

## SUPPORTING INFORMATION

for

### Structural Motifs in Aryl Organogermanium Ge-O Derivatives for Materials Design

#### Table of Contents

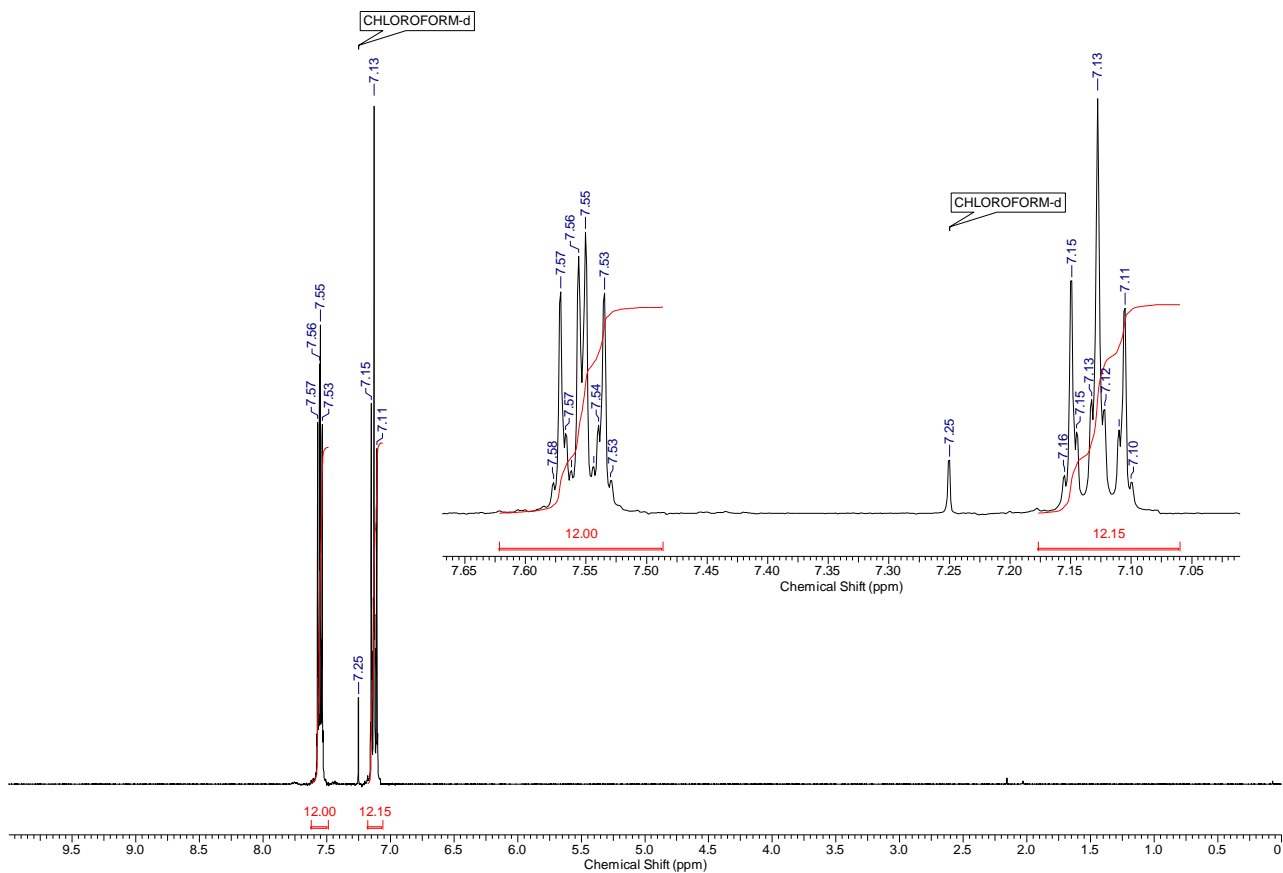
##### NMR Spectral Data

<b>Figure S1.</b> $^1\text{H}$ NMR spectrum of $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>1</b> ) ( $\text{CDCl}_3$ , RT).....	S2
<b>Figure S2.</b> $^{13}\text{C}$ NMR spectrum of $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>1</b> ) ( $\text{CDCl}_3$ , RT).....	S3
<b>Figure S3.</b> $^{19}\text{F}$ NMR spectrum of $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>1</b> ) ( $\text{CDCl}_3$ , RT).....	S4
<b>Figure S4.</b> $^1\text{H}$ NMR spectrum of $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>2</b> ) ( $\text{CDCl}_3$ , RT).....	S5
<b>Figure S5.</b> $^{13}\text{C}$ NMR spectrum of $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>2</b> ) ( $\text{CDCl}_3$ , RT).....	S6
<b>Figure S6.</b> $^{19}\text{F}$ NMR spectrum of $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>2</b> ) ( $\text{CDCl}_3$ , RT).....	S7

