Supporting Information

Structural Diversities in Ag(I) Complexes of Xylyl Platform Based Isomeric Bis-NHC Ligands: Effects of 2-Pyridine Wingtip Substituent

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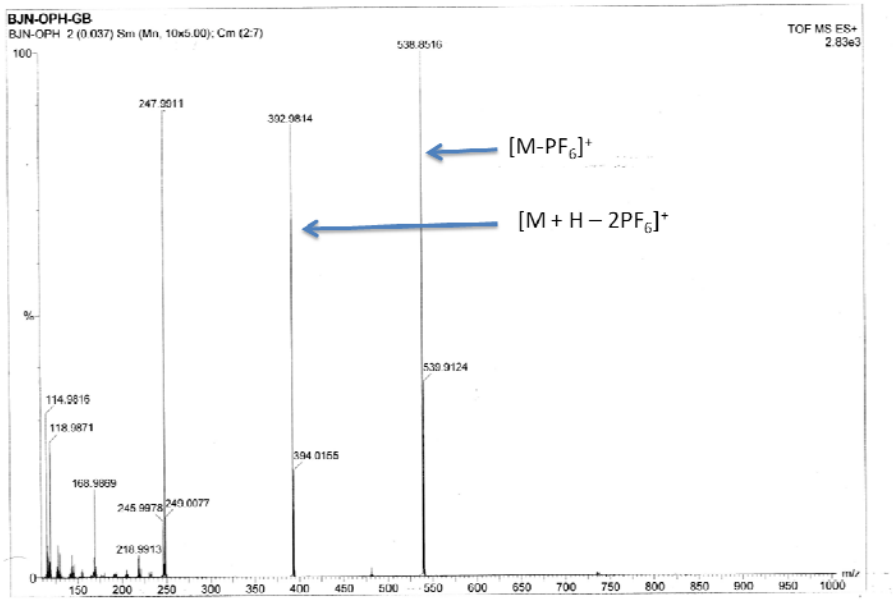


Figure 2S. ^{1}H-NMR spectrum of compound $\mathbf{H_2L1(PF_6)_2}$ in CD3CN at 25ºC (300 MHz).

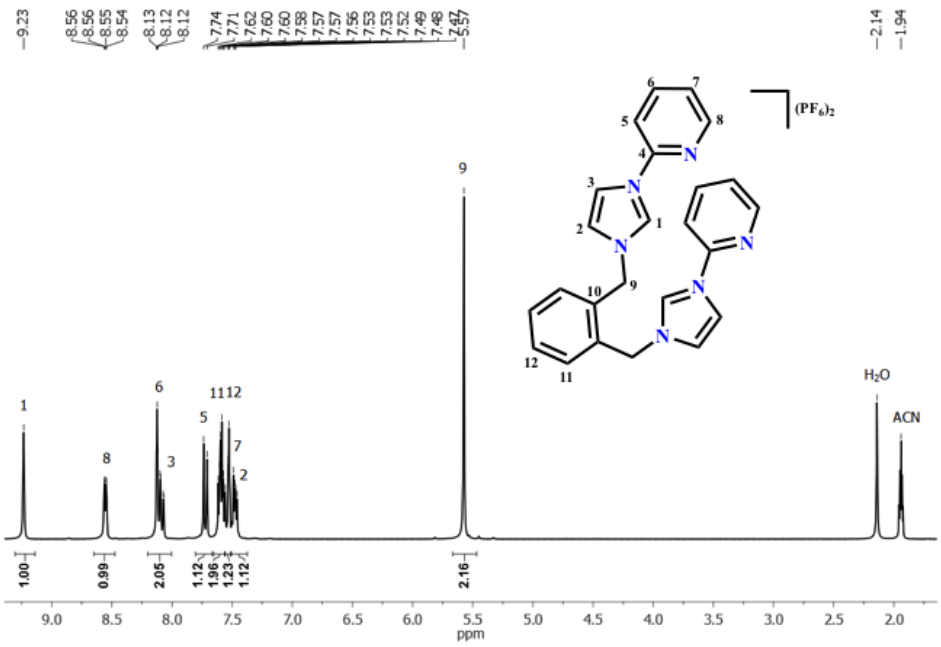


Figure 3S. ^{13}C-NMR spectrum of compound **$H_2L1(PF_6)_2$** in CD3CN at 25ºC (75 MHz).

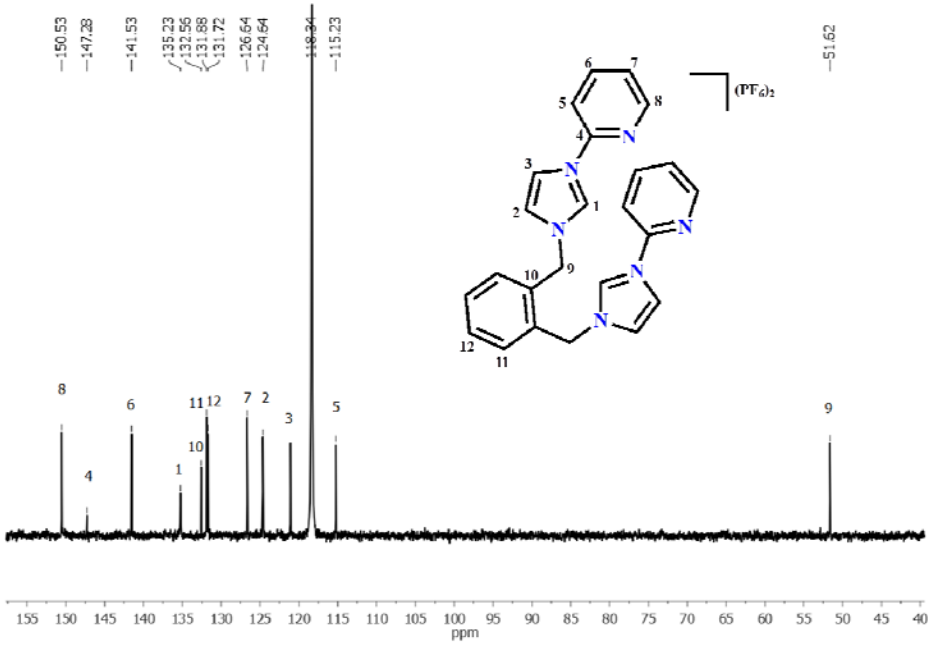
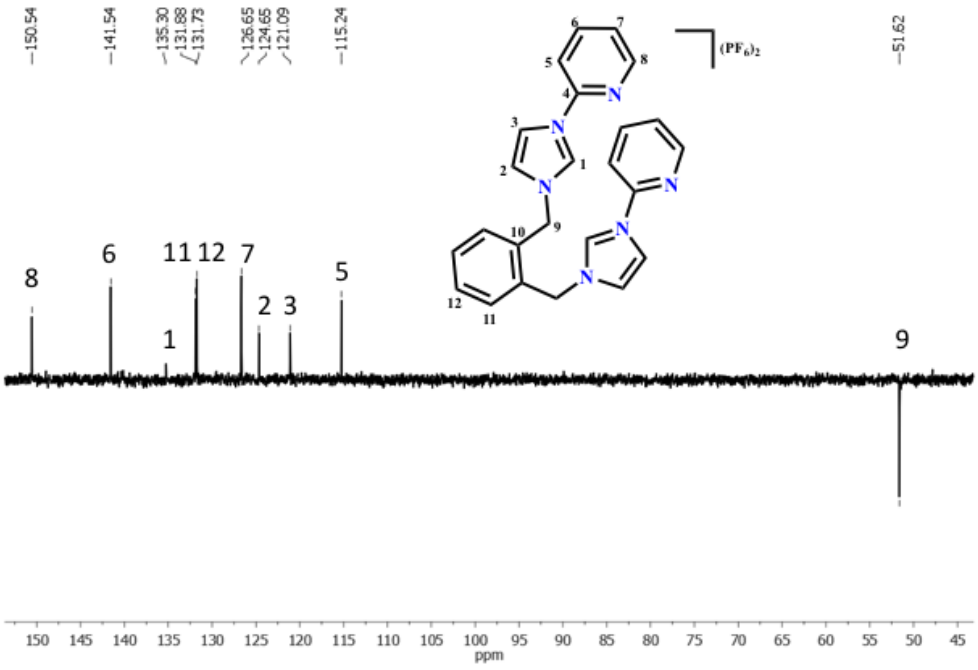


Figure 4S. DEPT-135-NMR spectrum of compound **$H_2L1(PF_6)_2$** in CD3CN at 25ºC.



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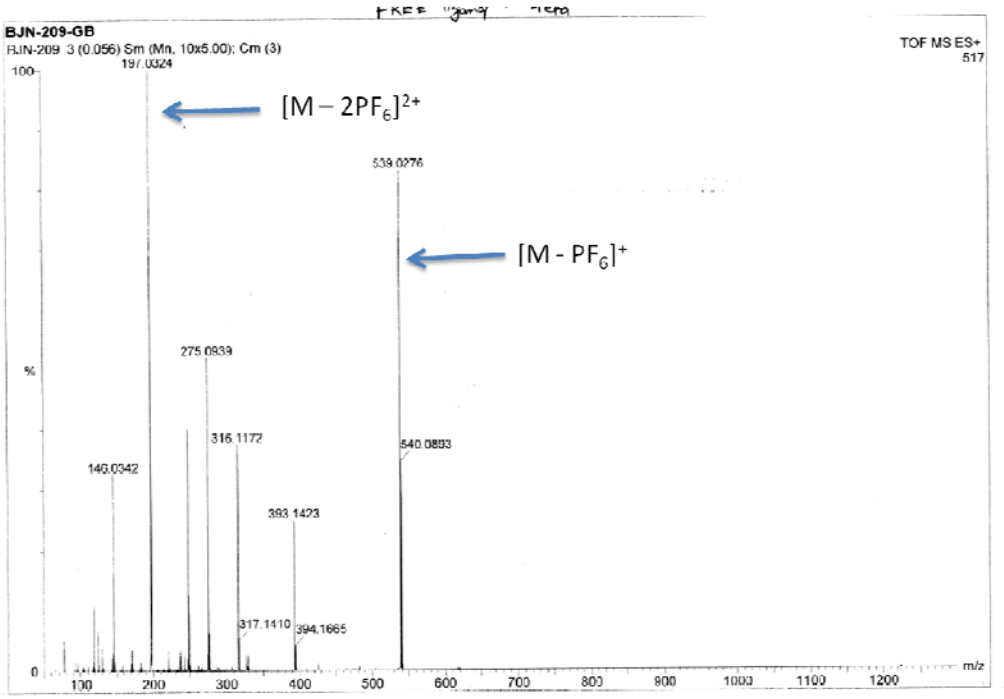


Figure 6S. ^{1}H-NMR spectrum of compound $\mathbf{H_2L2(PF_6)_2}$ in CD_3CN at 25ºC (500 MHz).

