

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 1S. ESI-MS (+ve) of compound **H₂L1(PF₆)₂**.

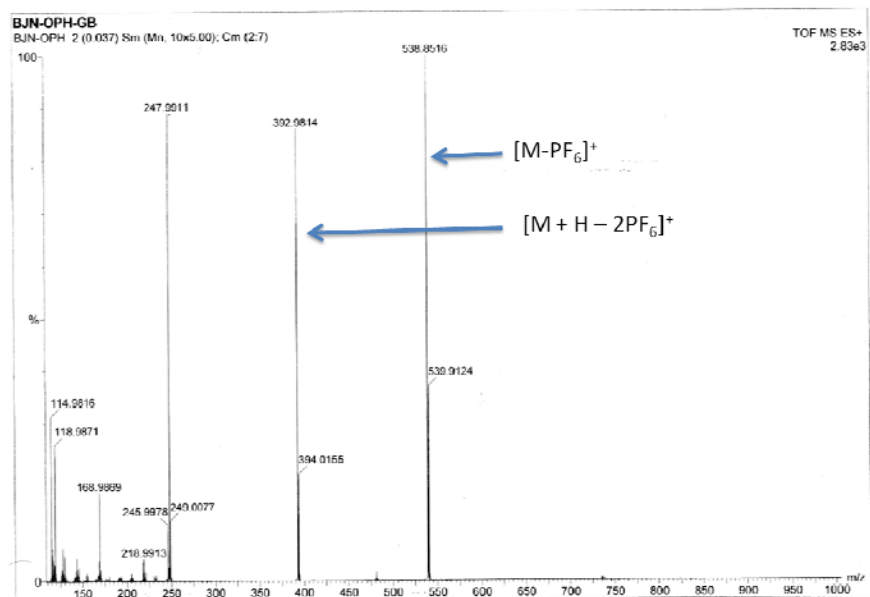


Figure 2S. ¹H-NMR spectrum of compound **H₂L1(PF₆)₂** in CD₃CN at 25°C (300 MHz).

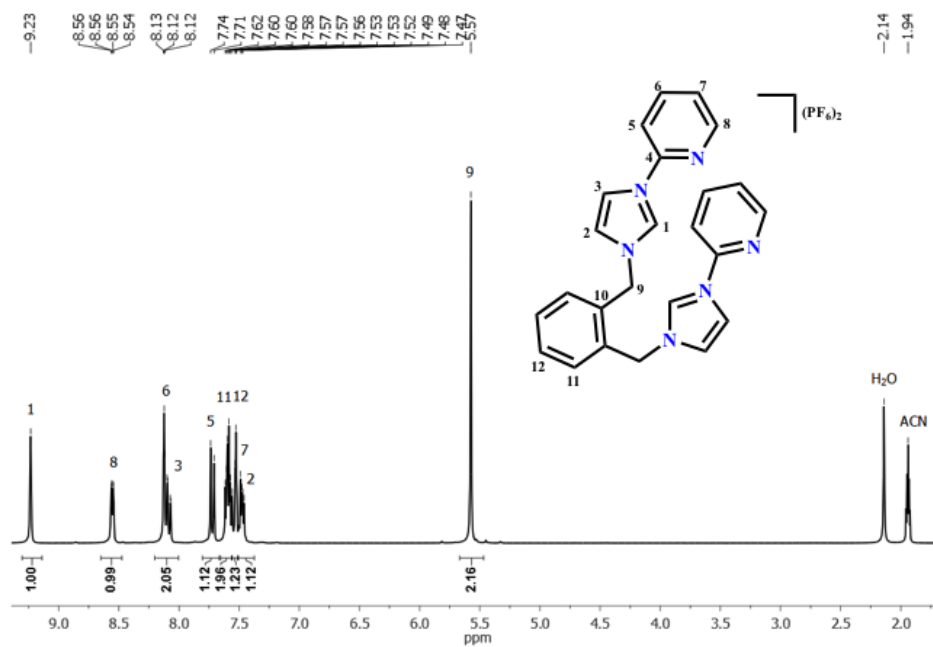


Figure 3S. ^{13}C -NMR spectrum of compound $\text{H}_2\text{L1}(\text{PF}_6)_2$ in CD_3CN at 25°C (75 MHz).

