Dalton Transactions - Full Article

Transition Metal Complexes of Antimony Centered Ligands based upon Acenaphthyl Scaffolds. Coordination Non-Innocent or Not?

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Received

Supporting Information

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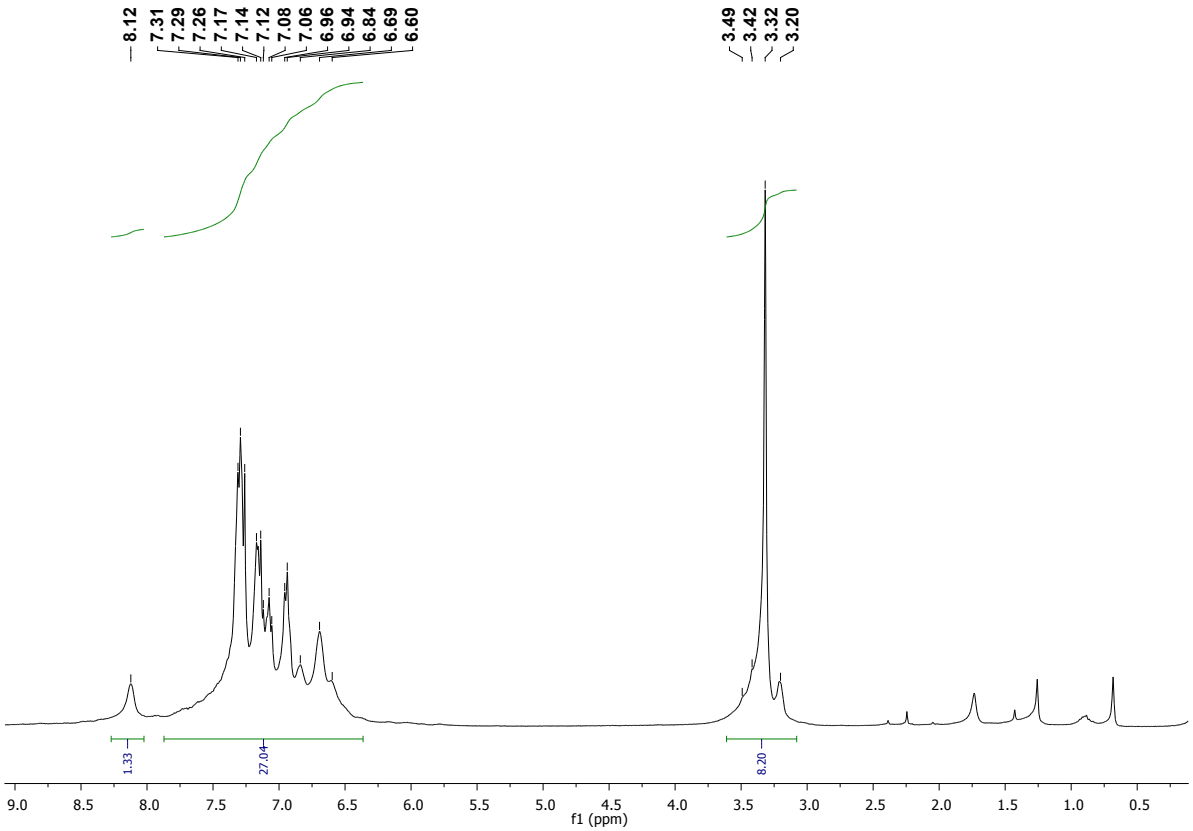


Figure S1a. ^{1}H-NMR spectrum ($CDCl_3$) of **1**.

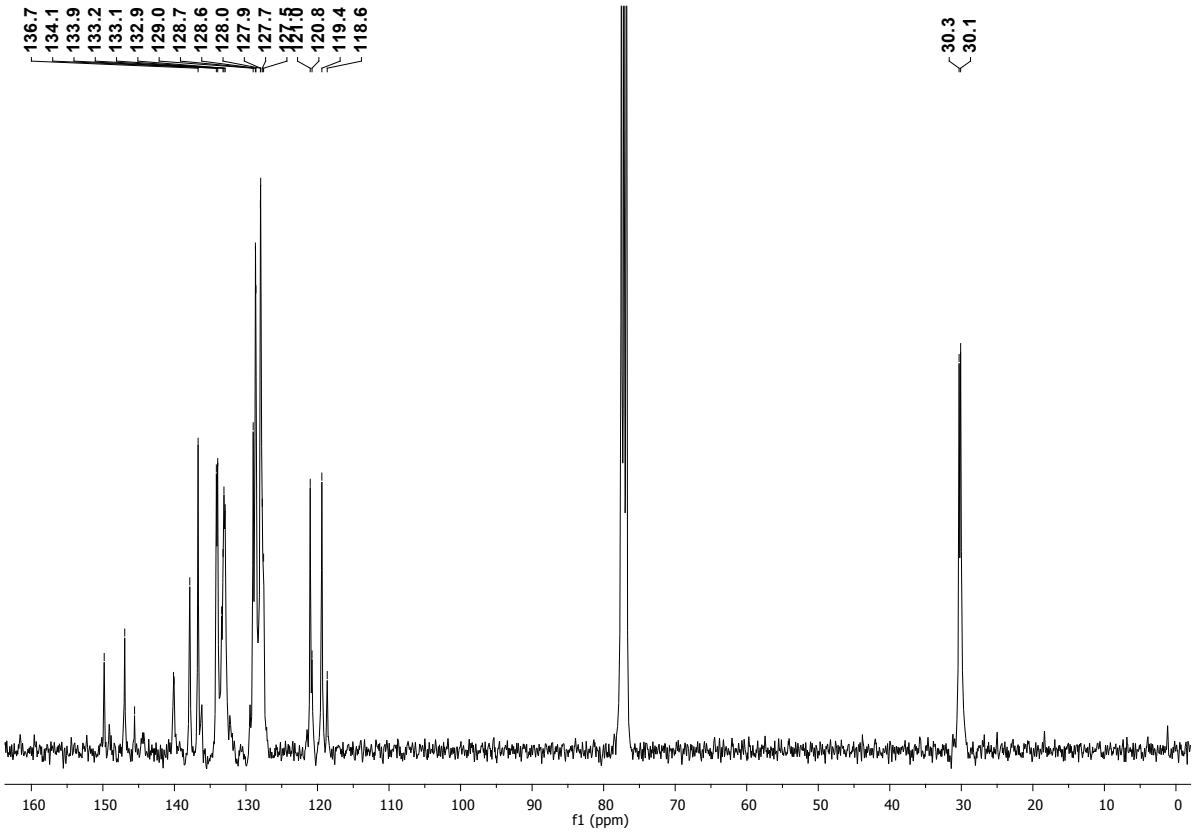


Figure S1b. ^{13}C{^{1}H}-NMR spectrum ($CDCl_3$) of **1**.

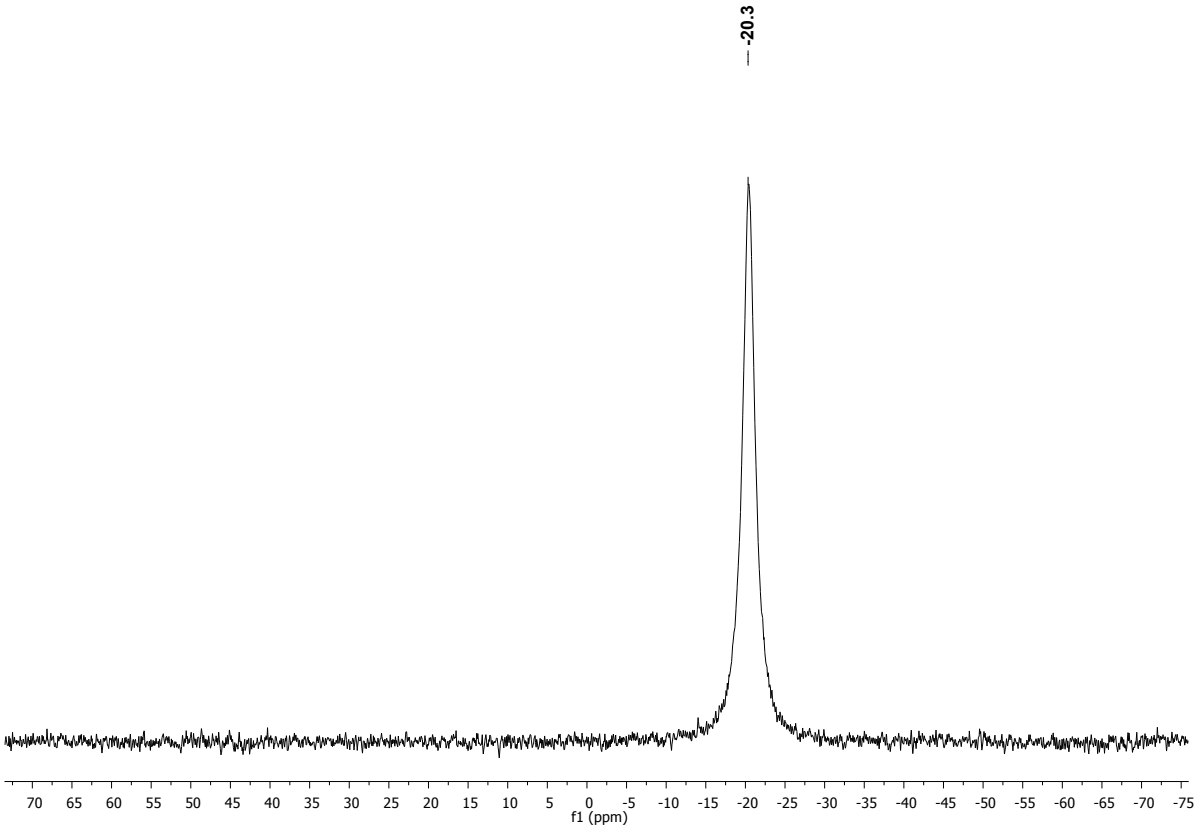


Figure S1c. $^{31}P\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **1**.

