ESI for:

Reactivity of Boraguanidinato Germylene Toward Carbonyl Compounds and Isocyanides: C-O, C-F and C-N Bond Activation.

*Jiří Böserle, Milan Erben, Roman Jambor, Aleš Růžička and Libor Dostál**

*E-mail: libor.dostal@upce.cz (L.D.)

Table of contents:

1) NMR spectra of studied compounds.

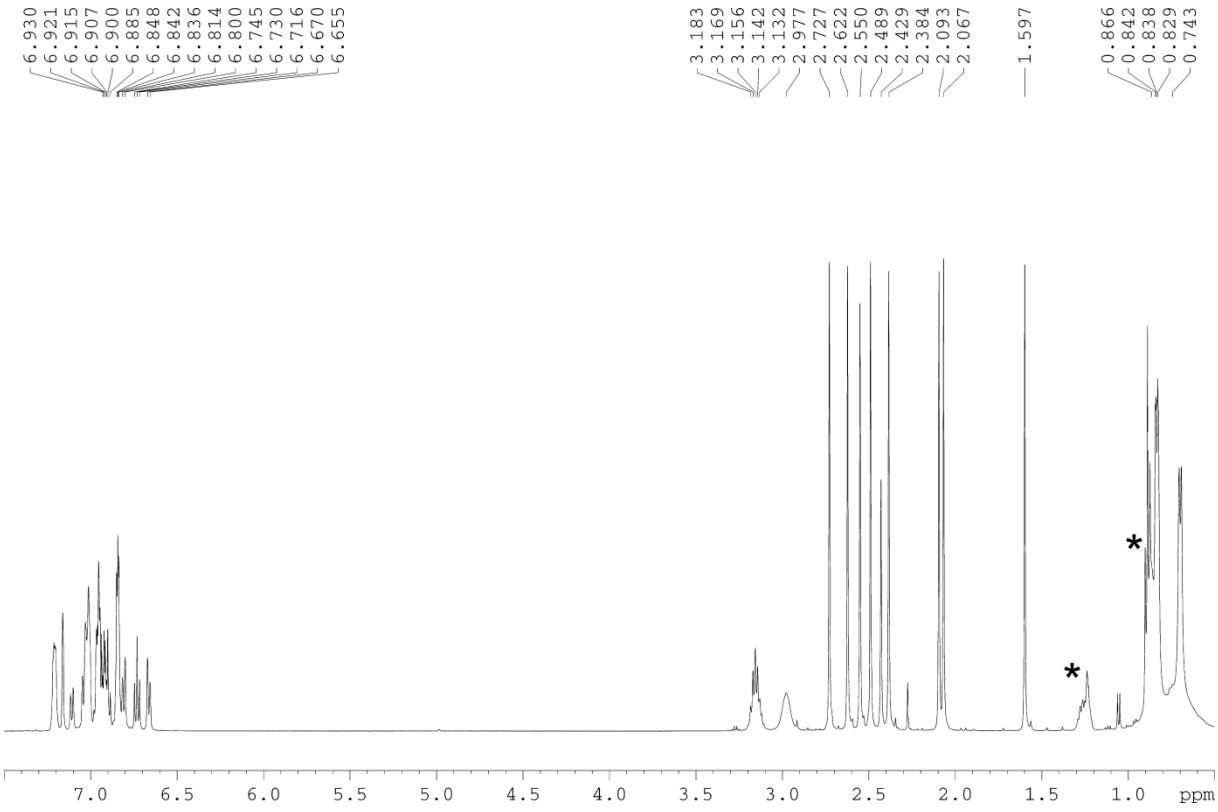

Figure S1: ^{1}H NMR spectrum of **2** in C_6D_6 (* traces of hexane).

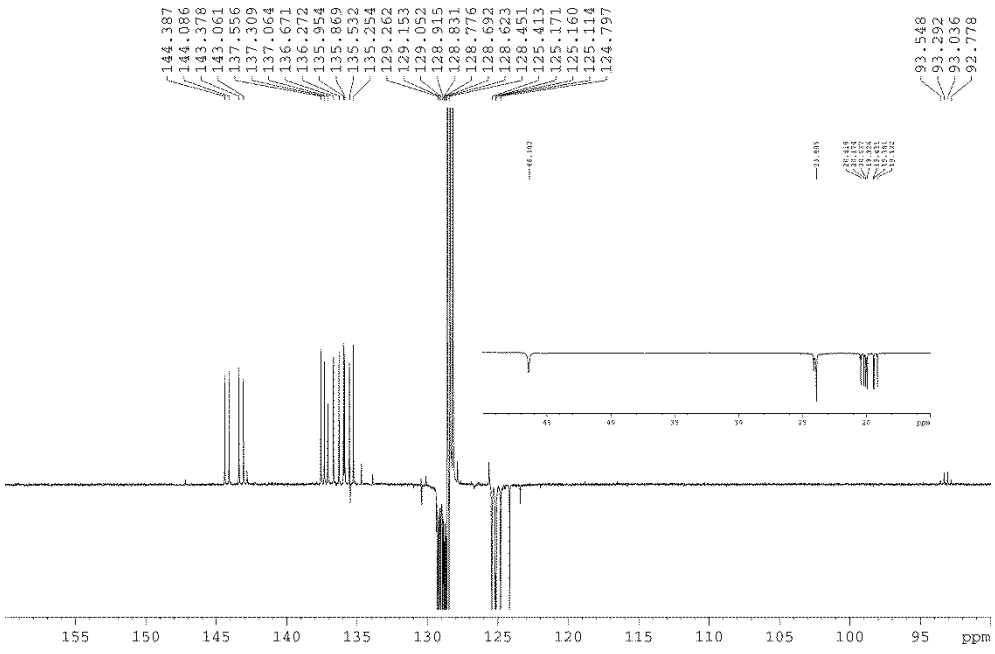

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

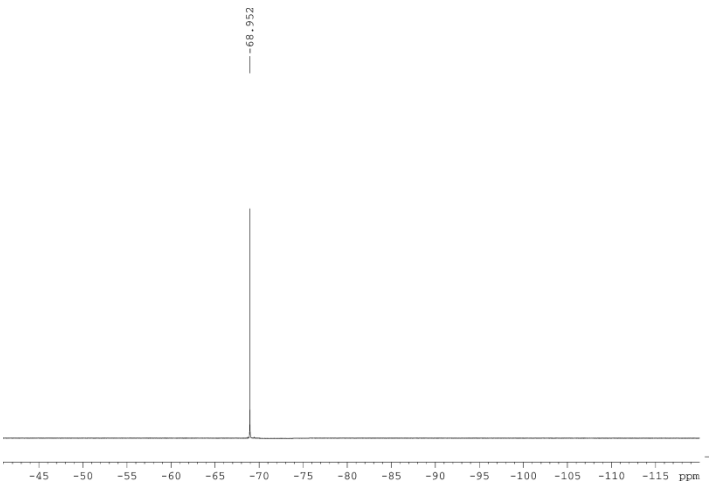

Figure S3: $^{19}F\{^{1}H\}$ NMR spectrum of **2** in C_6D_6.