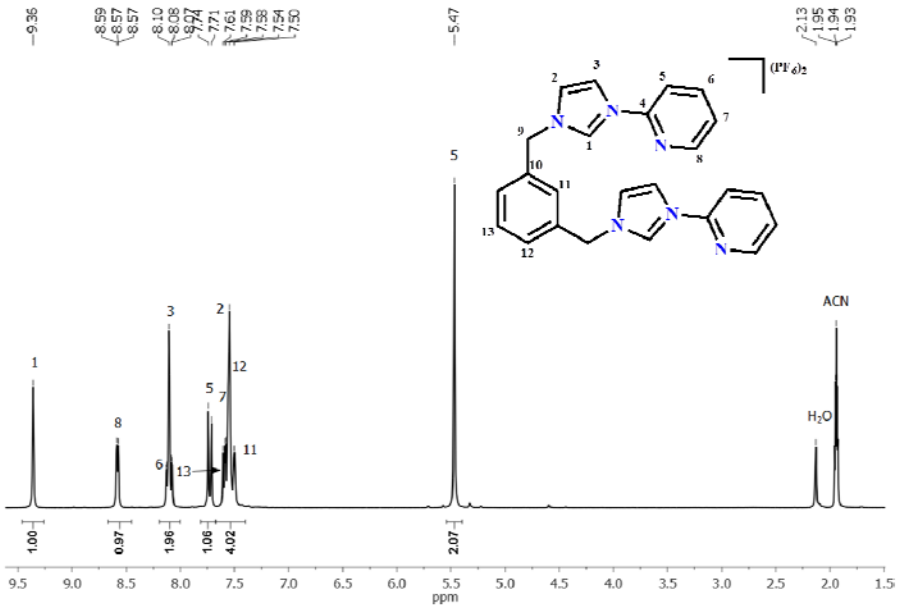


Figure 7S. ^{13}C-NMR spectrum of compound $\mathbf{H_2L_2(PF_6)_2}$ in CD_3CN at 25ºC (125 MHz).

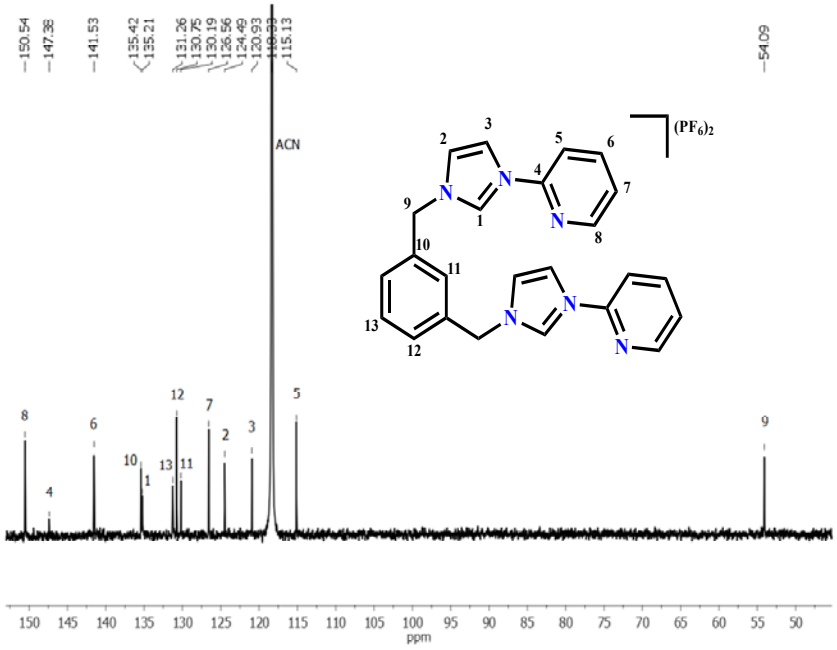


Figure 8S. DEPT-135-NMR spectrum of compound $\mathbf{H_2L_2(PF_6)_2}$ in CD_3CN at 25ºC.

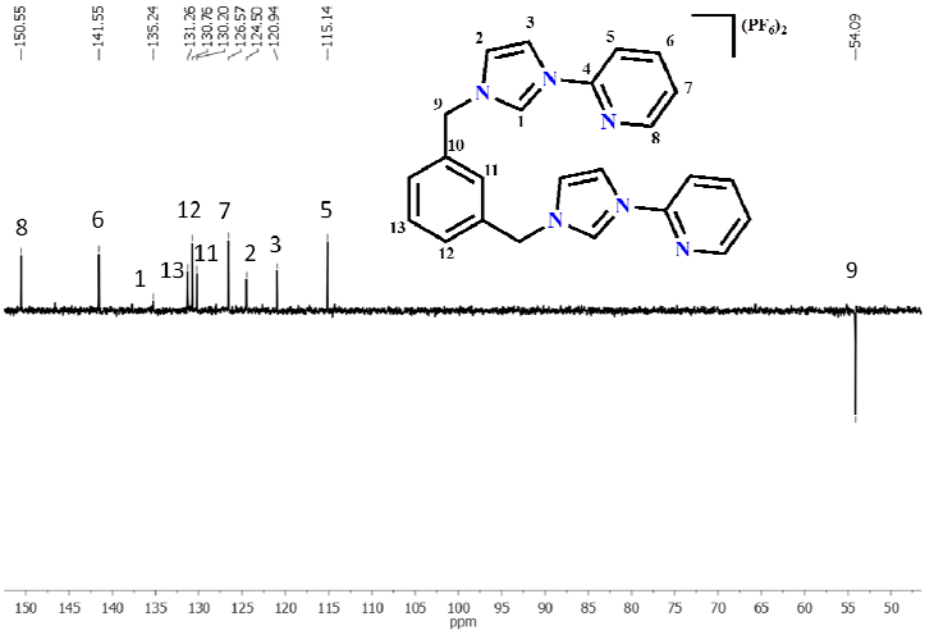


Figure 9S. ESI-MS (+ve) of $\mathbf{H_2L_3(PF_6)_2}$

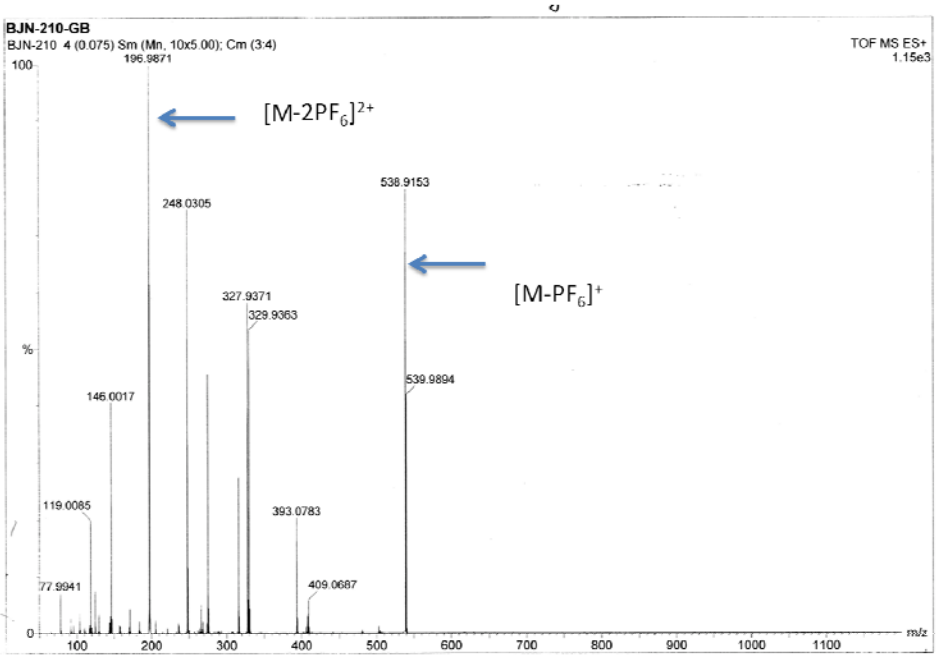
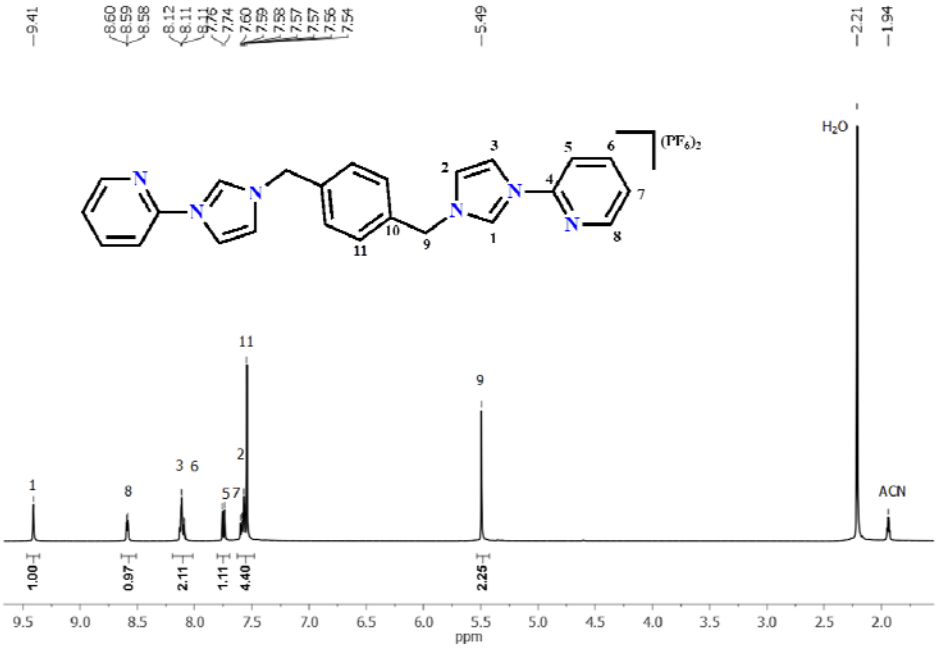


Figure 10S. ^{1}H-NMR spectrum of $\mathbf{H_2L_3(PF_6)_2}$ in CD_3CN at 25ºC (400 MHz)**.**



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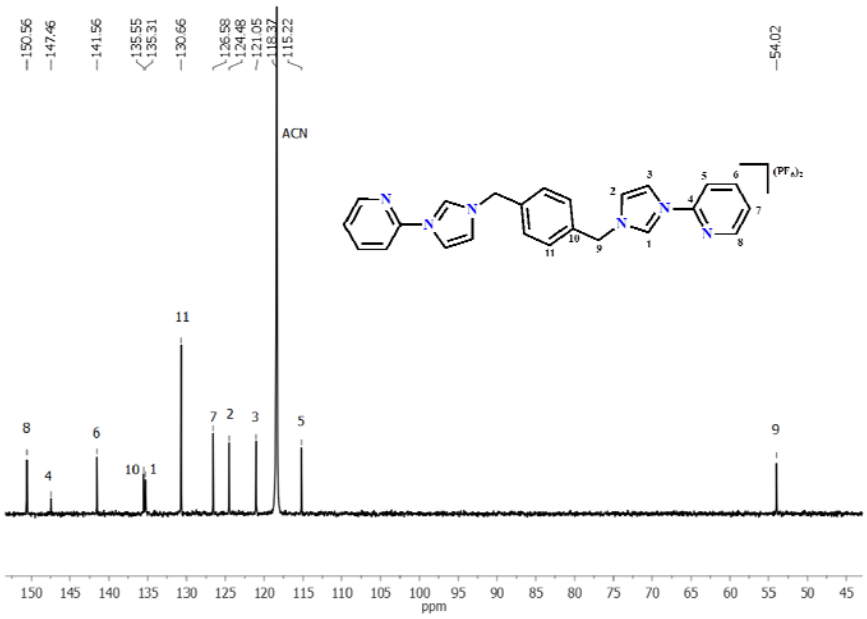


Figure 12S. DEPT-135-NMR spectrum of compound $\mathbf{H_2L_3(PF_6)_2}$ in CD_3CN at 25ºC.

