Supporting Information

Coordination Chemistry of Cyclic Disilylated Germylenes and Stannylenes with Group 11 Metals

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Table S1. Crystallographic data for compounds **3**, **4**, **5**, **6**, and **7**

	3	**4**	**5**	**6**	**7**
Empirical formula	$Au_2C_{45}H_{123}Ge_2Si_{16}P_2N_2$	$Au_2C_{46}H_{126}Ge_6Si_{12}P_2N_2$	$AuC_{41}H_{63}GeSi_8PNBF_{15}$	$AuC_{41}H_{63}Ge_3Si_6PNBF_{15}$	$AgC_{23}H_{63}GeSi_8PN$
M_w	1743.20	1935.98	1390.98	1479.98	789.89
Temperature [K]	100(2)	100(2)	100(2)	100(2)	100(2)
Size [mm]	0.28×0.22×0.16	0.36×0.30×0.22	0.36×0.28×0.22	0.45×0.30×0.20	0.50×0.35×0.35
Crystal system	monoclinic	monoclinic	orthorhombic	orthorhombic	monoclinic
Space group	P2(1)/c	P2(1)/c	Pna2(1)	Pna2(1)	P2(1)/n
a [Å]	31.802(6)	31.891(6)	22.063(4)	22.115(5)	12.630(3)
b [Å]	11.961(2)	11.972(2)	13.469(3)	13.491(3)	13.505(3)
c [Å]	23.279(5)	23.341(5)	20.265(4)	20.317(4)	27.281(6)
α [°]	90	90	90	90	90
β [°]	109.46(3)	109.47(3)	90	90	97.03(3)
γ [°]	90	90	90	90	90
V [Å ^{3}]	8349(3)	8402(3)	6022(2)	6062(2)	4619(2)
Z	4	4	4	4	4
ρ_{calc} [gcm^{-3}]	1.387	1.530	1.534	1.622	1.136
Absorption coefficient [mm^{-1}]	4.512	5.830	3.192	4.106	1.330
F(000)	3533	3856	2776	2920	1656
θ range	1.75<θ<26.38	1.75<θ<26.37	1.77<θ<26.36	1.77<θ<26.37	1.50<θ<26.37
Reflections collected/unique	65167/17040	65835/17165	46025/12169	32732/9936	36138/9419
Completeness to θ [%]	99.8	99.9	99.9	99.0	99.9
Data/restraints/parameters	17040/32/706	17165/30/754	12169/1/642	9936/1/642	9419/8/348
Goodness of fit on F^2	1.19	1.08	0.92	0.99	1.05
Final R indices [I>2σ(I)]	R1=0.075, *w*R2=0.142	R1=0.059, *w*R2=0.100	R1=0.023, *w*R2=0.051	R1=0.035, *w*R2=0.072	R1=0.064, *w*R2=0.159
R indices (all data)	R1=0.095, *w*R2=0.148	R1=0.066, *w*R2=0.106	R1=0.025, *w*R2=0.052	R1=0.039, *w*R2=0.073	R1=0.085 *w*R2=0.172
Largest diff. Peak/hole [$e^-/Å^3$]	2.15/-1.87	1.97/-1.79	1.22/-0.39	2.08/-1.06	1.58/-1.21

Table S2. Crystallographic data for compounds **8**, **10**, **12**, and **13**.

	8	**10**	**12**	**13**
Empirical formula	$CuC_{23}H_{63}GeSi_8PN$	$CuC_{41}H_{63}GeSi_8PNBF_{15}$	$Au_2Sn_2C_{45}H_{125}Si_{16}P_2N_2$	$AuC_{41}H_{63}SnSi_8PNBF_{15}$
M_w	745.56	1257.55	1839.66	1437.08
Temperature [K]	100(2)	100(2)	180(2)	100(2)
Size [mm]	0.36×0.30×0.22	0.45×0.36×0.18	0.35×0.26×0.24	0.24×0.18×0.14
Crystal system	monoclinic	orthorhombic	monoclinic	monoclinic
Space group	P2(1)/n	Pna2(1)/c	P2(1)/c	P2(1)/c
a [Å]	12.587(3)	22.059(3)	32.214(6)	13.099(3)
b [Å]	13.373(3)	13.517(3)	12.094(2)	25.632(5)
c [Å]	26.515(5)	19.985(4)	23.532(5)	18.775(4)
α [°]	90	90	90	90
β [°]	96.89(3)	90)	109.54(3)	106.54(3)
γ [°]	90	90	90	90
V [Å ^{3}]	4431(2)	5959(3)	8639(3)	6043(2)
Z	4	4	4	4
ρ_{calc} [gcm^{-3}]	1.118	1.402	1.414	1.579
Absorption coefficient [mm^{-1}]	1.424	1.125	4.243	3.098
F(000)	1584	2576	3688	2848
θ range	1.55<θ<25.00	1.77<θ<26.36	1.81<θ<26.38	1.38<θ<26.35
Reflections collected/unique	30694/7777	30611/11727	67534/17576	48105/12315
Completeness to θ [%]	100	99.8	99.5	99.8
Data/restraints/parameters	7777/48/335	11727/1/642	17576/0/688	12315/0/641
Goodness of fit on F^2	1.03	0.97	1.00	1.05
Final R indices [I>2σ(I)]	R1=0.097, *w*R2=0.222	R1=0.028, *w*R2=0.060	R1=0.0413, *w*R2=0.084	R1=0.033, *w*R2=0.076
R indices (all data)	R1=0.154, *w*R2=0.250	R1=0.031, *w*R2=0.0618	R1=0.064, *w*R2=0.091	R1=0.038, *w*R2=0.078
Largest diff. Peak/hole [e^-/ $Å^3$]	1.19/-0.96	0.64/-0.26	1.18/-0.80	1.16/-4.01

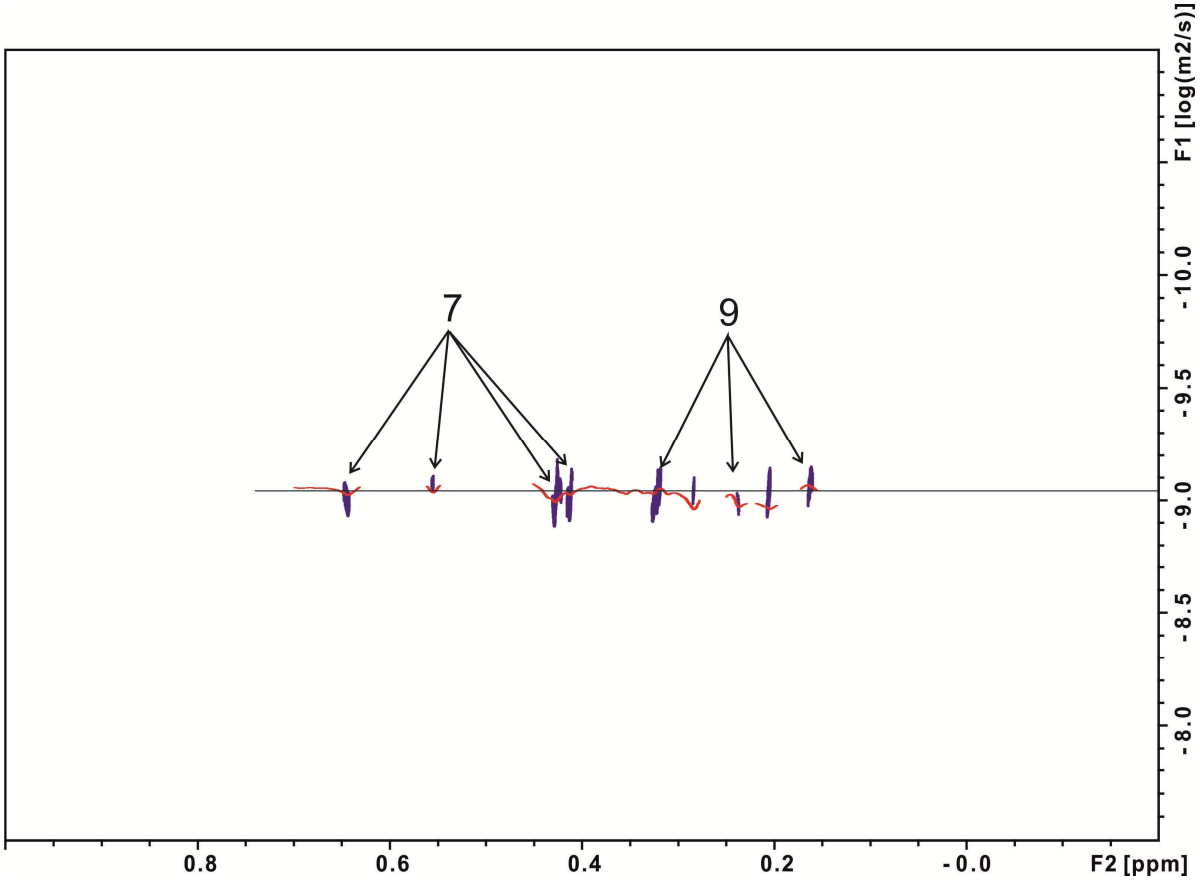


Figure S1. Overlay of a regular (red) and a homonuclear broadband decoupled 2D DOSY (blue). Signals belonging to compounds **7** and **9** are indicated.