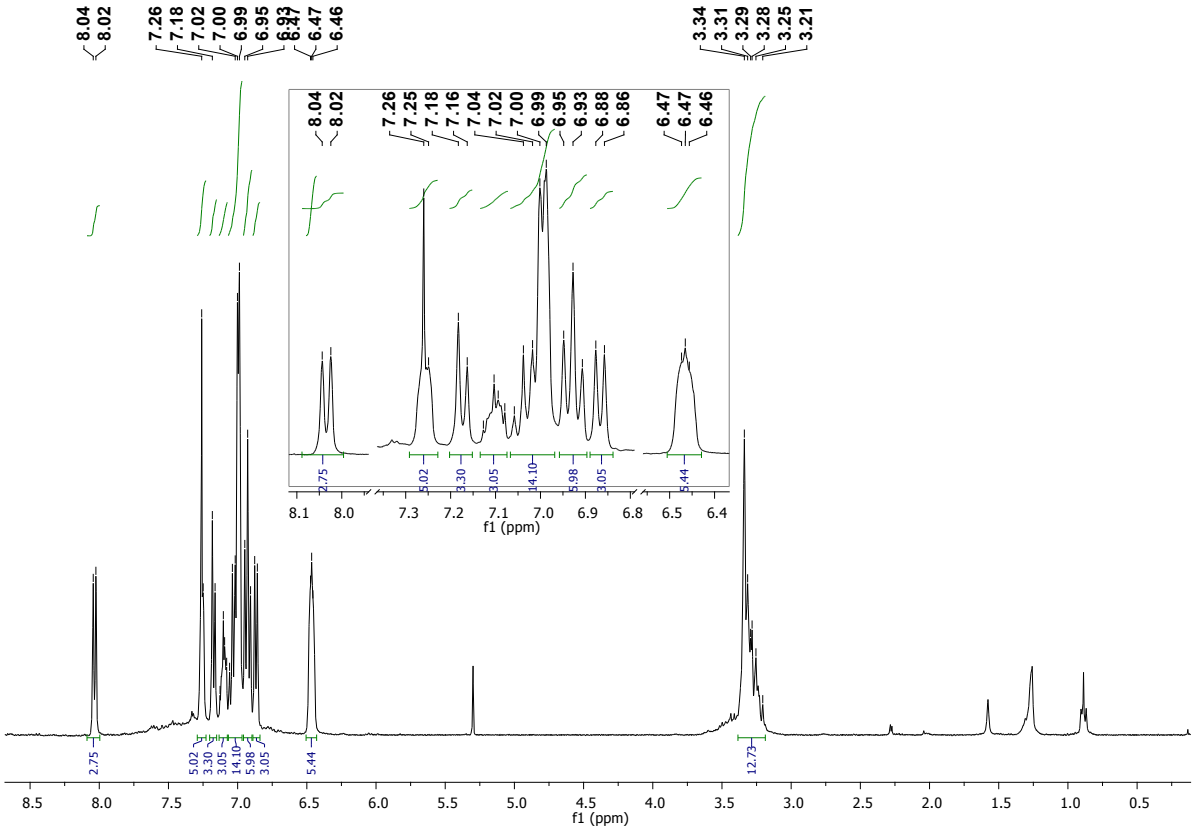


Figure S2a. ^{1}H-NMR spectrum ($CDCl_3$) of **2**.

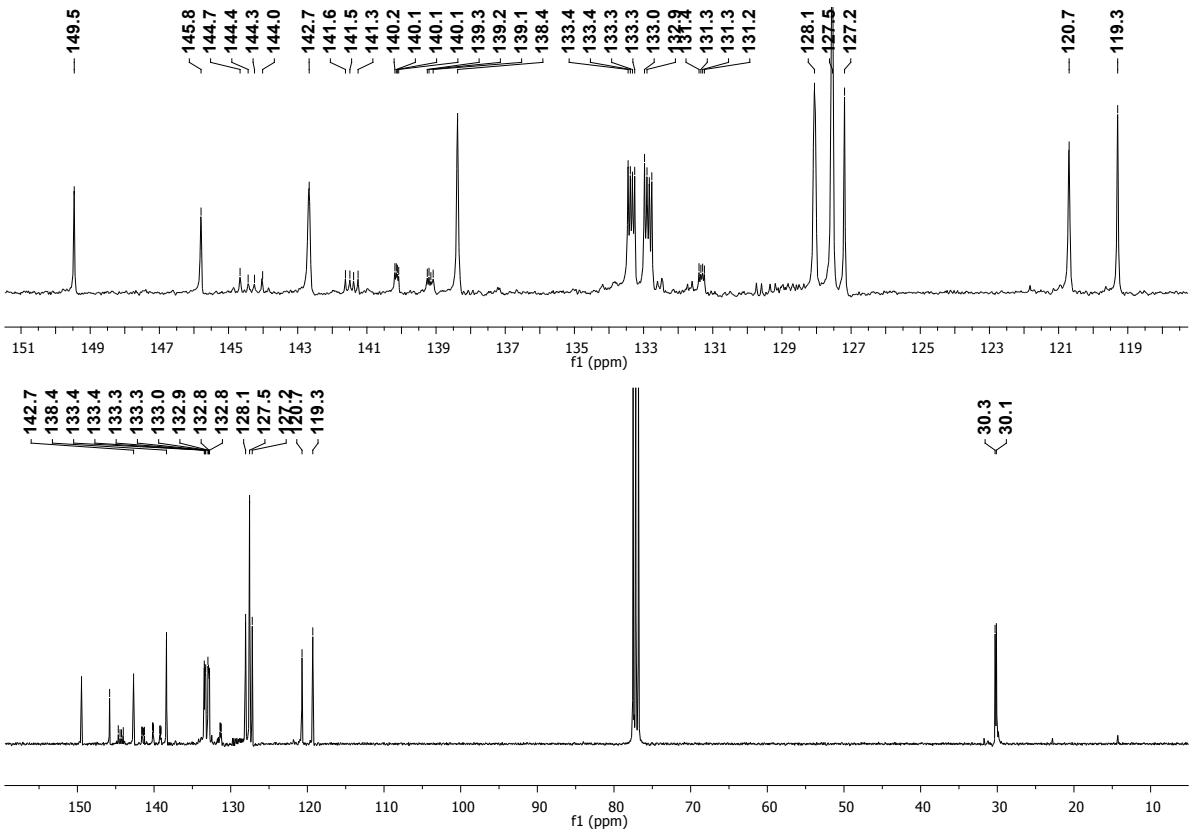


Figure S2b. $^{13}C\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **2**.

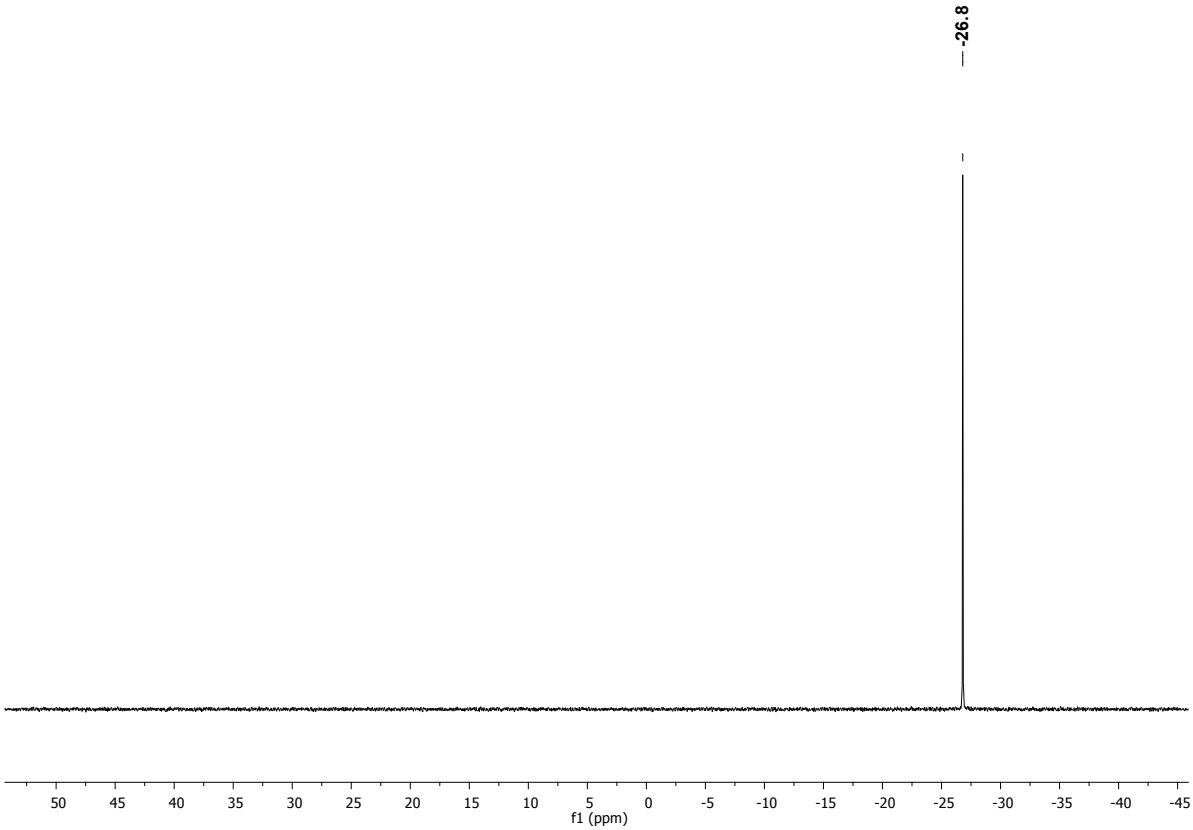


Figure S2c. $^{31}P\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **2**.