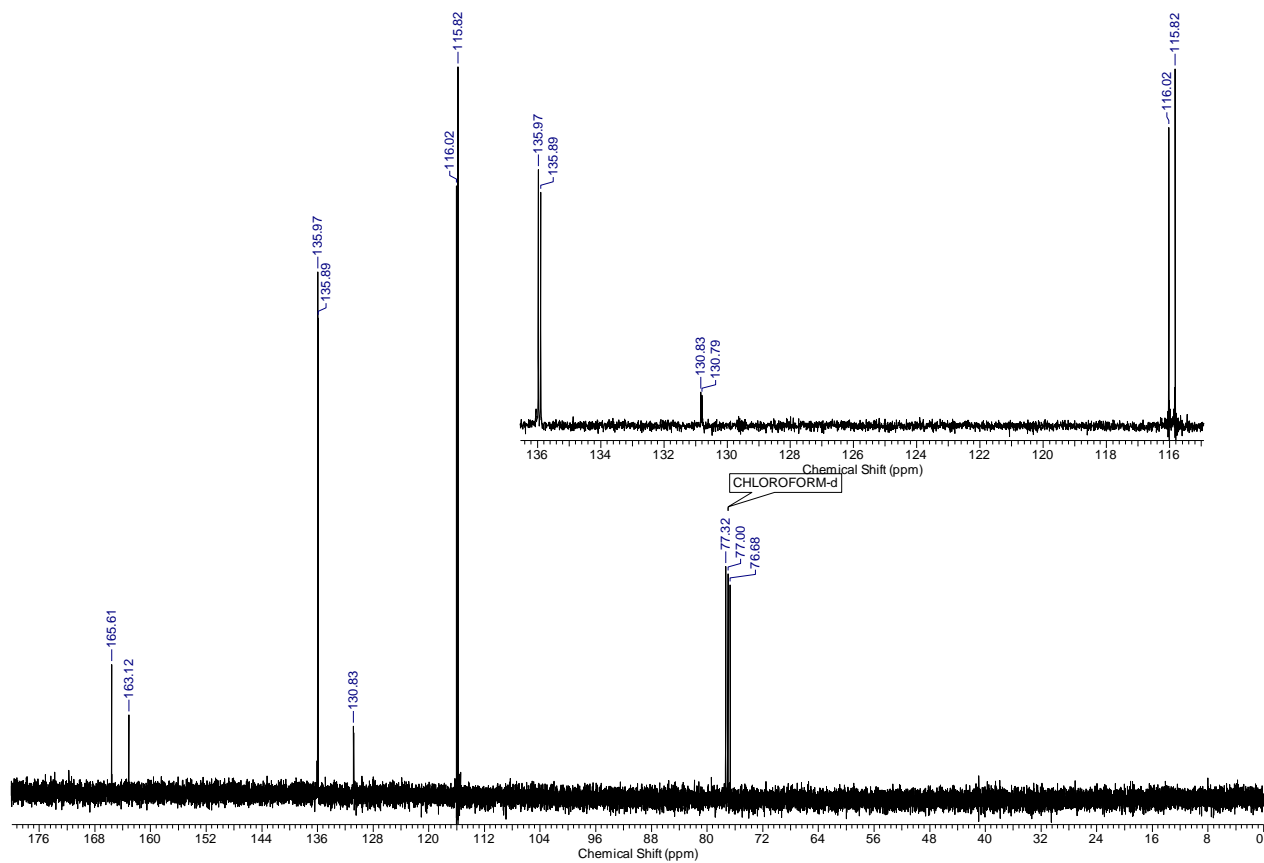
##### X-Ray Diffraction Analysis Data

<b>Table S1.</b> The crystallographic data for compounds $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>1</b> ), $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$ ( <b>2</b> ) (structural type <b>A</b> ).....	S8
<b>Table S2.</b> The crystallographic data for compound <i>cyclo</i> - $[(p\text{-F}_3\text{CC}_6\text{H}_4)_2\text{GeO}]_4$ ( <b>3</b> ) (structural type <b>F</b> ).....	S9
<b>Table S3.</b> The crystallographic data for compound $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{GeO}]_4\text{Ge}$ ( <b>4</b> ) (structural type <b>K</b> ).....	S10