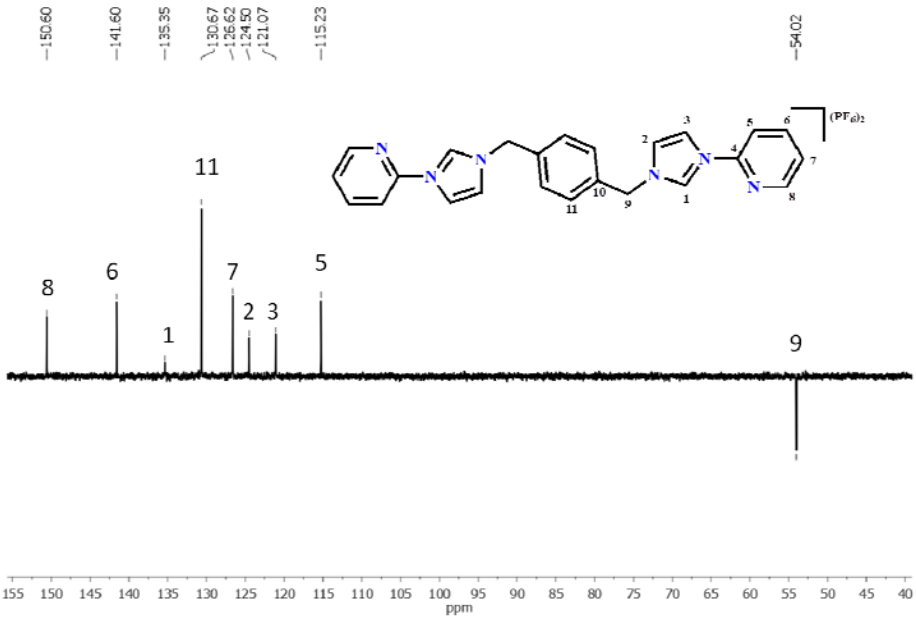


Figure 13S. ^{1}H-^{1}H COSY spectrum of $\mathbf{H_2L_3(PF_6)_2}$ in CD_3CN at 25ºC (400 MHz).

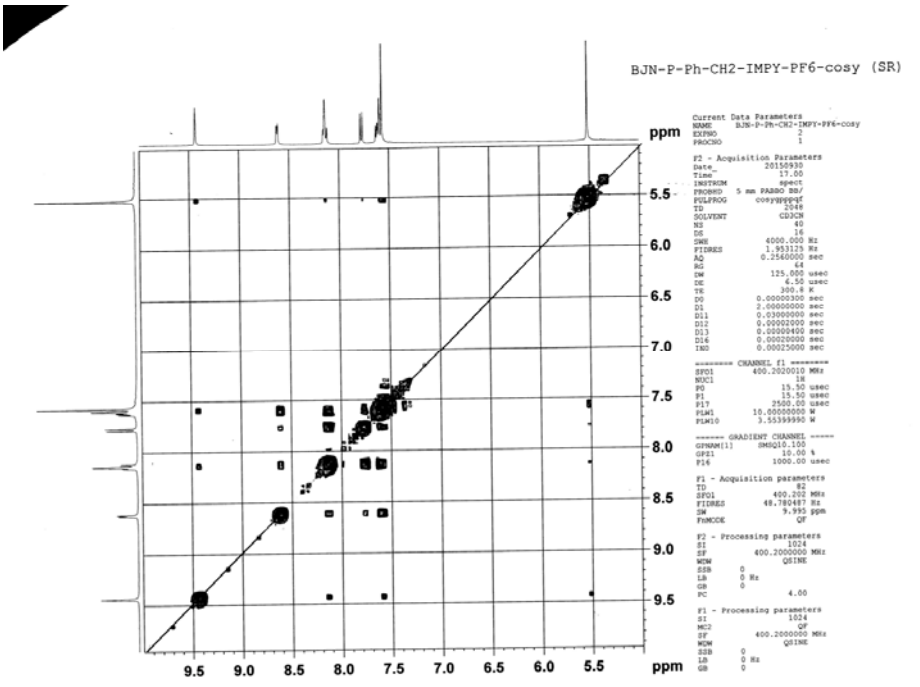
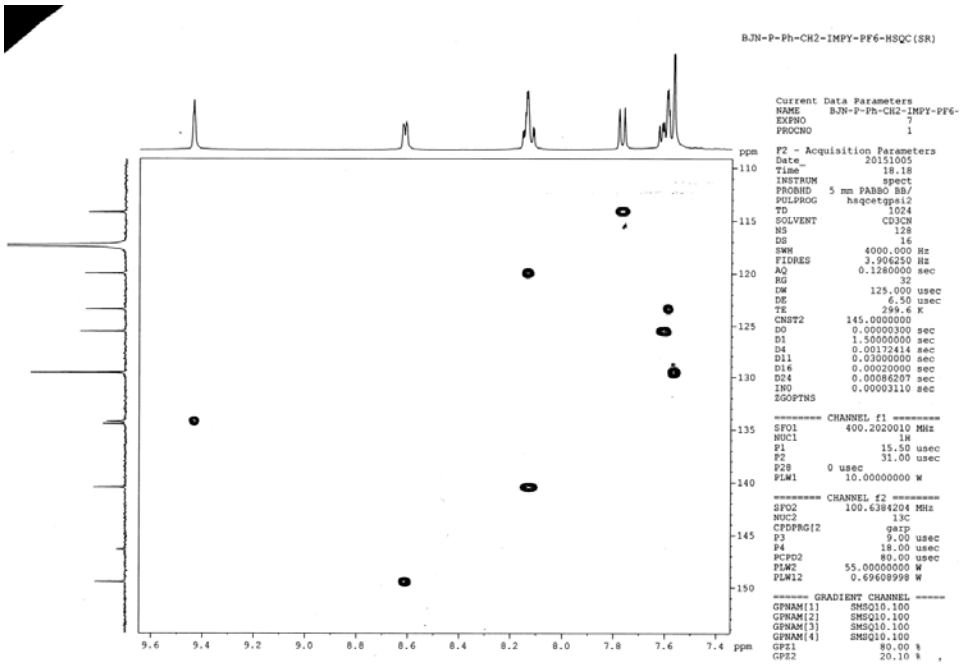


Figure 14S. ^{1}H-^{13}C HSQC spectrum of $\mathbf{H_2L_3(PF_6)_2}$ in CD_3CN at 25ºC (400 MHz)



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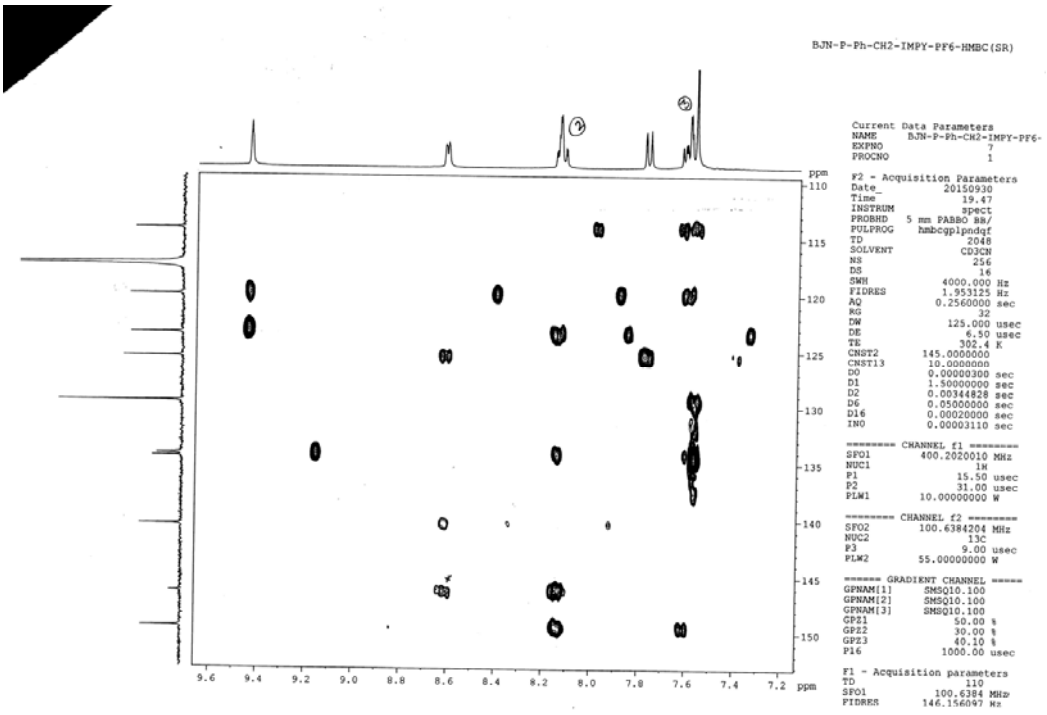

Figure 16S. Molecular structures of the ligands showing the cationic part H_2L_1 (a) H_2L_2 (b) and H_2L_3 (c) in 40% ellipsoids. PF_6 counter anions are omitted for clarity. Selected bond lengths [Å] and angles [°] with estimated standard deviation are given in Table 1 in supporting information.

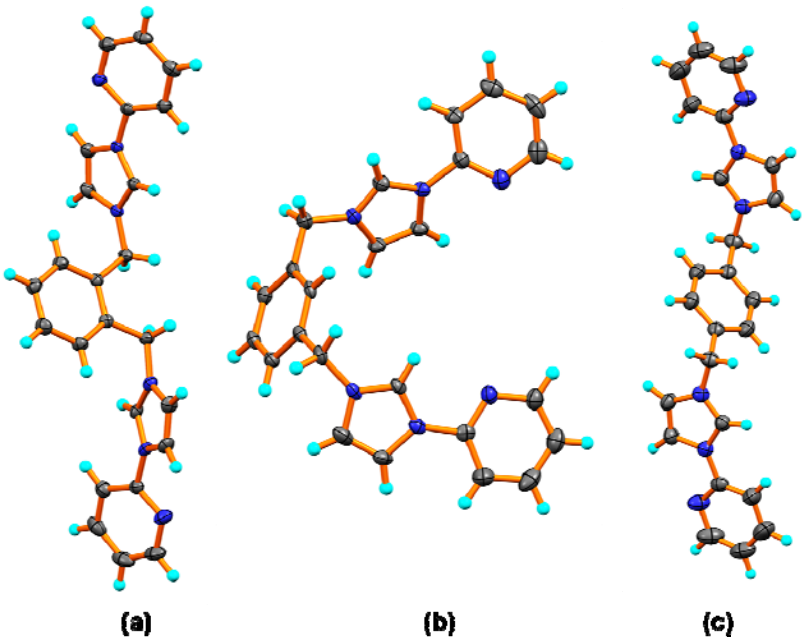

Figure 17S. Molecular structure of $H_2L_1(PF_6)_2$ in 40% ellipsoids. C-H…F interactions between cationic and anionic parts of the ligand are shown. Selected bond lengths [Å] and angles [°] with estimated standard deviations are tabulated in Table S1.