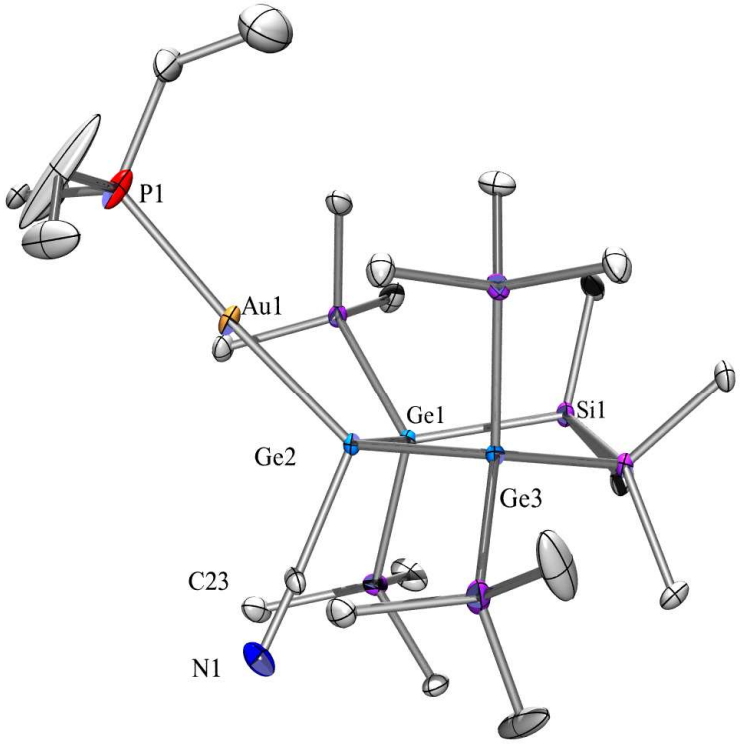


Figure S2. Crystal structure of **4**. Displacement ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity (bond lengths in Å, angles in deg). Au(1)-P(1) 2.320(2), Au(1)-Ge(2) 2.4292(8), C(1)-Si(1) 1.880(7), C(17)-P(1) 1.813(8), C(19)-C(20) 1.254(18), C(23)-N(1) 1.147(8), C(23)-Ge(2) 1.979(7), Ge(1)-Si(4) 2.3751(19), Ge(1)-Ge(2) 2.4520(10), Si(1)-Si(2) 2.354(3), P(1)-Au(1)-Ge(2) 175.70(7), N(1)-C(23)-Ge(2) 177.7(6), C(23)-Ge(2)-Au(1) 108.27(19).

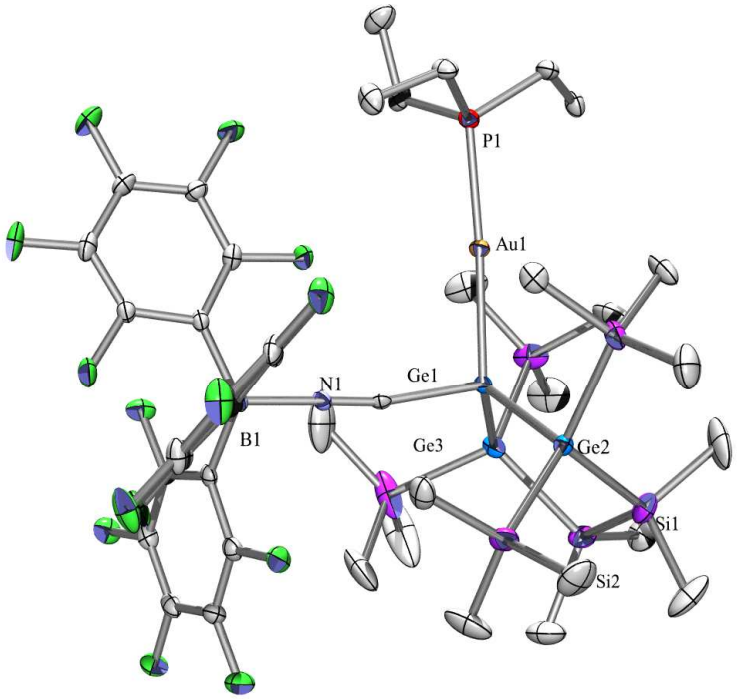


Figure S3. Crystal structure of **6**. Displacement ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity (bond lengths in Å, angles in deg). Au(1)-P(1) 2.3025(17), Au(1)-Ge(1) 2.4145(7), P(1)-C(18) 1.815(7), N(1)-C(17) 1.134(6), N(1)-B(1) 1.582(7), Ge(1)-C(17) 2.018(5), Ge(1)-Ge(3) 2.4475(11), Ge(2)-Si(1) 2.3733(19), Si(1)-C(1) 1.883(10), Si(1)-Si(2) 2.350(3), C(24)-B(1) 1.628(9), C(31)-F(1) 1.365(6), P(1)-Au(1)-Ge(1) 176.61(4), C(17)-N(1)-B(1) 179.2(6), C(17)-Ge(1)-Au(1) 97.12(15), Au(1)-Ge(1)-Ge(3) 118.70(3), Au(1)-Ge(1)-Ge(2) 115.99(3), Ge(3)-Ge(1)-Ge(2) 110.08(3).

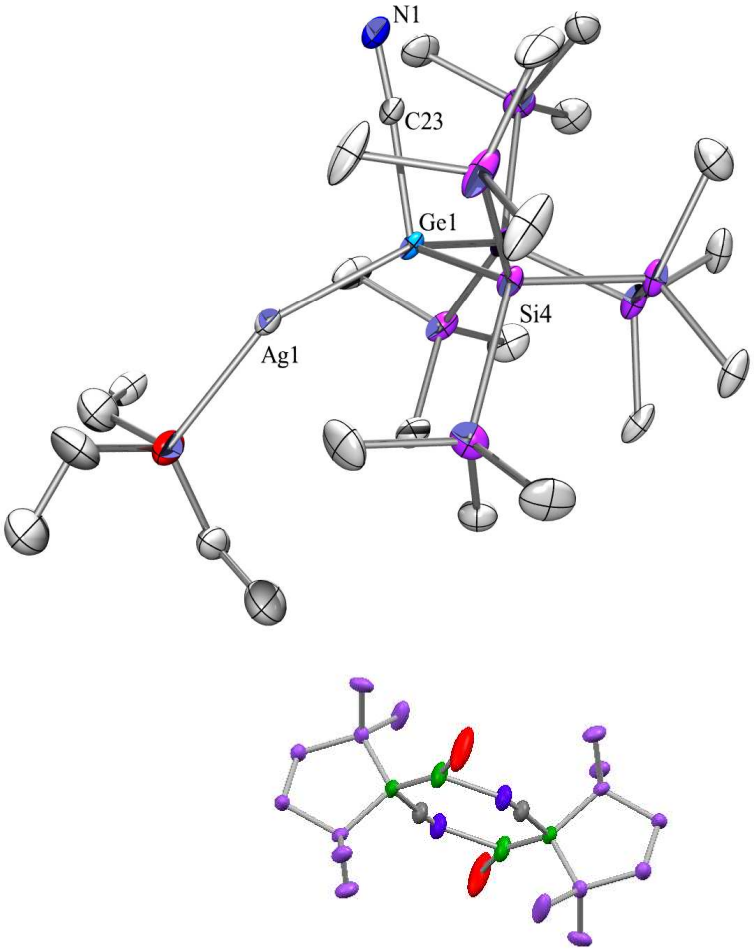


Figure S4. Crystal structure of **7**. Displacement ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity (bond lengths in Å, angles in deg). Ag(1)-P(1) 2.427(3), Ag(1)-N(1-1) 2.477(5), Ag(1)-Ge(1) 2.4850(8), Ge(1)-C(23) 1.986(5), Ge(1)-Si(4) 2.4271(16), C(23)-N(1) 1.146(7), Si(3)-Si(4) 2.340(2), Si(5)-C(5) 1.851(7), P(1)-C(17) 1.839(9), P(1)-Ag(1)-N(1-1) 94.81(13), P(1)-Ag(1)-Ge(1) 156.65(6), N(1-1)-Ag(1)-Ge(1) 108.43(12), C(23)-Ge(1)-Ag(1) 107.89(16), N(1)-C(23)-Ge(1) 176.4(5), C(23)-N(1)-Ag(1-1) 147.1(5).

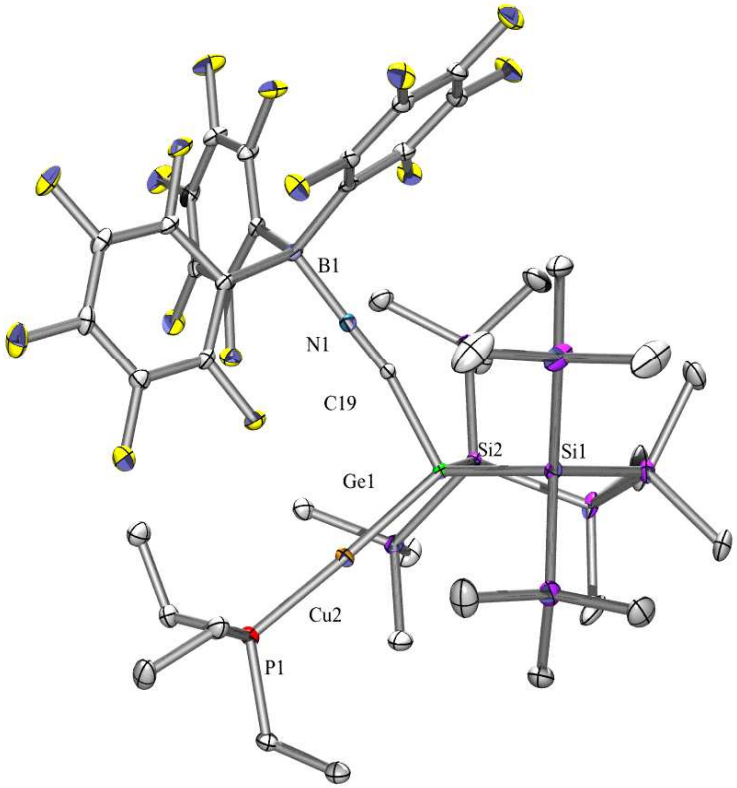


Figure S5. Crystal structure of **10**. Displacement ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity (bond lengths in Å, angles in deg). Ge(1)-C(19) 1.997(2), Ge(1)-Cu(2) 2.3166(5), Ge(1)-Si(1) 2.4102(8), Ge(1)-Si(2) 2.4134(8), Cu(2)-P(1) 2.2010(7), P(1)-C(20) 1.823(3), F(1)-C(2) 1.359(3), N(1)-C(19) 1.143(3), N(1)-B(1) 1.575(3), Si(1)-Si(5) 2.3348(11), Si(5)-C(41) 1.874(3), C(19)-Ge(1)-Cu(2) 98.02(6), Si(1)-Ge(1)-Si(2) 108.43(2), P(1)-Cu(2)-Ge(1) 176.97(2), N(1)-C(19)-Ge(1) 168.68(19).