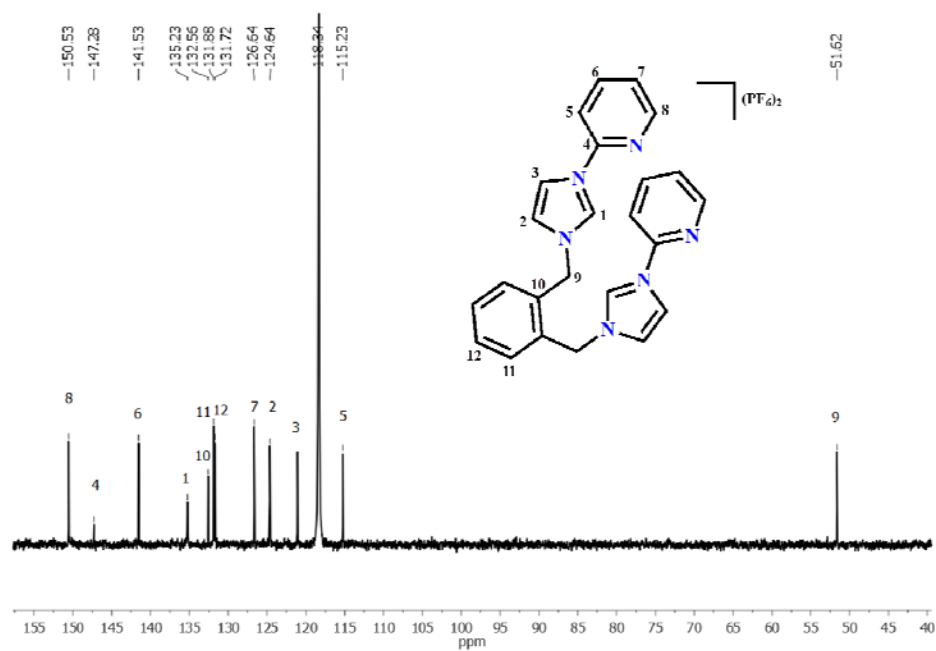


Figure 4S. DEPT-135-NMR spectrum of compound $\text{H}_2\text{L1}(\text{PF}_6)_2$ in CD_3CN at 25°C .

