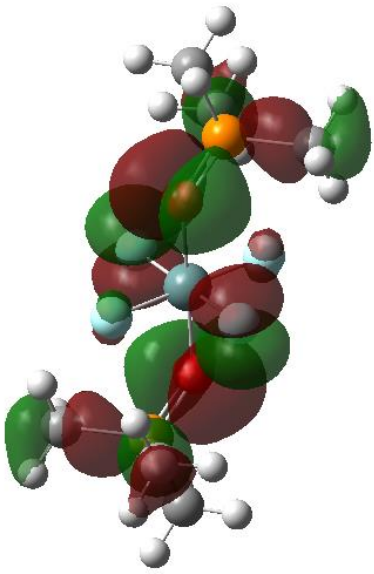
Table S1. X-ray crystallographic data <sup>a</sup>

Compound	[GeF <sub>3</sub> (OPPh <sub>3</sub> ) <sub>3</sub> ][OTf]·CH <sub>2</sub> Cl <sub>2</sub>	14{[GeFe(Me <sub>4</sub> -cyclen)][OTf] <sub>2</sub> }·4CH <sub>3</sub> NO <sub>2</sub>
Formula	C <sub>55</sub> H <sub>45</sub> F <sub>6</sub> GeO <sub>6</sub> P <sub>3</sub> S·CH <sub>2</sub> Cl <sub>2</sub>	C <sub>200</sub> H <sub>399</sub> F <sub>112</sub> Ge <sub>14</sub> N <sub>60</sub> O <sub>92</sub> S <sub>28</sub>
<i>M</i>	1198.39	9158.71
Crystal system	Triclinic	Monoclinic
Space group (no.)	<i>P</i> -1 (2)	<i>P</i> 2 <sub>1</sub> (4)
<i>a</i> /Å	17.9880(3)	25.1422(2)
<i>b</i> /Å	18.9588(2)	30.1462(2)
<i>c</i> /Å	19.7554(3)	25.2492(2)
$\alpha$ /°	61.380(1)	90
$\beta$ /°	70.394(1)	110.2850(10)
$\gamma$ /°	64.978(1)	90
<i>U</i> /Å <sup>3</sup>	5283.71(15)	17950.5(3)
<i>Z</i>	4	2
$\mu$ (Mo-K $\alpha$ ) /mm <sup>-1</sup>	3.570	1.456
<i>F</i> (000)	2448	9318
Total number reflns	100585	495295
<i>R</i> <sub>int</sub>	0.040	0.069
Unique reflns	21188	107372
No. of params, restraints	1351, 0	4677, 4781
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] <sup>b</sup>	0.033, 0.083	0.086, 0.228
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> (all data)	0.037, 0.094	0.123, 0.255

<sup>a</sup> Common items: *T* = 293 K;  $\lambda$ (Mo-K $\alpha$ ) = 0.71073 Å;  $\theta$ (max) = 27.5°; <sup>b</sup>  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ ;  $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$

Figure S15. Frontier orbitals of *cis/trans*-[GeF<sub>4</sub>(OPMe<sub>3</sub>)<sub>2</sub>]



LUMO (0.01187)	(0.01521)
	
HOMO (-0.29209)	(-0.28990)
	