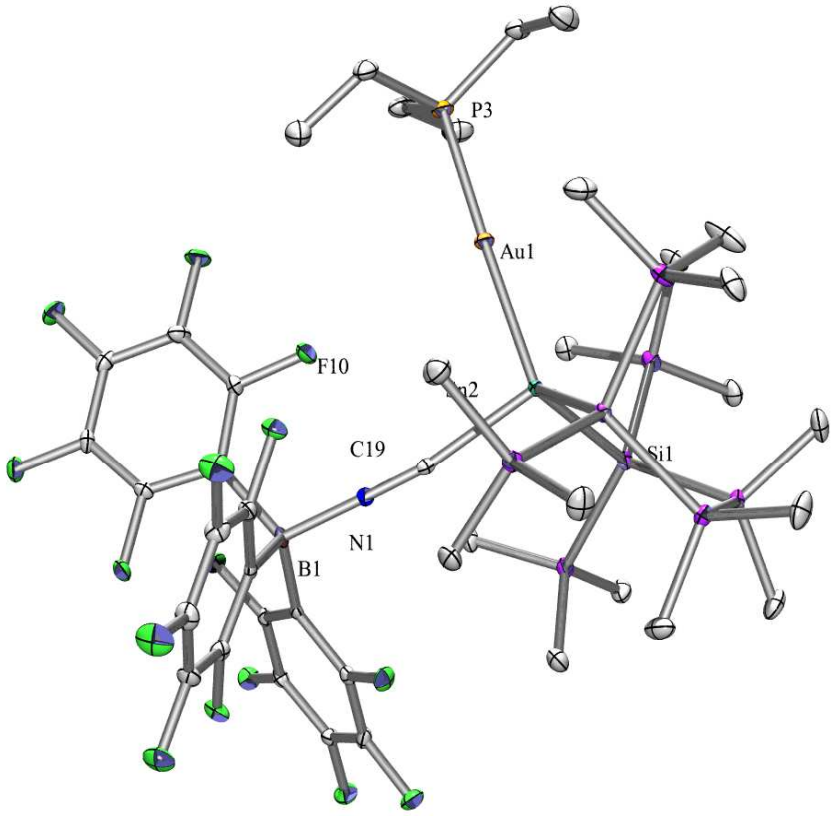
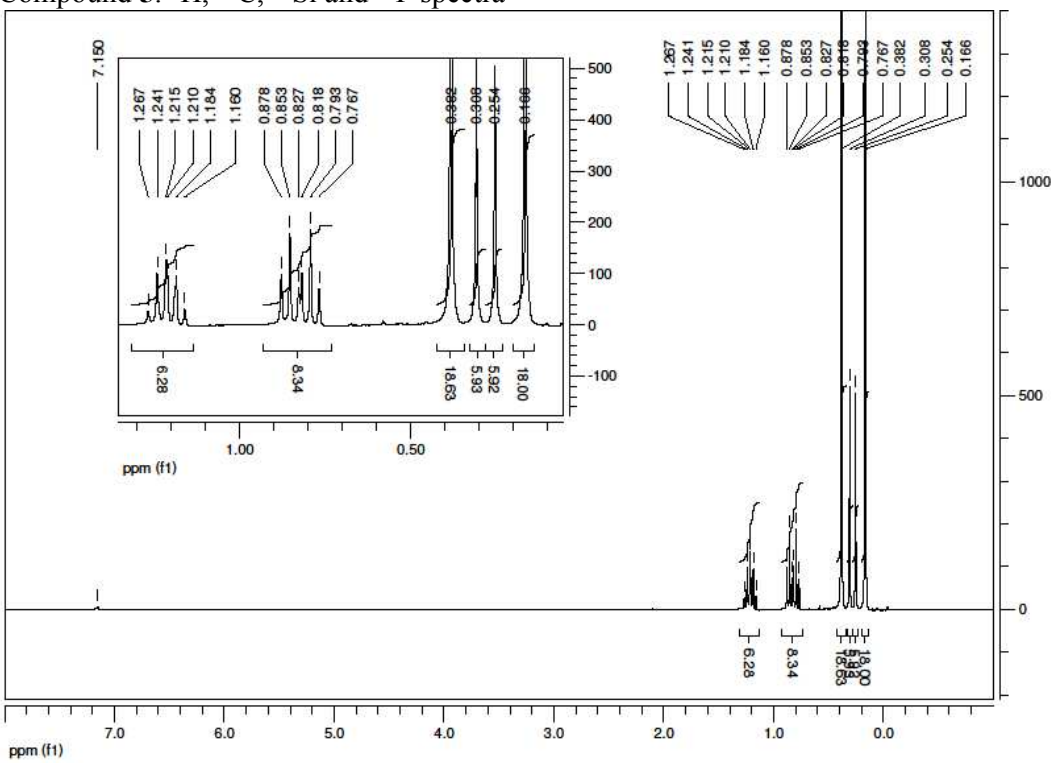
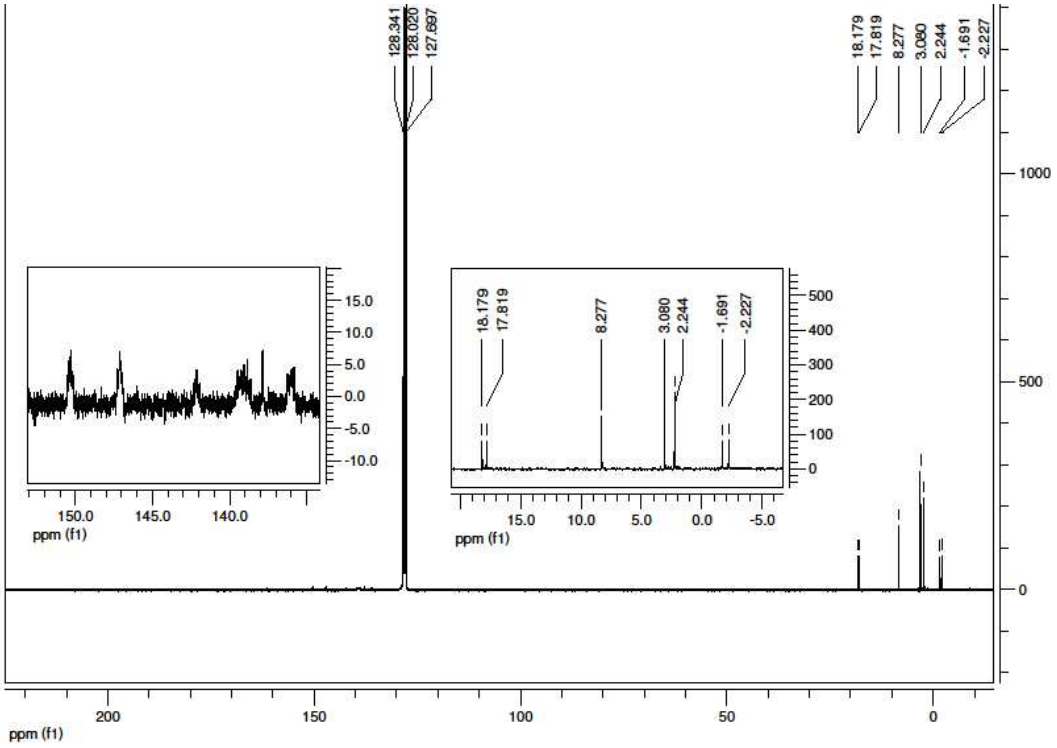
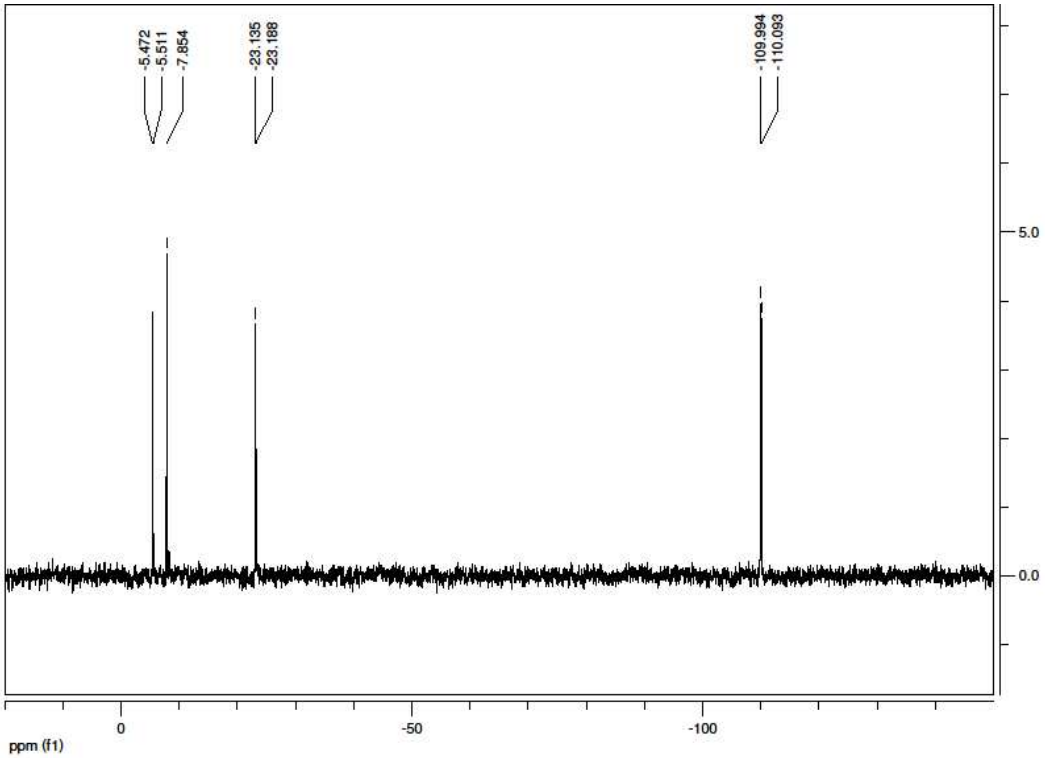


Figure S6. Crystal structure of **13**. Displacement ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity (bond lengths in Å, angles in deg). Au(1)-P(3) 2.3074(11), Au(1)-Sn(2) 2.5756(7), B(1)-N(1) 1.573(4), B(1)-C(7) 1.632(5), Si(1)-Si(5) 2.3514(14), Si(1)-Sn(2) 2.5888(11), Si(2)-C(21) 1.885(4), Si(4)-Sn(2) 2.5829(10), Sn(2)-C(19) 2.241(4), C(2)-F(1) 1.358(4), C(19)-N(1) 1.144(4), C(36)-P(3) 1.824(4), P(3)-Au(1)-Sn(2) 177.67(3), C(19)-Sn(2)-Au(1) 103.28(9), Si(4)-Sn(2)-Si(1) 105.32(4), N(1)-C(19)-Sn(2) 171.1(3).