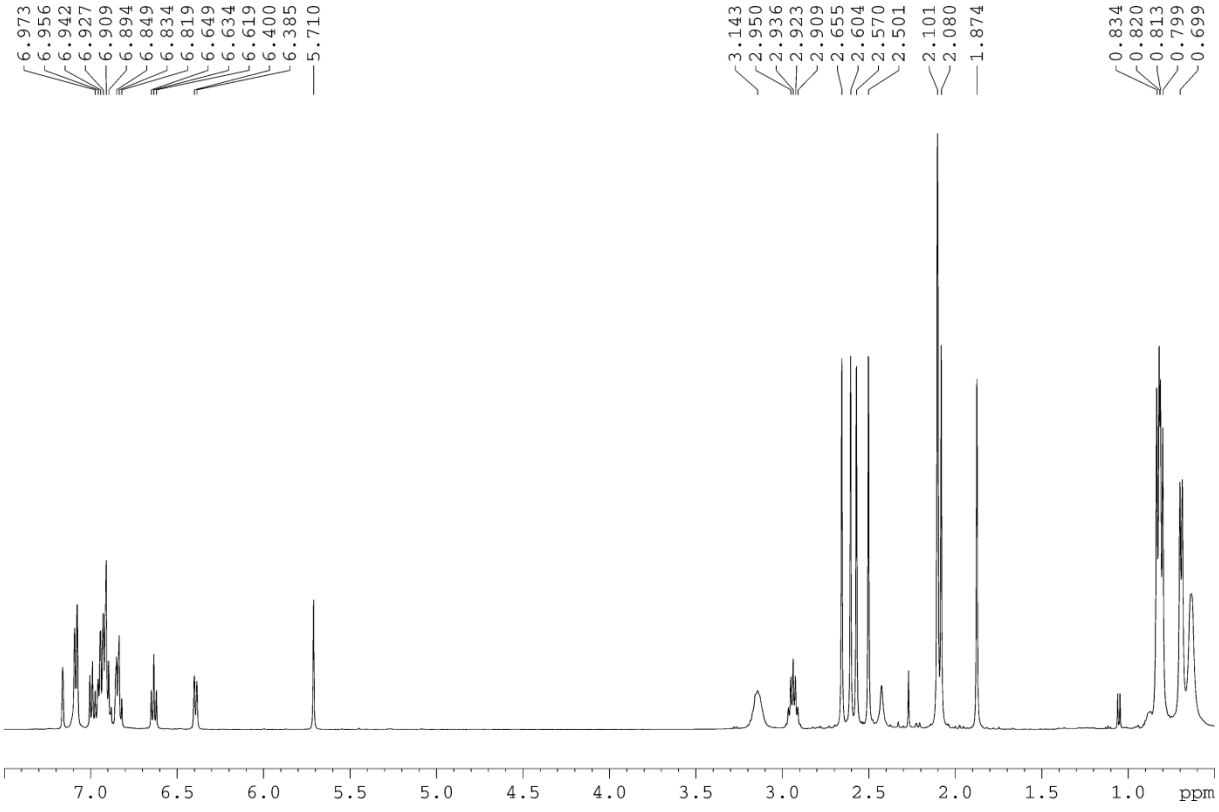

Figure S4: ^{1}H NMR spectrum of **3** in C_6D_6.

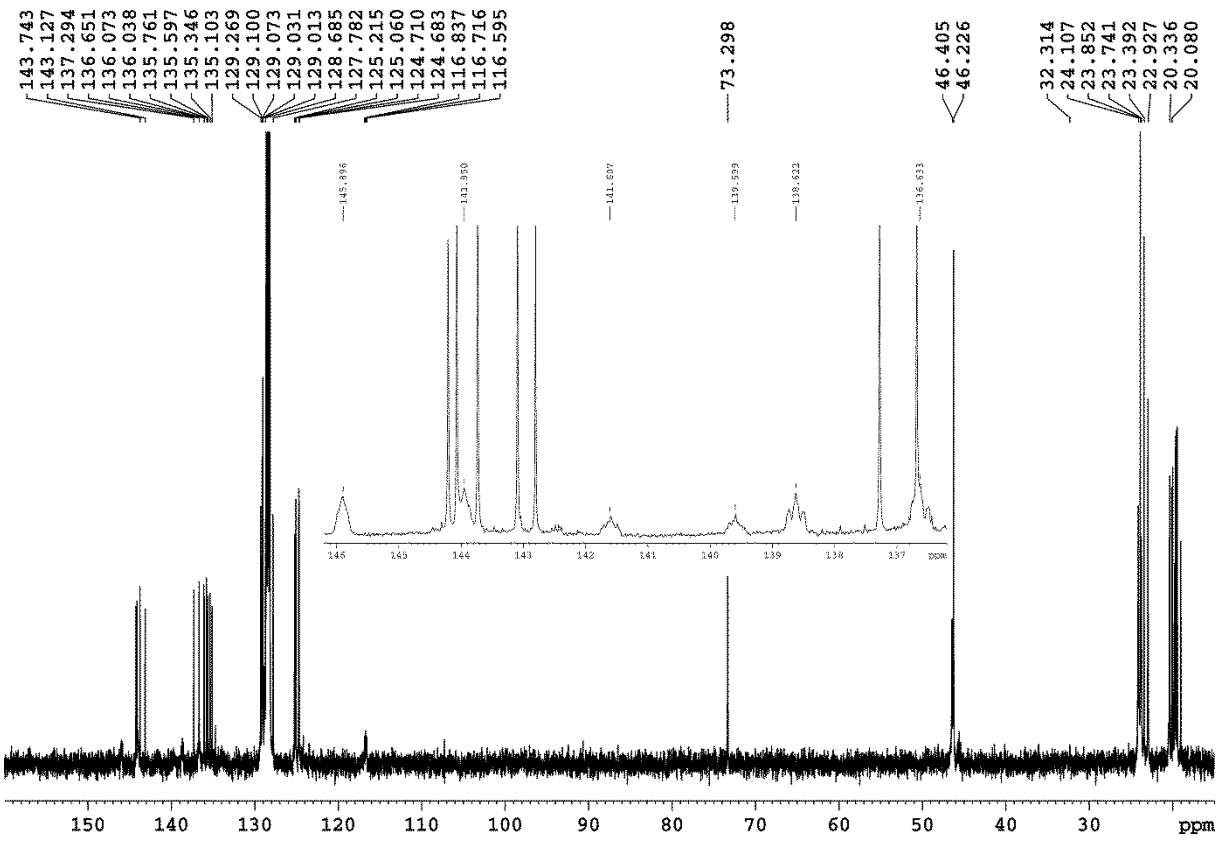

Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6.

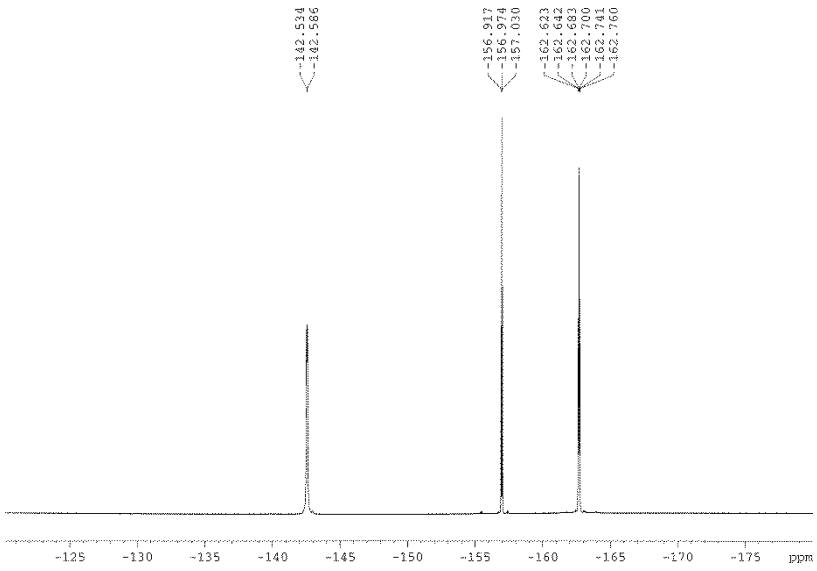

Figure S6: $^{19}F\{^{1}H\}$ NMR spectrum of **3** in C_6D_6.