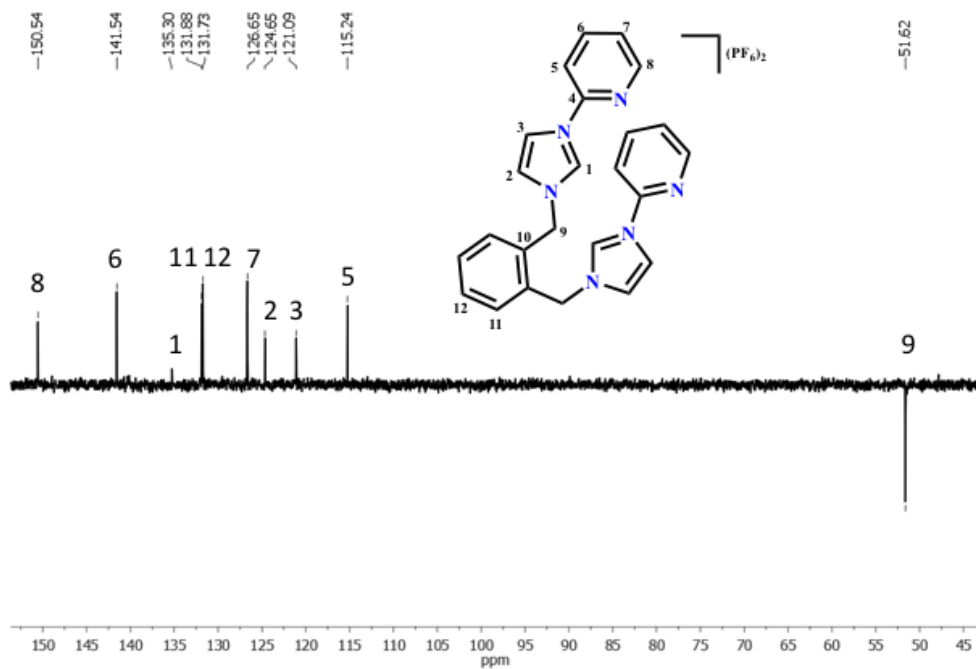


Figure 5S. ESI-MS (+ve) of compound **H₂L₂(PF₆)₂**.

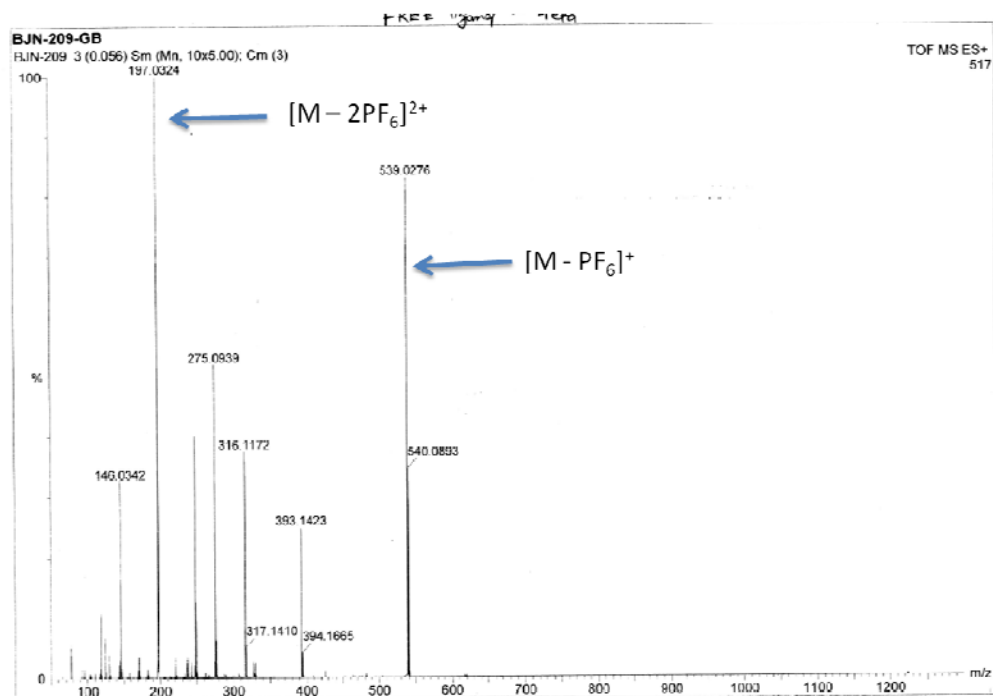


Figure 6S. ¹H-NMR spectrum of compound **H₂L₂(PF₆)₂** in CD₃CN at 25°C (500 MHz).