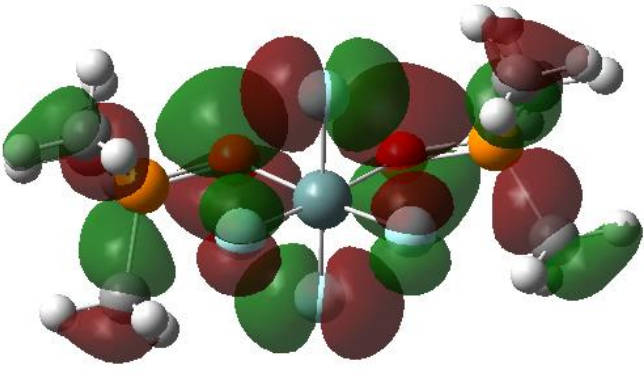
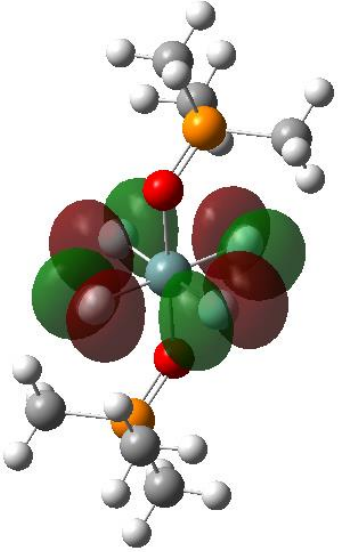
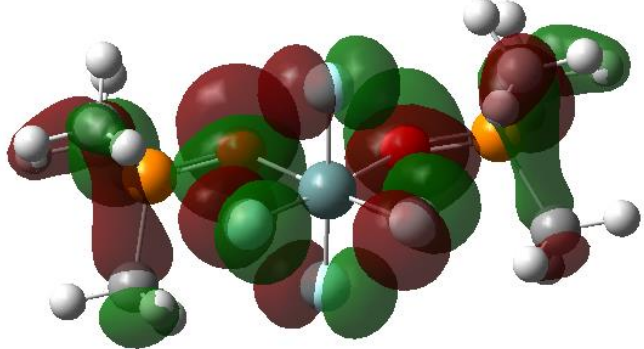
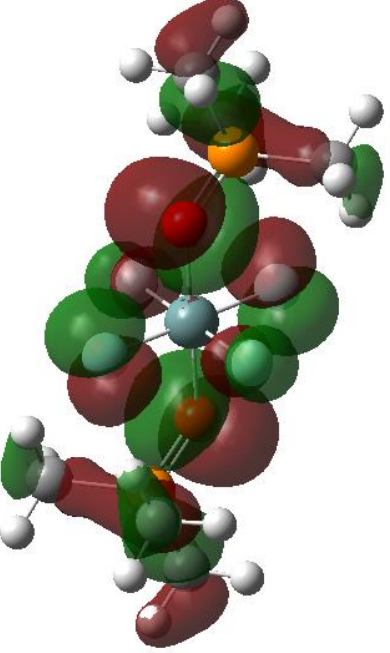
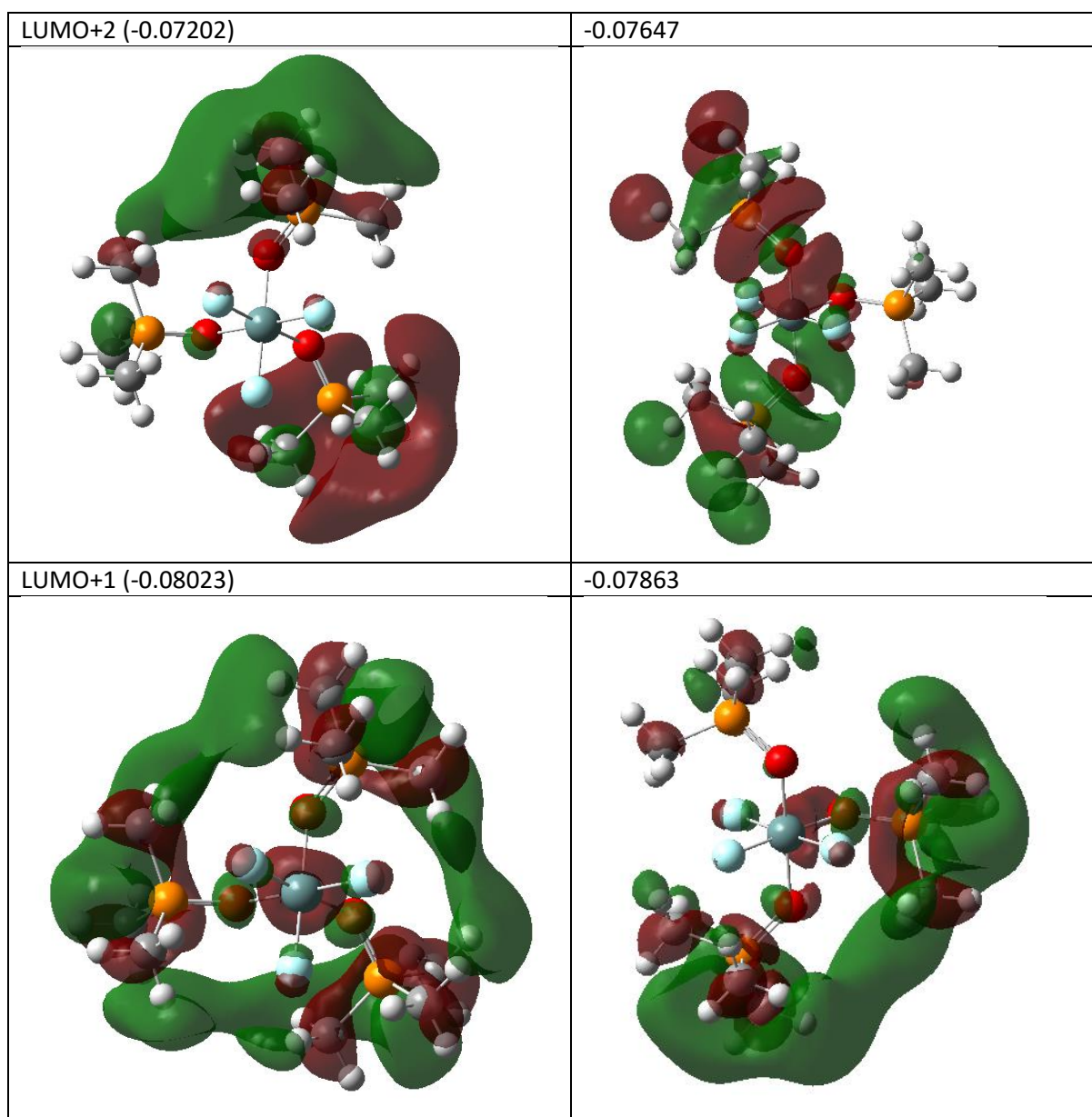