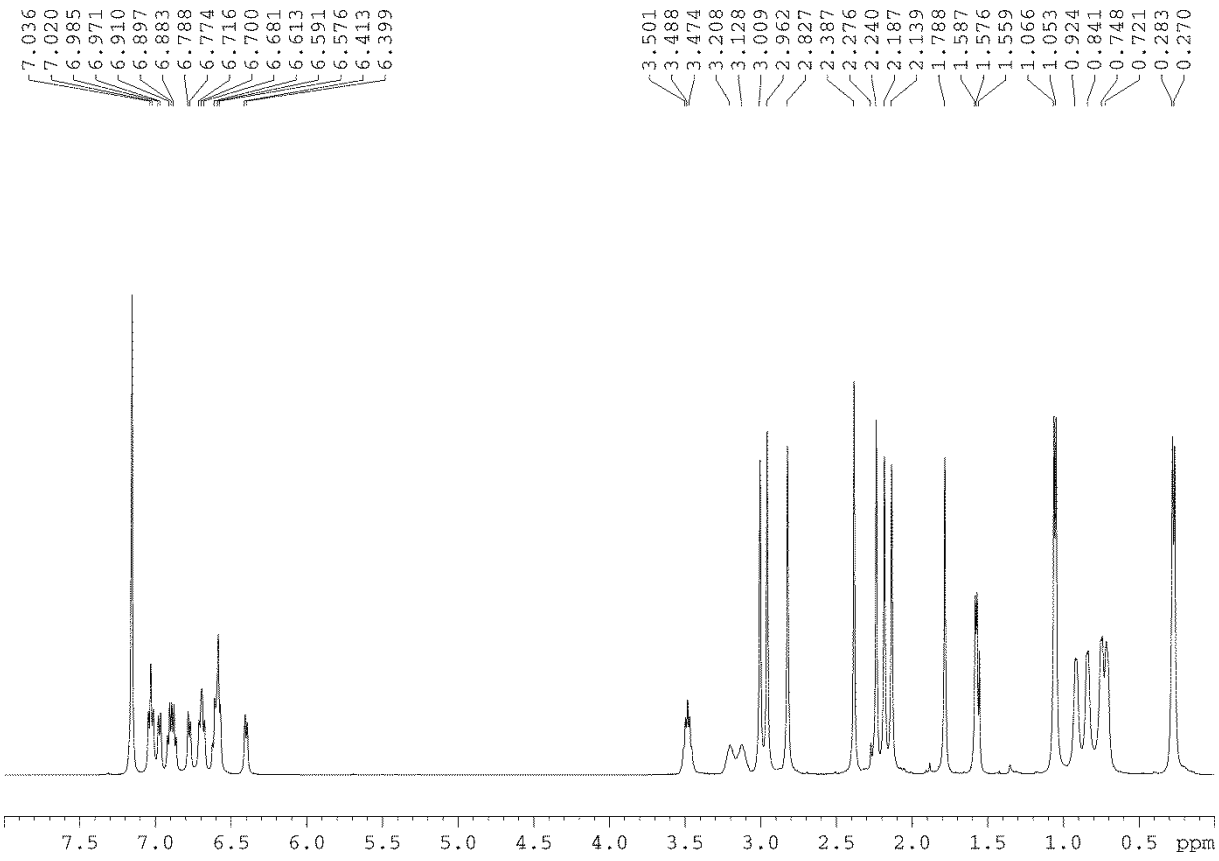

Figure S7: ^{1}H NMR spectrum of **4** in C_6D_6.

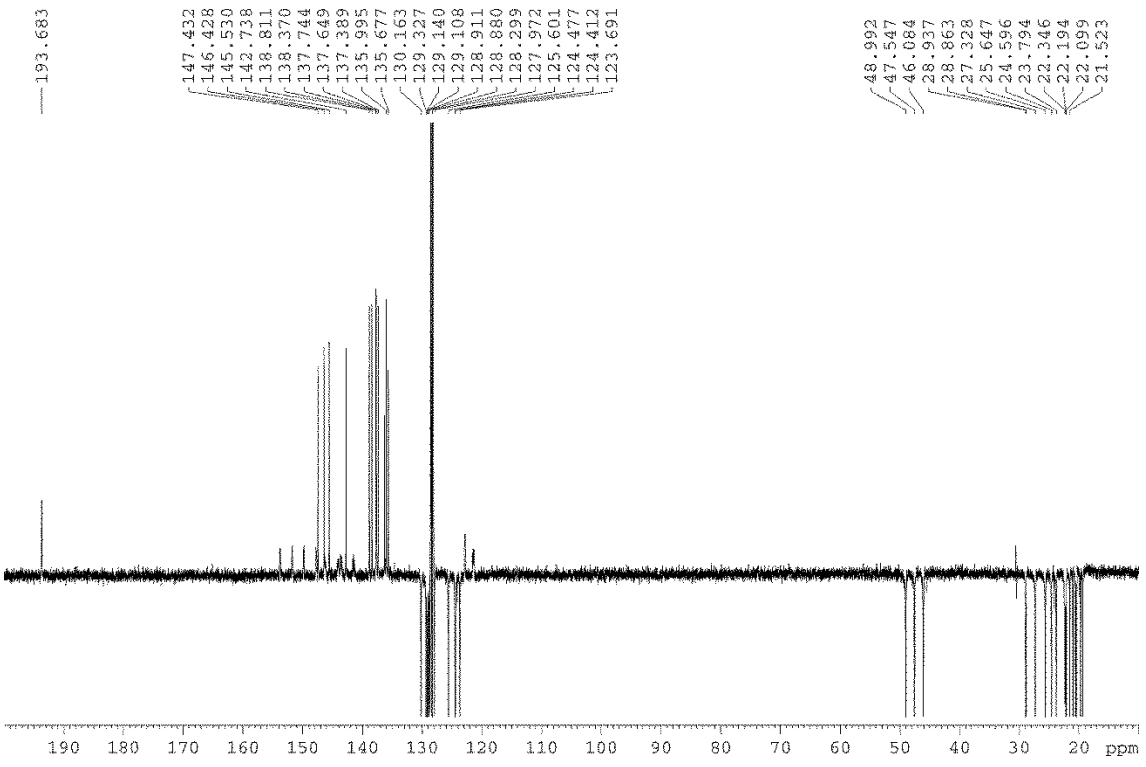

Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6.

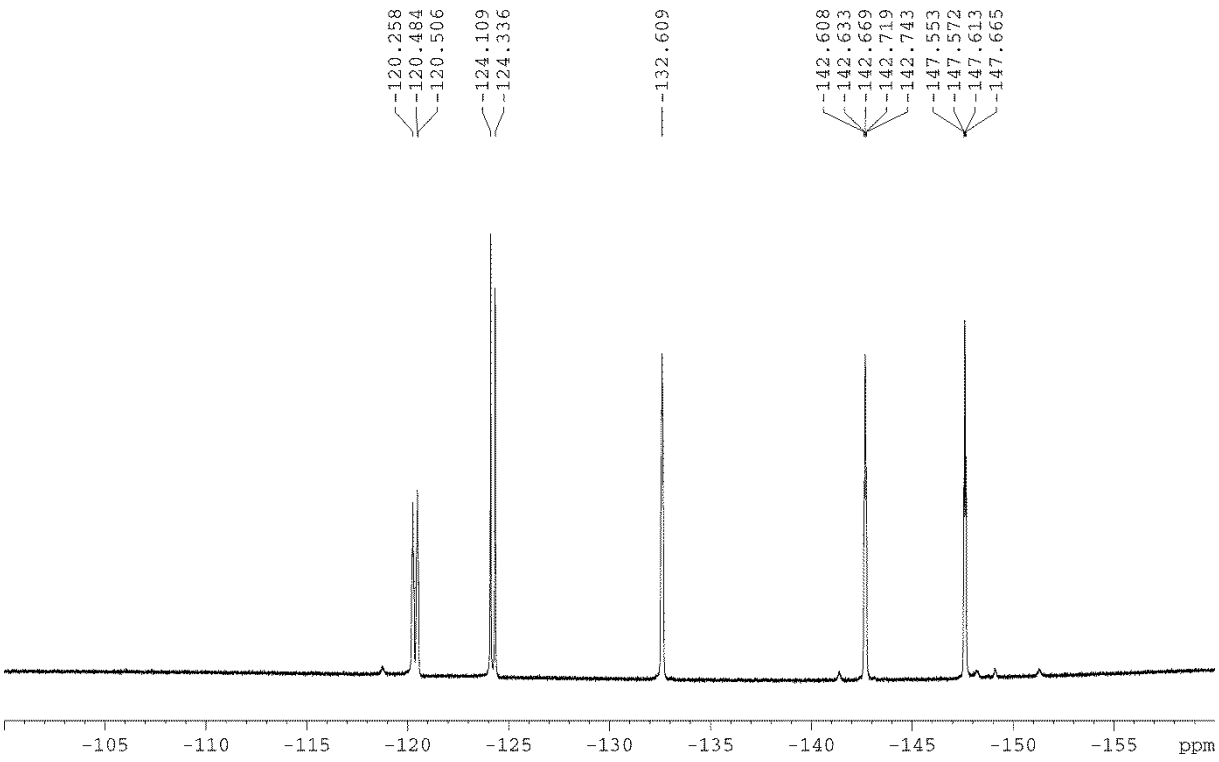

Figure S9: $^{19}F\{^{1}H\}$ NMR spectrum of **4** in C_6D_6.

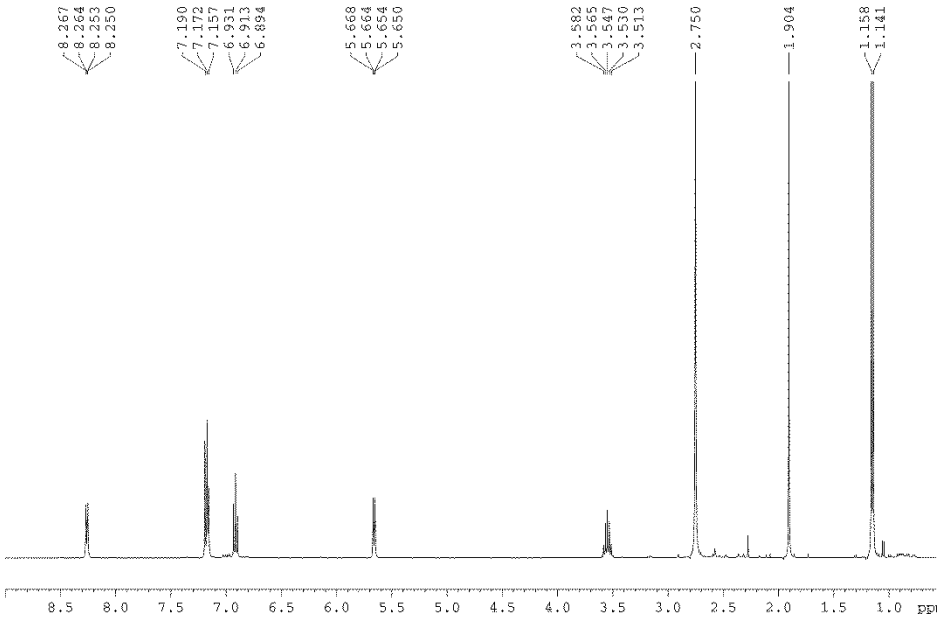

Figure S10: ^{1}H NMR spectrum of **5** in C_6D_6.