Compound **5**: ^{1}H, ^{13}C, ^{29}Si and ^{19}F spectra



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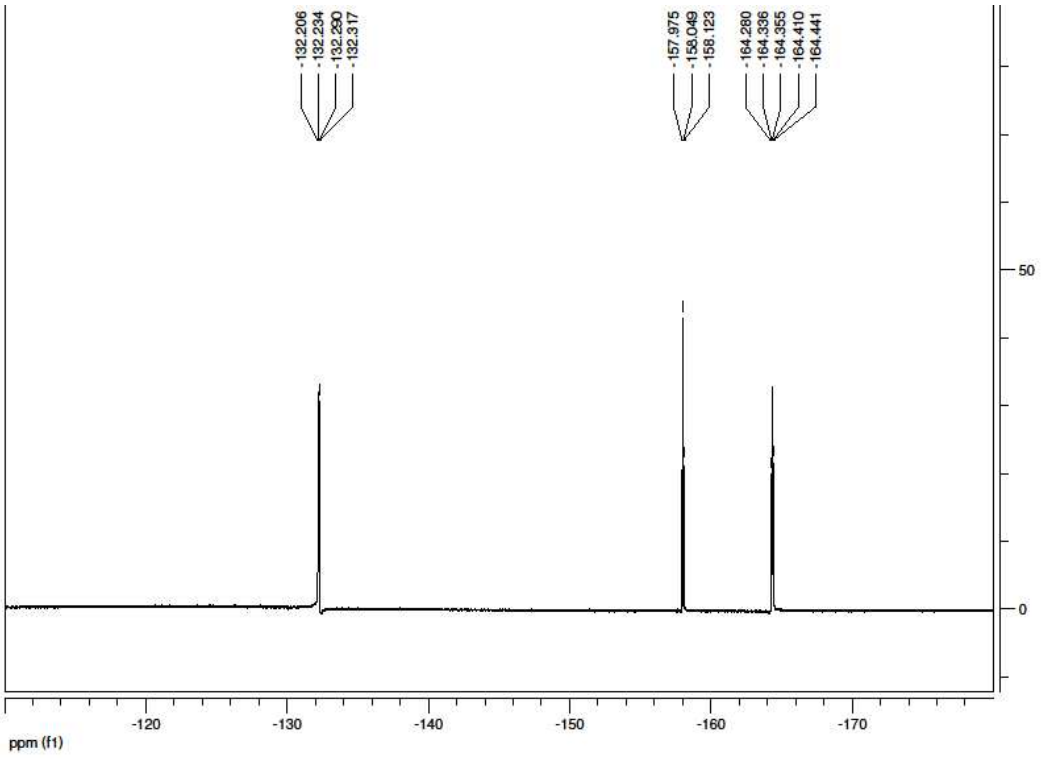
-100
ppm (f1)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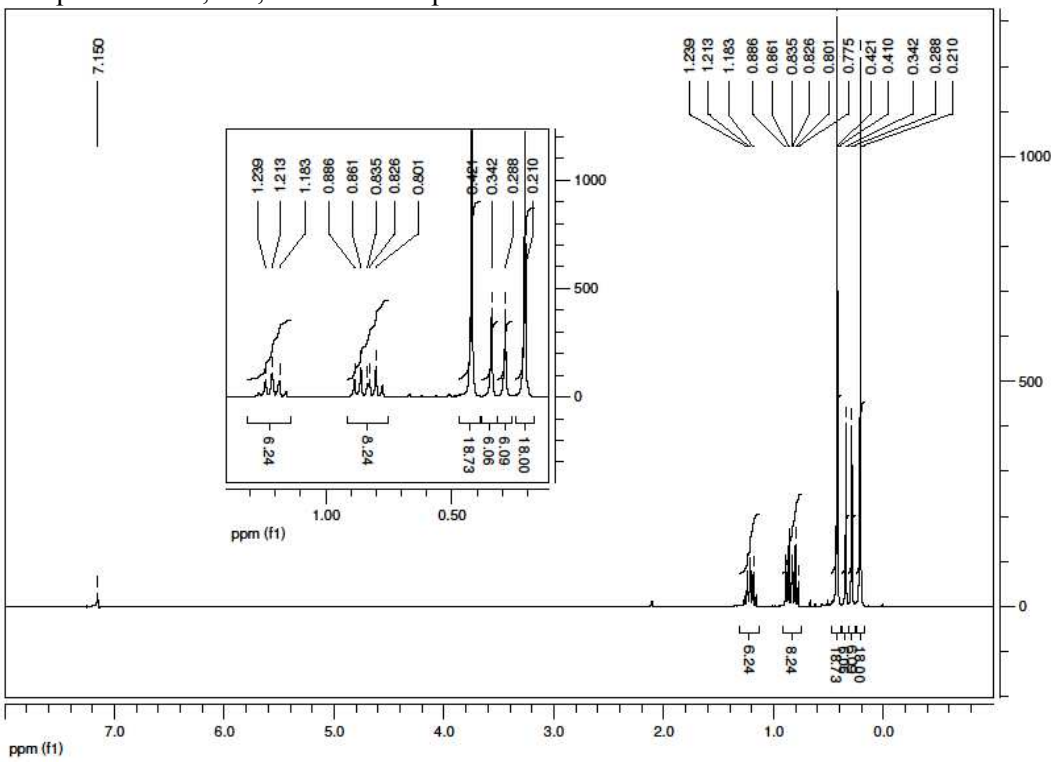
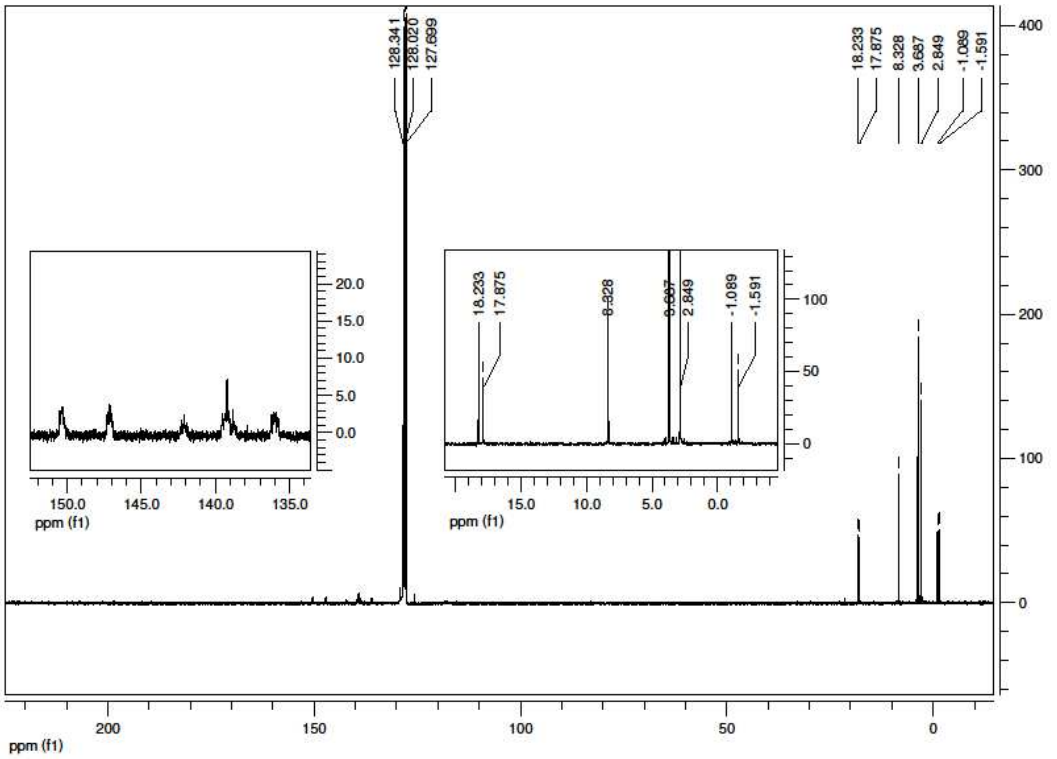
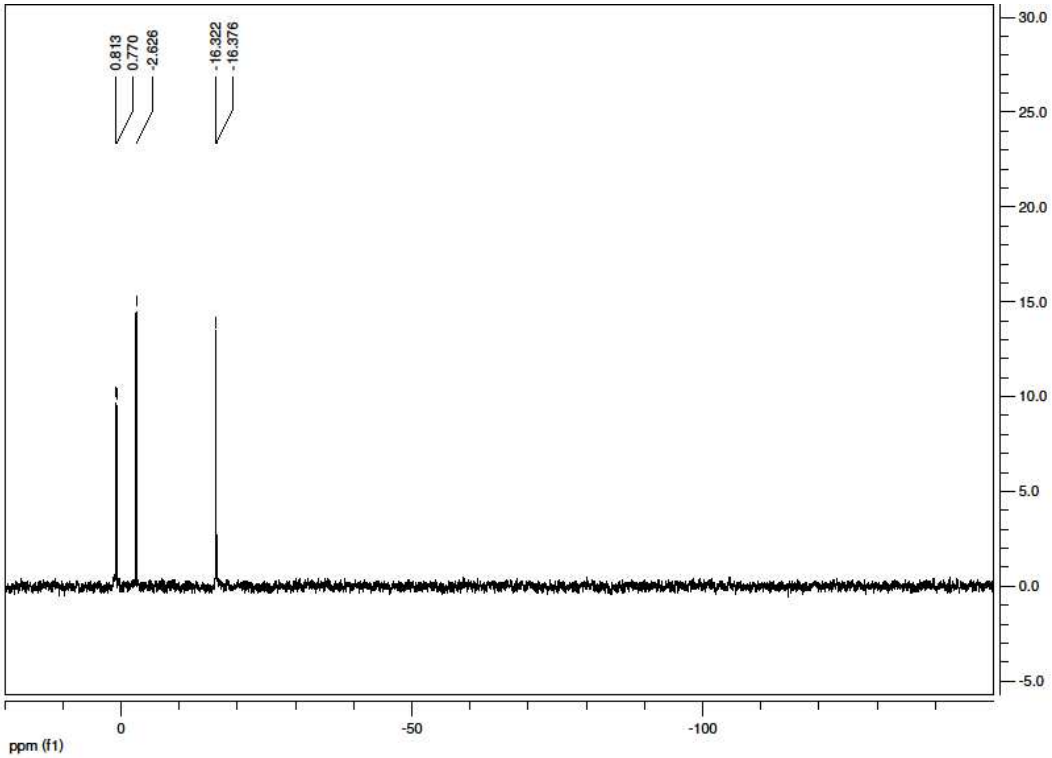
-164.410
-164.441
50
0
-120
-130
-140
-150
-160
-170
ppm (f1)