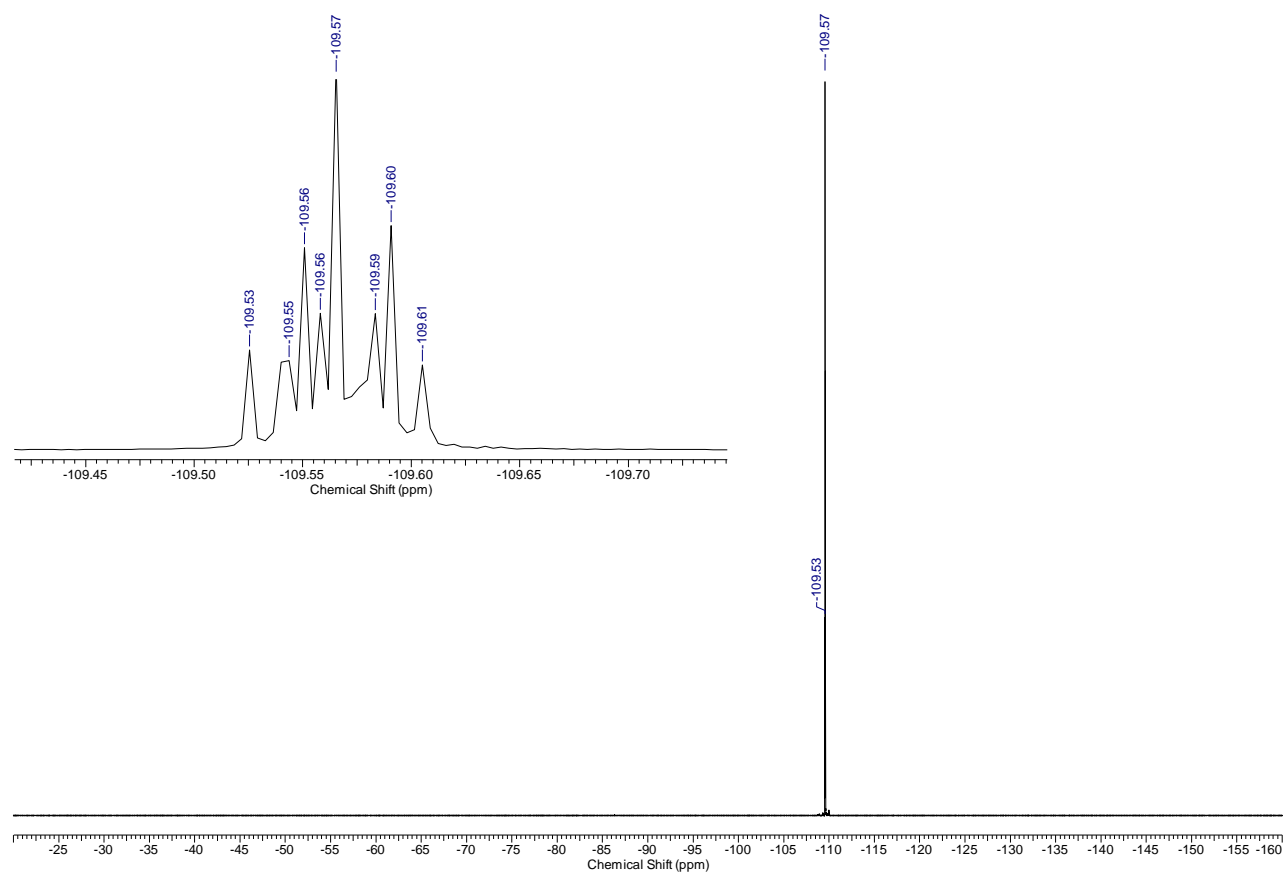
### NMR Spectral Data



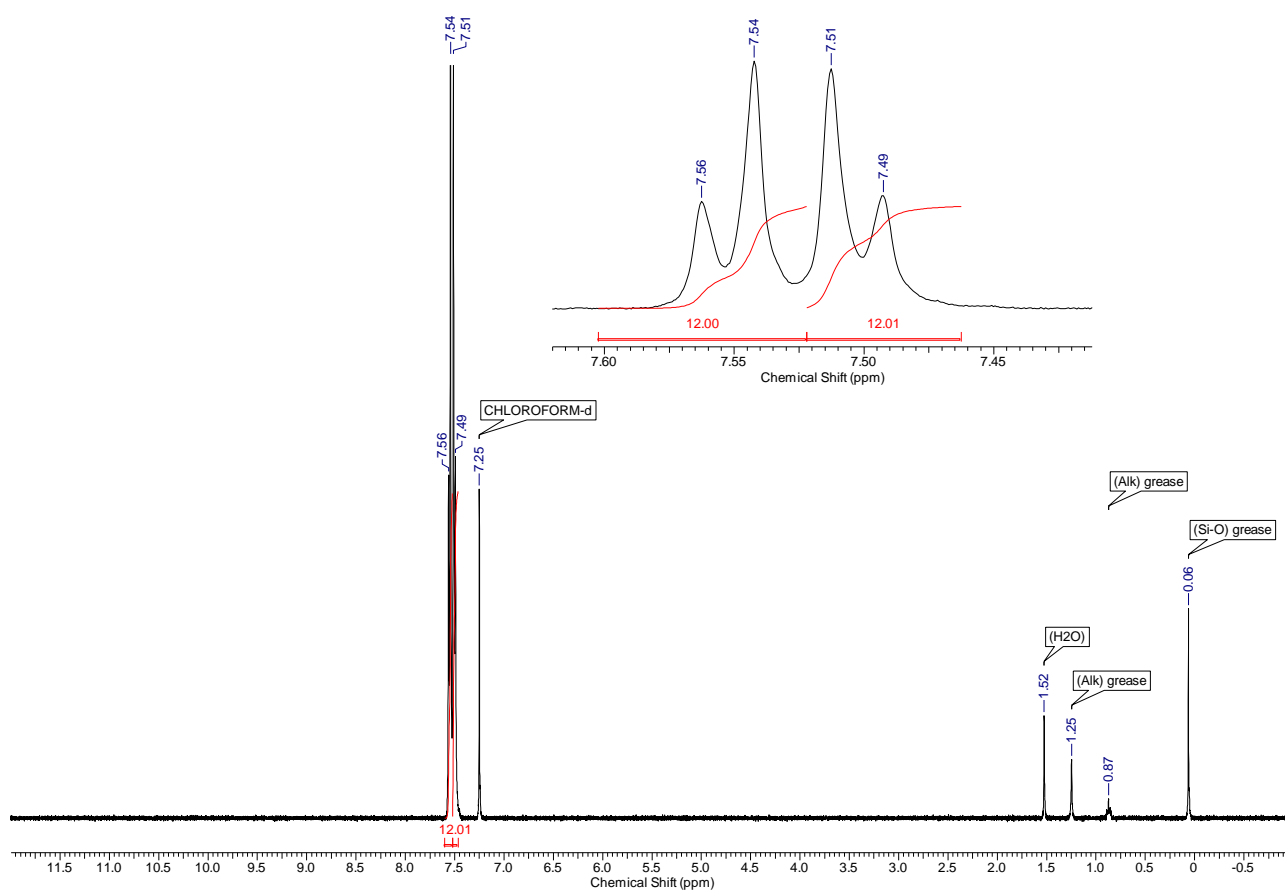
**Figure S1.**  $^1\text{H}$  NMR spectrum of  $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (1) ( $\text{CDCl}_3$ , RT).