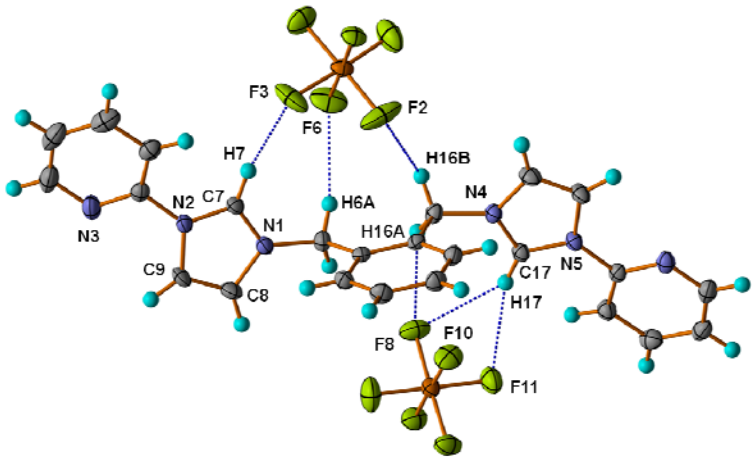

Figure 18S. ESI-MS (+ve) of **1**

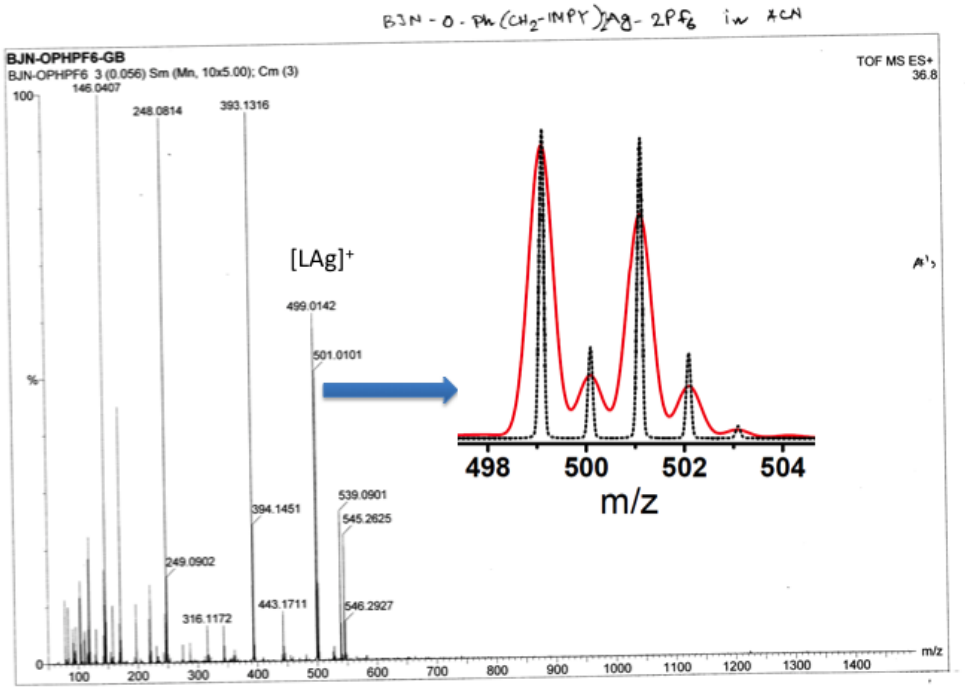

Figure 19S. ^{1}H-NMR spectrum of **1** in CD_3CN at 25ºC (300 MHz)

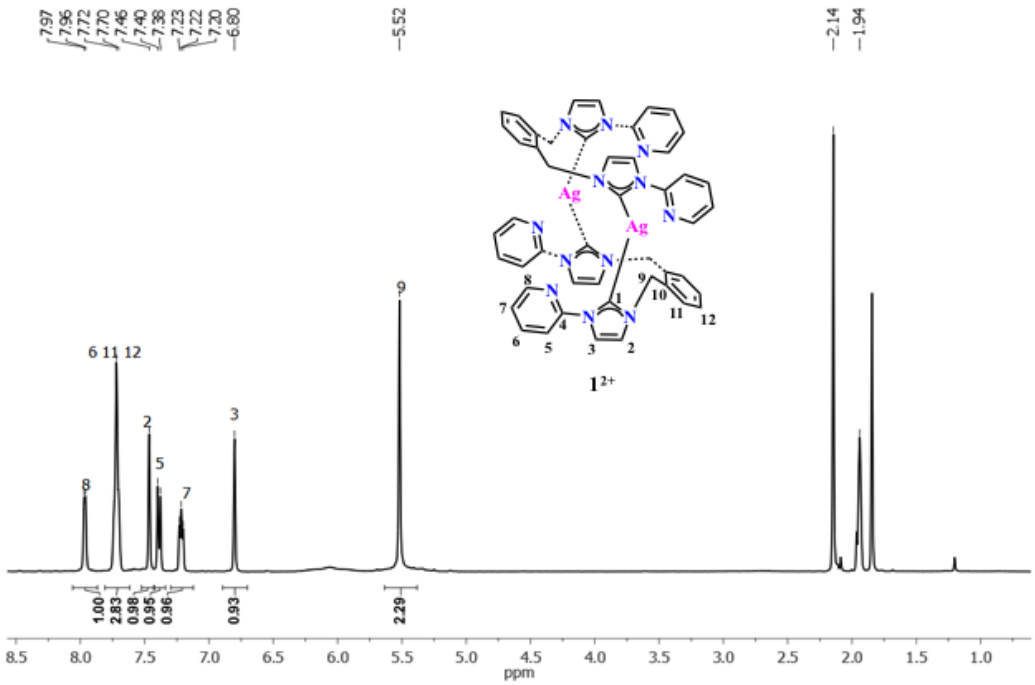

Figure 20S. ^{13}C-NMR spectrum of **1** in CD_3CN at 25ºC (75 MHz)

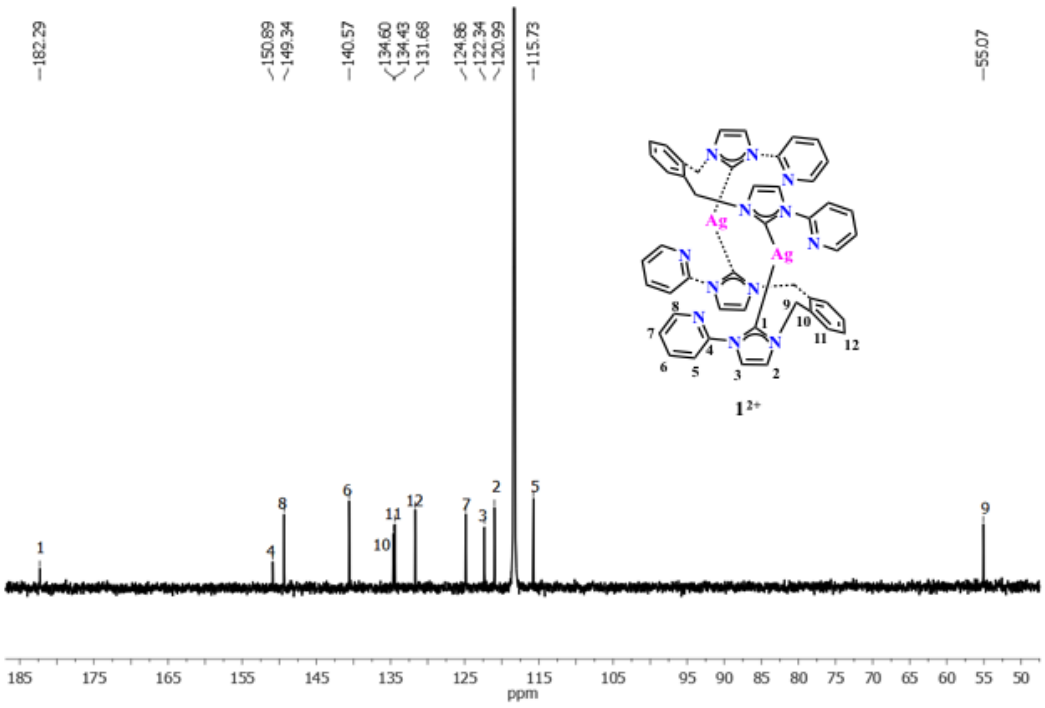

Figure 21S. DEPT-135 spectrum of **1** in CD_3CN at 25ºC (75 MHz)

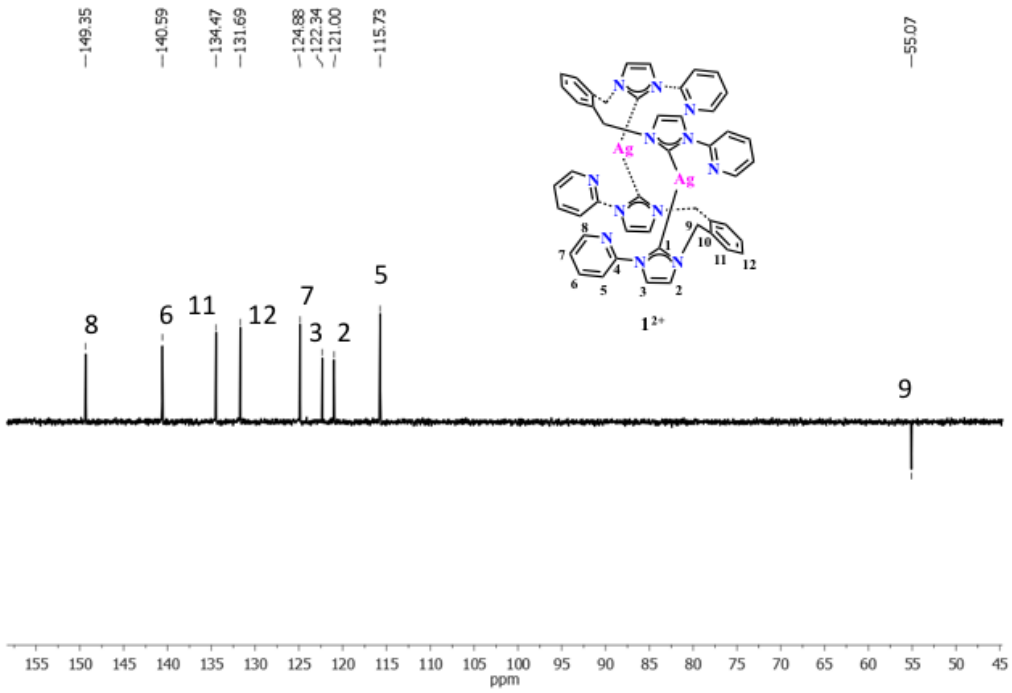

Figure 22S. ^{1}H-^{1}H COSY spectrum of **1** in CD_3CN at 25ºC (400 MHz)