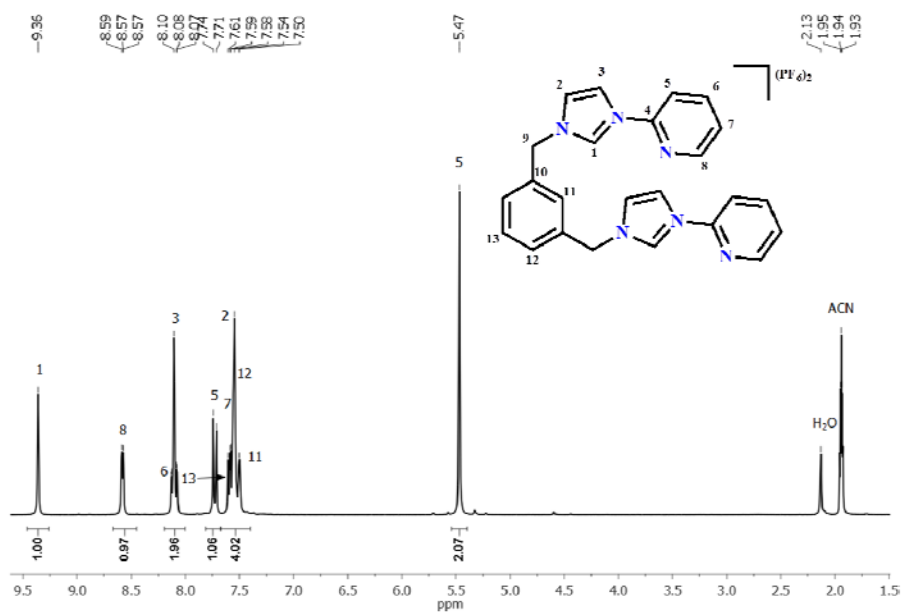


Figure 7S. ^{13}C -NMR spectrum of compound $\text{H}_2\text{L}_2(\text{PF}_6)_2$ in CD_3CN at 25°C (125 MHz).

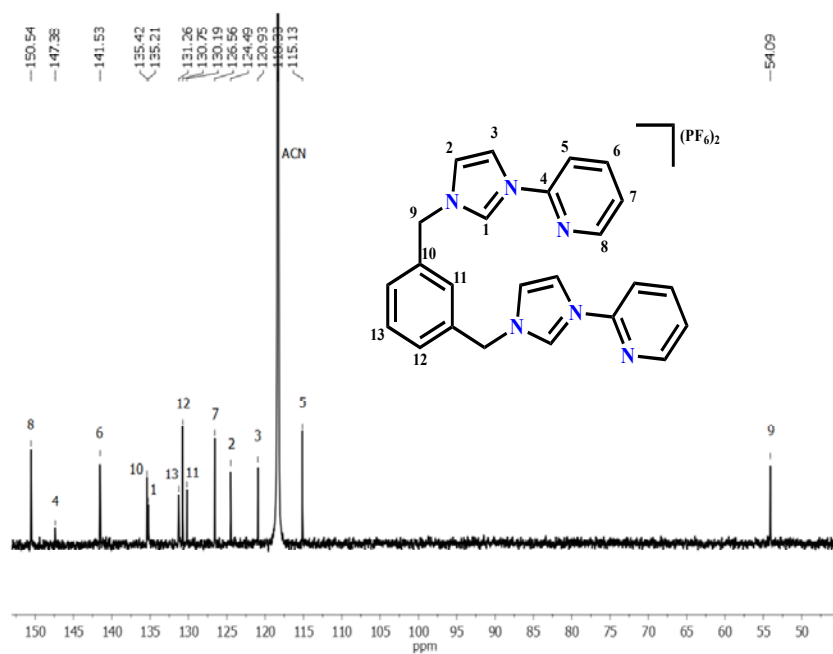


Figure 8S. DEPT-135-NMR spectrum of compound $\text{H}_2\text{L}_2(\text{PF}_6)_2$ in CD_3CN at 25°C .