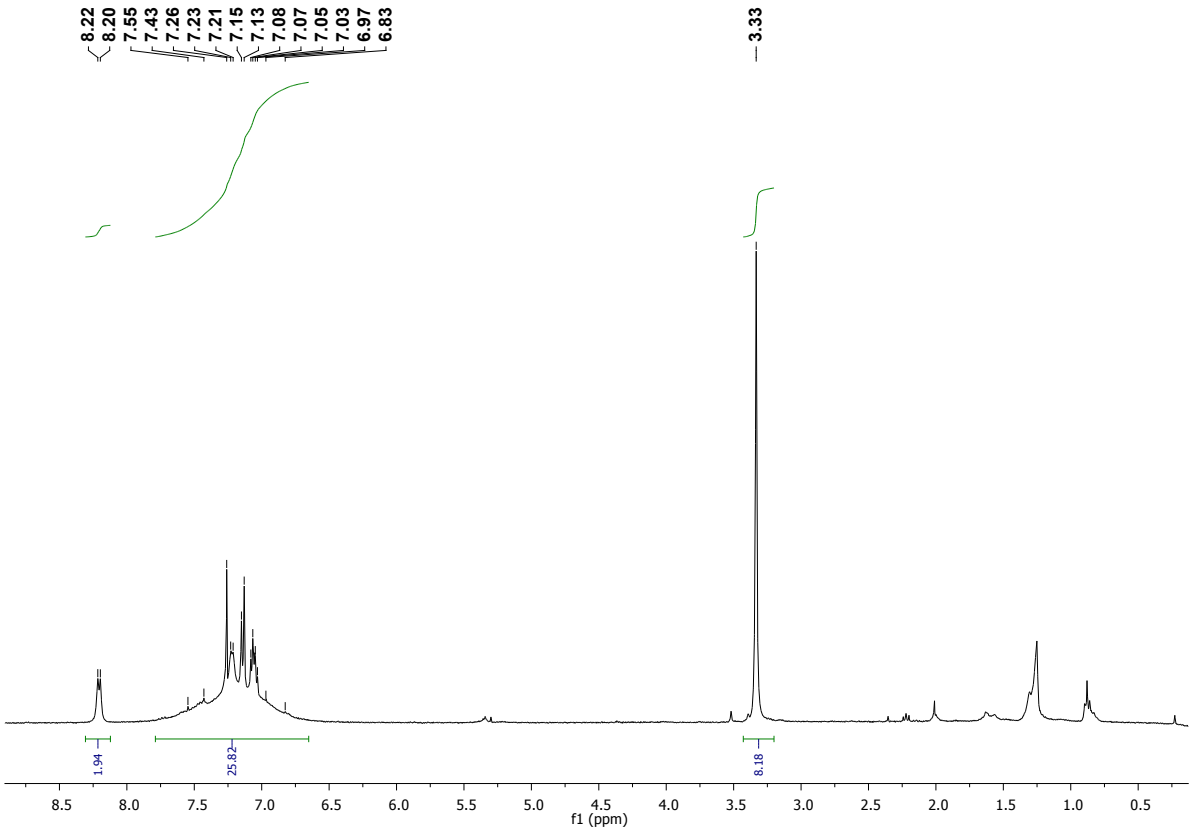


Figure S3a. ^{1}H-NMR spectrum ($CDCl_3$) of **3**.

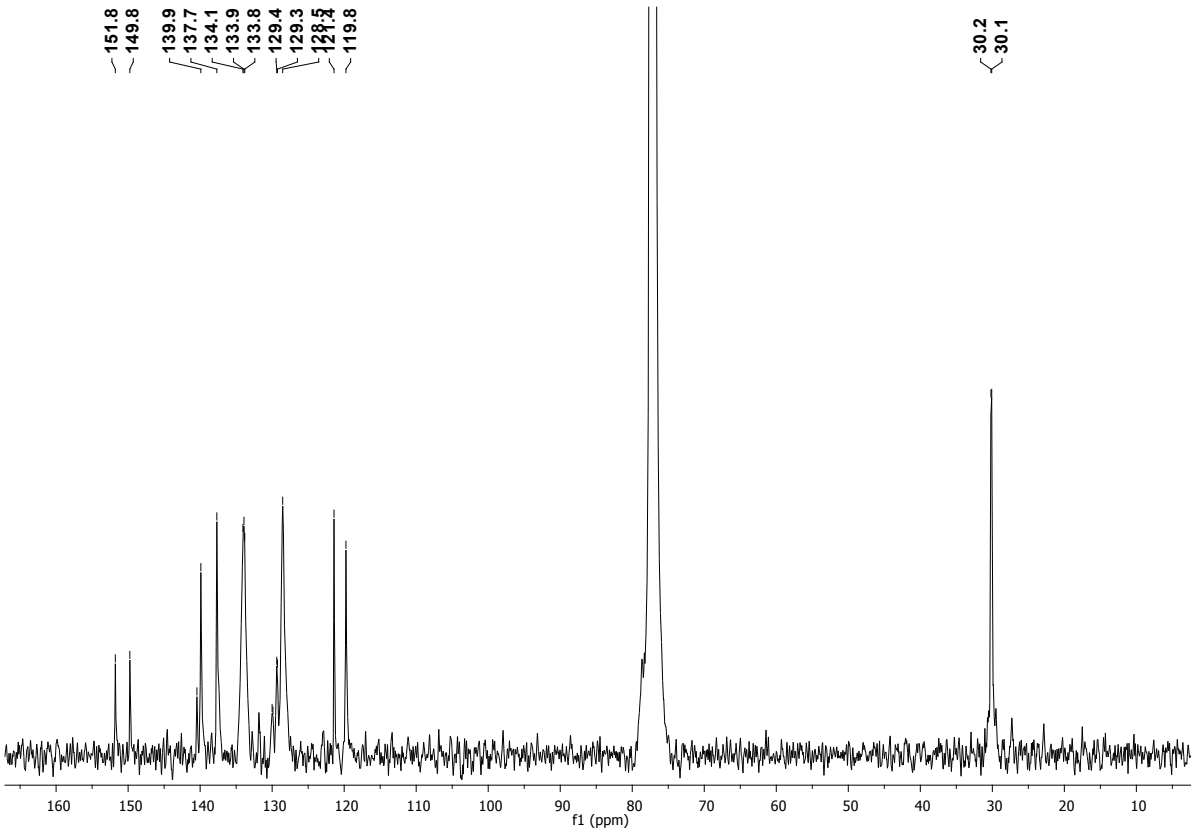
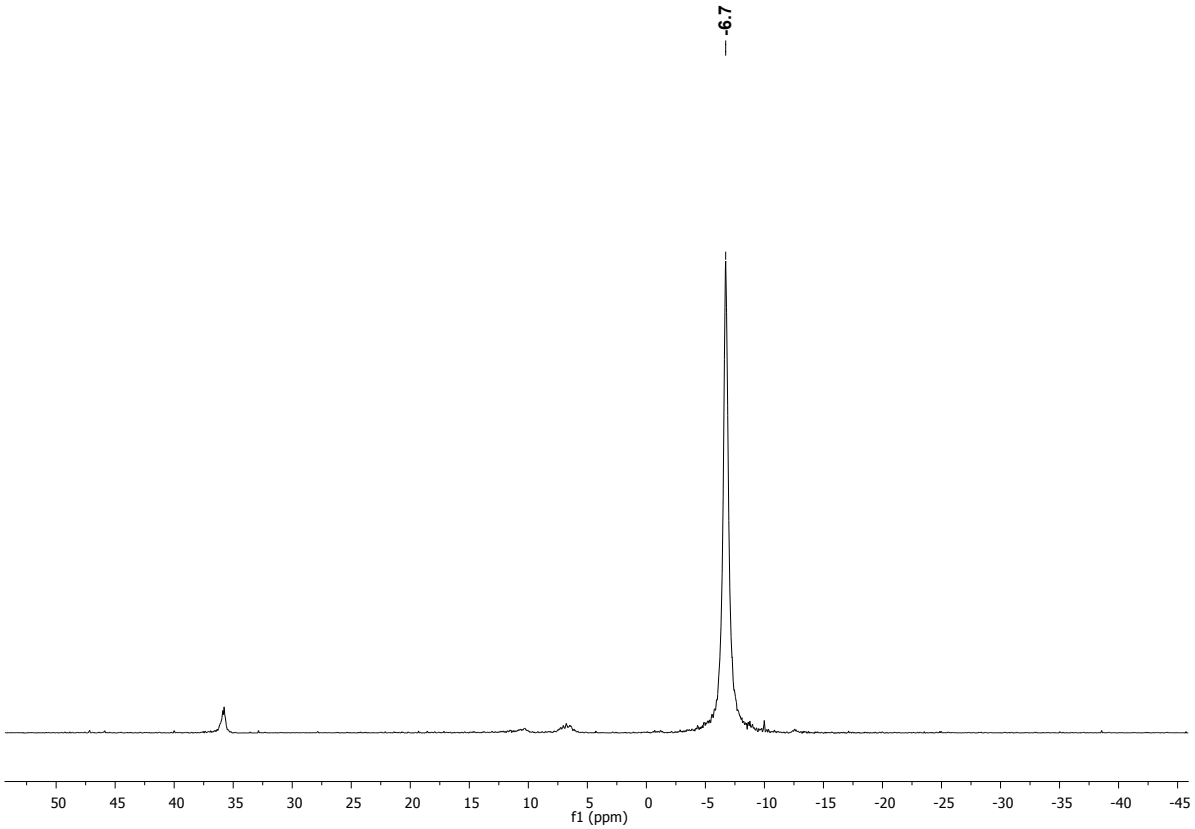


Figure S3b. ^{13}C{^{1}H}-NMR spectrum ($CDCl_3$) of **3** (poor solubility, acquisition time 48 h).