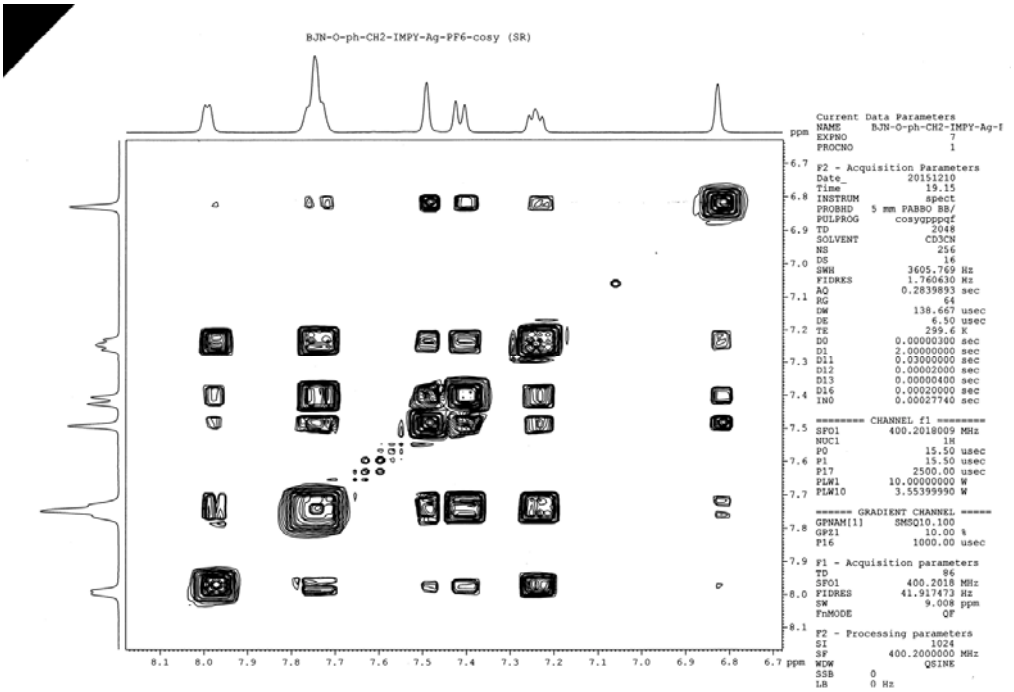

Figure 23S. ^{1}H-^{1}H HSQC spectrum of **1** in CD_3CN at 25ºC (500 MHz)

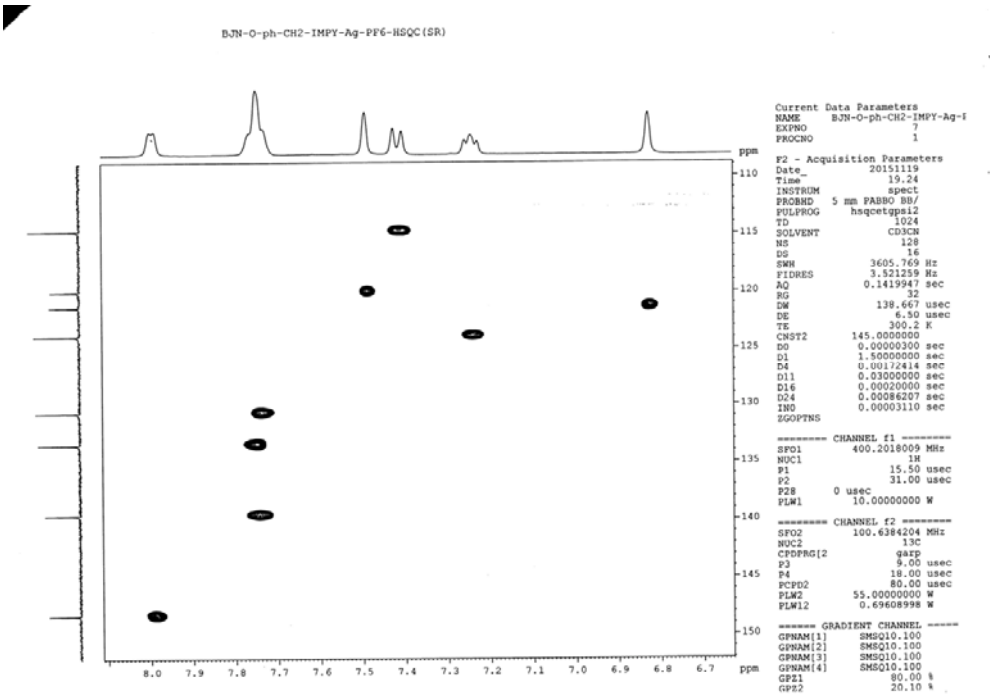

Figure 24S. ^{1}H-^{13}C HMBC spectrum of **1** in CD_3CN at 25ºC (500 MHz)

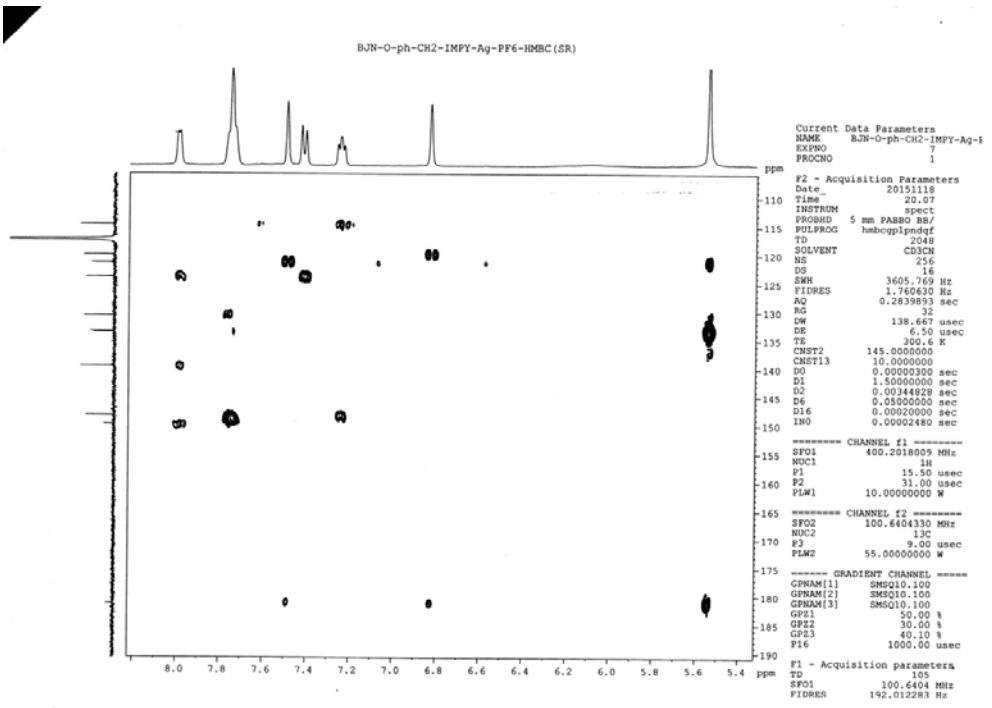

Figure 25S. ESI-MS (+ve) of **2**

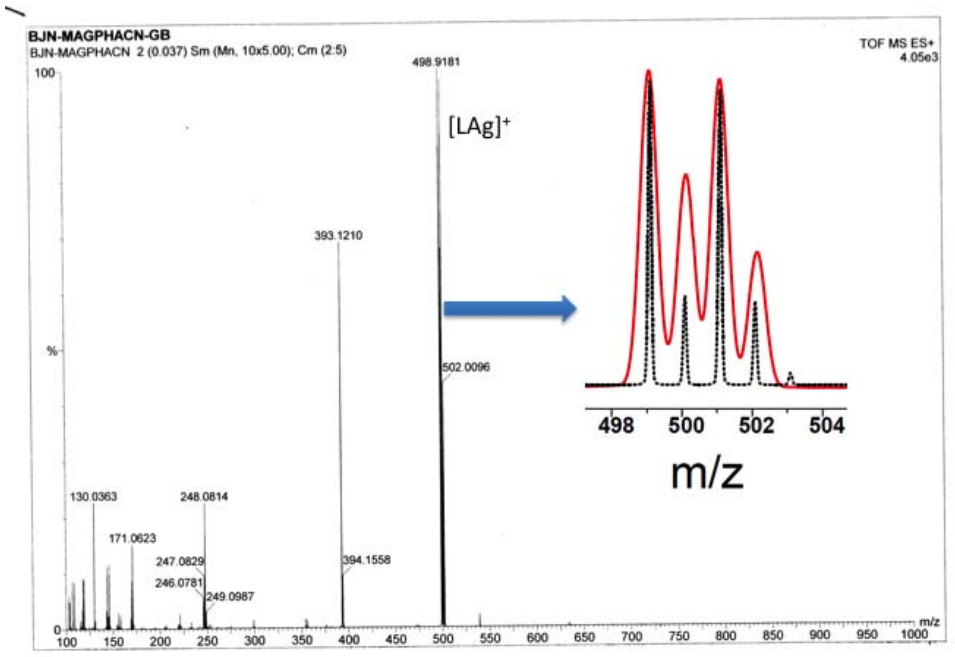

Figure 26S. ^{1}H-NMR spectrum of **2** in CD_3CN at 25ºC (500 MHz)

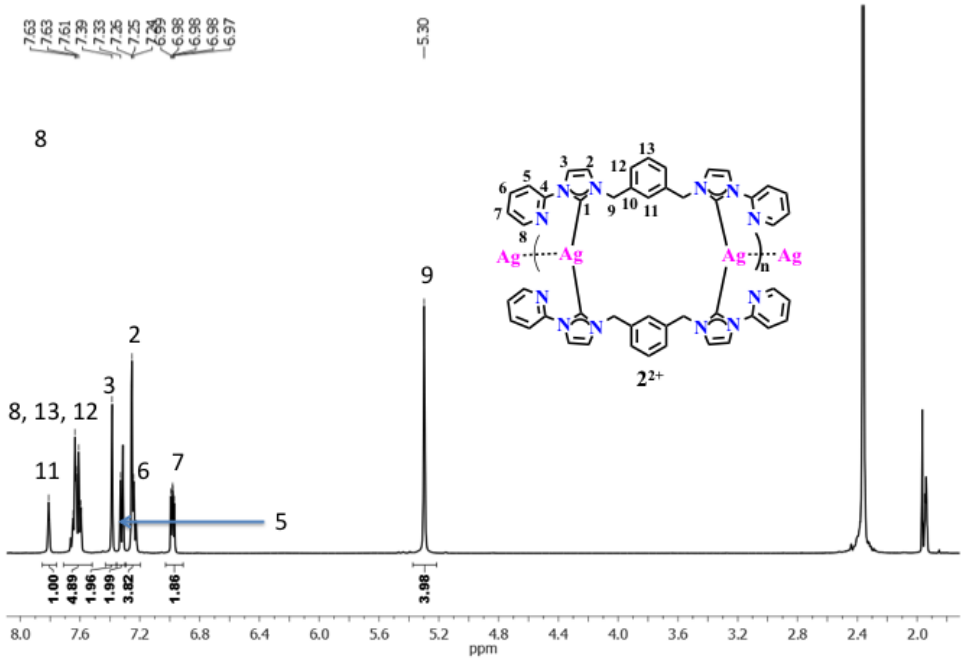

Figure 27S. ^{13}C-NMR spectrum of **2** in CD_3CN at 25ºC (75 MHz)