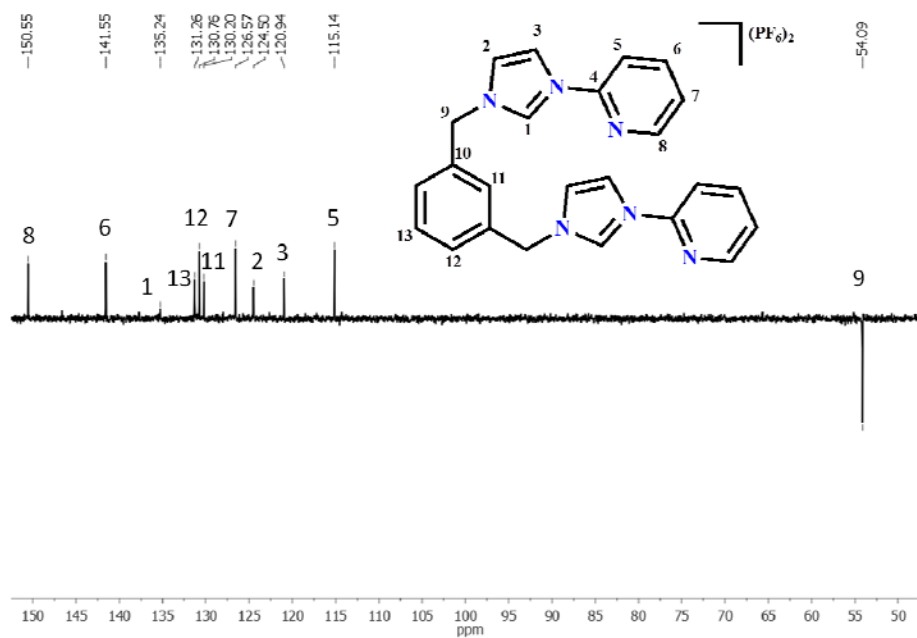


Figure 9S. ESI-MS (+ve) of $\text{H}_2\text{L}_3(\text{PF}_6)_2$

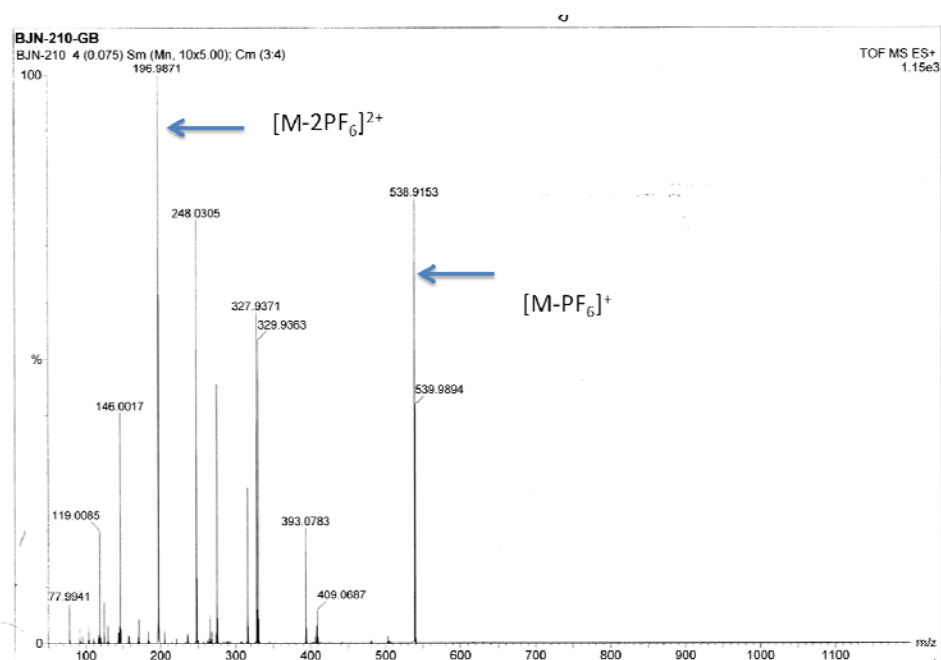


Figure 10S. ^1H -NMR spectrum of $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C (400 MHz).