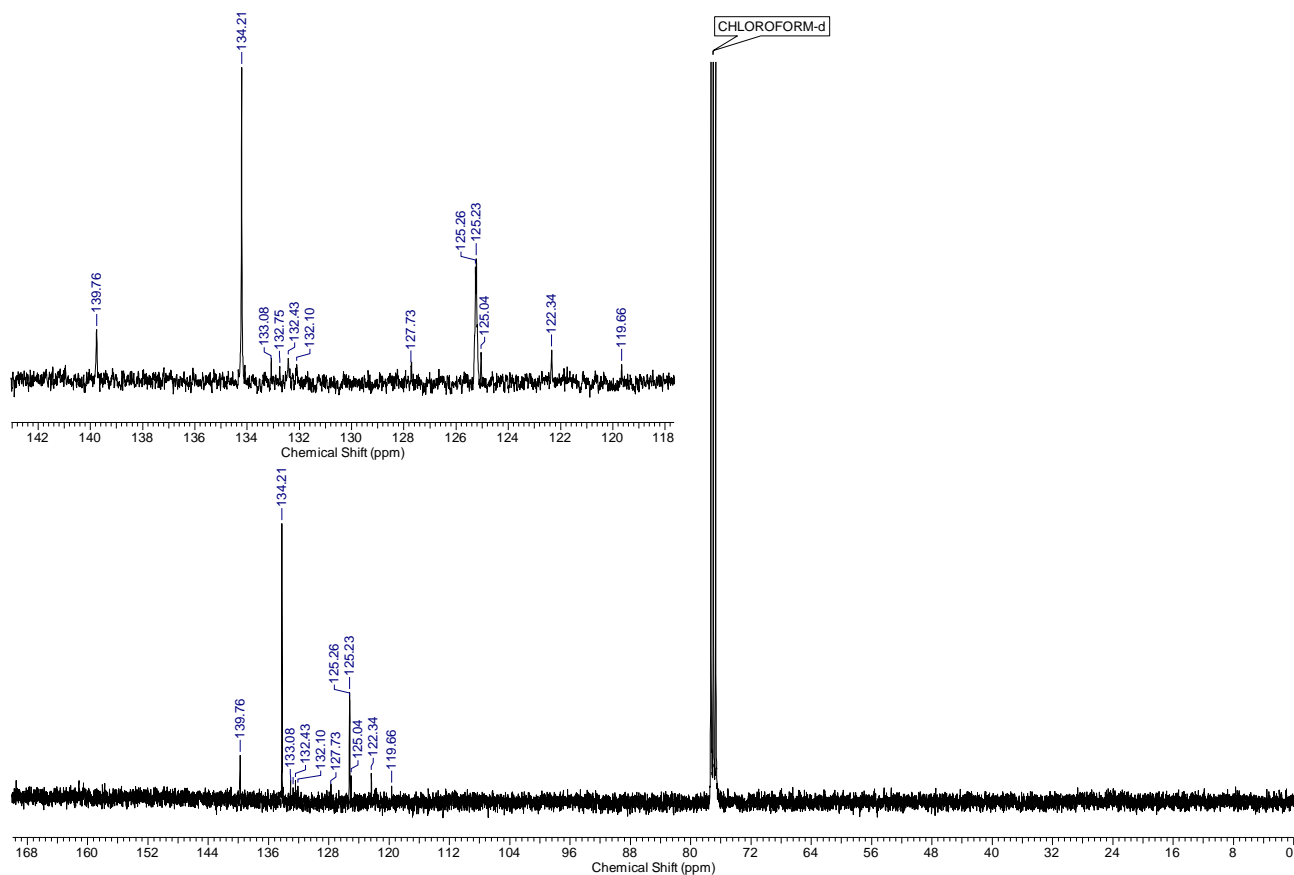
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of  $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (**1**) ( $\text{CDCl}_3$ , RT).