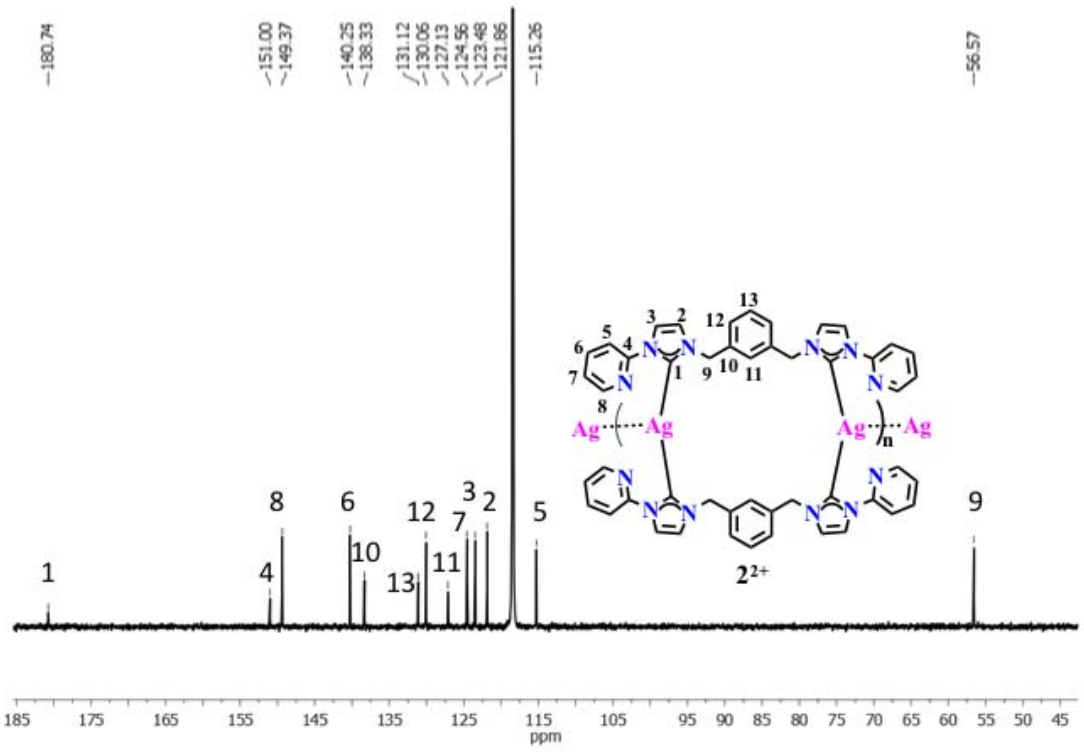

Figure 28S. DEPT-135 spectrum of **2** in CD_3CN at 25ºC (500 MHz)

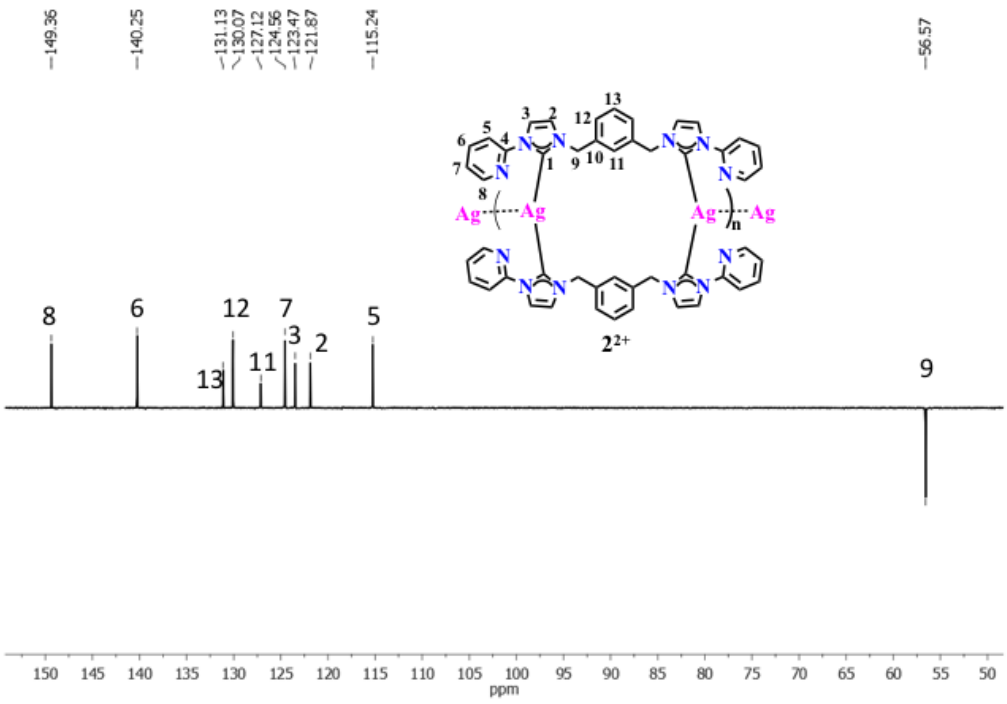

Figure 29S. ^1H-^1H COSY spectrum of **2** in CD_3CN at 25ºC (500 MHz)

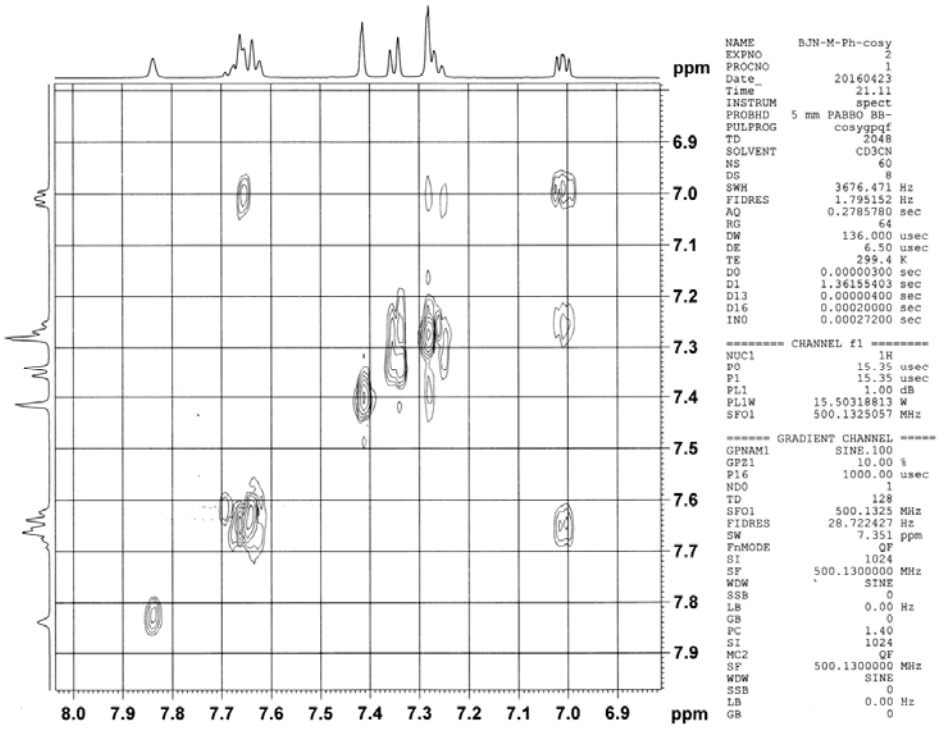

Figure 30S. ^{1}H-^{13}C HSQC spectrum of **2** in CD_3CN at 25ºC (500 MHz)

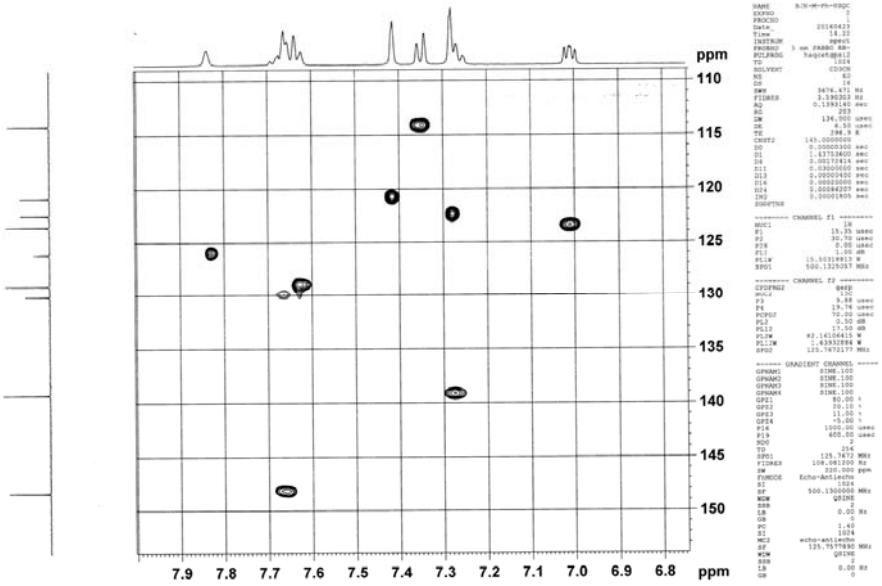

Figure 31S. ^{1}H-^{13}C HMBC spectrum of **2** in CD_3CN at 25ºC (500 MHz)