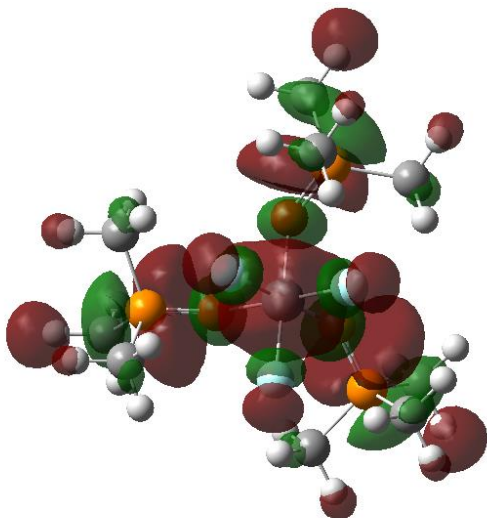
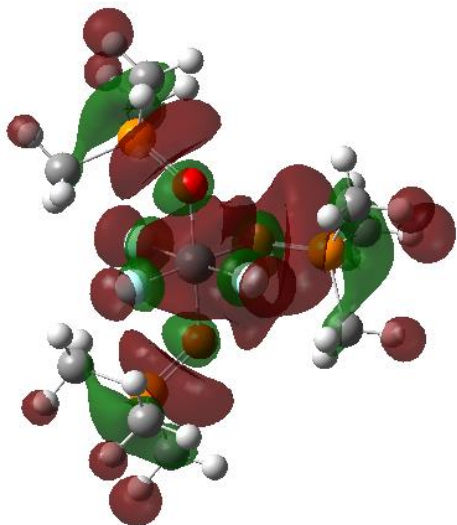
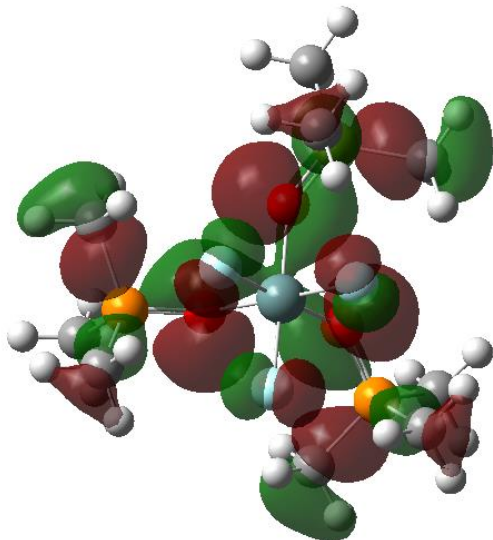
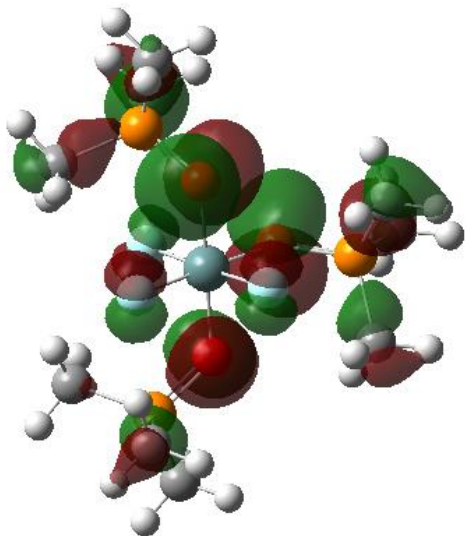
HOMO-1 (-0.29275)	(-0.29438)
	