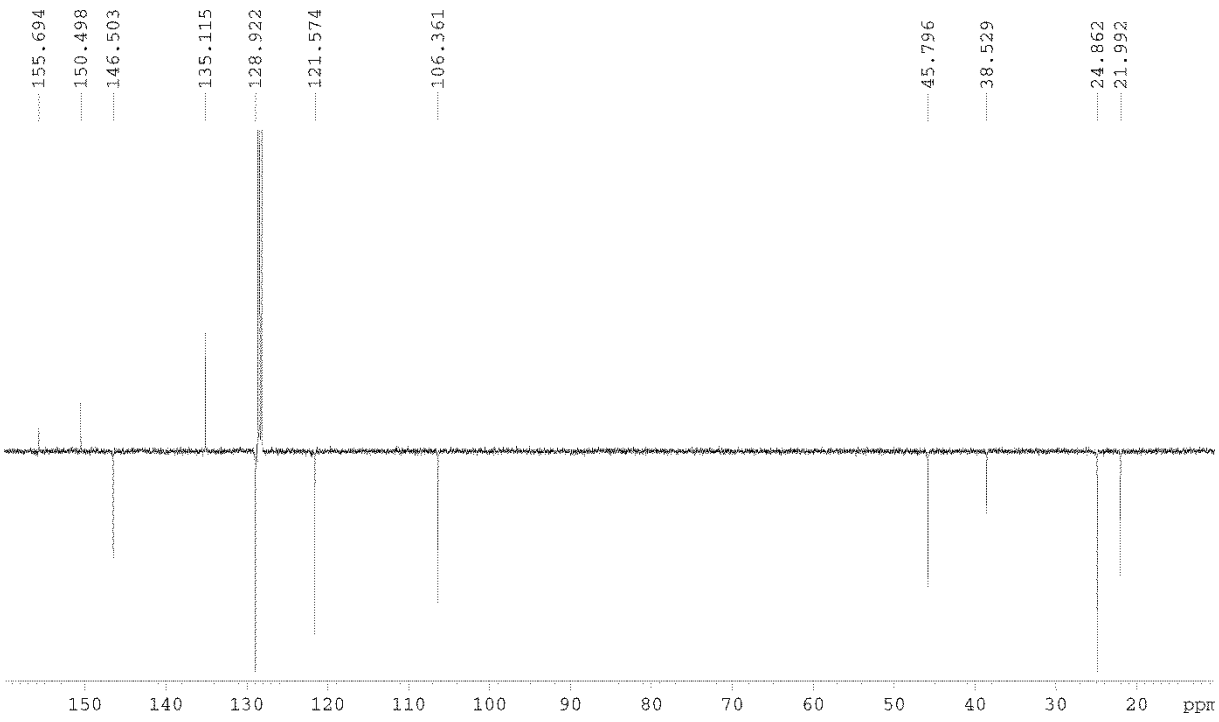

Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

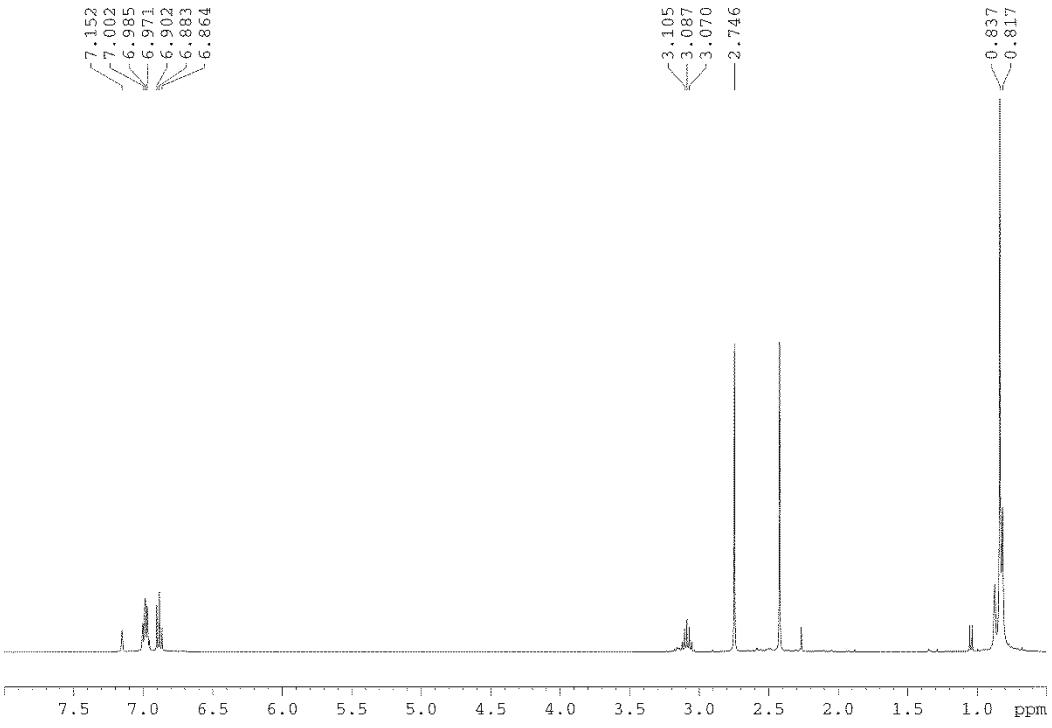

Figure S12: ^{1}H NMR spectrum of **6** in C_6D_6.

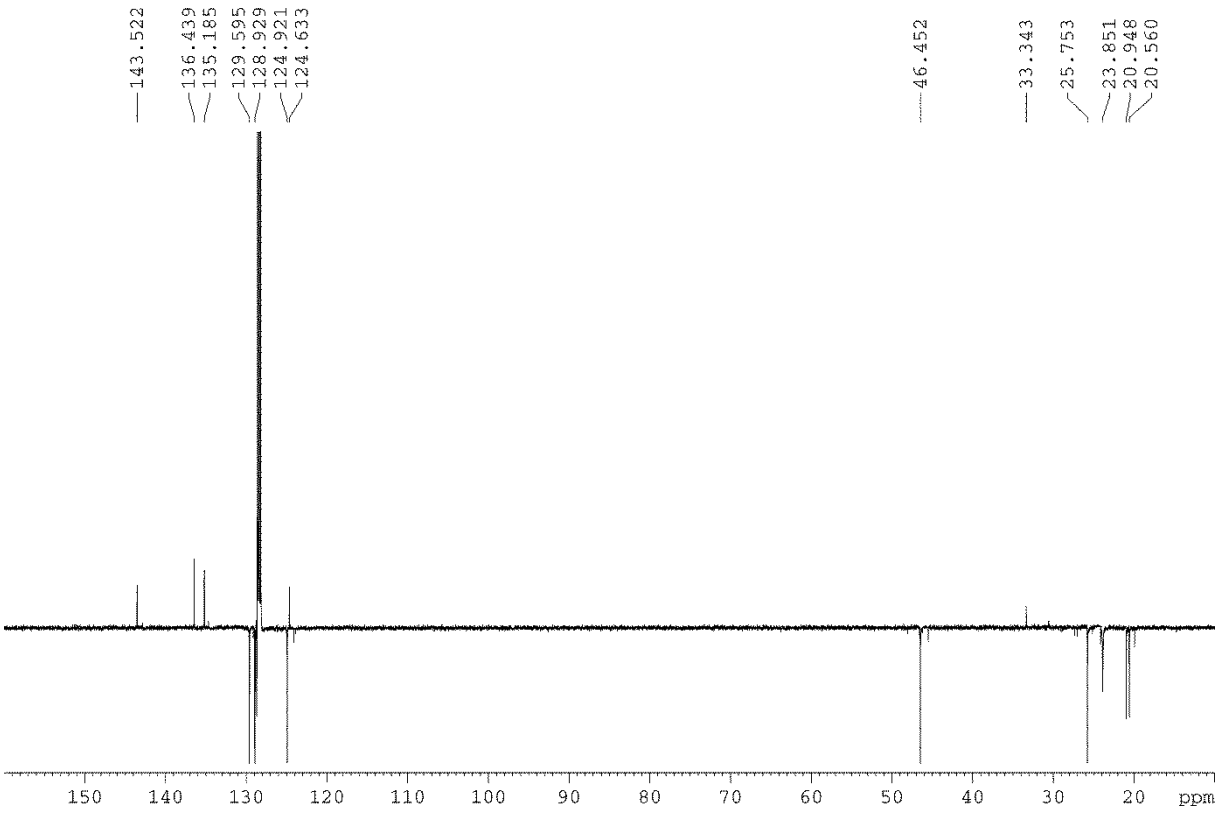

Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum of **6** in C_6D_6.