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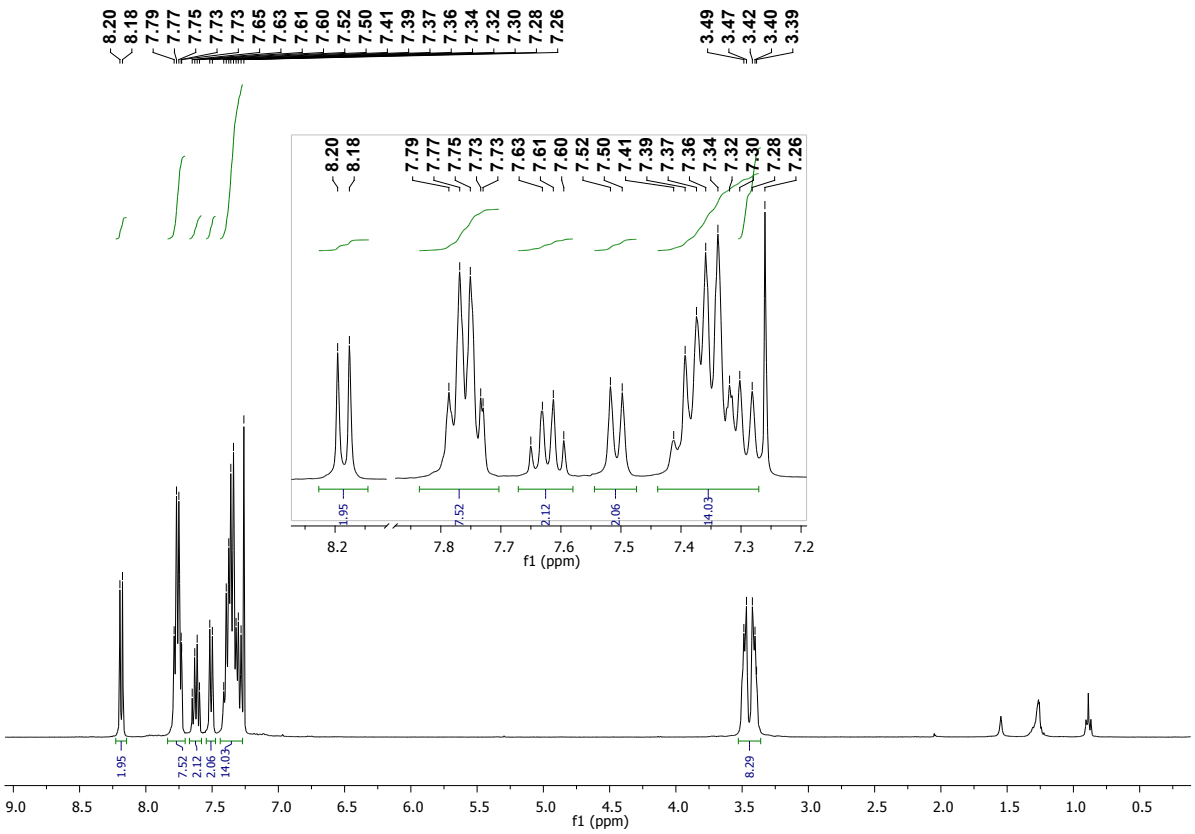

Figure S4a. ^{1}H-NMR spectrum ($CDCl_3$) of **4**.

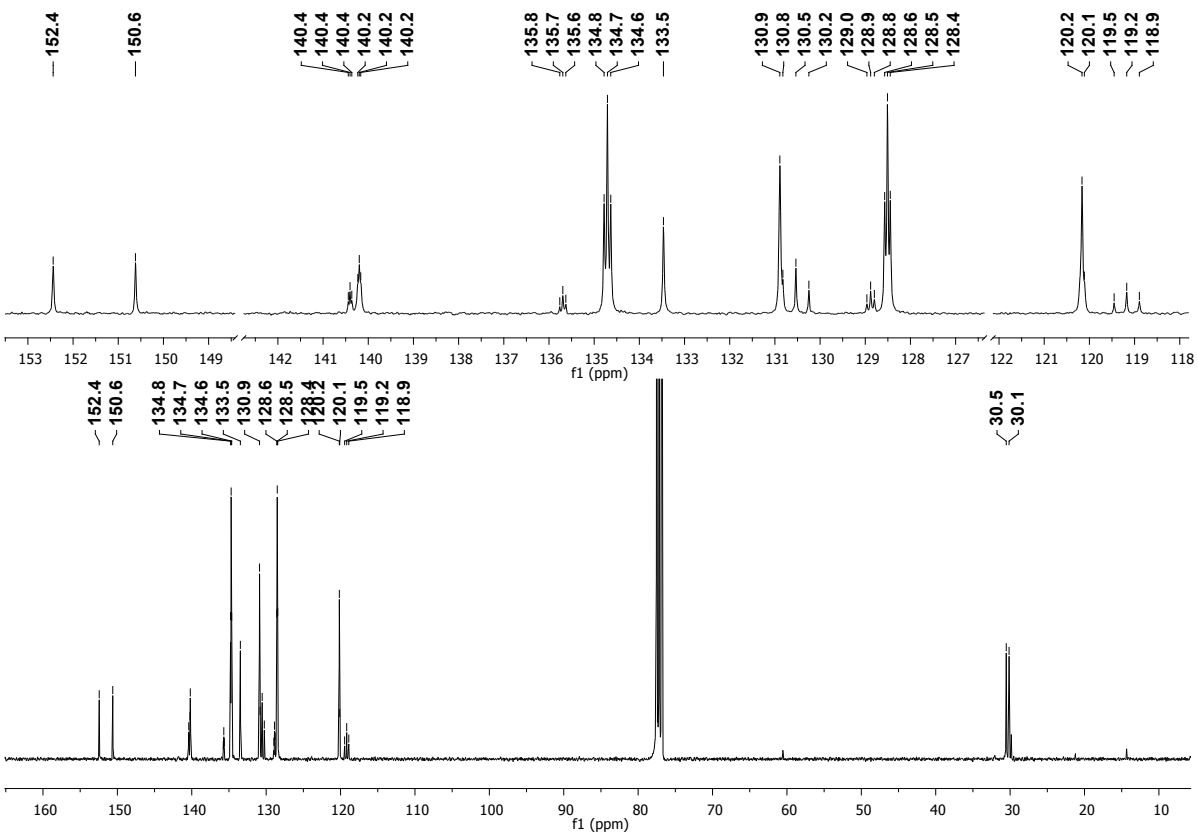

Figure S4b. $^{13}C\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **4**.