HOMO-2 (-0.30315)	(-0.30489)
	

Figure S16. Frontier orbitals of *fac/mer*-[GeF<sub>3</sub>(OPMe<sub>3</sub>)<sub>3</sub>]<sup>+</sup>





LUMO (-0.10779)	(-0.11364)
	
HOMO (-0.41760)	-0.38878
	

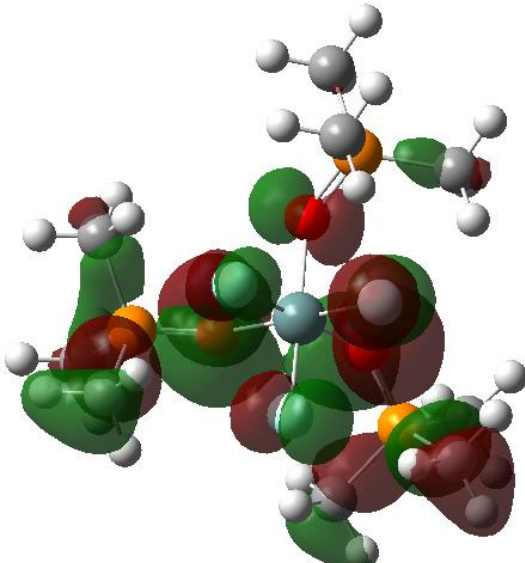