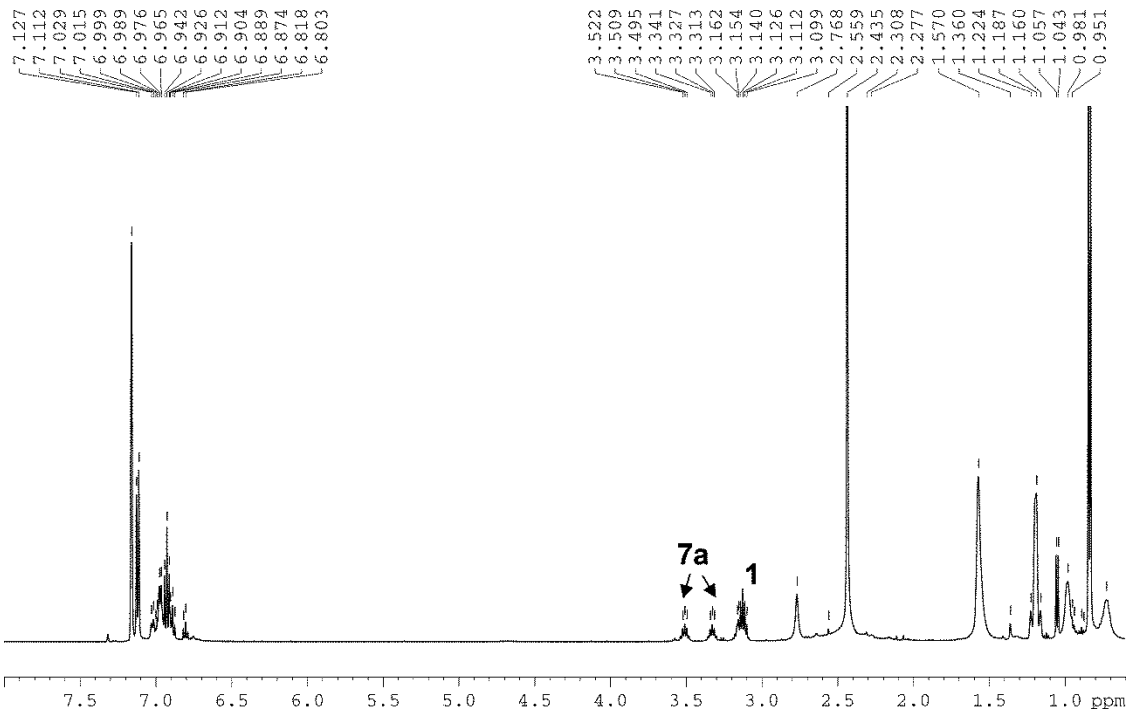

Figure S14: ^{1}H NMR spectrum of single-crystals of **7** in C_6D_6 showing two set of signals assigned to starting **1** proposed complex **7a.**

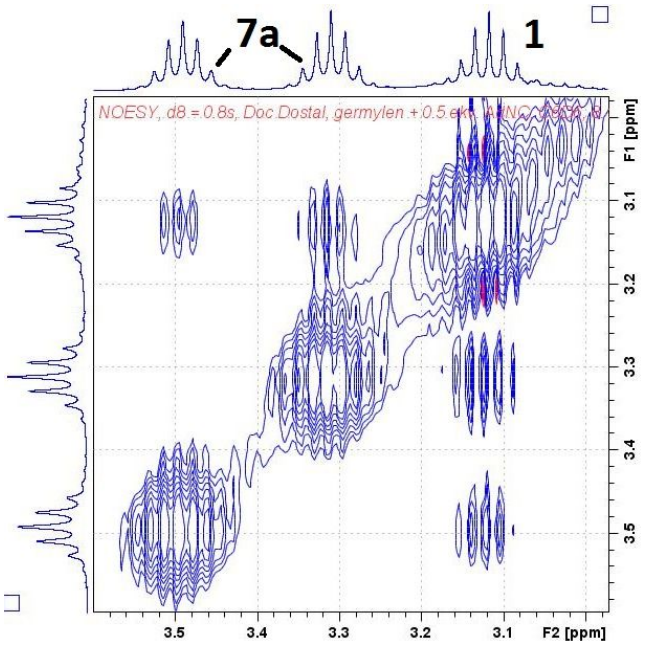

Figure S15: ^{1}H, ^{1}H EXSY NMR spectrum of single-crystals of **7** in C_6D_6 (region of NC***H***$(CH_3)_2$ group) showing mutual dynamic exchange between starting **1** and proposed complex **7a**.

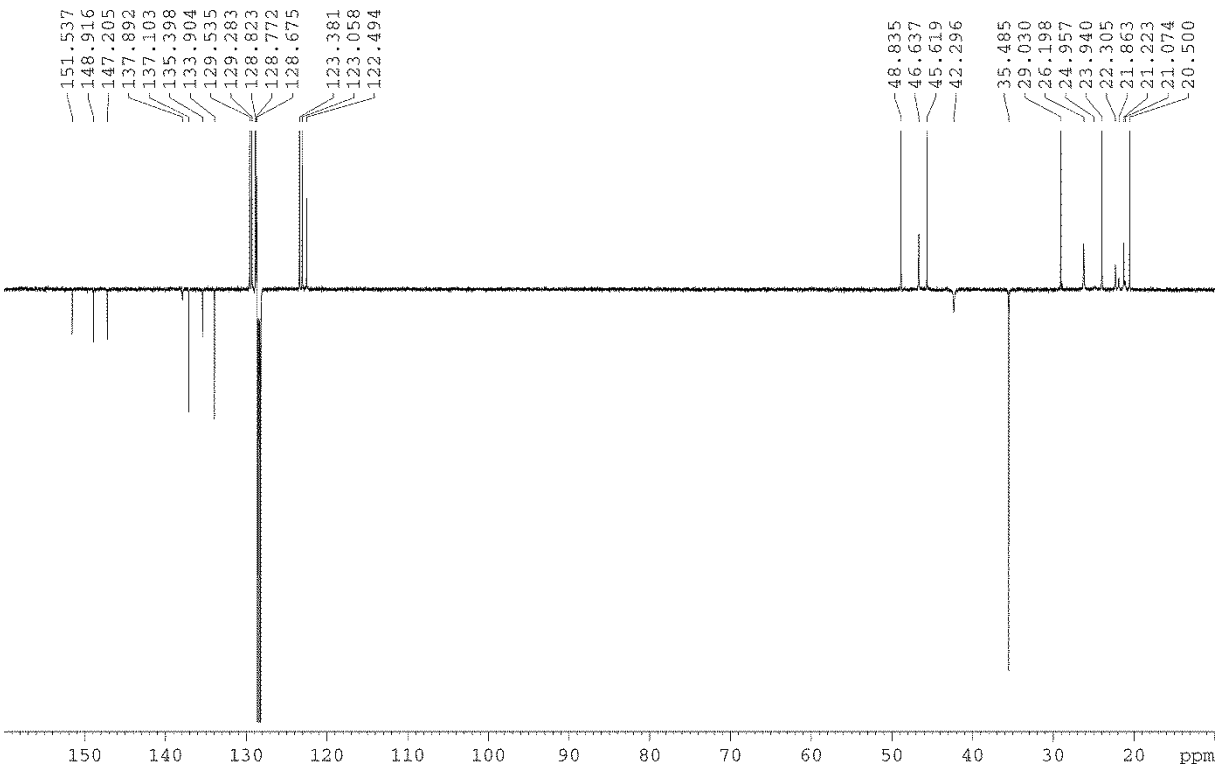

Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of single-crystals of **7** in C_6D_6 showing two set of signals assigned to starting **1** proposed complex **7a**.