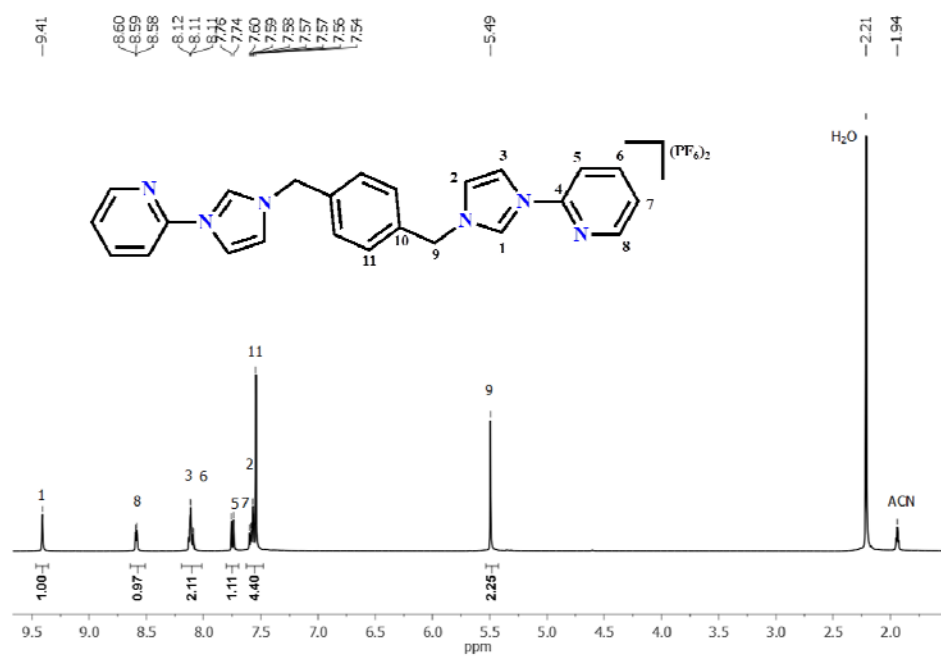


Figure 11S. ^{13}C -NMR spectrum of $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C (100 MHz).

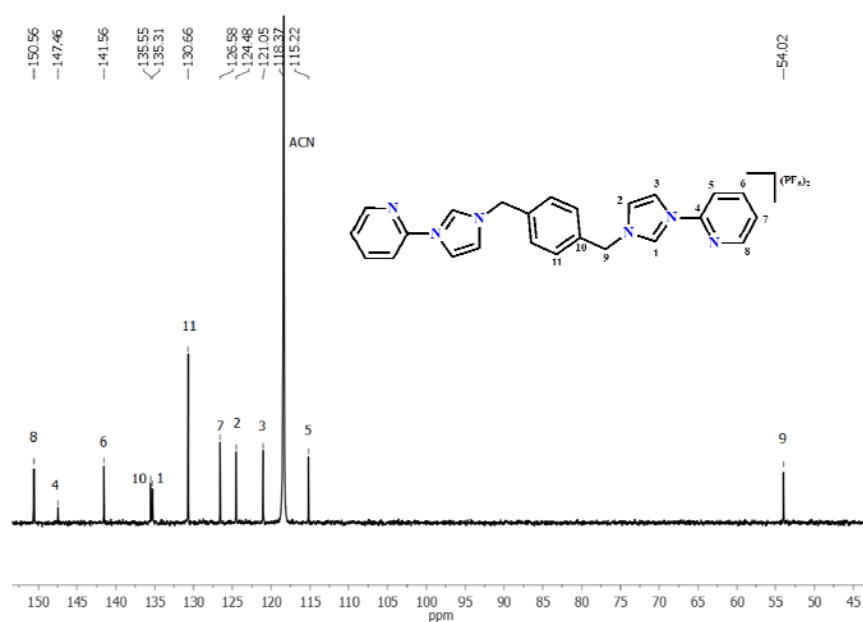


Figure 12S. DEPT-135-NMR spectrum of compound $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C .