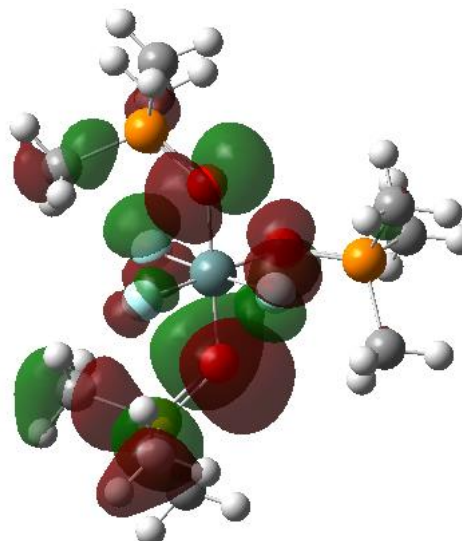
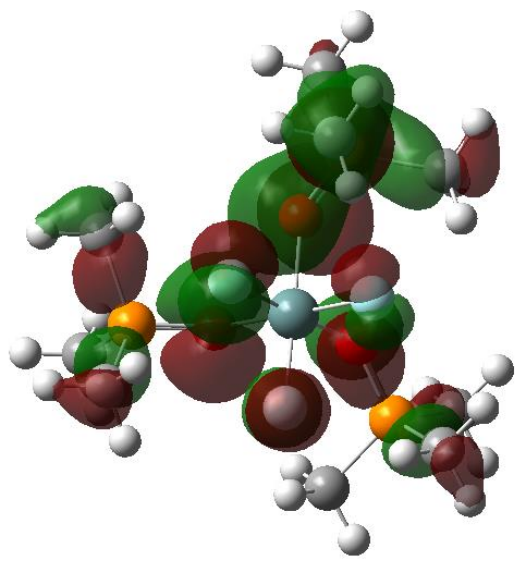
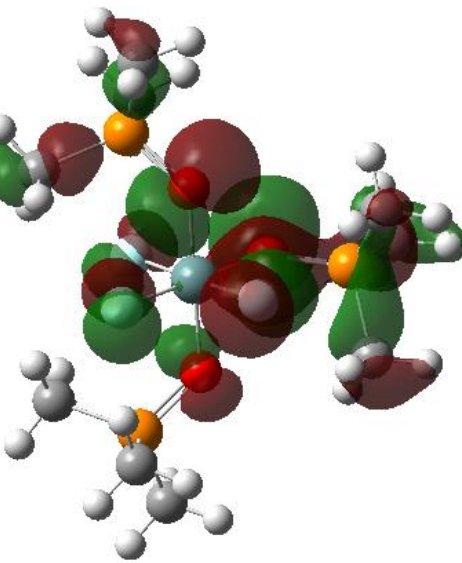
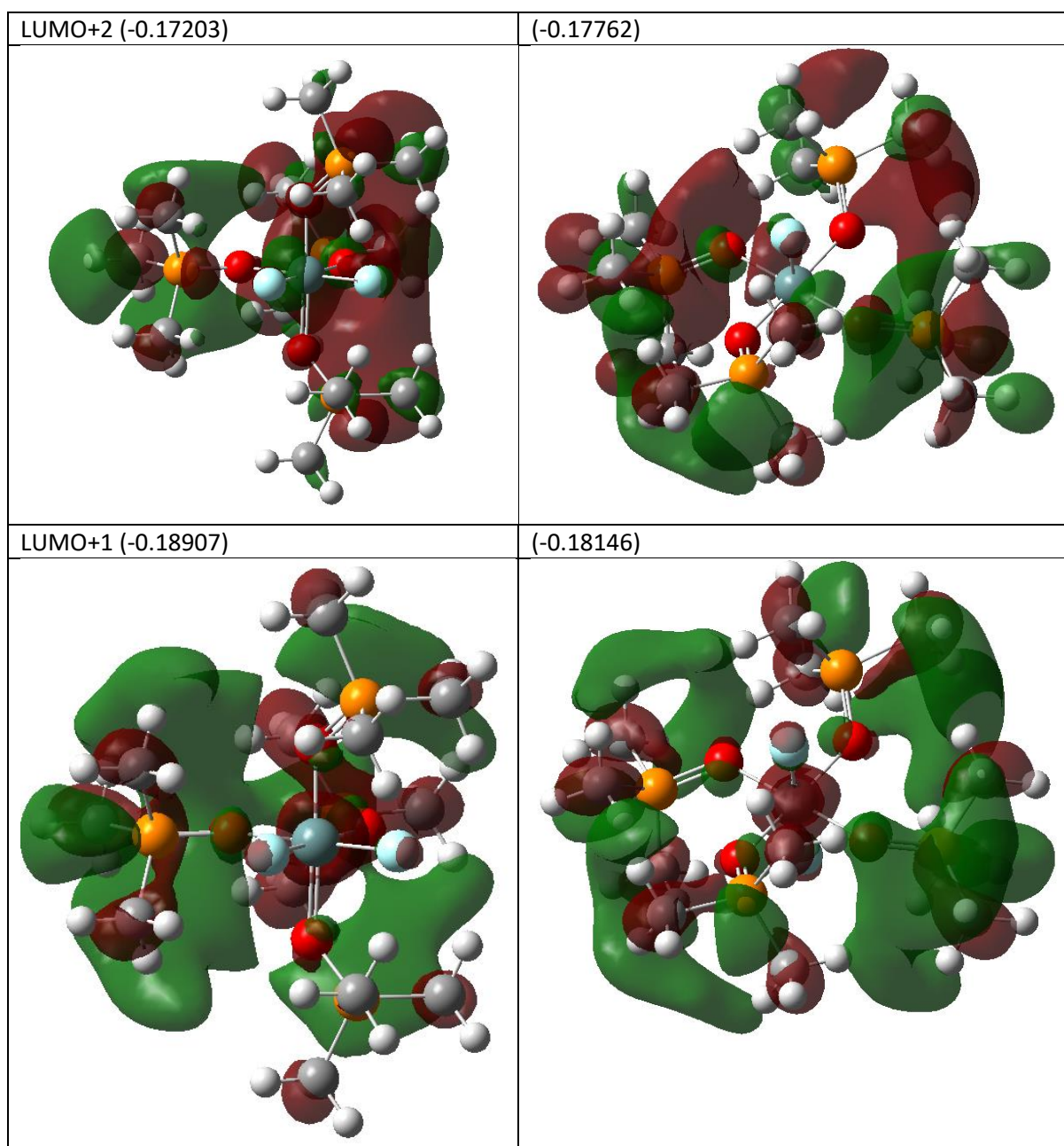
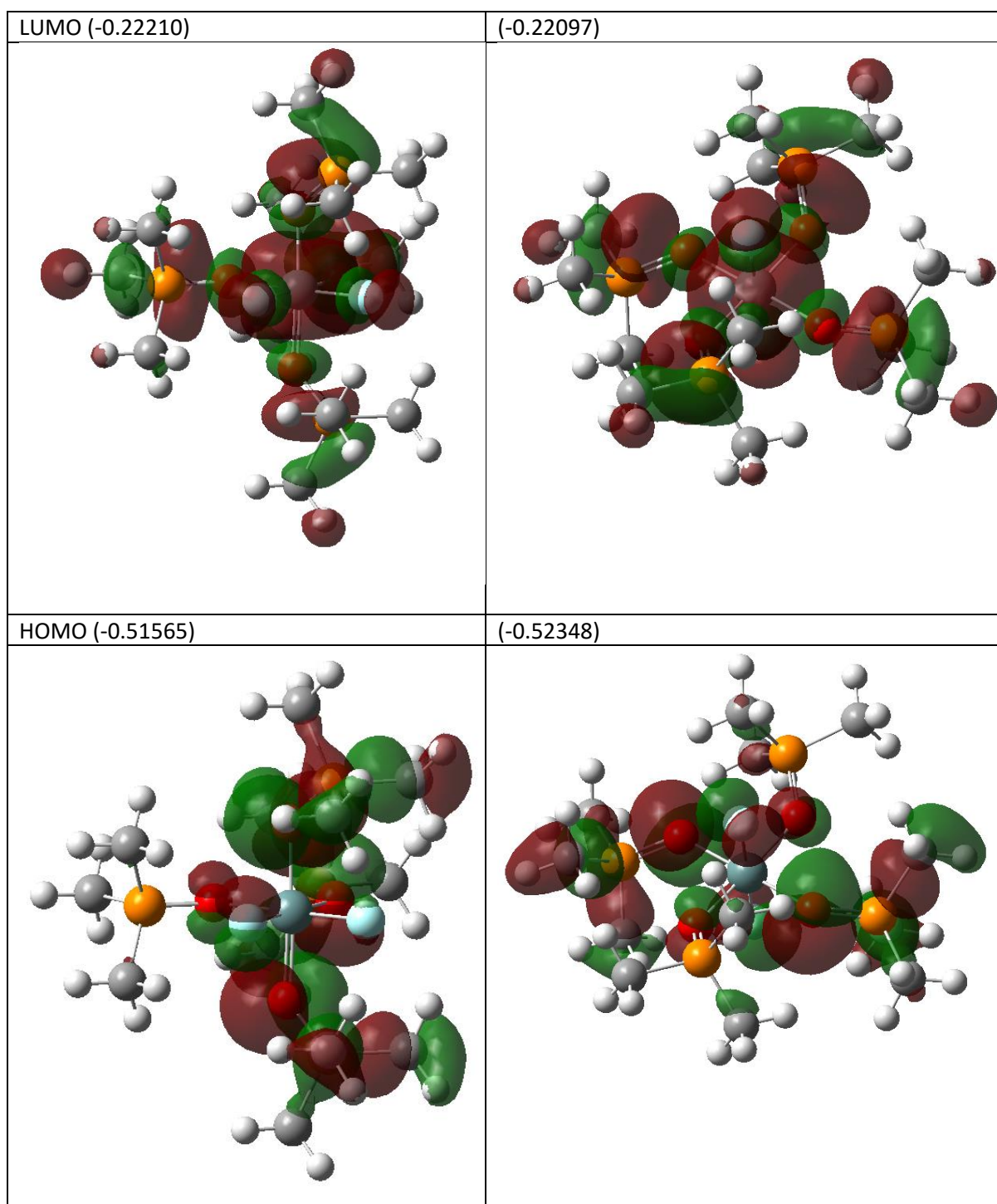
HOMO-1 (-0.41978)	(-0.44048)
	