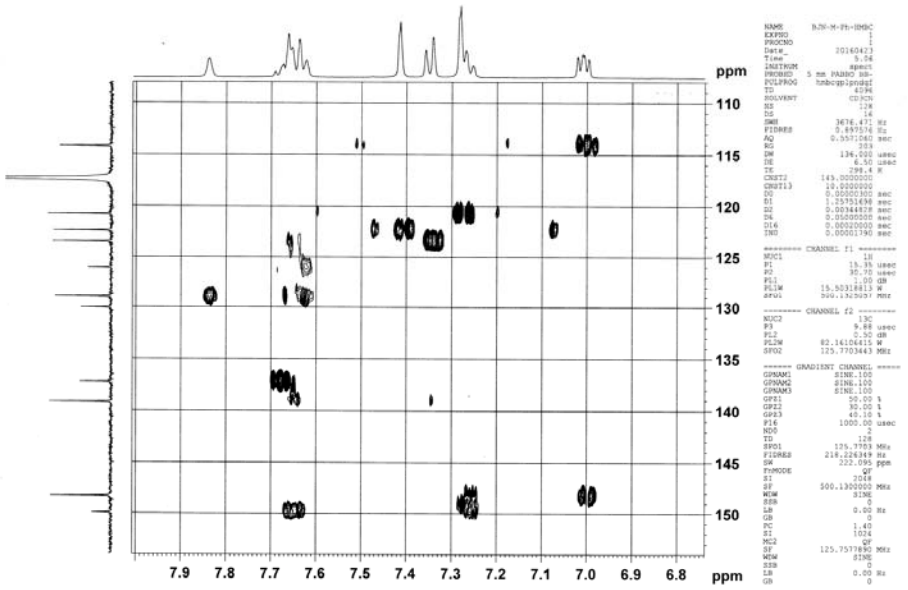

Figure 32S. ESI-FTICR-MS (+ve) of **3**

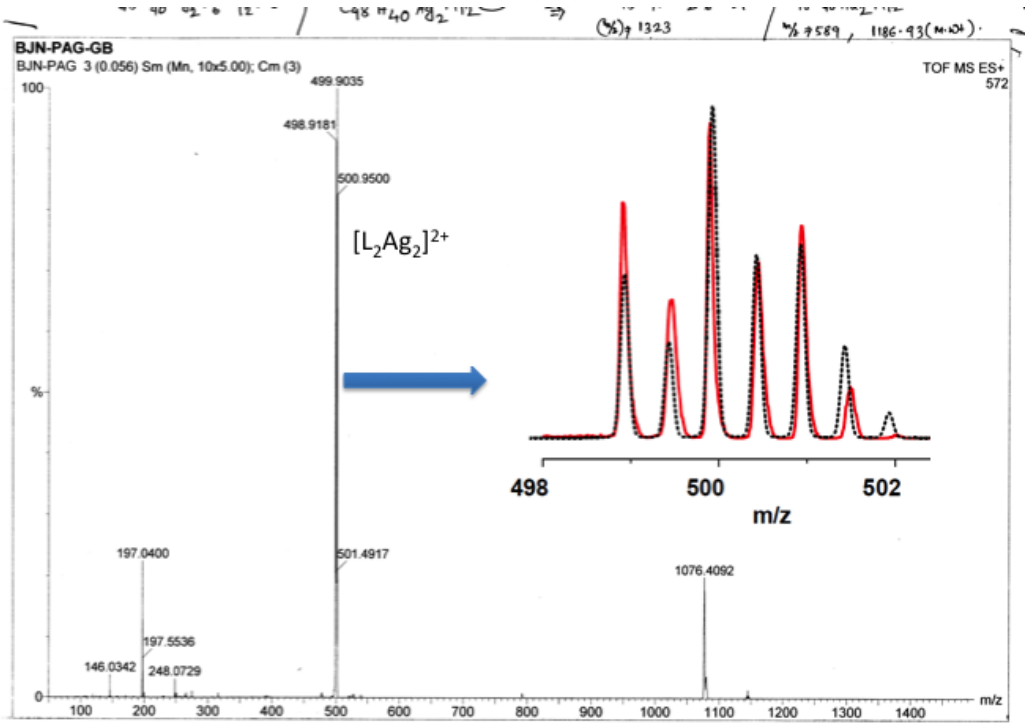

Figure 33S. ^{1}H-NMR spectrum of **3** in CD_3CN at 25ºC (300 MHz)

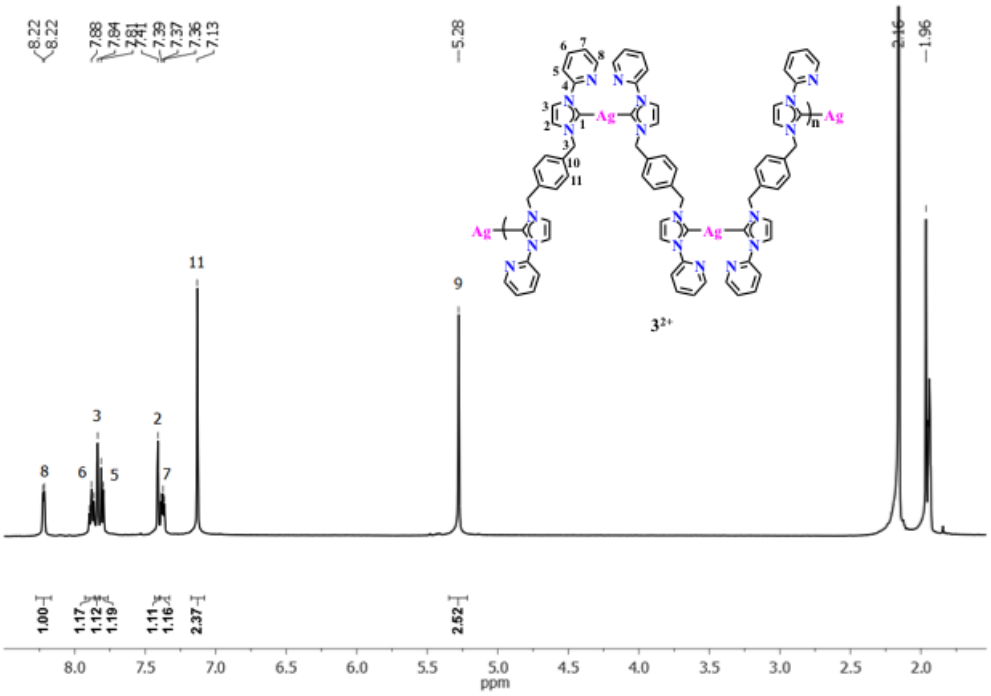

Figure 34S. ^{13}C-NMR spectrum of **3** in CD_3CN at 25ºC (75 MHz)

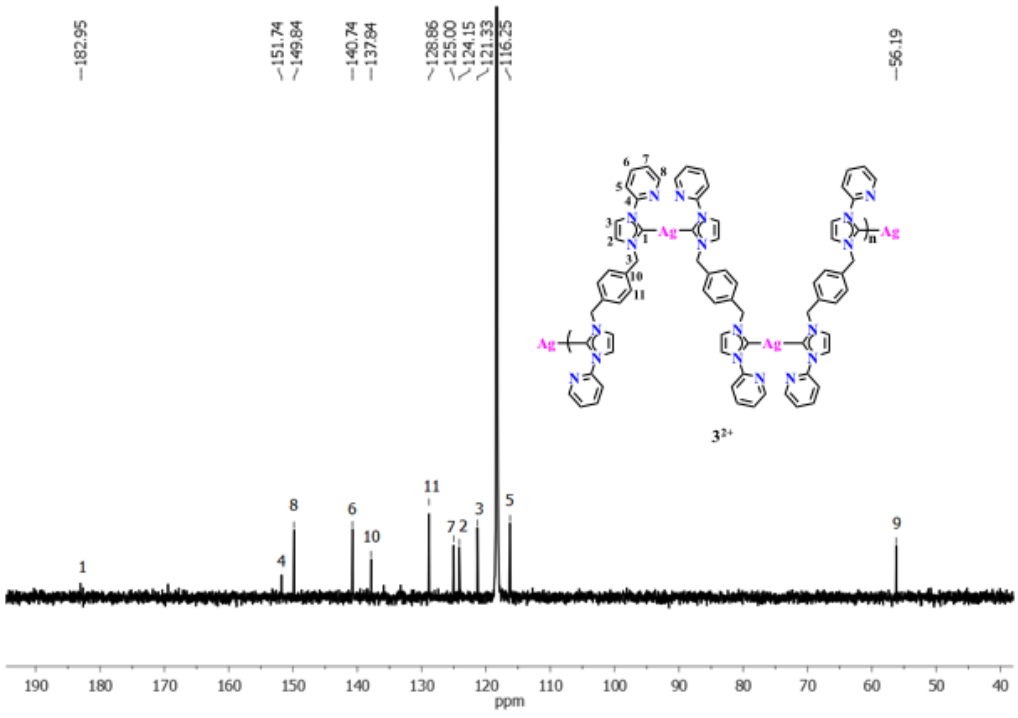

Figure 35S. ^{13}C-NMR spectrum of **3** in CD_3CN at 25ºC (75 MHz)

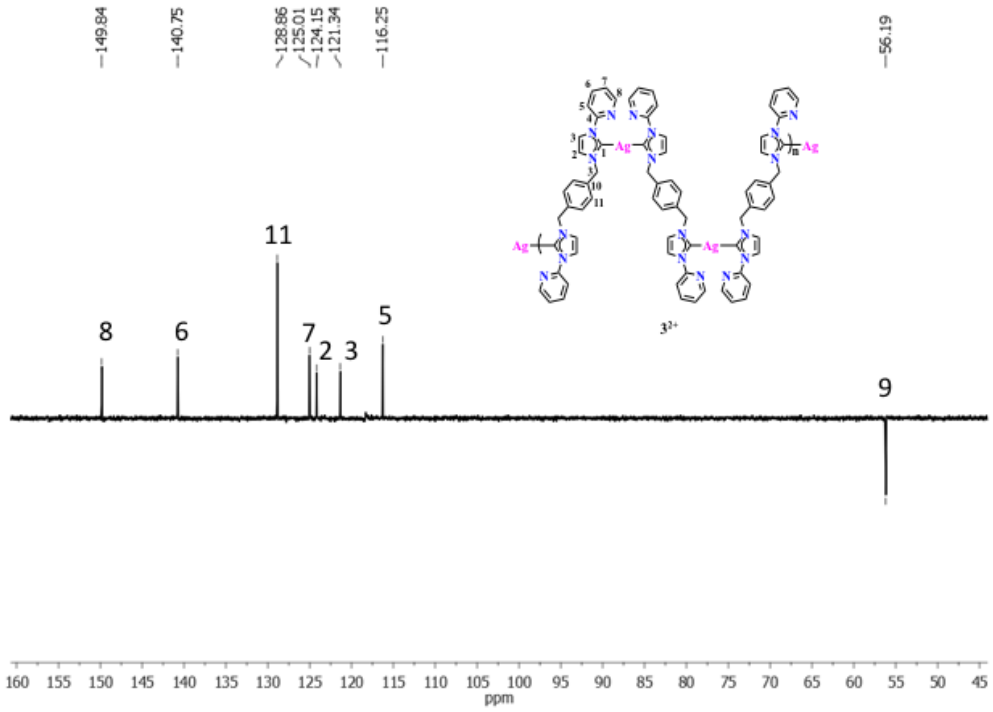

Figure 36S. ^{1}H-^{1}H COSY spectrum of **3** in CD_3CN at 25ºC (500 MHz)

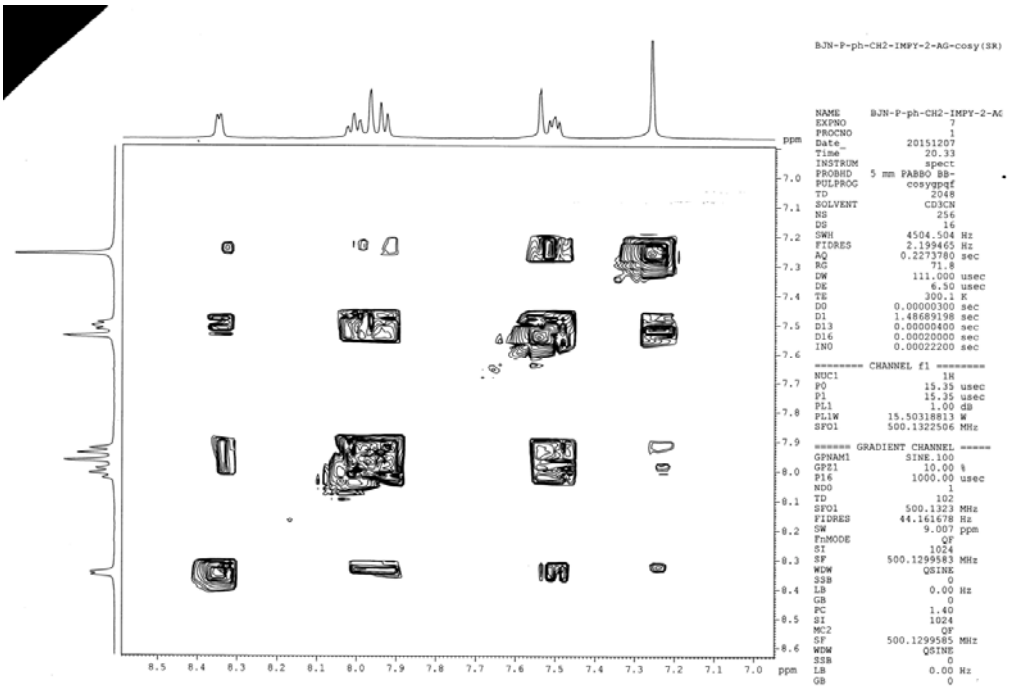

Figure 37S. ^{1}H-^{13}C HSQC spectrum of **3** in CD_3CN at 25ºC (500 MHz)