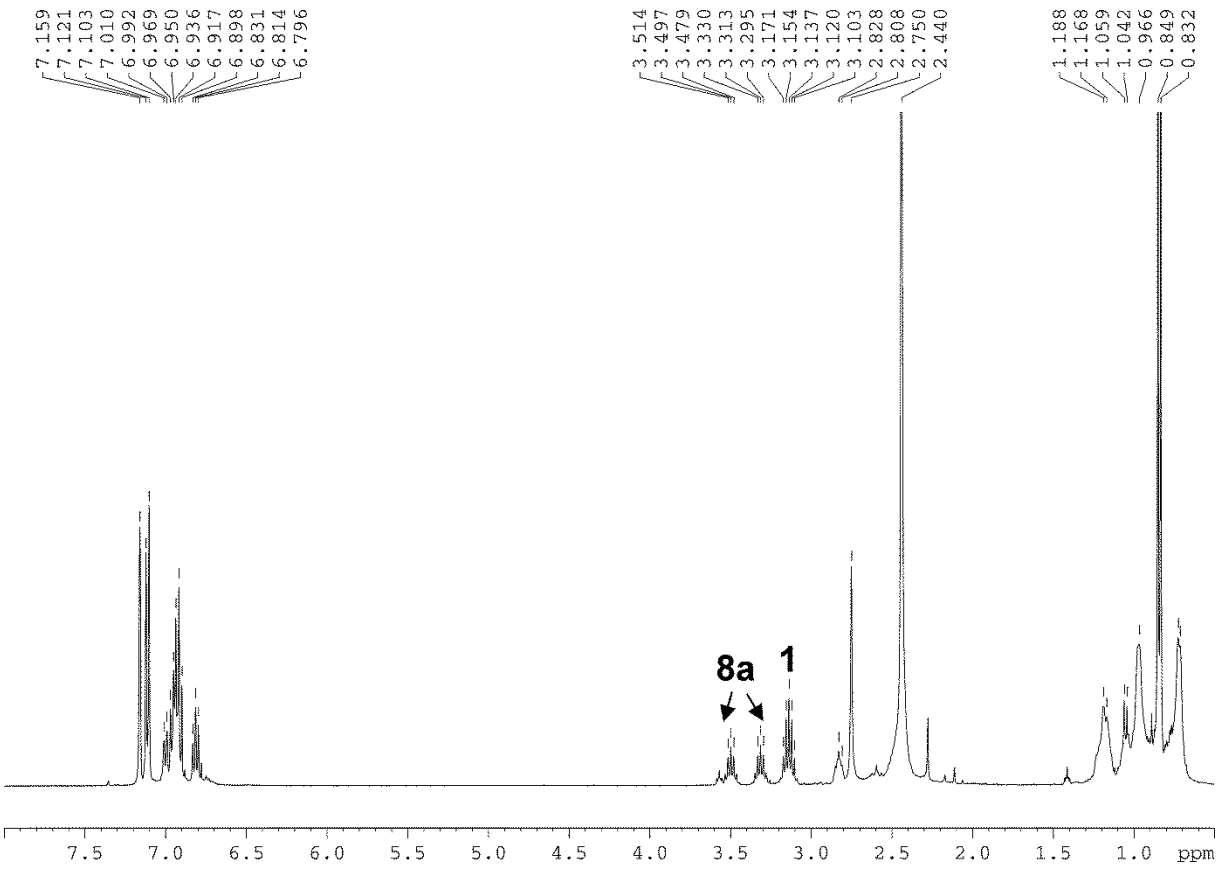

Figure S17: ^{1}H NMR spectrum of single-crystals of **8** in C_6D_6 showing two set of signals assigned to starting **1** proposed complex **8a**.

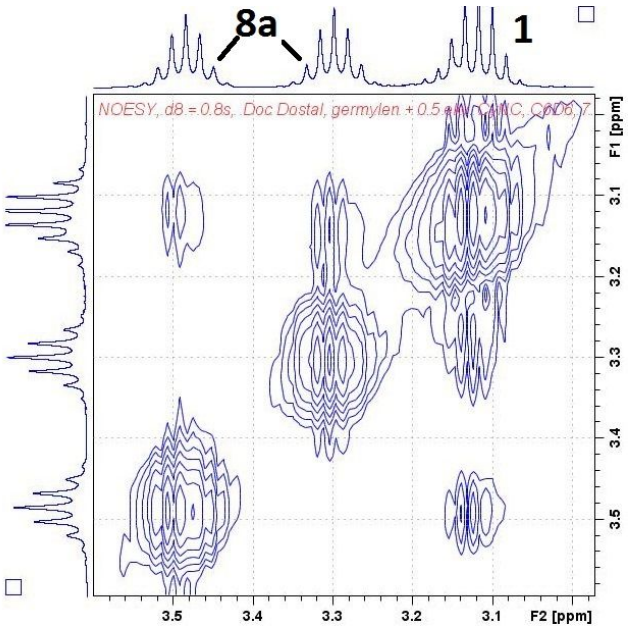

Figure S18: ^{1}H, ^{1}H EXSY NMR spectrum of single-crystals of **8** in C_6D_6 (region of NC***H***$(CH_3)_2$ group) showing mutual dynamic exchange between starting **1** and proposed complex **8a**.

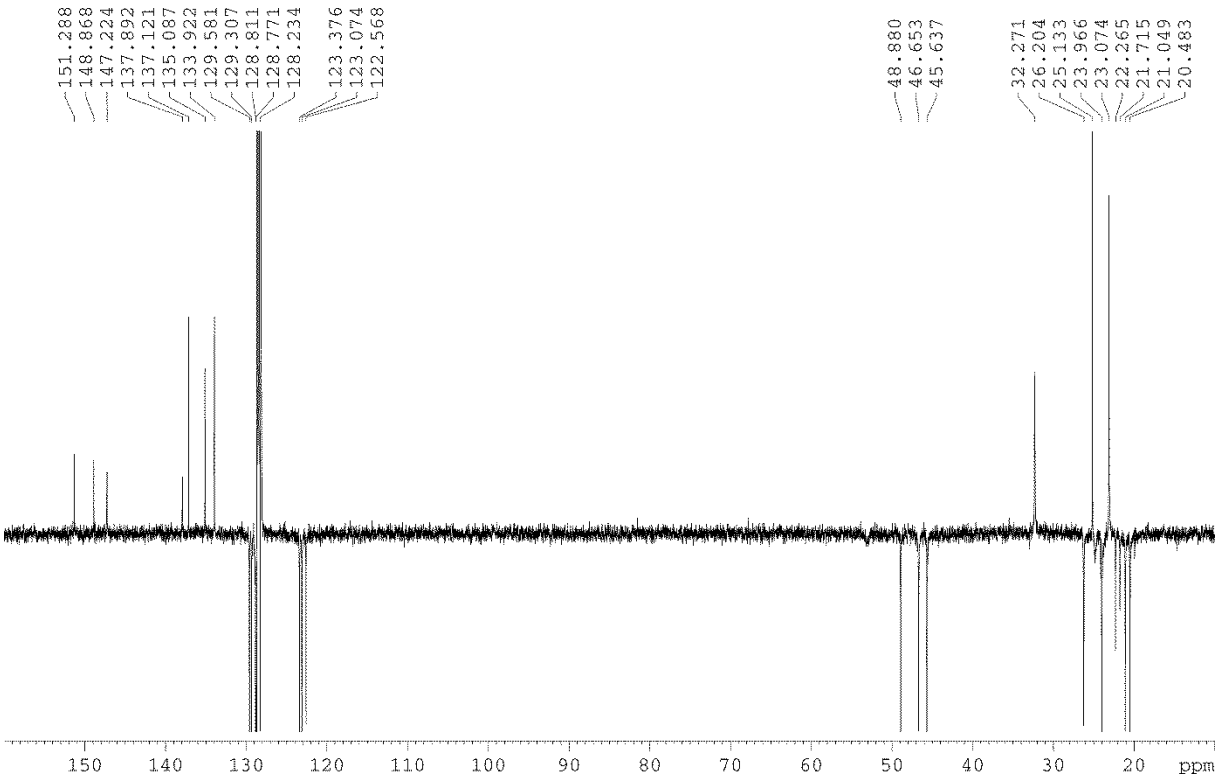

Figure S19: $^{13}C\{^{1}H\}$ NMR spectrum of single-crystals of **8** in C_6D_6 showing two set of signals assigned to starting **1** proposed complex **8a**.

2) IR and Raman spectra of studied compounds.