HOMO-2 (-0.41985)	(-0.40885)
	

Figure S17. Frontier orbitals of *cis/trans*-[GeF<sub>2</sub>(OPMe<sub>3</sub>)<sub>4</sub>]<sup>2+</sup>







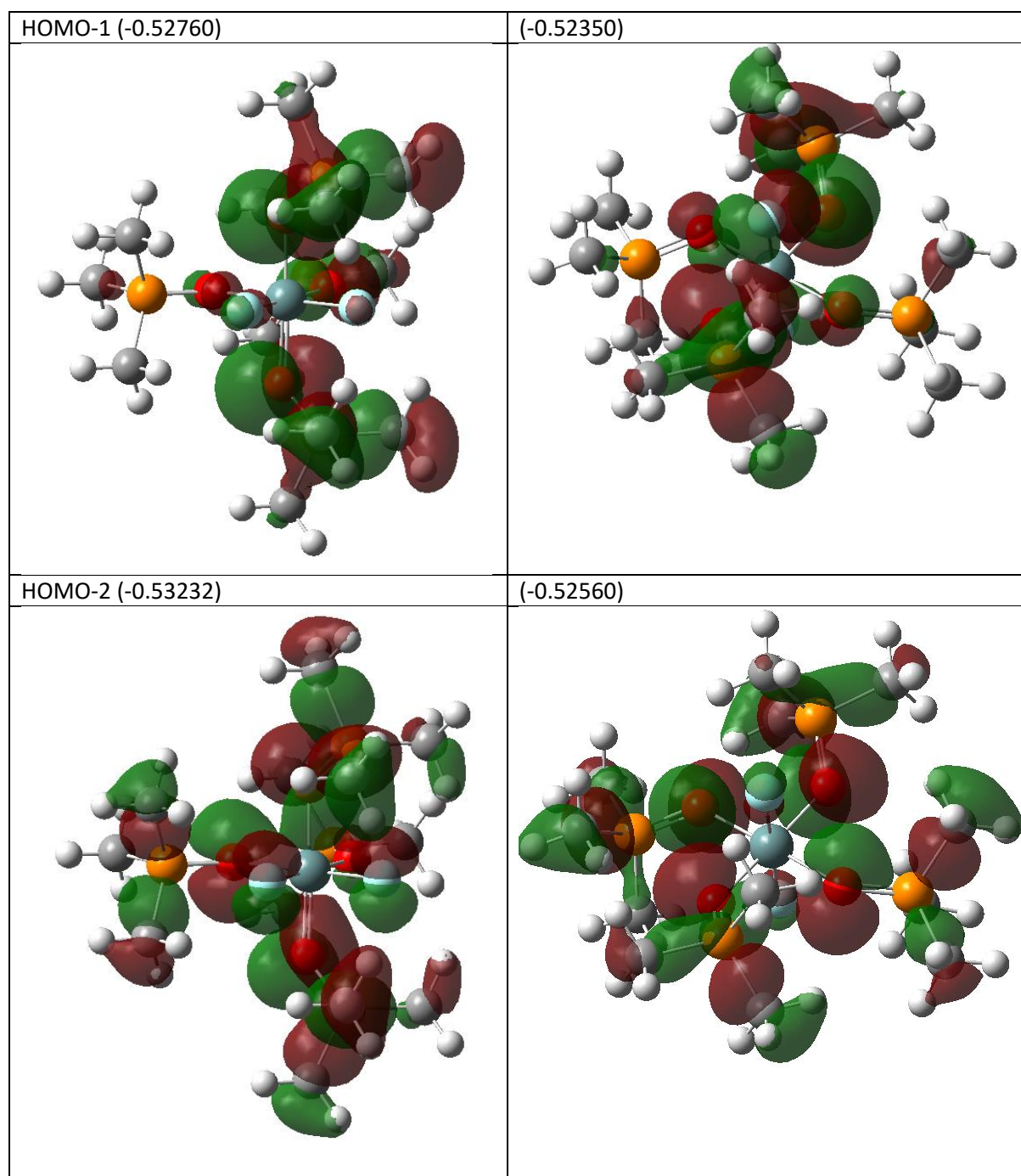


Table S2. xyz coordinates from DFT calculations

33

trans-[GeF4(OPMe3)2]

Ge	-0.0000070	0.0000490	-0.0000150
P	3.0943670	-0.0012970	0.0844670
F	0.1822370	1.7487870	-0.3514200
F	-0.7901840	0.3920000	1.5893130
O	1.7637600	0.0031820	0.8571560
C	3.4148920	-1.5809230	-0.7347140
H	3.3743110	-2.3803020	0.0065170
H	4.3904220	-1.5813510	-1.2254130
H	2.6202030	-1.7352750	-1.4629060
C	4.4097970	0.2576780	1.3020210
H	4.2600300	1.2217730	1.7895370
H	5.3936340	0.2396470	0.8292640
H	4.3574350	-0.5262340	2.0585490
C	3.2211820	1.3205820	-1.1415650
H	2.4786460	1.1305220	-1.9138050
H	4.2258590	1.3585930	-1.5682430
H	2.9784470	2.2689380	-0.6622110
P	-3.0943690	0.0012730	-0.0844550
F	-0.1822090	-1.7487030	0.3513890
F	0.7901650	-0.3920170	-1.5893200
O	-1.7637700	-0.0031310	-0.8571630
C	-3.4152150	1.5810010	0.7344050
H	-3.3747820	2.3802310	-0.0069950
H	-4.3907510	1.5813430	1.2250940
H	-2.6205570	1.7356600	1.4625640
C	-4.4097700	-0.2582080	-1.3019340
H	-4.2599160	-1.2224400	-1.7891520
H	-5.3936120	-0.2401180	-0.8291870
H	-4.3574680	0.5254760	-2.0587030
C	-3.2208620	-1.3203680	1.1418610
H	-2.4782550	-1.1300510	1.9139720
H	-4.2254800	-1.3584000	1.5686740
H	-2.9780720	-2.2688010	0.6626890

33

cis-[GeF4(OPMe3)2]

Ge	0.0000170	-0.6404210	0.0000270
F	-0.2365350	-0.5369730	-1.7716210
F	1.3436910	-1.8407720	-0.1645730
F	-1.3436800	-1.8397630	0.1720230
P	2.8412010	0.6159010	-0.0154440
F	0.2359660	-0.5267860	1.7713490
O	1.3255330	0.8206590	-0.1681680
C	3.5725230	-0.2369400	-1.4326030
H	3.3375960	0.3161300	-2.3431040
H	4.6555070	-0.3257600	-1.3243990
H	3.1143920	-1.2231200	-1.4909240
C	3.5902630	2.2635590	0.0694080
H	3.2012900	2.7877570	0.9432440

H	4.6777590	2.1997170	0.1404300
H	3.3192680	2.8273280	-0.8240980
C	3.3169220	-0.2679460	1.4879670
H	2.9565470	-1.2910900	1.4055300
H	4.4010020	-0.2476190	1.6192450
H	2.8223830	0.1963090	2.3407660
O	-1.3250310	0.8221010	0.1601480
P	-2.8411270	0.6159670	0.0138780
C	-3.5910840	2.2628830	-0.0773320
H	-4.6787430	2.1982590	-0.1450560
H	-3.3178830	2.8313190	0.8125380
H	-3.2047080	2.7827560	-0.9548940
C	-3.5675420	-0.2294250	1.4380090
H	-3.1095840	-1.2154620	1.4997590
H	-3.3289760	0.3282230	2.3447630
H	-4.6509600	-0.3182610	1.3342270
C	-3.3211530	-0.2759900	-1.4833720
H	-2.8296360	0.1842300	-2.3401210
H	-2.9598470	-1.2984610	-1.3967180
H	-4.4056370	-0.2570830	-1.6114600
46			
fac-[GeF3(OPMe3)3]+			
Ge	-0.0013240	0.0005020	-0.5361310
P	1.8111870	2.3548100	0.3785230
P	1.1367520	-2.7442010	0.3782620
F	1.4162020	-0.5407150	-1.5122930
F	-0.2405710	1.4993870	-1.5110110
O	0.2220780	-1.5125570	0.6291220
O	1.1967710	0.9492080	0.6306840
F	-1.1790970	-0.9557660	-1.5121550
C	0.7621020	-3.9302250	1.6869170
H	-0.2866980	-4.2228460	1.6245240
H	1.3860540	-4.8205500	1.5915840
H	0.9413350	-3.4693840	2.6590130
C	2.8889340	-2.3242140	0.4911240
H	3.1294190	-1.6408220	-0.3209970
H	3.0772990	-1.8315310	1.4458960
H	3.5057380	-3.2217690	0.4180900
C	0.8279690	-3.5354800	-1.2130390
H	1.4402300	-4.4336590	-1.3147510
H	-0.2264990	-3.8020920	-1.2875370
H	1.0650060	-2.8279170	-2.0054480
C	0.5759600	3.6665420	0.4906430
H	-0.1372330	3.5343670	-0.3207320
H	0.0555150	3.5864370	1.4459140
H	1.0480860	4.6478240	0.4159030
C	2.6513520	2.4789980	-1.2128830
H	3.1276580	3.4560880	-1.3147350
H	3.4057920	1.6955510	-1.2872430
H	1.9196360	2.3338980	-2.0055440
C	3.0267710	2.6197380	1.6868490