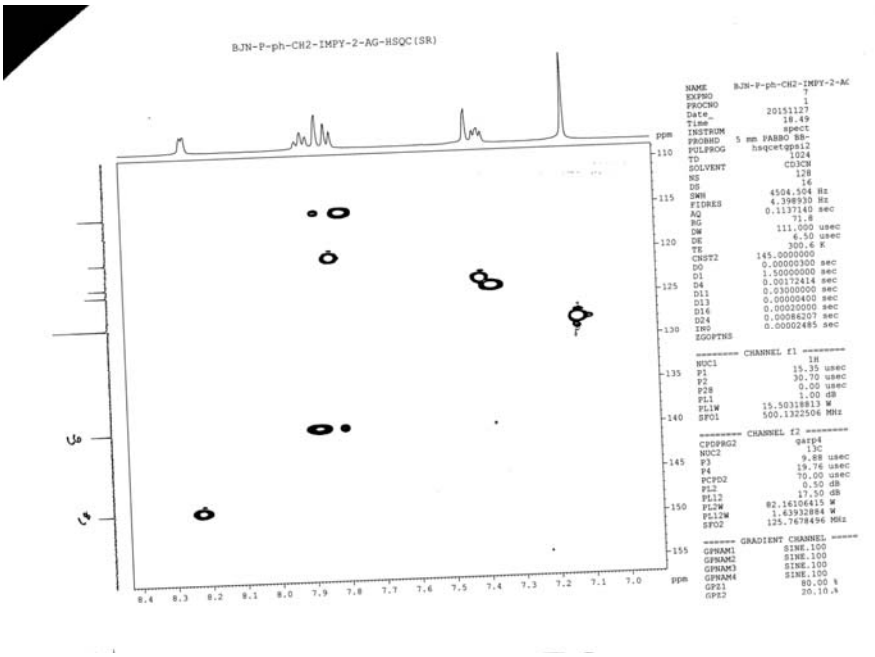

Figure 38S. ^{1}H-^{13}C HMBC spectrum of **3** in CD_3CN at 25ºC (500 MHz)

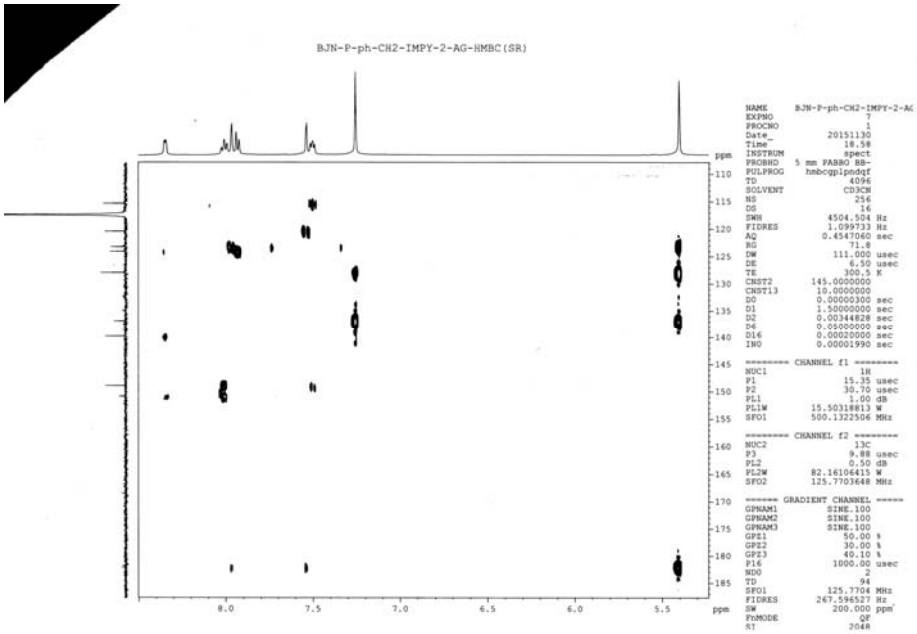

Figure 39S. Molecular structure with numbering scheme of compound **1**

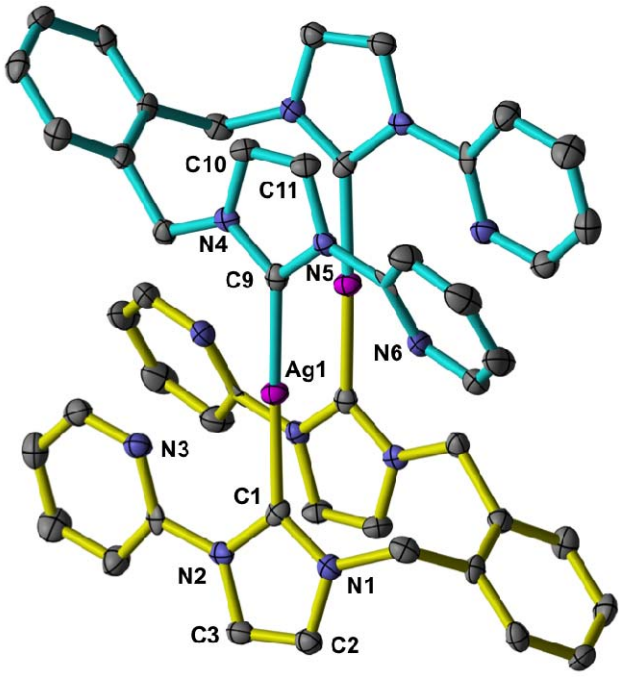

Figure 40S. Molecular structure with numbering scheme of compound **2**

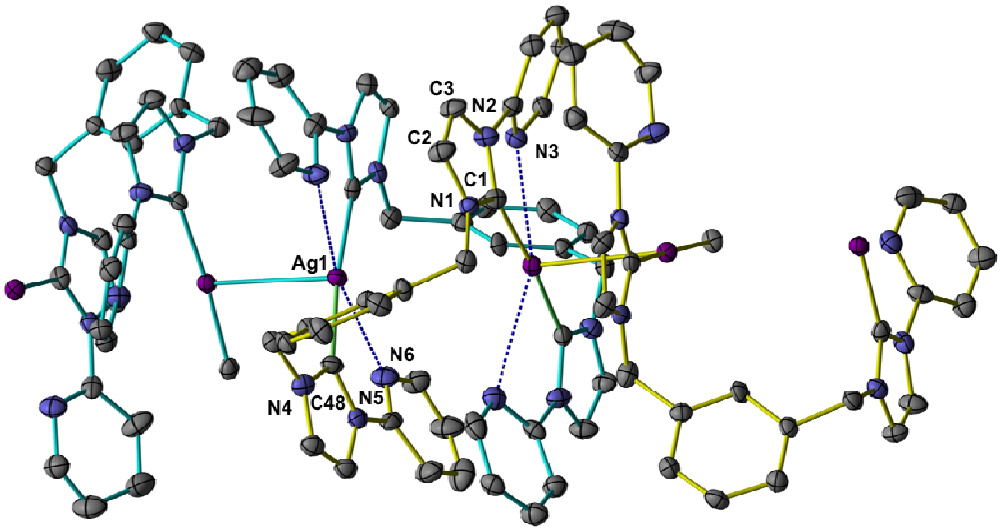

Figure 41S. Molecular structure with numbering scheme of compound **3**

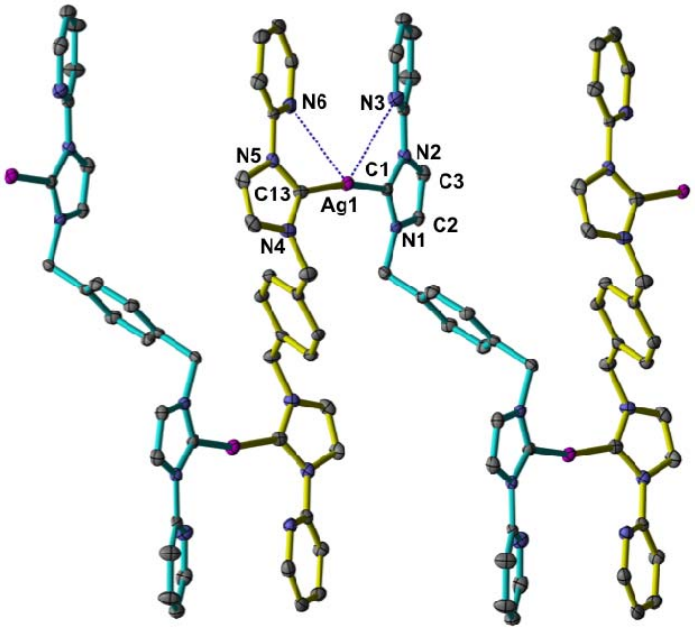

Table 1S. Selected bond lengths [Å] and angles [°] with estimated standard deviation for compounds **1**, **2** and **3**

1		2		3	
Ag1…Ag1(intramolecular)	3.257(9),	Ag2-C1	2.064(3)	Ag1-C1	2.104(2)
Ag1…Ag1(intermolecular)	4.281	Ag1-C24	2.085(3)	Ag1-C13	2.109(2)
Ag1…N3	3.120(9)	Ag2-C39	2.122(3)	Ag1…N3	3.074(3)
Ag1…N6	2.908(8)	Ag1…Ag2	3.18(14)	Ag1…N6	2.959(1)
Ag1-C1	2.086(7)	Ag1…N9	3.051(4)	π – π (pyridyl-imidazole)	3.740
Ag1-C9	2.103(6)	Ag1…N6	2.962(4)	π – π (imidazole - pyridyl)	3.862
C1-C9	4.183	Ag2...N3	3.103(4)	C1-C13	4.185
C14...C18	3.637	Ag2...N12	3.054(4)	C13-N5-C16-N6	28.45(1)
C14...H18b-C18	137.4	C1-Ag2-C39	175.2(1)	C1-N2-C4-N3	18.74(1)
C1-Ag1-C9	173.9(3)	C24-Ag1-C48	172.9(1)	C1-Ag1-C13	166.8(1)
N4-C9-N5	103.8(5)	N1-C1-N2	104.3(1)	N1-C1-N2	103.5(3)
N1-C1-N2	104.2(5)	N5-C19-N6	118.71(1)	N4-C13-N5	104.2(3)