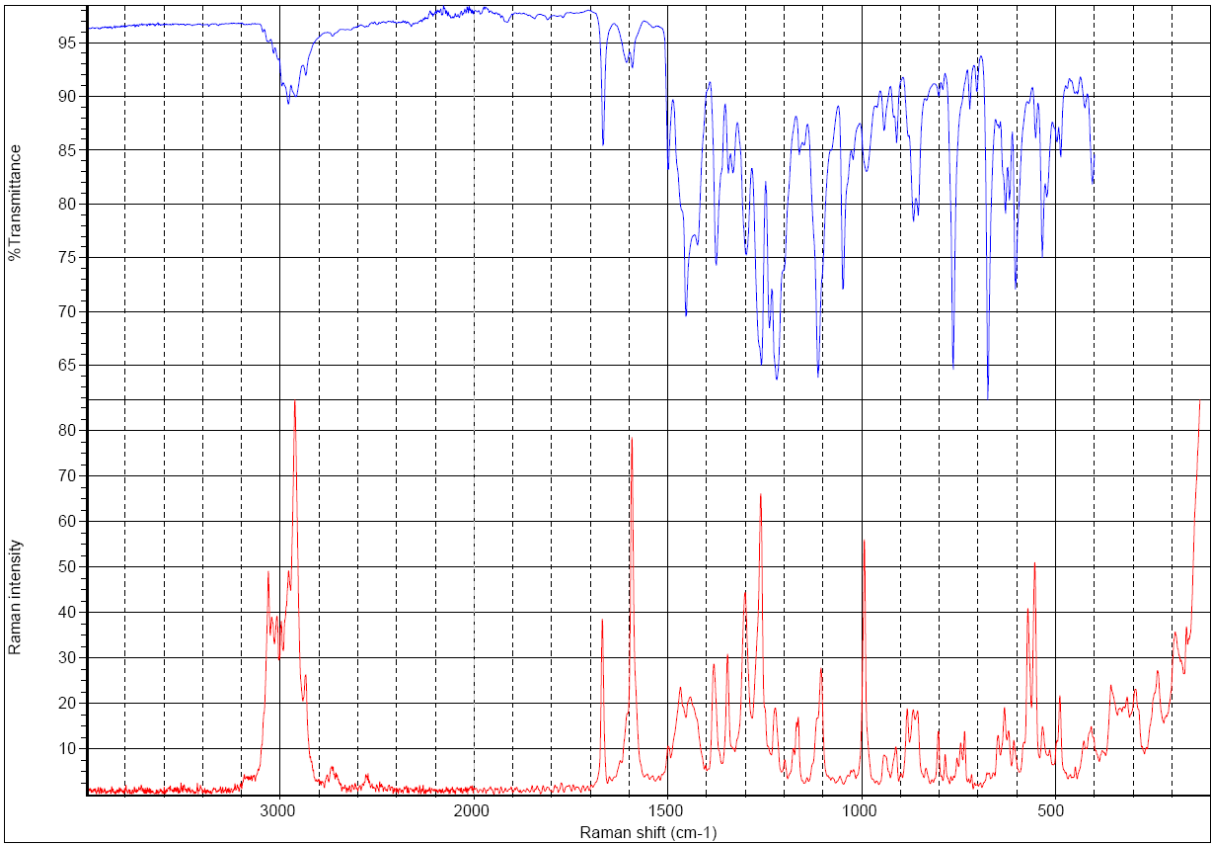

Figure S20: IR (top) and Raman (bottom) spectra of solid **4**.

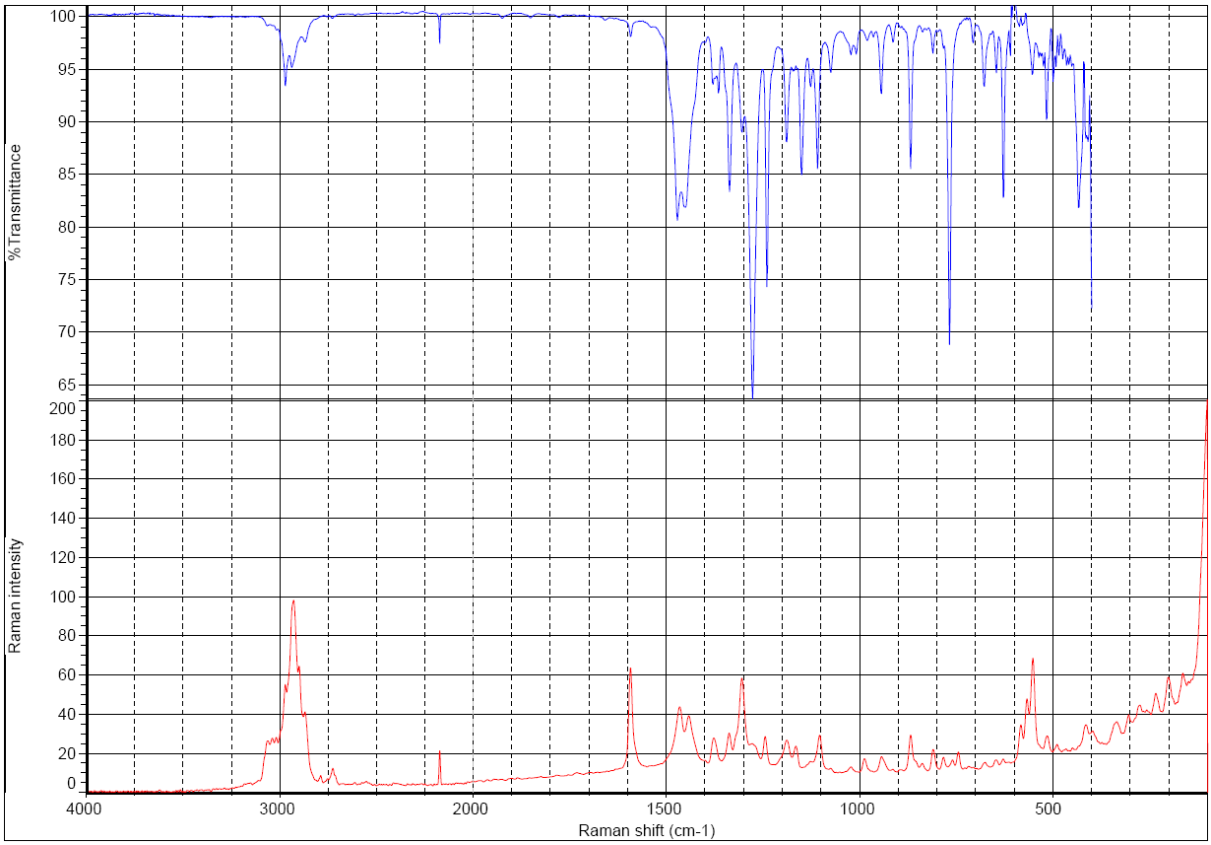

Figure S21: IR (top) and Raman (bottom) spectra of solid **6**.

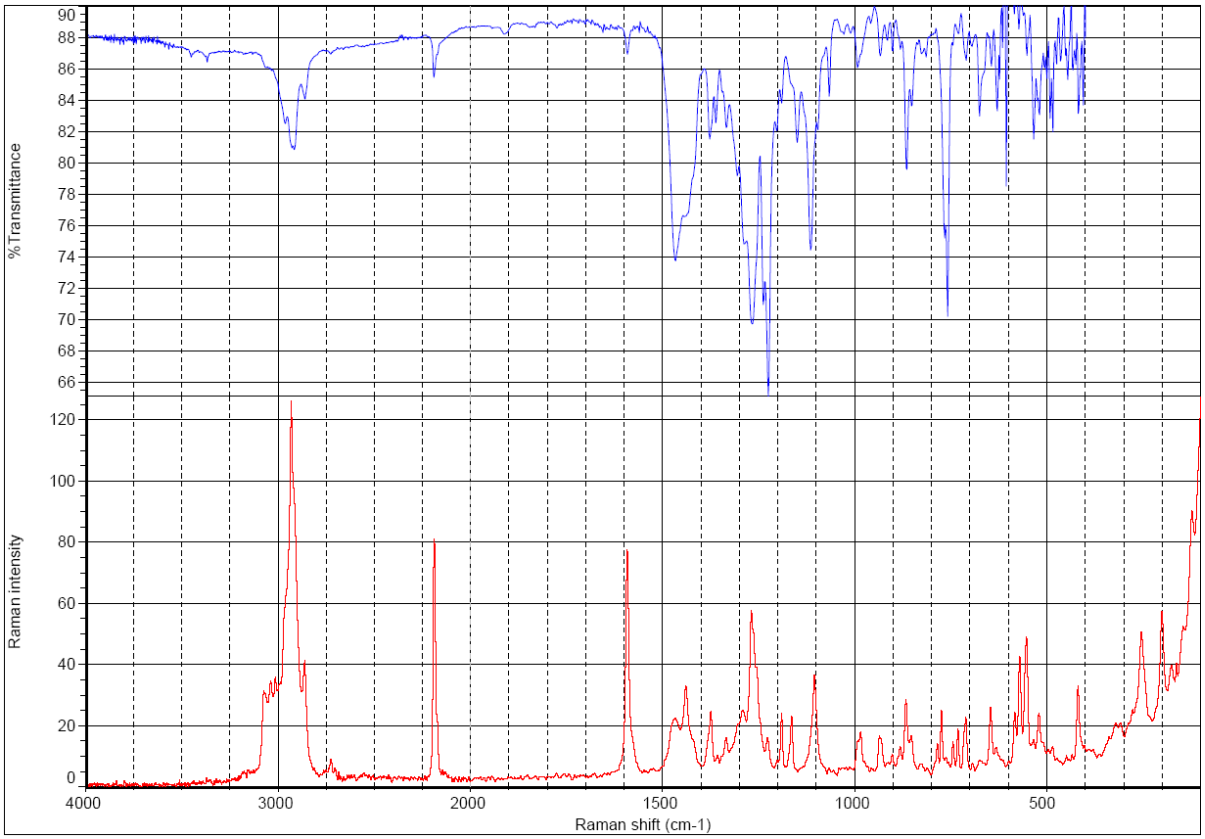

Figure S22: IR (top) and Raman (bottom) spectra of solid **7**.