H	3.8023780	1.8555320	1.6241050
H	3.4886530	3.6039480	1.5915000
H	2.5381370	2.5458750	2.6590810
O	-1.4225590	0.5627540	0.6302130
P	-2.9469250	0.3886810	0.3790720
C	-3.4773830	1.0542610	-1.2113960
H	-4.5616610	0.9756600	-1.3122330
H	-3.1788670	2.1001850	-1.2852110
H	-2.9853760	0.4948600	-2.0049750
C	-3.7853120	1.3057060	1.6888720
H	-3.5118530	2.3597900	1.6284480
H	-4.8685010	1.2131200	1.5927720
H	-3.4771960	0.9176770	2.6604520
C	-3.4609880	-1.3382480	0.4898630
H	-2.9883360	-1.8877720	-0.3219640
H	-3.1304550	-1.7488690	1.4448280
H	-4.5466430	-1.4228820	0.4148710

46

mer-[GeF3(OPMe3)3]+

Ge	-0.0139130	-0.1266480	0.1868510
P	2.9120360	-1.2946790	-0.1362920
P	-0.0064540	3.0096510	-0.1385260
P	-2.9441480	-1.2828570	-0.0690770
F	0.2662510	0.8457640	1.7094790
F	-0.3527390	-1.0639680	-1.3648170
F	0.3134750	-1.7375330	1.0291030
O	-0.2742770	1.4938930	-0.7478440
O	1.8449260	-0.0296490	-0.2289200
O	-1.8589710	-0.2261720	0.5981130
C	-0.2530340	4.1394900	-1.5773810
H	-1.2572110	3.9977330	-1.9656460
H	-0.1179020	5.1715270	-1.2625610
H	0.4687880	3.8865050	-2.3482610
C	1.7144700	3.2171230	0.5044030
H	1.8053340	2.6209430	1.4048720
H	2.4045890	2.8454830	-0.2465490
H	1.8980430	4.2694870	0.7089050
C	-1.2238700	3.4323440	1.1863090
H	-1.0499560	4.4506880	1.5269030
H	-2.2280790	3.3395310	0.7833240
H	-1.0838310	2.7239010	1.9955420
C	2.2983630	-2.7995550	-1.0196520
H	1.5038000	-3.2322890	-0.4238390
H	1.8976310	-2.4925120	-1.9806550
H	3.1195390	-3.5009580	-1.1484250
C	3.3029350	-1.7098510	1.6213490
H	4.0343420	-2.5143940	1.6522690
H	3.6986790	-0.8260980	2.1137020
H	2.3754710	-2.0117770	2.0961720
C	4.4401060	-0.6862280	-0.9761570
H	4.7864970	0.2102170	-0.4702690

H	5.2110900	-1.4522200	-0.9384140
H	4.2009470	-0.4512170	-2.0092100
C	-4.4410610	-1.1679130	1.0044270
H	-4.7776930	-0.1357630	1.0284360
H	-5.2274200	-1.8069490	0.6096670
H	-4.1735360	-1.4823500	2.0089770
C	-3.3753480	-0.7743290	-1.7924530
H	-2.4553660	-0.7795520	-2.3677100
H	-4.0977410	-1.4720570	-2.2100320
H	-3.7940980	0.2276400	-1.7714330
C	-2.3333140	-3.0287180	-0.0721860
H	-1.9149710	-3.2480690	0.9049530
H	-3.1617780	-3.6962740	-0.2981040
H	-1.5532500	-3.1072730	-0.8200240