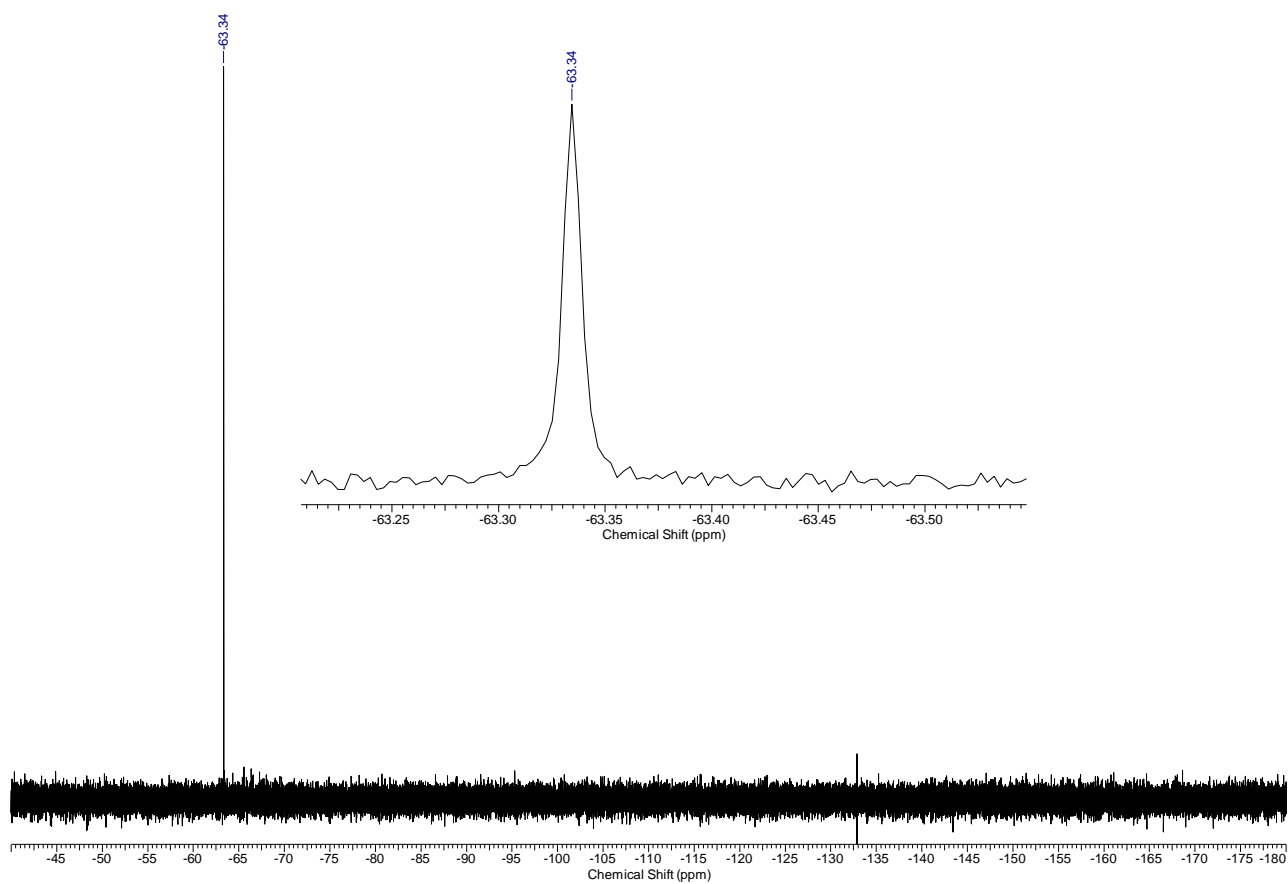
**Figure S3.**  $^{19}\text{F}$  NMR spectrum of  $[(p\text{-FC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (1) ( $\text{CDCl}_3$ , RT).



**Figure S4.**  $^1\text{H}$  NMR spectrum of  $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (**2**) ( $\text{CDCl}_3$ , RT).



**Figure S5.**  $^{13}\text{C}$  NMR spectrum of  $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (**2**) ( $\text{CDCl}_3$ , RT).



**Figure S6.**  $^{19}\text{F}$  NMR spectrum of  $[(p\text{-F}_3\text{CC}_6\text{H}_4)_3\text{Ge}]_2\text{O}$  (**2**) ( $\text{CDCl}_3$ , RT).

**X-Ray Diffraction Analysis Data**

**Table S1.** The crystallographic data for compounds [(*p*-FC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>Ge]<sub>2</sub>O (**1**), [(*p*-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>Ge]<sub>2</sub>O (**2**) (structural type **A**).