Compound **6**: ^{1}H, ^{13}C, ^{29}Si and ^{19}F spectra



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0
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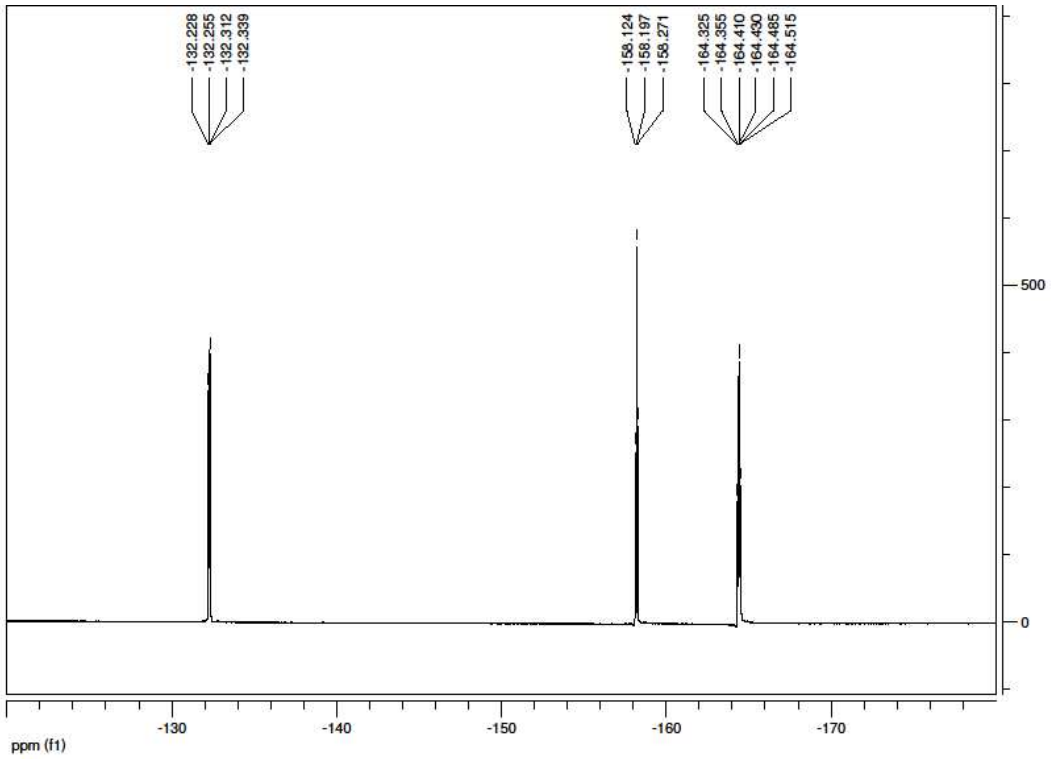
-100
ppm (f1)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-132.339
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-164.325
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-164.430
-164.485
-164.515
500
0
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-140
-150
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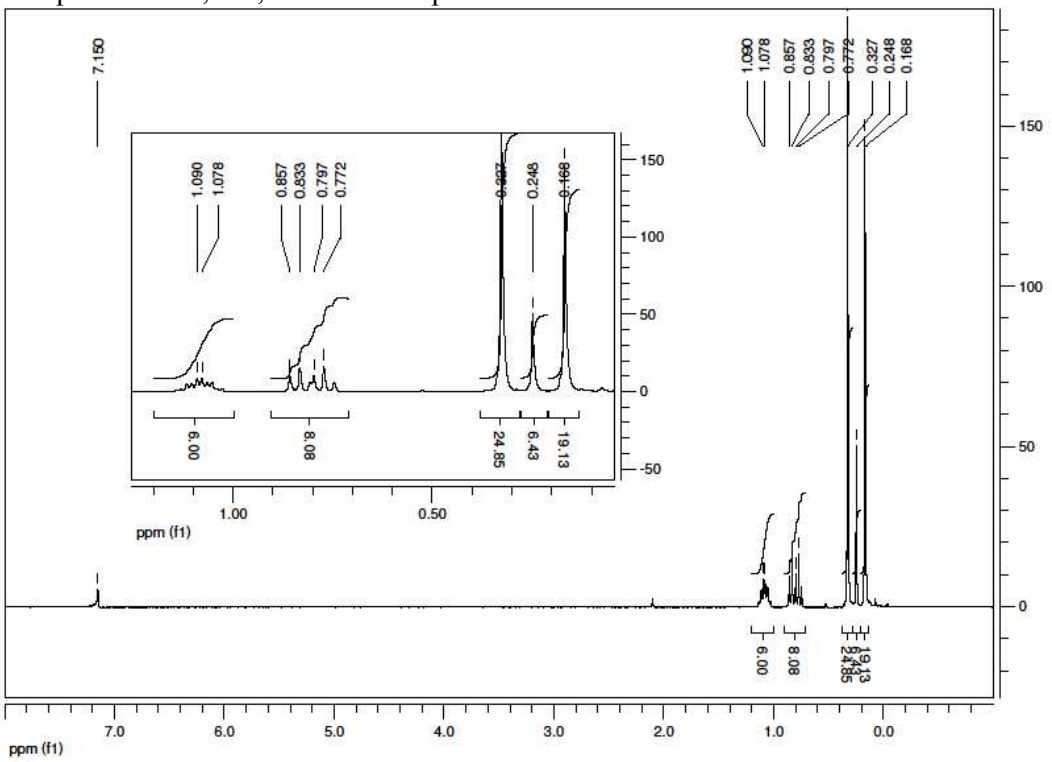
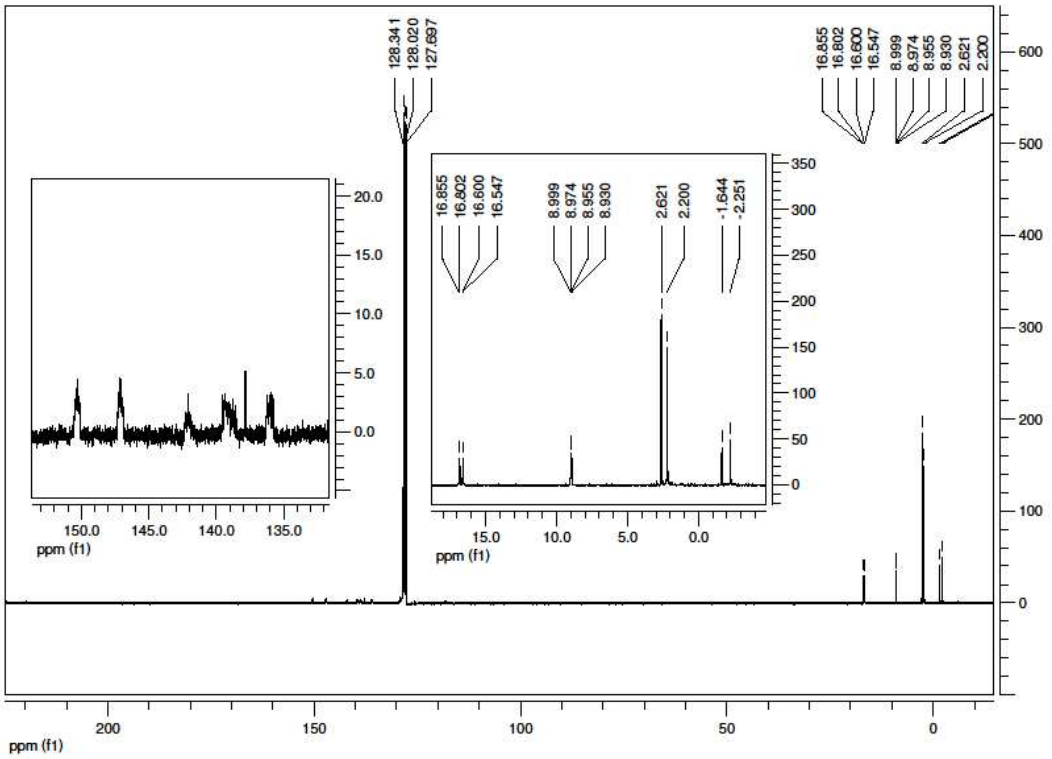
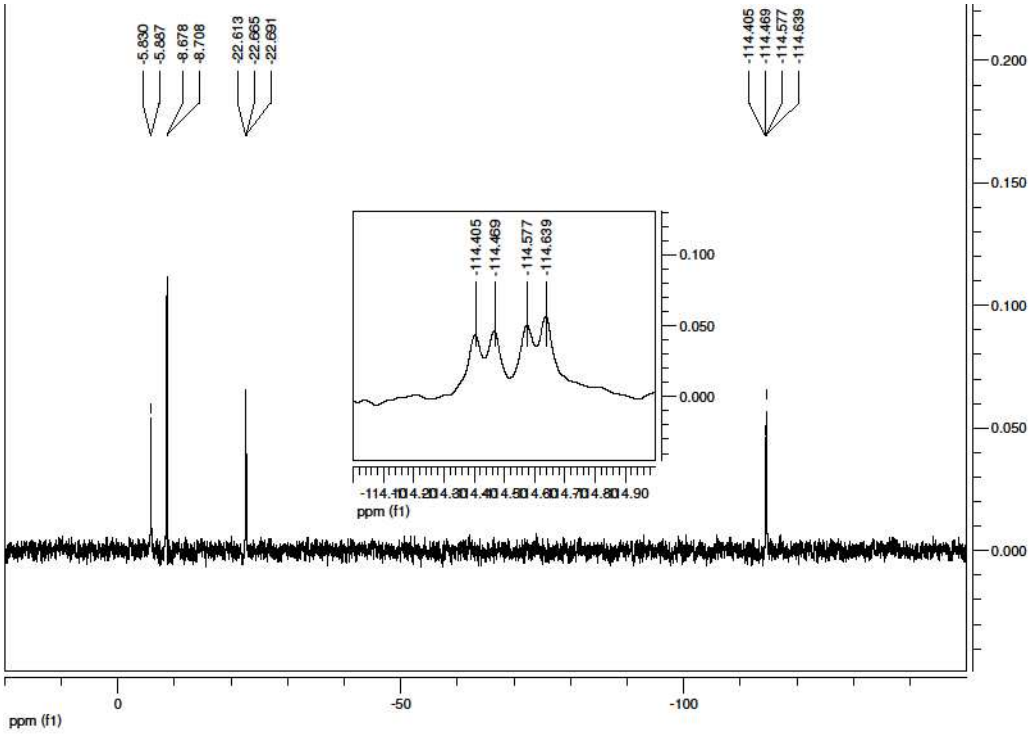
ppm (f1)