59

cis-[GeF2(OPMe3)4]2+

Ge	0.0000048	-0.3040243	-0.1631384
F	0.0000035	-2.0976846	0.0616616
F	0.0000840	-0.4668580	-1.9645257
O	-1.9046937	-0.2566489	-0.1597744
O	-0.0000080	-0.1093802	1.7205111
O	-0.0000184	1.5992639	-0.3295207
O	1.9047116	-0.2566406	-0.1596542
P	-2.9078268	-1.4534183	-0.3113311
P	-0.0001236	1.0855672	2.7179944
P	2.9078912	-1.4533656	-0.3111877
P	0.0000179	2.4552102	-1.6465429
C	-2.5416891	-2.4823415	-1.7447014
H	-1.5830024	-2.9754186	-1.5973713
H	-3.3247343	-3.2322980	-1.8730466
H	-2.4862809	-1.8627832	-2.6397887
C	-2.9212878	-2.4861447	1.1660533
H	-1.9232636	-2.8939156	1.3196914
H	-3.2058702	-1.8873895	2.0323742
H	-3.6363169	-3.3032281	1.0522464
C	-4.5414222	-0.7236279	-0.5262003
H	-4.7771103	-0.0801807	0.3223290
H	-4.5647452	-0.1293390	-1.4405395
H	-5.2997558	-1.5056908	-0.5964371
C	1.4685606	2.1153722	2.5280628
H	2.3607932	1.5105061	2.6932049
H	1.4952990	2.5147011	1.5163254
H	1.4572973	2.9341605	3.2498595
C	-0.0003237	0.3856690	4.3770350
H	0.0000468	1.1791294	5.1268321
H	-0.8868649	-0.2340202	4.5172267
H	0.8857545	-0.2347158	4.5170848
C	-1.4686958	2.1154708	2.5277257
H	-1.4948861	2.5152670	1.5161598
H	-2.3610198	1.5105328	2.6920945
H	-1.4578018	2.9339176	3.2499154

C	1.4706384	2.1597687	-2.6442399
H	1.4493459	1.1340752	-3.0069689
H	1.4944059	2.8491110	-3.4904749
H	2.3606337	2.3118122	-2.0325707
C	-1.4703426	2.1595454	-2.6445539
H	-2.3605086	2.3115366	-2.0331208
H	-1.4939635	2.8488564	-3.4908194
H	-1.4488488	1.1338377	-3.0072266
C	-0.0001502	4.1794760	-1.1189043
H	0.0000024	4.8400145	-1.9879897
H	-0.8892591	4.3900360	-0.5230075
H	0.8887269	4.3900646	-0.5226704
C	4.5414551	-0.7235037	-0.5260719
H	4.7772060	-0.0801776	0.3225326
H	5.2998088	-1.5055254	-0.5965211
H	4.5646582	-0.1290595	-1.4403150
C	2.5418541	-2.4823588	-1.7445355
H	1.5832061	-2.9755126	-1.5972172
H	2.4864050	-1.8628166	-2.6396316
H	3.3249702	-3.2322452	-1.8728506
C	2.9213605	-2.4860156	1.1662443
H	1.9233975	-2.8939802	1.3197774
H	3.6365673	-3.3029662	1.0525857
H	3.2057107	-1.8871511	2.0325651

59

trans-[GeF2(OPMe3)4]2+

Ge	-0.0002930	-0.0000369	-0.0006974
P	0.9381636	2.9842555	0.5908214
P	2.9851349	-0.9368425	-0.5899848
P	-0.9366585	-2.9846077	0.5896184
P	-2.9854550	0.9372770	-0.5898887
F	0.0012415	0.0030830	-1.7861337
F	-0.0032866	-0.0019513	1.7844456
O	1.1498176	1.5379925	0.0347033
O	1.5393540	-1.1479031	-0.0320228
O	-1.5397934	1.1487745	-0.0315292
O	-1.1477617	-1.5403693	0.0271465
C	-2.5694317	-3.6847723	0.9000699
H	-3.1790054	-3.6315374	-0.0030846
H	-2.4783868	-4.7317482	1.1958964
H	-3.0654546	-3.1417018	1.7056652
C	-0.1026695	-4.0197451	-0.6281929
H	0.8799202	-3.5987303	-0.8315066
H	0.0081341	-5.0398534	-0.2557784
H	-0.6791412	-4.0397178	-1.5541235
C	-0.0062778	-3.0148987	2.1316594
H	-0.4743796	-2.3466538	2.8535856
H	0.0124994	-4.0322212	2.5278945
H	1.0085795	-2.6665675	1.9526234
C	3.6871423	-2.5696108	-0.8961437
H	3.1427248	-3.0693589	-1.6985119

H	4.7332423	-2.4780122	-1.1948834
H	3.6371849	-3.1760632	0.0092982
C	4.0166790	-0.1004716	0.6291055
H	5.0376755	0.0102589	0.2591567
H	3.5942696	0.8820629	0.8295829
H	4.0343610	-0.6754351	1.5560432
C	3.0180890	-0.0078644	-2.1328098
H	2.6631080	1.0052070	-1.9561195
H	4.0371027	0.0166698	-2.5243698
H	2.3561174	-0.4802924	-2.8576811
C	-3.0179839	0.0121340	-2.1350465
H	-2.6546253	-0.9986243	-1.9626856
H	-4.0383943	-0.0187086	-2.5224873
H	-2.3627114	0.4915343	-2.8614846
C	-4.0154761	0.0972008	0.6279759
H	-4.0283556	0.6674693	1.5578953
H	-5.0380364	-0.0089367	0.2610360
H	-3.5951399	-0.8874443	0.8220092
C	-3.6906366	2.5692550	-0.8927448
H	-4.7366117	2.4751867	-1.1912824
H	-3.6419675	3.1745610	0.0135074
H	-3.1483065	3.0715624	-1.6949275
C	0.0221079	3.0146523	2.1413629
H	-0.0126425	4.0352836	2.5278224
H	-0.9876421	2.6453643	1.9749416
H	0.5089043	2.3630508	2.8662183
C	0.0872948	4.0121723	-0.6212999
H	-0.8970511	3.5886754	-0.8092995
H	-0.0196732	5.0338527	-0.2521260
H	0.6517073	4.0282143	-1.5547180
C	2.5712304	3.6923064	0.8805968
H	3.0825418	3.1479136	1.6756416
H	3.1675838	3.6472728	-0.0317862
H	2.4785379	4.7371252	1.1834736