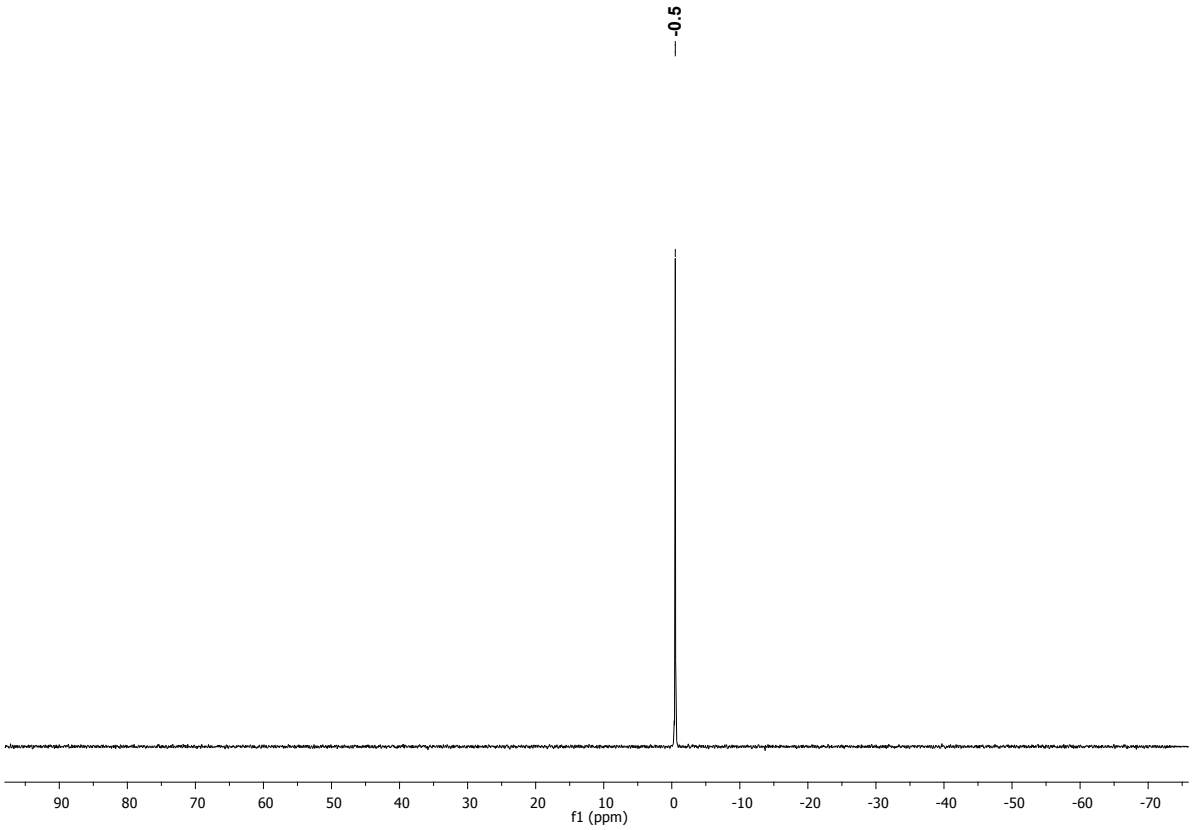

Figure S4c. $^{31}P\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **4**.

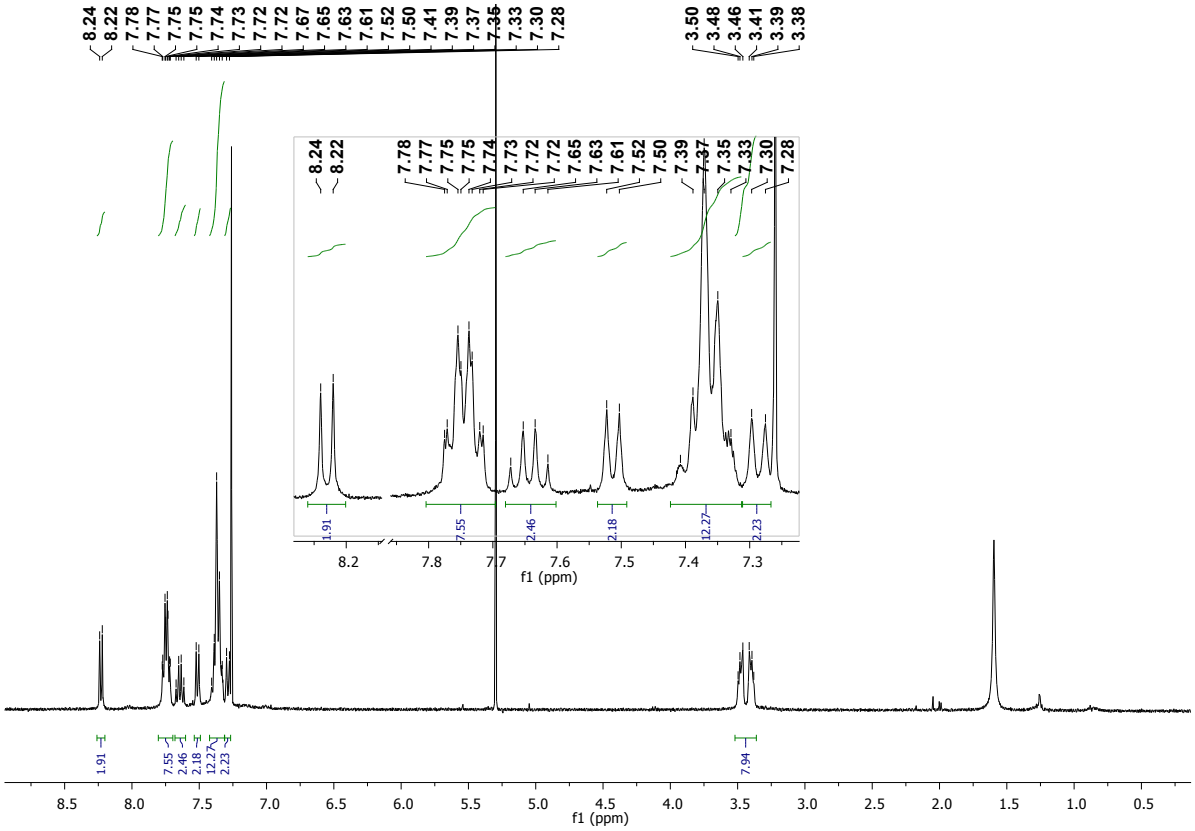

Figure S5a. ^{1}H-NMR spectrum ($CDCl_3$) of **5**.

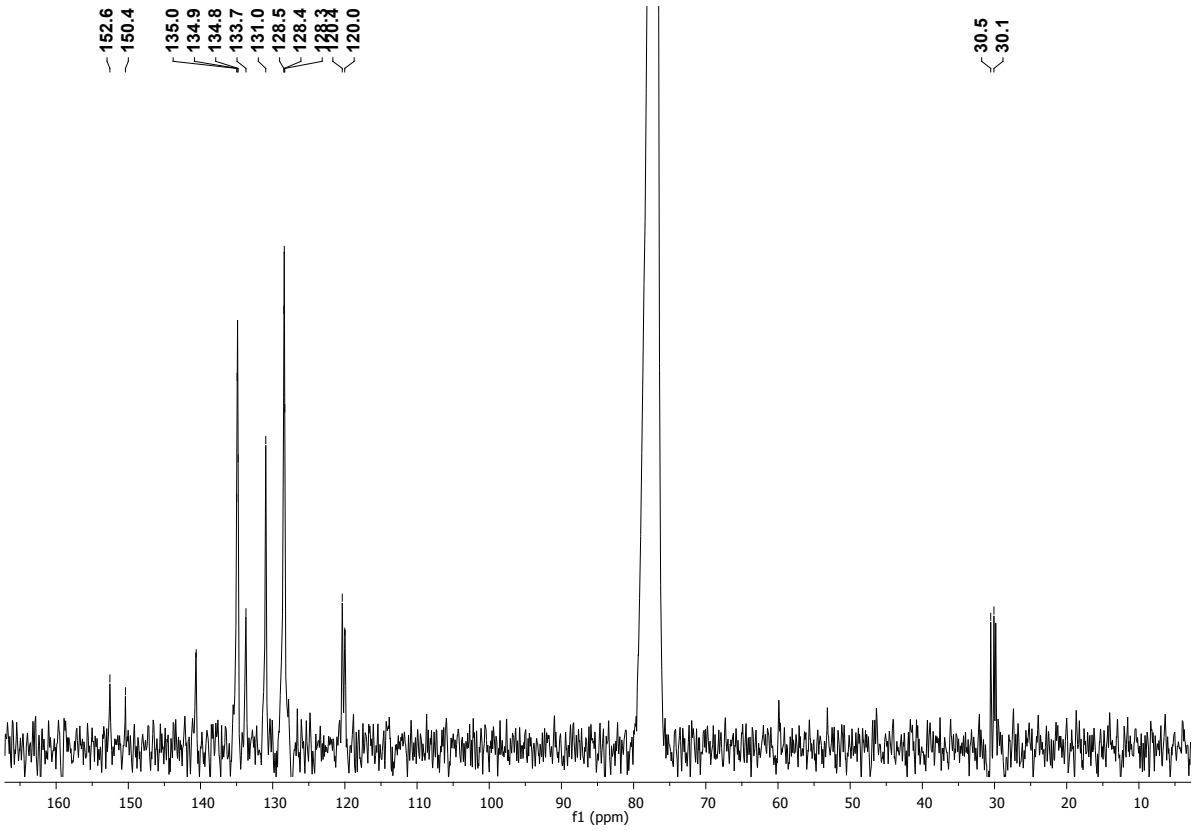

Figure S5b. ^{13}C{^{1}H}-NMR spectrum ($CDCl_3$) of **5** (poor solubility, acquisition time 72 h).