Compound **9**: ^{1}H, ^{13}C, ^{29}Si and ^{19}F spectra



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0.000
ppm (f1)
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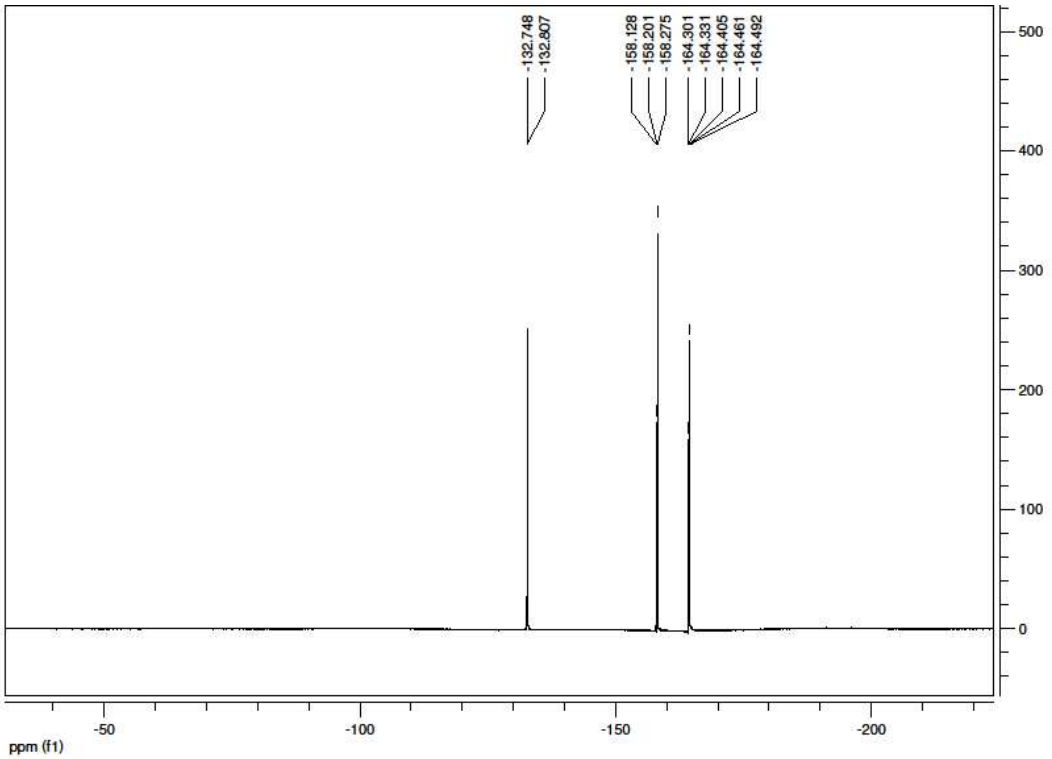
-100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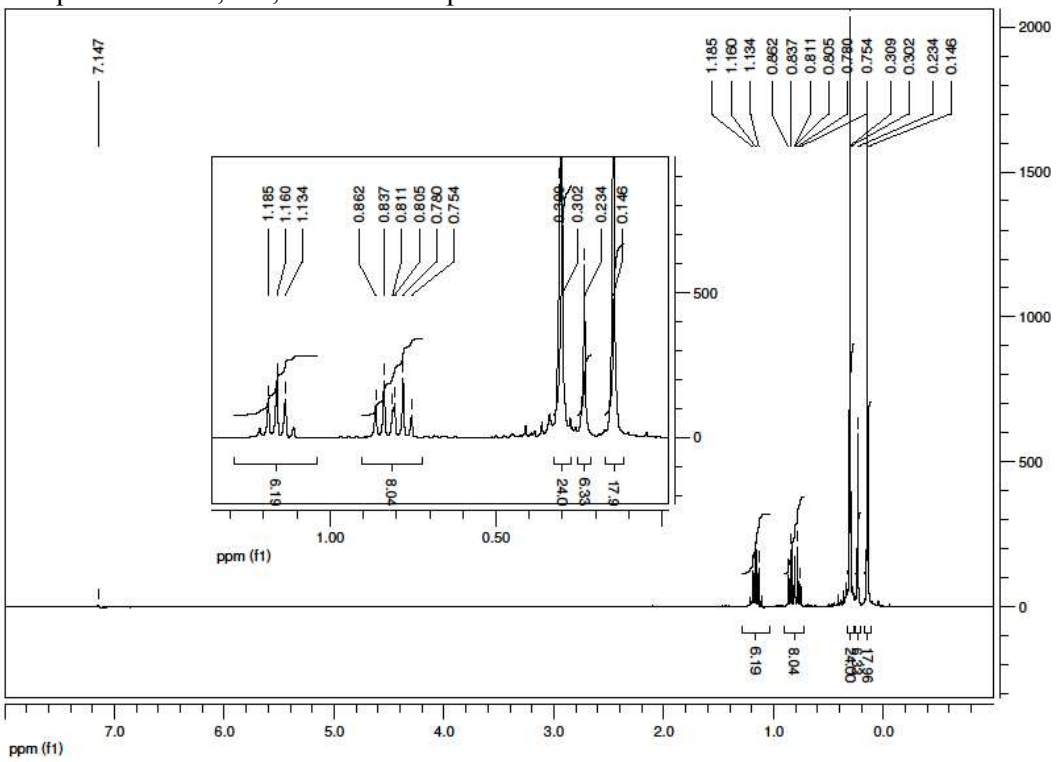
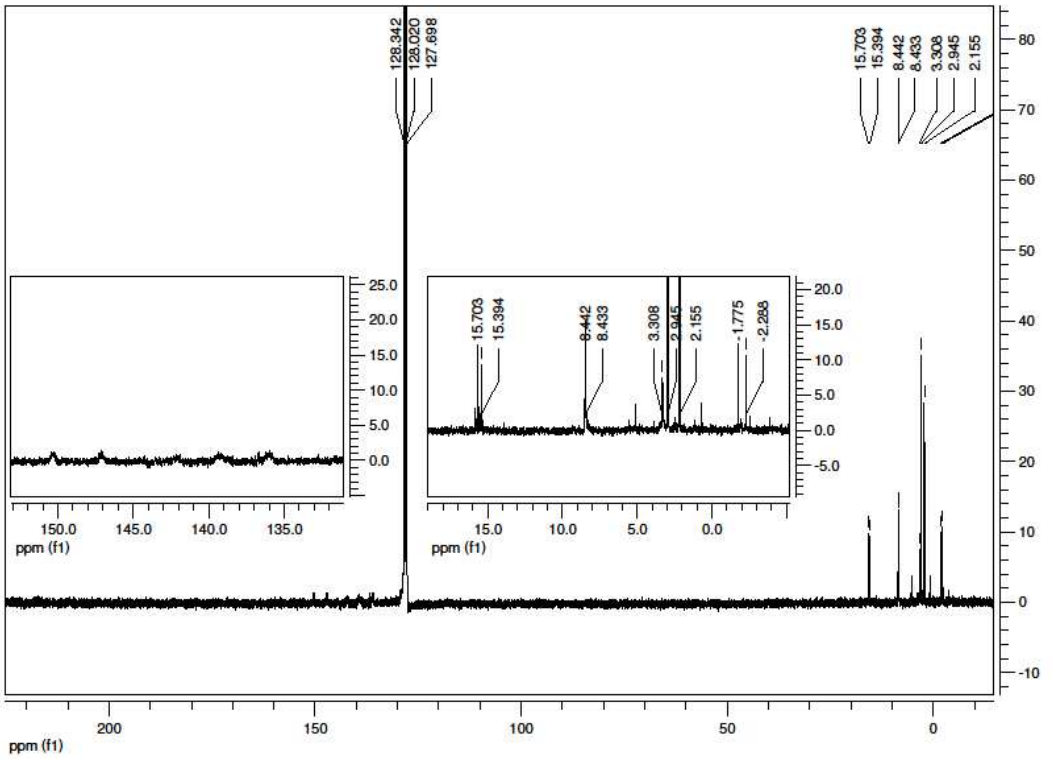
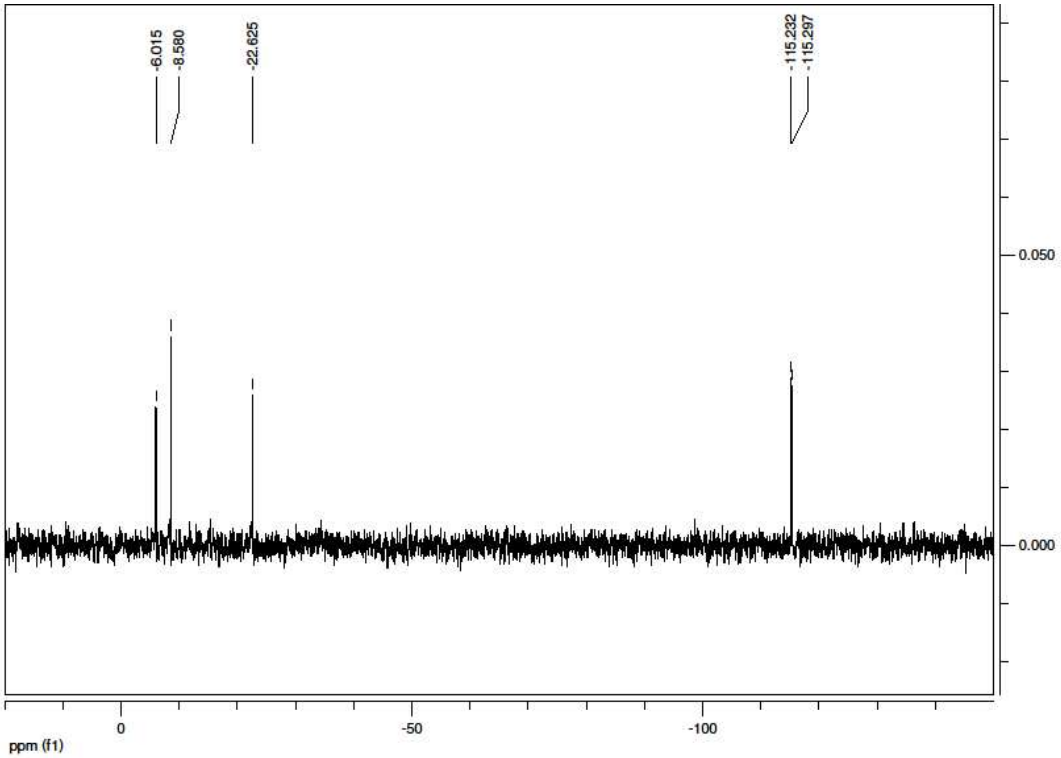
-158.128
-158.201
-158.275
-164.301
-164.331
-164.405
-164.461
-164.492
500
400
300
200
100
0
ppm (f1)
-50
-100
-150
-200