	<b>1</b>	<b>2</b>
empirical formula	C <sub>36</sub> H <sub>24</sub> F <sub>6</sub> Ge <sub>2</sub> O	C <sub>42</sub> H <sub>24</sub> F <sub>18</sub> Ge <sub>2</sub> O
$M_w$	731.73	1031.79
temperature (K)	120	150
size (mm)	0.15 x 0.10 x 0.08	0.21 x 0.15 x 0.10
cryst. system	monoclinic	monoclinic
space group	<i>C2/c</i>	<i>P2<sub>1</sub>/c</i>
<i>a</i> (Å)	9.7200(4)	16.4116(13)
<i>b</i> (Å)	20.9864(8)	18.5115(14)
<i>c</i> (Å)	15.2582(6)	13.8675(11)
$\beta$ (deg)	99.143(1)	107.325(1)
<i>V</i> (Å <sup>3</sup> )	3072.9(2)	4021.9(5)
<i>Z</i>	4	4
$\rho_{\text{cald}}$ (g*cm <sup>-3</sup> )	1.582	1.704
abs coeff. (mm <sup>-1</sup> )	2.022	1.613
<i>F</i> (000)	1464	2040
$\theta$ range (deg)	2.33 - 28.00	2.54 - 27.00
no. of collected/unique rflns.	12118 / 3681	31468 / 8762
<i>R</i> <sub>int</sub>	0.0193	0.0549
data/restraints/params.	3681 / 9 / 272	8762 / 1026 / 838
goodness of fit on <i>F</i> <sup>2</sup>	1.074	1.107
final <i>R</i> indices ( <i>I</i> > 2σ( <i>I</i> ))	<i>R</i> <sub>1</sub> = 0.0552, w <i>R</i> <sub>2</sub> = 0.1196	<i>R</i> <sub>1</sub> = 0.0412, w <i>R</i> <sub>2</sub> = 0.0925
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0701, w <i>R</i> <sub>2</sub> = 0.1298	<i>R</i> <sub>1</sub> = 0.0637, w <i>R</i> <sub>2</sub> = 0.1020
largest diff. peak/hole (e/Å <sup>3</sup> )	1.754 / -1.771	0.766 / -0.715



**Table S2.** The crystallographic data for compound *cyclo*-[(*p*-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>)<sub>2</sub>GeO]<sub>4</sub> (**3**)  
(structural type **F**).

empirical formula	C <sub>56</sub> H <sub>32</sub> F <sub>24</sub> Ge <sub>4</sub> O <sub>4</sub>
$M_w$	1515.17
temperature (K)	120
size (mm)	0.30 x 0.20 x 0.20
cryst. system	tetragonal
space group	<i>I</i> 4 <sub>1</sub> /a
<i>a</i> (Å)	11.2193(5)
<i>c</i> (Å)	44.188(4)
<i>V</i> (Å <sup>3</sup> )	5562.1(7)
<i>Z</i>	4
$\rho_{\text{cald}}$ (g*cm <sup>-3</sup> )	1.809
abs coeff. (mm <sup>-1</sup> )	2.269
<i>F</i> (000)	2976
$\theta$ range (deg)	2.57 - 27.99
no. of collected/unique rflns.	14852 / 3351
<i>R</i> <sub>int</sub>	0.0786
data/restraints/params.	3351 / 282 / 234
goodness of fit on <i>F</i> <sup>2</sup>	1.144
final <i>R</i> indices ( <i>I</i> > 2σ( <i>I</i> ))	<i>R</i> <sub>1</sub> = 0.1030, w <i>R</i> <sub>2</sub> = 0.2147
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.1170, w <i>R</i> <sub>2</sub> = 0.2218
largest diff. peak/hole (e/Å <sup>3</sup> )	1.002 / -1.015

**Table S3.** The crystallographic data for compound [(*p*-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>)<sub>3</sub>GeO]<sub>4</sub>Ge (**4**) (structural type **K**).

empirical formula	C <sub>84</sub> H <sub>48</sub> F <sub>36</sub> Ge <sub>5</sub> O <sub>4</sub> *2(C <sub>6</sub> H <sub>6</sub> )
$F_w$	2324.39
temperature (K)	183
size (mm)	0.25 x 0.25 x 0.20
cryst. system	tetragonal
space group	$P4_32_12$
$a$ (Å)	16.5336(8)
$c$ (Å)	34.892(3)
$V$ (Å <sup>3</sup> )	9538.1(9)
$Z$	4
$\rho_{\text{cald}}$ (g*cm <sup>-3</sup> )	1.619
abs coeff. (mm <sup>-1</sup> )	1.679
$F(000)$	4608
$\theta$ range (deg)	2.10 - 27.00
no. of collected/unique rflns.	92313 / 10419
$R_{\text{int}}$	0.0416
data/restraints/params.	10419 / 1194 / 894
goodness of fit on $F^2$	1.108
final $R$ indices ( $I > 2\sigma(I)$ )	$R_1 = 0.0445$ , $wR_2 = 0.1199$
$R$ indices (all data)	$R_1 = 0.0528$ , $wR_2 = 0.1199$
largest diff. peak/hole (e/Å <sup>3</sup> )	0.809 / -0.561
Flack param.	0.001(3)