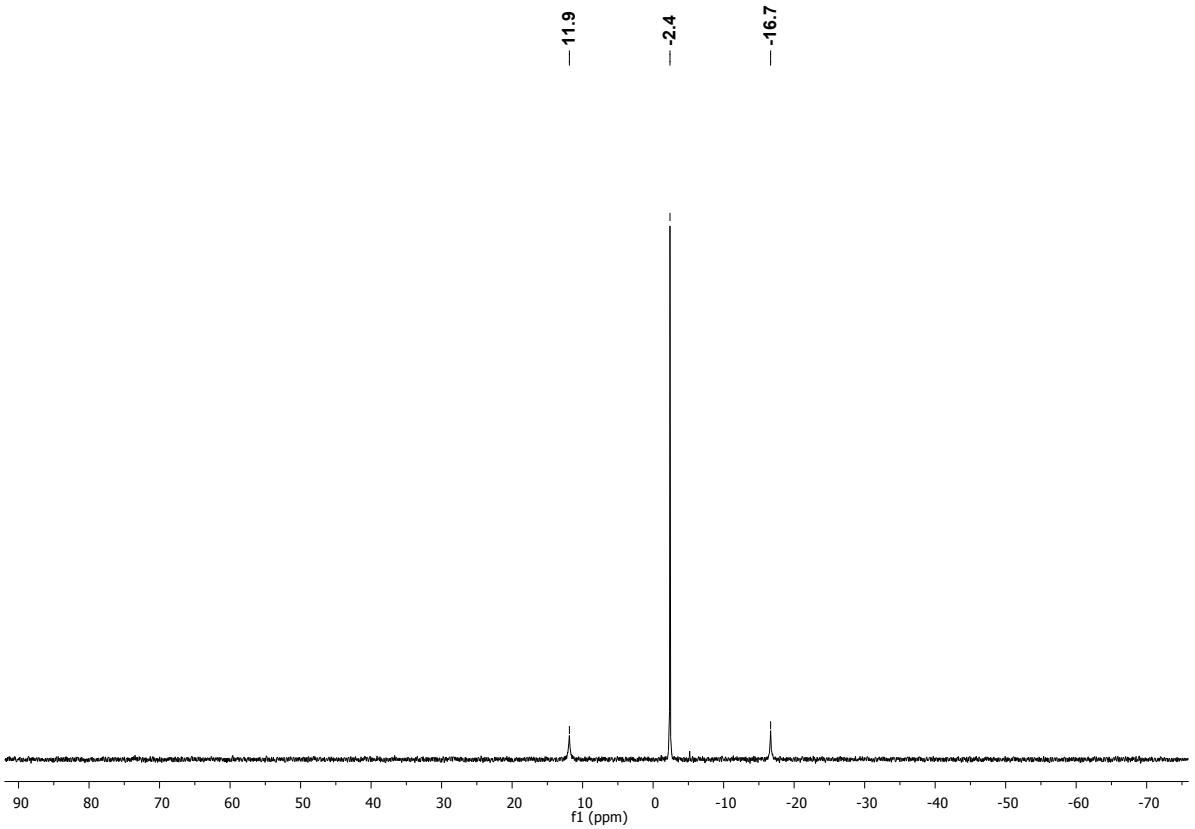

Figure S5c. $^{31}P\{^{1}H\}$-NMR spectrum ($CDCl_3$) of **5**.

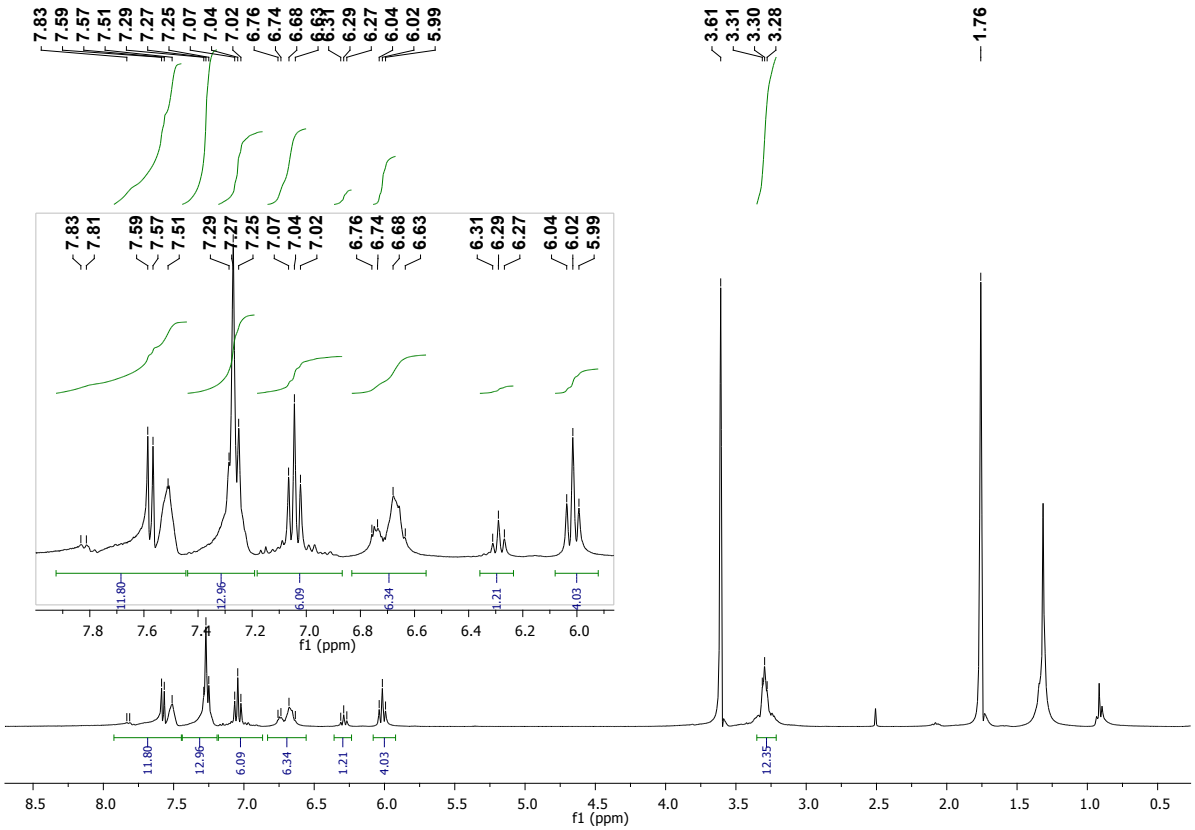

Figure S6a. ^{1}H-NMR spectrum (THF-d_8) of **6**.

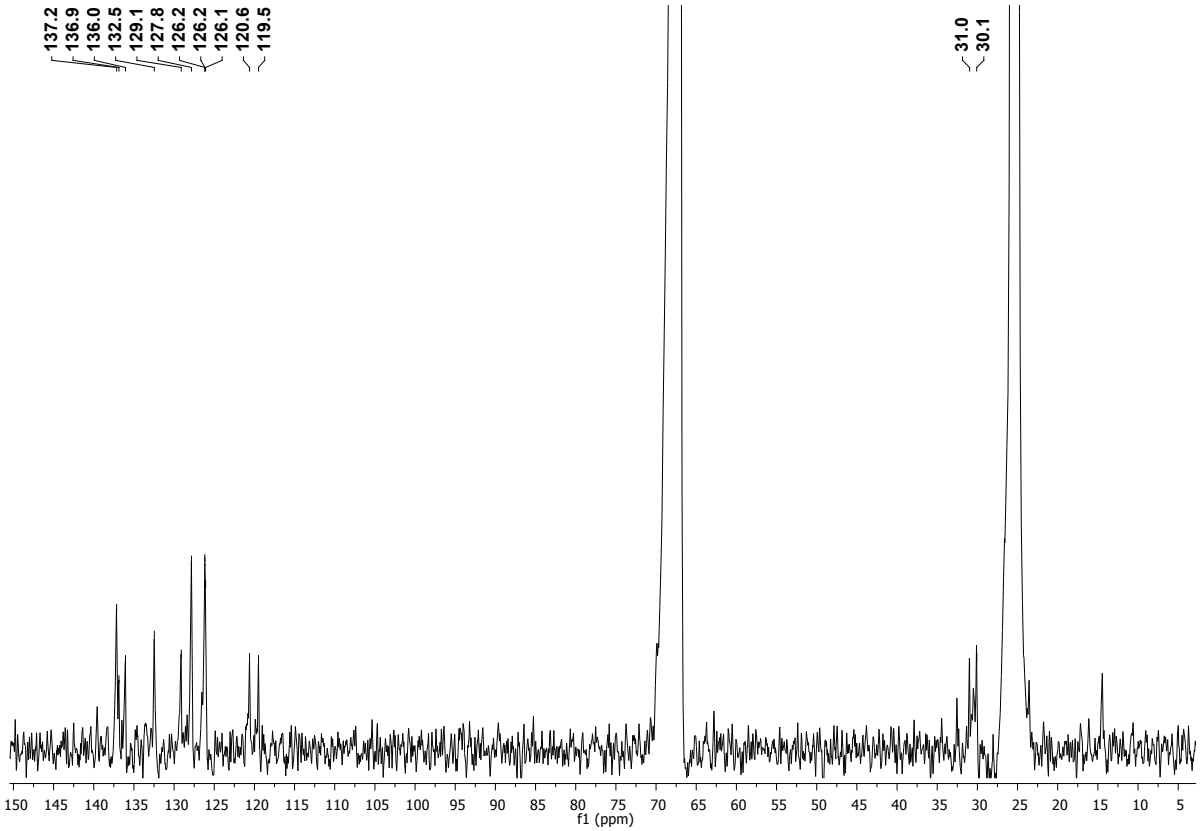

Figure S6b. $^{13}C\{^{1}H\}$-NMR spectrum (THF-d_8) of **6** (poor solubility, acquisition time 24 h, decomposition in $CDCl_3$ and CD_2Cl_2).