Compound **10**: ^{1}H, ^{13}C, ^{29}Si and ^{19}F spectra



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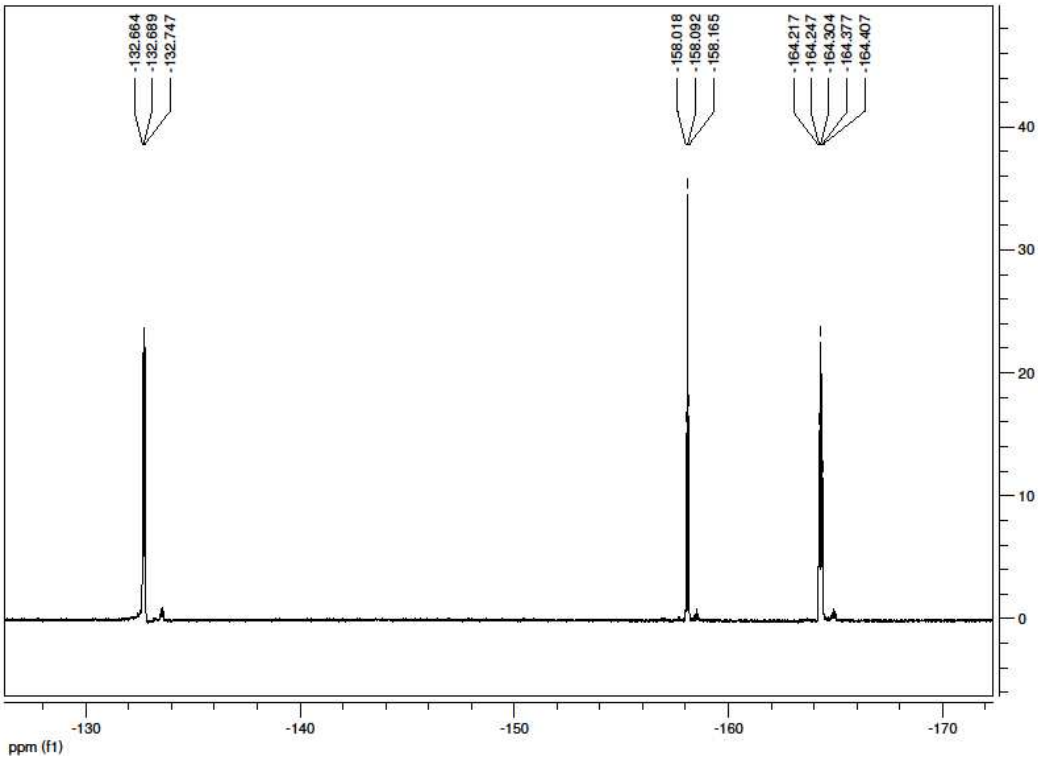
-115.297
0.050
0.000
0
-50
-100
ppm (f1)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-158.092
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-164.217
-164.247
-164.304
-164.377
-164.407
40
30
20
10
0
-130
-140
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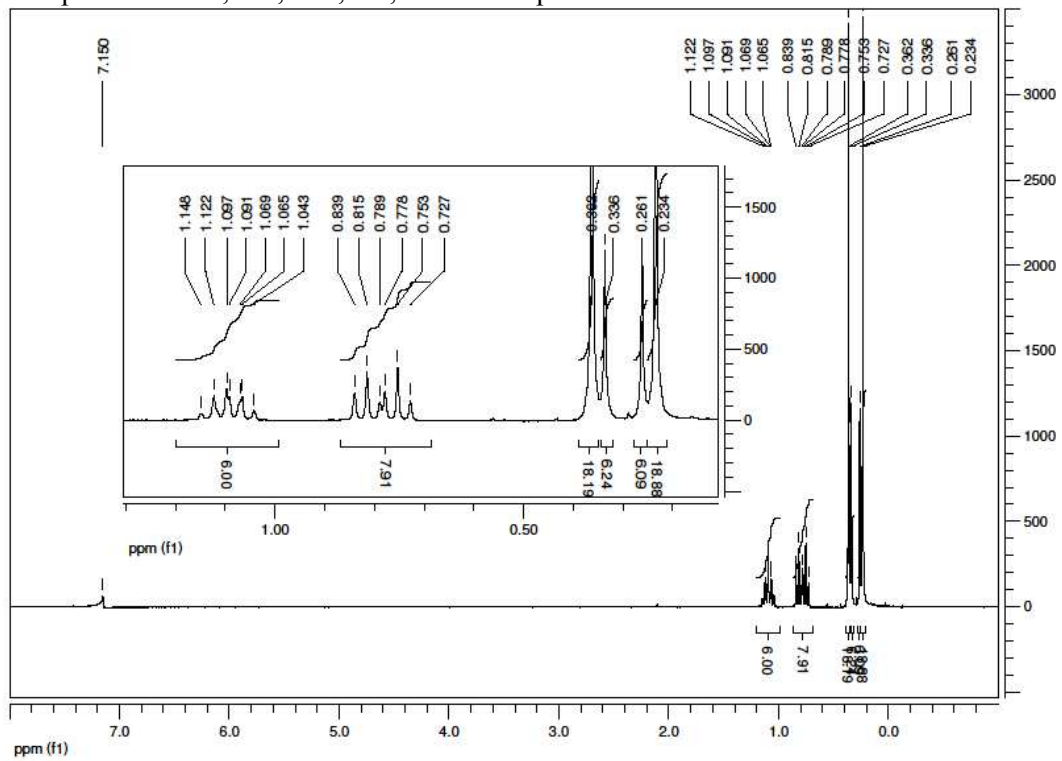
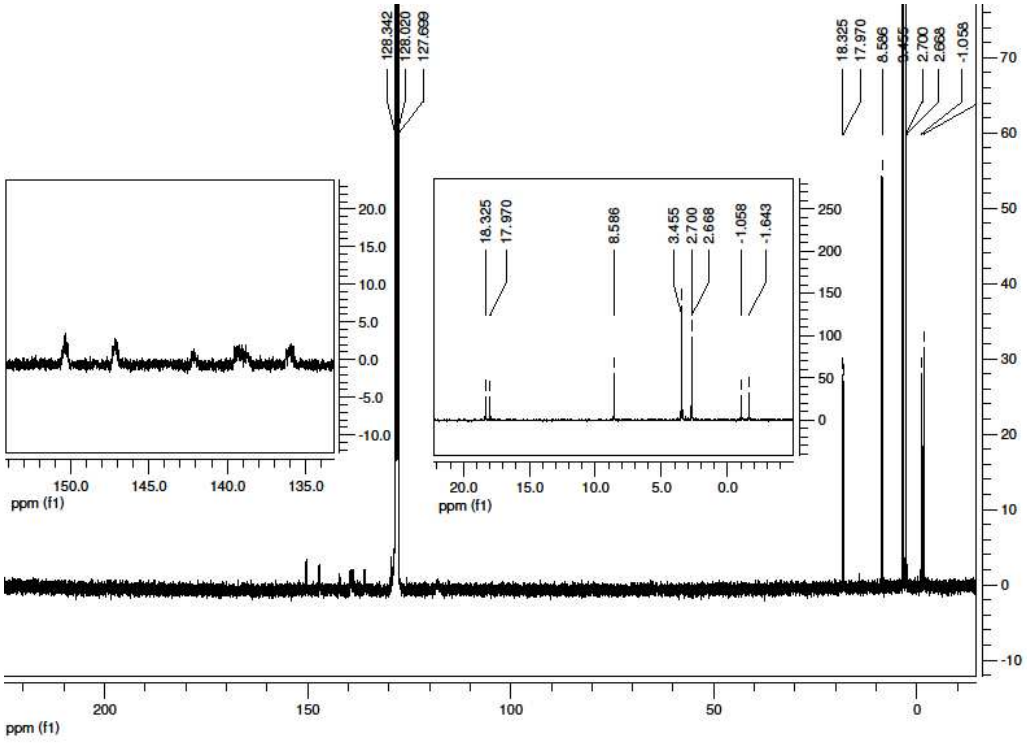
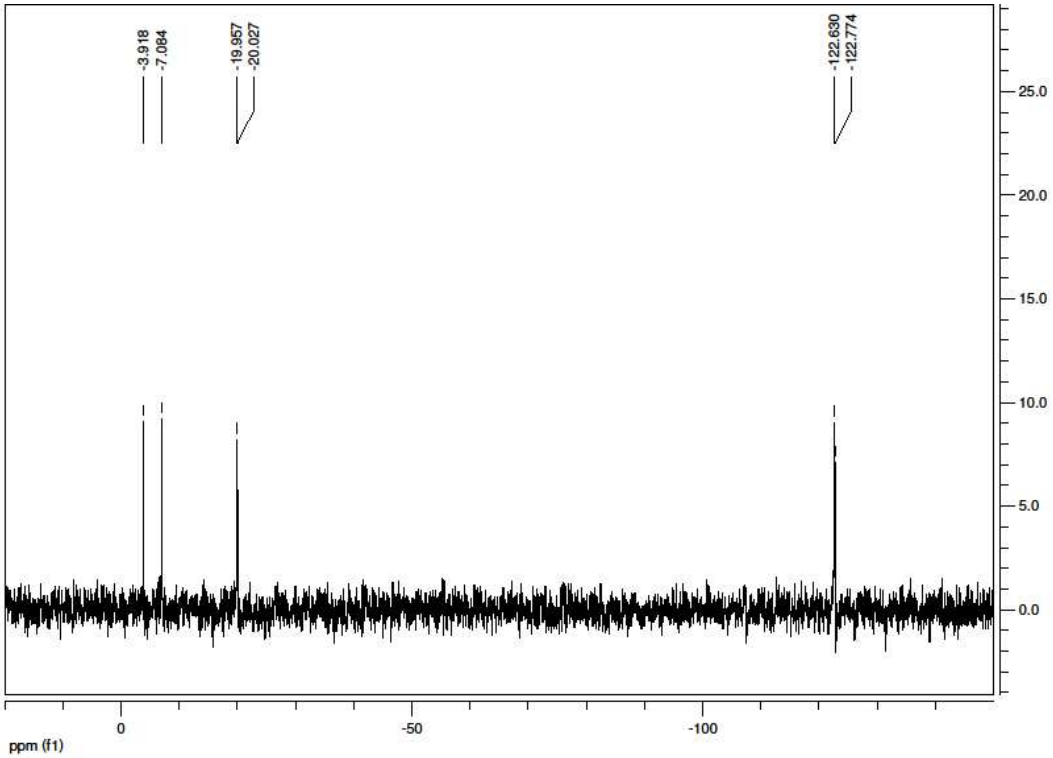
-160
-170
ppm (f1)