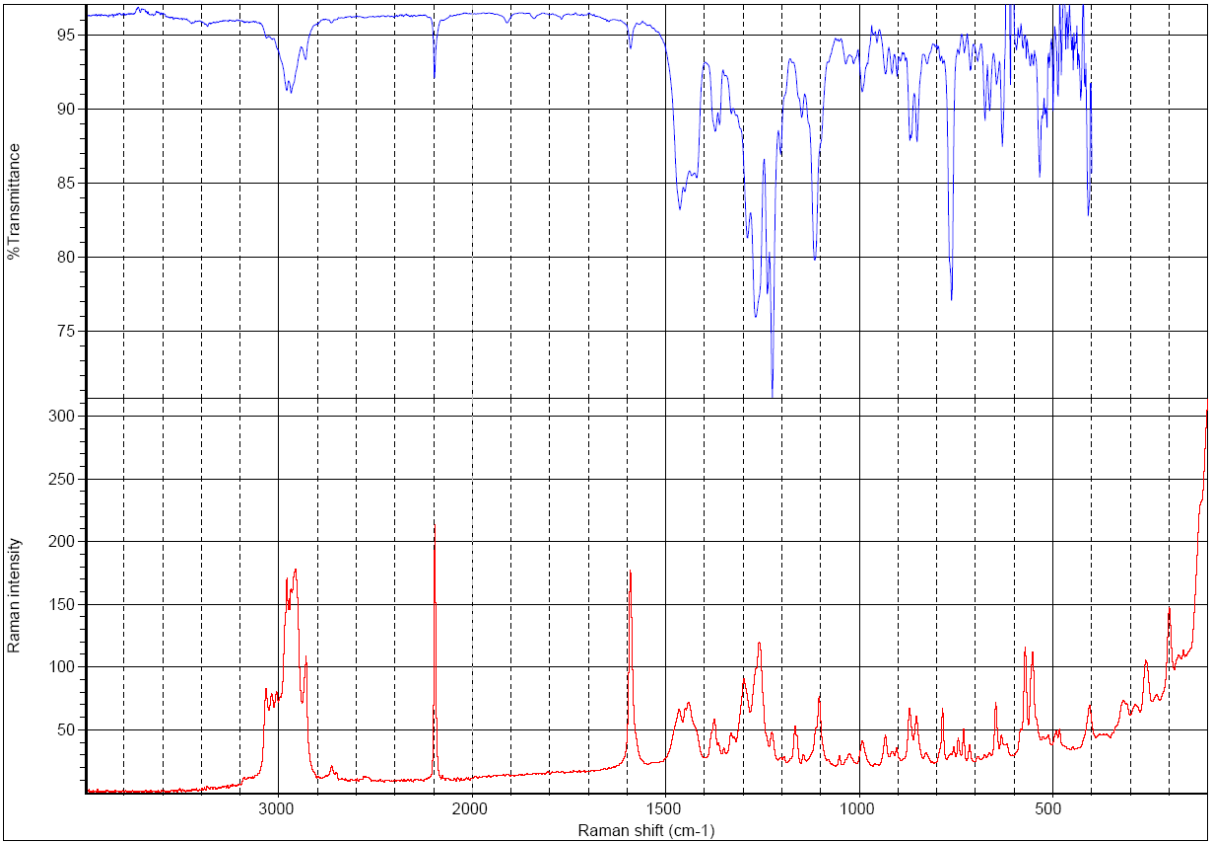

Figure S23: IR (top) and Raman (bottom) spectra of solid **8**.

3) Crystallographic data.

Table S1. Relevant crystallographic data for the studied compounds.

	2	**4**	**5**
chemical formula	$C_{52}H_{69}B_2F_3Ge_2N_6O.0.5(C_6H_6)$	$C_{67}H_{82}B_2F_5Ge_2N_6O$	$C_{29}H_{42}BGeN_5$
Cryst syst	monoclinic	Triclinic	monoclinic
Space group	$P2_1/c$	$P\text{-}1$	$P2_1/c$
a[Å]	13.3959(8)	13.2217(10)	16.9688(11)
b[Å]	10.9681(6)	13.5451(11)	11.0690(6)
c[Å]	19.050(2)	20.1024(15)	15.7622(13)
α[°]	90	78.791(2)	90
β[°]	100.283(7)	74.532(2)	102.325(6)
γ[°]	90	66.824(2)	90
Z	4	2	4
μ[mm^{-1}]	1.133	1.009	1.085
D_x [Mg m^{-3}]	1.218	1.307	1.249
Cryst size [mm]	0.59×0.51×0.39	0.29x0.20x0.19	0.37×0.19×0.13
ϑ range, [deg]	1-27	1-27.5	1-27.5
T_{min}, T_{max}	0.635, 0.763	0.5596, 0.7456	0.797, 0.900
no. of reflns measd	24 311	120 008	29 521
no. of unique reflns, R_{int}	5924, 0.029	14674, 0.035	6529, 0.033
no. of obsd reflns	5027	12670	5274
no. of params	298	763	325
S all data	1.111	1.038	1.115
final R indices [$I>2\sigma(I)$]	0.033	0.042	0.034
wR2 indices (all data)	0.074	0.098	0.065
Δρ, max., min. [e $Å^{-3}$]	0.406, -0.443	0.837, -0.676	0.308, -0.362
Diffractometer	Bruker D8 - Venture	Bruker D8 - Venture	Bruker Nonius KappaCCD area detector
Absorption correction	Multi-scan; *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction.	Multi-scan; *SADABS2016*/2 - Bruker AXS area detector scaling and absorption correction	Integration Gaussian integration (Coppens, 1970)

Definitions: $R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Table S1 (continuation). Relevant crystallographic data for the studied compounds.

	6	**7**	**8**
chemical formula	$C_{27}H_{41}BGeN_4$	$C_{55}H_{79}B_2Ge_2N_7$	$C_{51}H_{74}B_2Ge_2N_7$
Cryst syst	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a[Å]	17.935(4)	14.1030(17)	16.2361(11)
b[Å]	13.777(3)	22.561(2)	14.0029(13)
c[Å]	22.017(4)	18.1100(18)	23.556(3)
α[°]	90	90	90
β[°]	95.854(8)	112.285(6)	106.592(7)
γ[°]	90	90	90
Z	4	4	4
μ[mm^{-1}]	1.164	1.170	1.211
D_x [Mg m^{-3}]	1.297	1.252	1.232
Cryst size [mm]	0.60×0.54×0.41	0.35x0.19x0.15	0.43×0.27×0.25
ϑ range, [deg]	1-27.5	1-27.5	1-27
T_{min}, T_{max}	0.4836, 0.7455	0.764, 0.880	0.736, 0.830
no. of reflns measd	89 593	61 097	54 633
no. of unique reflns, R_{int}	12206, 0.103	12060, 0.081	11084, 0.056
no. of obsd reflns	8277	7887	8035
no. of params	611	595	559
S all data	1.044	1.093	1.106
final R indices [$I>2\sigma(I)$]	0.084	0.068	0.046
wR2 indices (all data)	0.23	0.121	0.086
Δρ, max., min. [e $Å^{-3}$]	1.407, -1.721	3.109, -2.445	0.795, -0.606
Diffractometer	Bruker Nonius KappaCCD area detector	Bruker Nonius KappaCCD area detector	Bruker Nonius KappaCCD area detector
Absorption correction	Integration Gaussian integration (Coppens, 1970)	Integration Gaussian integration (Coppens, 1970)	Integration Gaussian integration (Coppens, 1970)

Definitions: $R_{int} = \sum | F_o^2 - F_{o,mean}^2 | / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum | | F_o | - | F_c | | / \sum | F_o |$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.