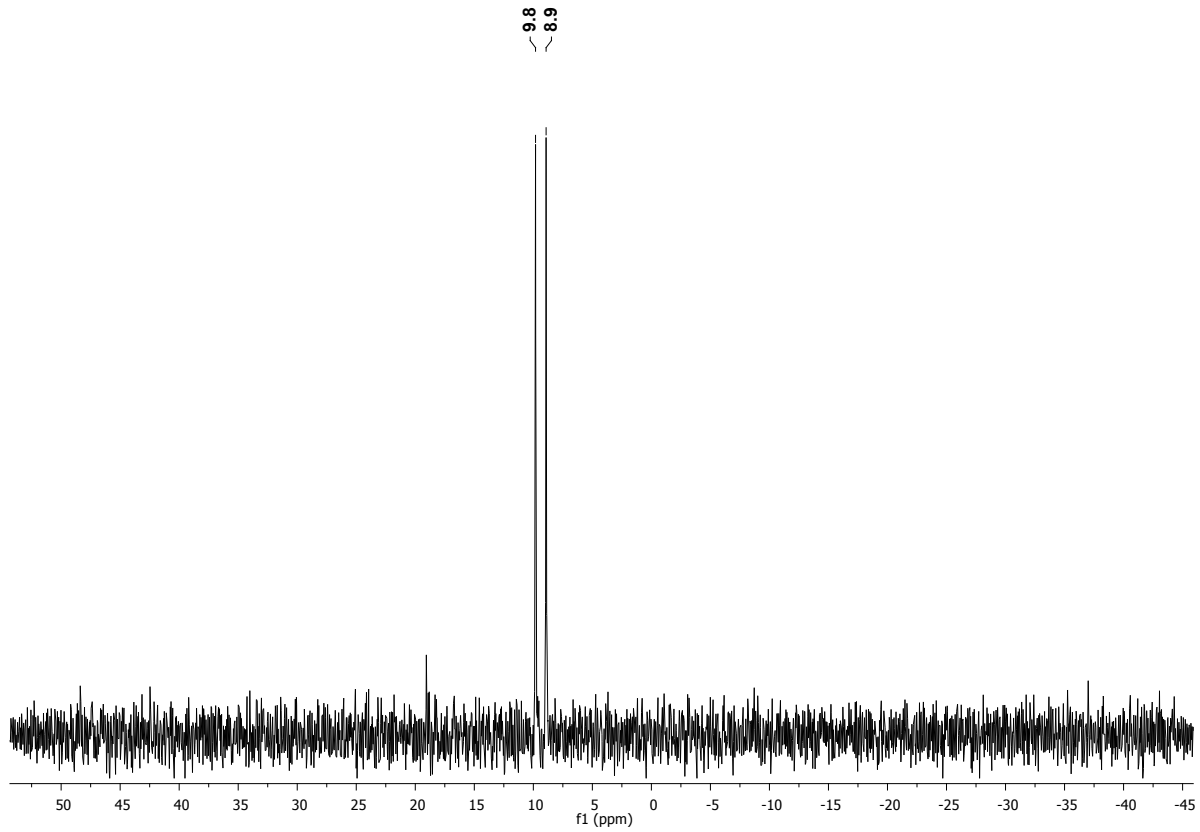

Figure S6c. $^{31}P\{^{1}H\}$-NMR spectrum (THF-d_8) of **6**.

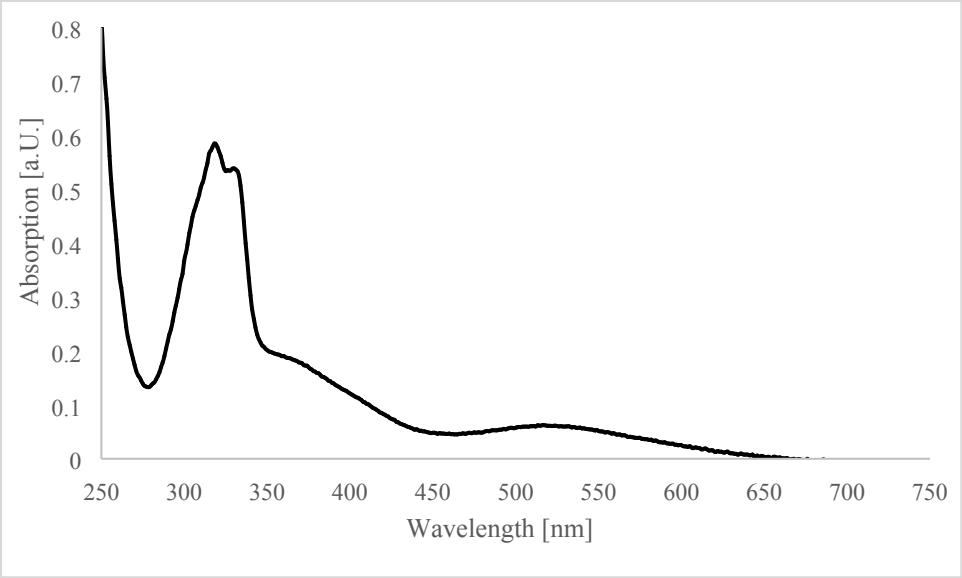

Figure S6d. UV/Vis spectrum (THF) of **6**.

Table S1. Selected interatomic distances (Å) and angles (°) of **1** and **2**.

	1	**2**
	Bond Lengths and Angles	
Sb(1)−C(10)	2.187(2)	2.201(2)
Sb(1)−Cl(1)/C(70)	2.632(1)	2.192(2)
Sb(1)−C(40)	2.181(2)	2.203(3)
C(10)−Sb(1)−C(40)	93.14(9)	96.4(2)
C(10)−Sb(1)−Cl(1)/C(70)	91.68(7)	92.6(2)
C(40)−Sb(1)−Cl(1)/C(70)	92.28(7)	94.8(4)
	peri Region Distances	
Sb(1)−P(1)	2.774(1)	3.171(1)
Sb(1)−P(2)	3.266(1)	3.229(1)
Sb(1)−P(3)		3.243(1)
	peri Region Bond Angles	
Sb(1)−C(10)−C(19)	121.7(2)	125.3(3)
Sb(1)−C(40)−C(49)	126.8(2)	126.7(2)
Sb(1)−C(70)−C(79)		124.3(3)
C(10)−C(19)−C(18)	126.9(3)	129.1(3)
C(40)−C(49)−C(48)	129.4(2)	129.1(3)
C(70)−C(79)−C(78)		128.9(2)
P(1)−C(18)−C(19)	115.1(2)	120.9(2)
P(1)−C(48)−C(49)	117.8(2)	121.1(3)
P(1)−C(78)−C(79)		120.5(3)
Σ of bay angles	363.7(7)	375.3(7)
	374.0(6)	376.9(8)
		373.7(8)
Splay angle[a]	3.7(7)	15.3(7)
	14(6)	16.9(8)
		13.7(8)
	Out-of-Plane Displacement	
P(1)	0.271(1)	0.016(1)
P(2)	0.510(1)	0.014(1)
P(3)		0.287(1)
Sb(1)	0.242(1)	0.019(1)
	0.462(1)	0.040(1)
		0.652(1)
	Central Acenaphthyl Ring Torsion Angles	
C: (13)−(14)−(19)−(18)	178.9(3)	178.6(3)
C: (43)−(44)−(49)−(48)	–173.6(2)	–179.9(4)
C: (73)−(74)−(79)−(78)		173.4(3)
C: (15)−(14)−(19)−(10)	178.1(3)	–177.6(3)
C: (45)−(44)−(49)−(40)	–175.6(3)	–175.4(3)
C: (75)−(74)−(79)−(70)		176.3(5)

[a] Splay angle: sum of the three bay region angles – 360.