Compound **13**: ^{1}H, ^{13}C, ^{29}Si, ^{19}F, and ^{119}Sn spectra



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-20.027
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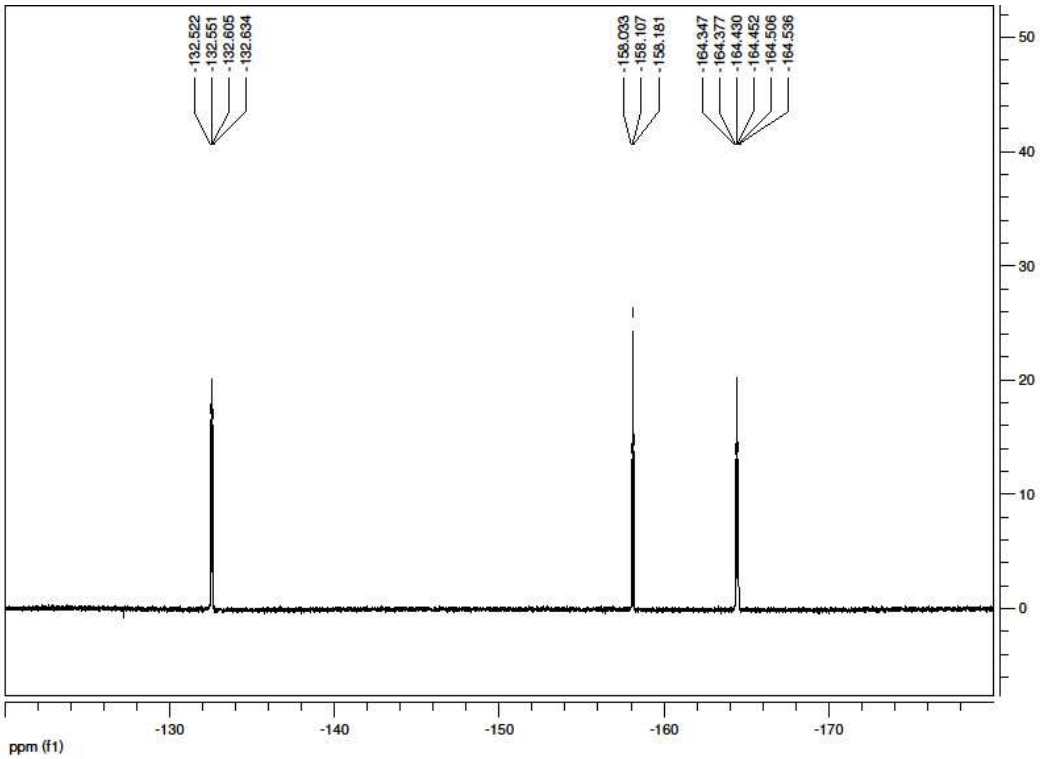
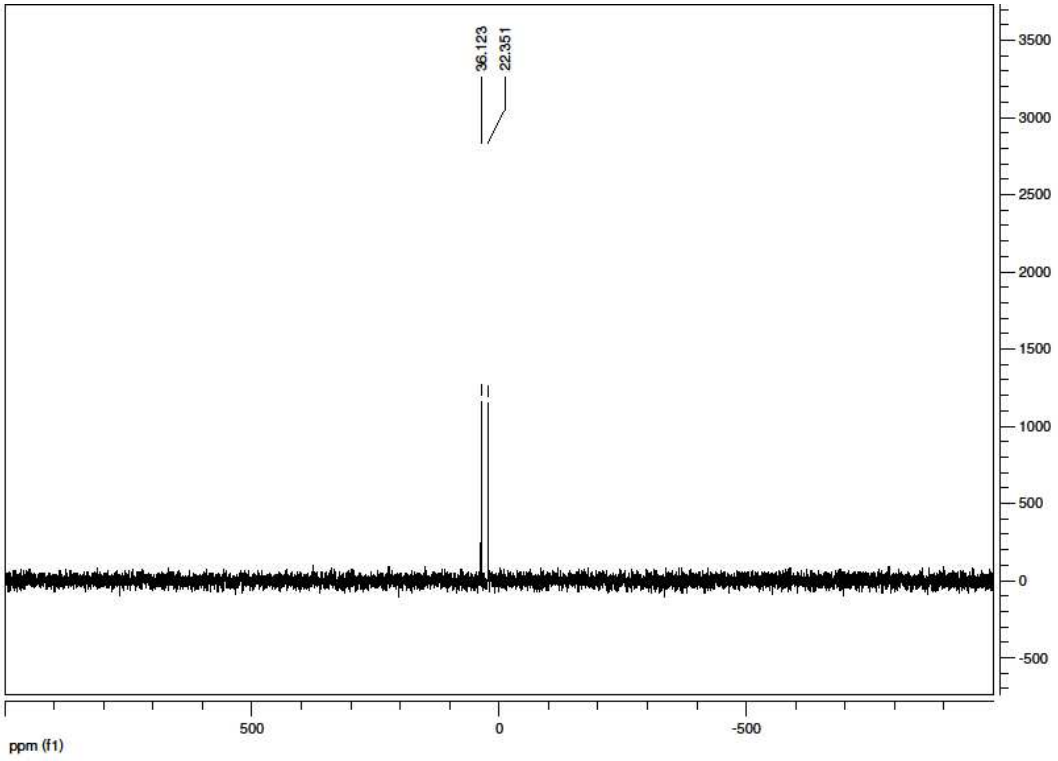
20.0
15.0
10.0
5.0
0.0
0
-50
-100
ppm (f1)


-132.522
-132.551
-132.605
-132.634
-158.033
-158.107
-158.181
-164.347
-164.377
-164.430
-164.452
-164.506
-164.536
50
40
30
20
10
0
-130
-140
-150
-160
-170
ppm (f1)


36.123
22.351
3500
3000
2500
2000
1500
1000
500
0
-500
500
0
-500
ppm (f1)