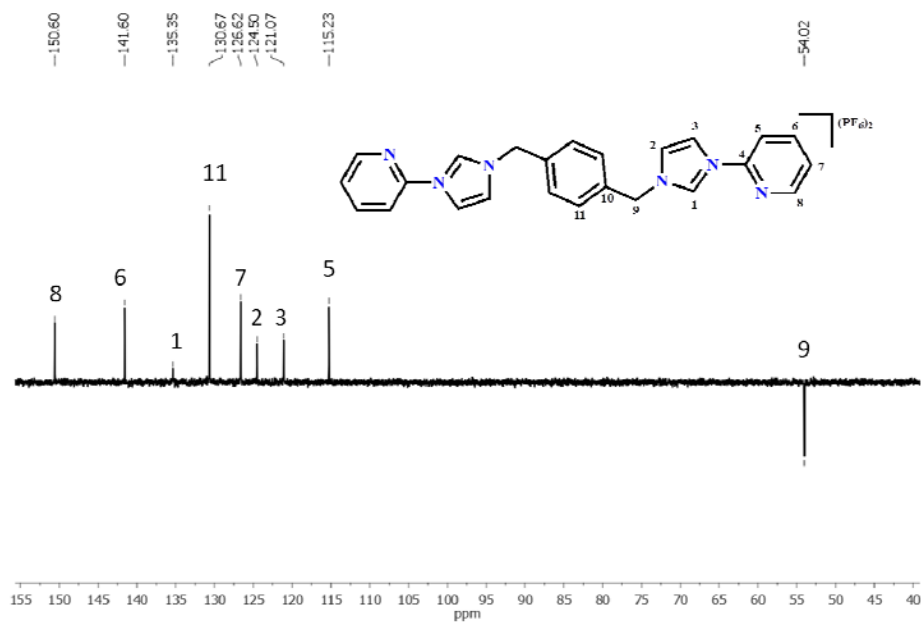


Figure 13S. ^1H - ^1H COSY spectrum of $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C (400 MHz).

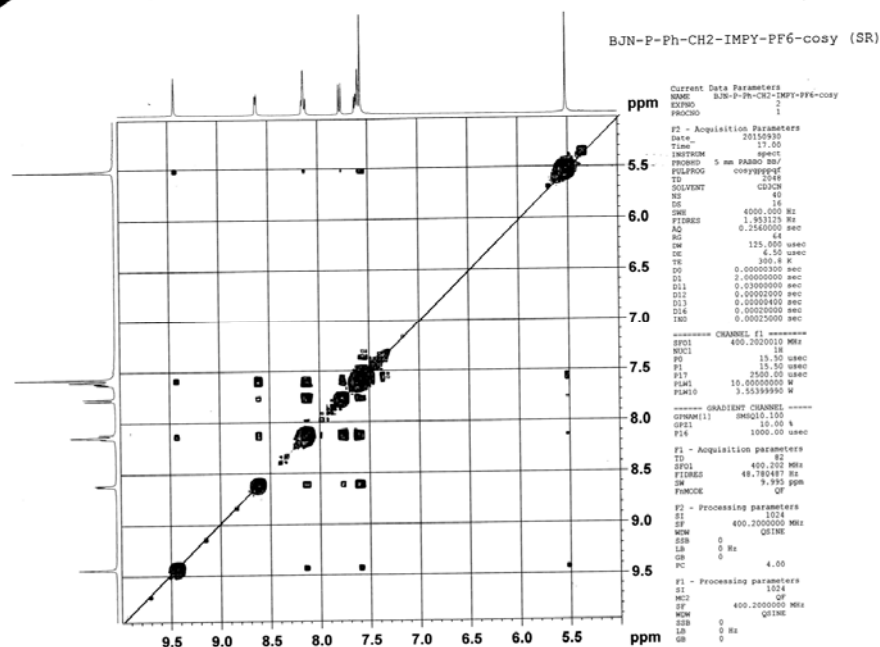


Figure 14S. ^1H - ^{13}C HSQC spectrum of $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C (400 MHz)