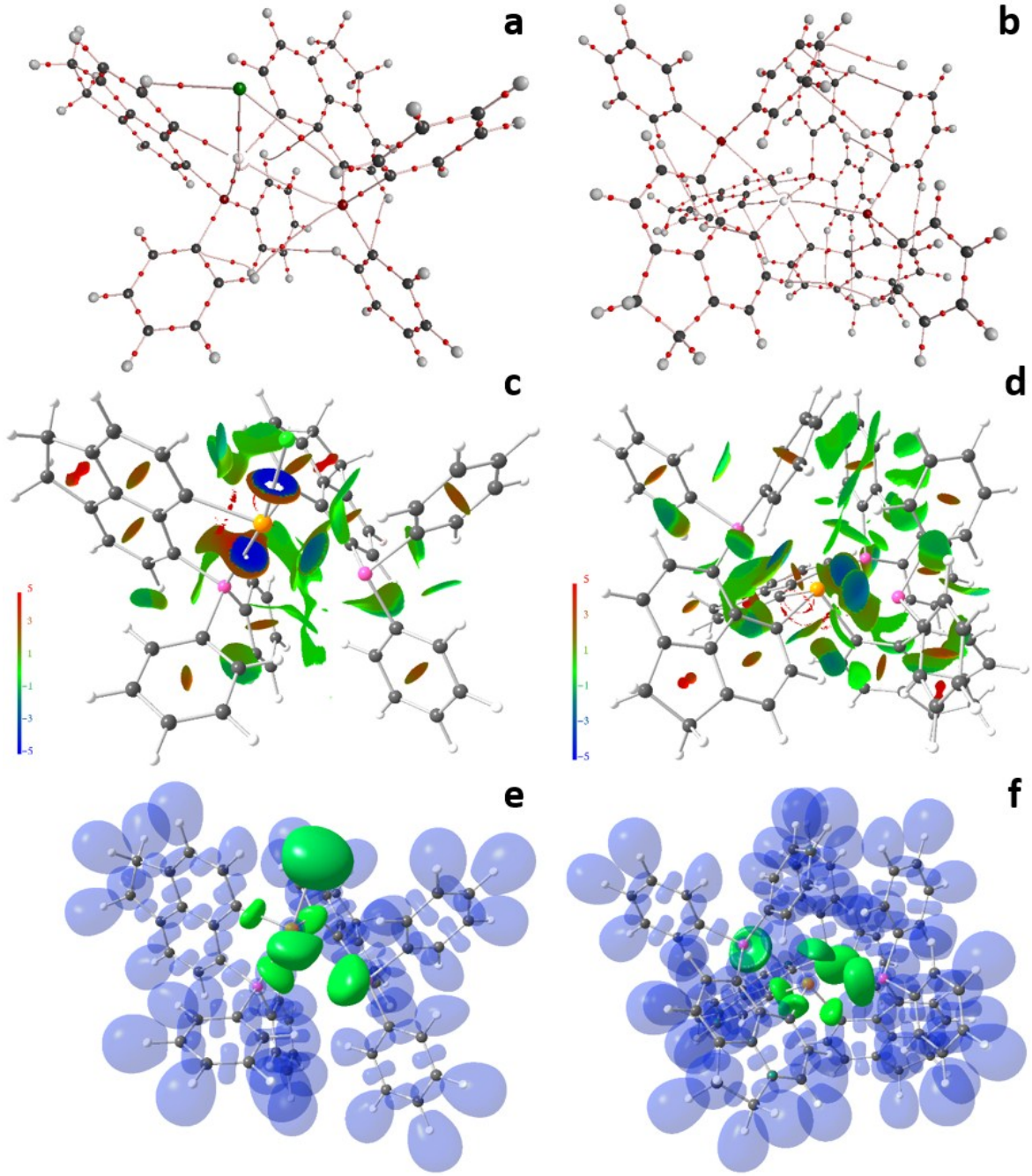

Figure S7. AIM topologies, NCI *iso*-surfaces (**s** = 0.5), and ELI-D *iso*-surfaces (γ = 1.3) of **1** (left column) and **2** (right column).

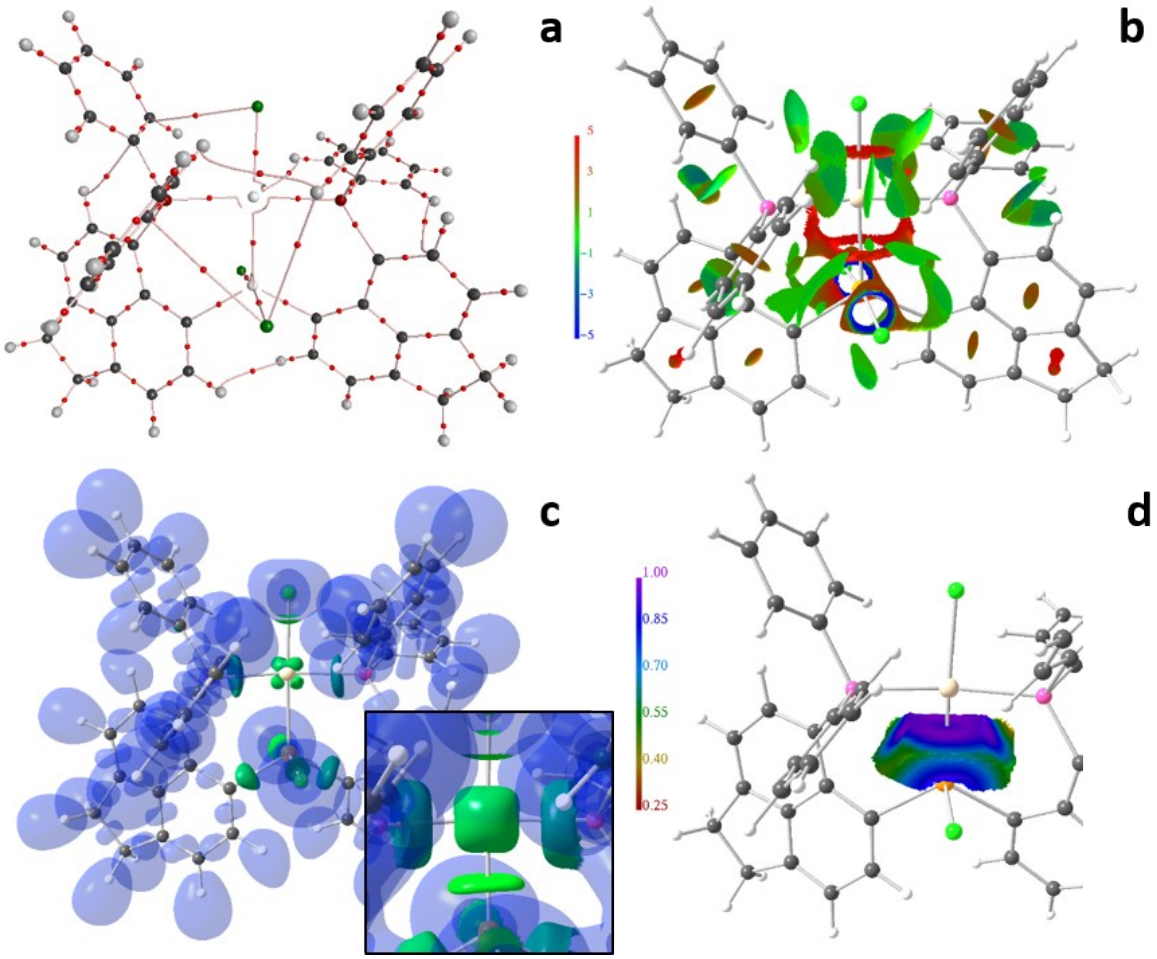

Figure S8. AIM topology, NCI *iso*-surface (**s** = 0.5), ELI-D *iso*-surface (γ = 1.3; inset shows magnification around the metal center at γ = 1.25), and ELI-D distribution mapped on the Sb–Pt ELI-D basin in **5**.

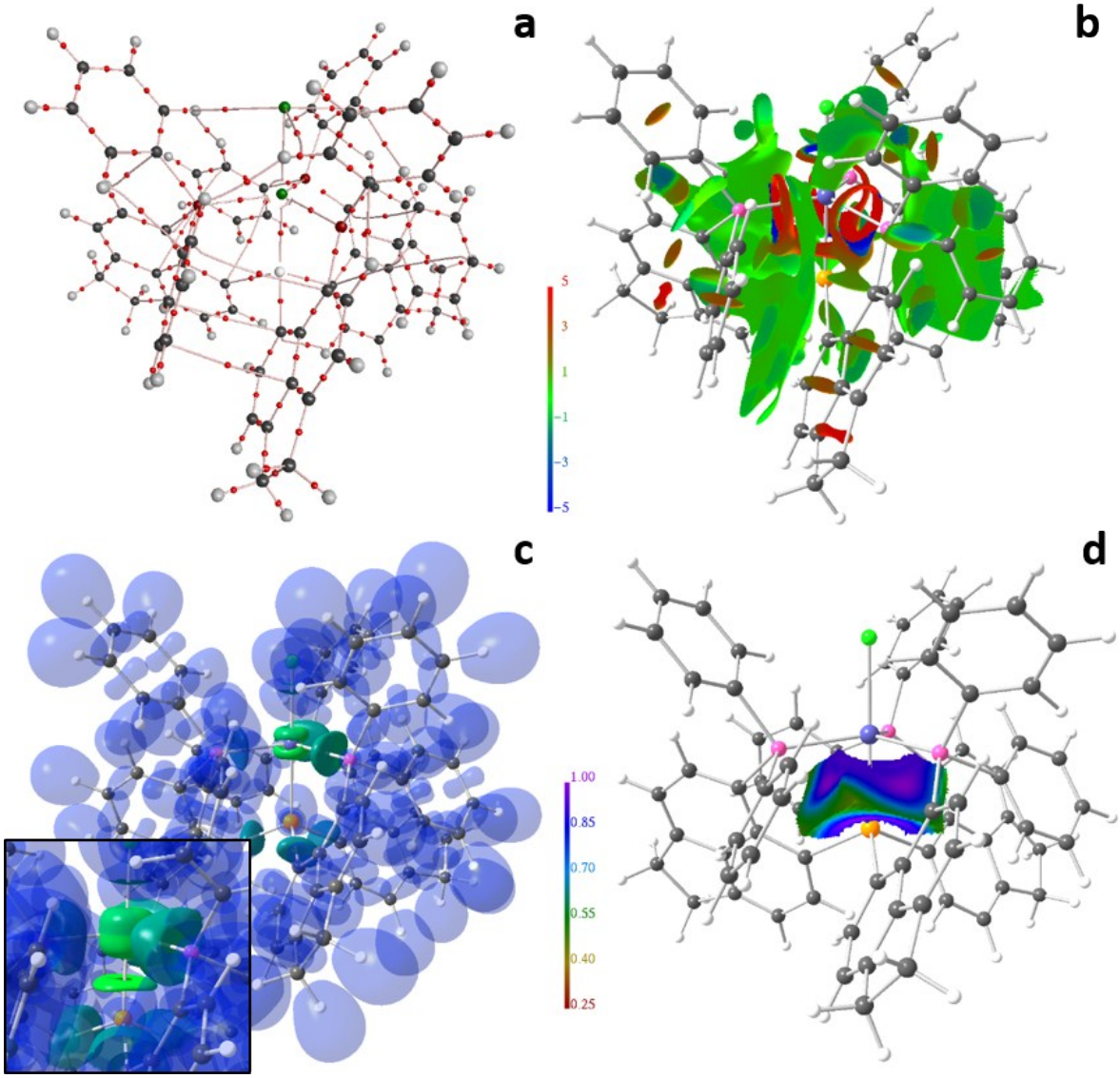

Figure S9 AIM topology, NCI *iso*-surface (**s** = 0.5), ELI-D *iso*-surface (γ = 1.3; inset shows magnification around the metal center at γ = 1.25), and ELI-D distribution mapped on the Sb–Rh ELI-D basin in **6**.