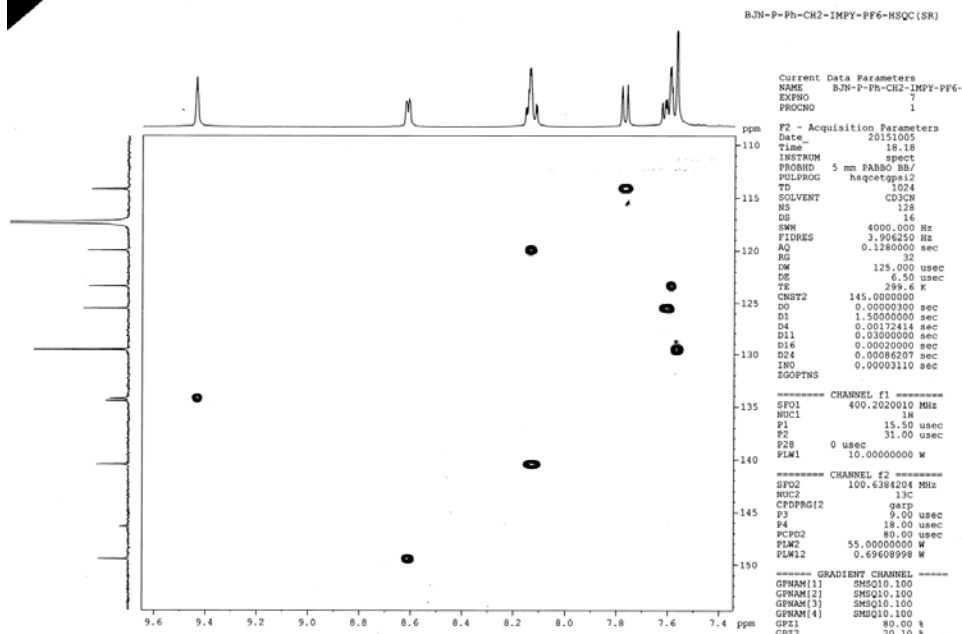


Figure 15S. ^1H - ^{13}C HMBC spectrum of $\text{H}_2\text{L}_3(\text{PF}_6)_2$ in CD_3CN at 25°C (400 MHz)

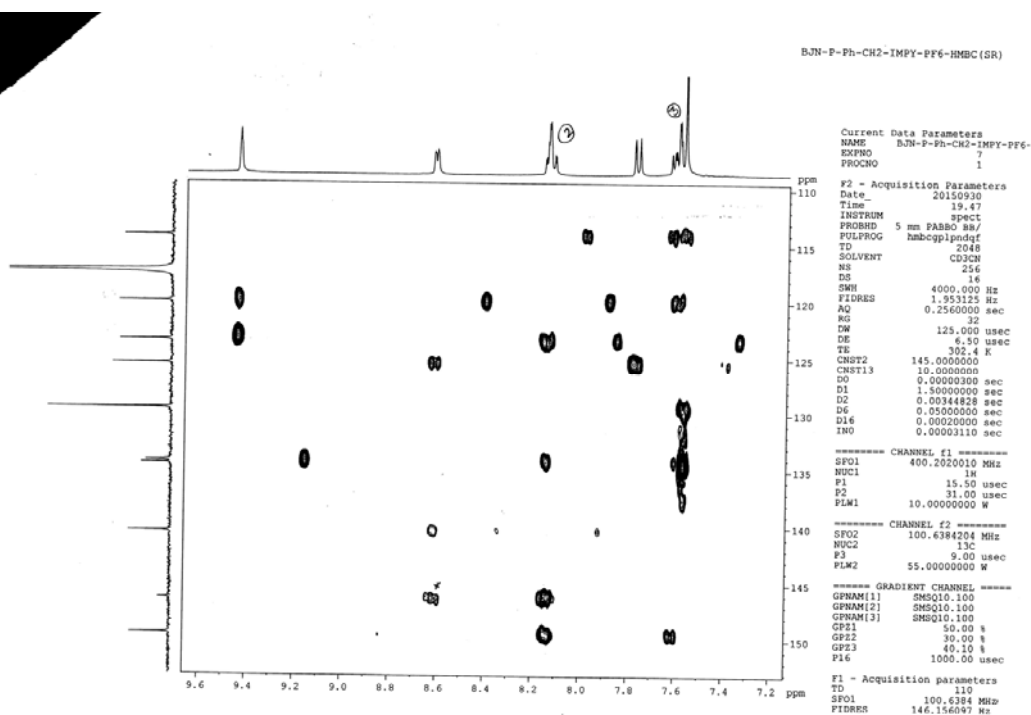


Figure 16S. Molecular structures of the ligands showing the cationic part H₂L₁ (a) H₂L₂ (b) and H₂L₃ (c) in 40% ellipsoids. PF₆ counter anions are omitted for clarity. Selected bond lengths [Å] and angles [°] with estimated standard deviation are given in Table 1 in supporting information.

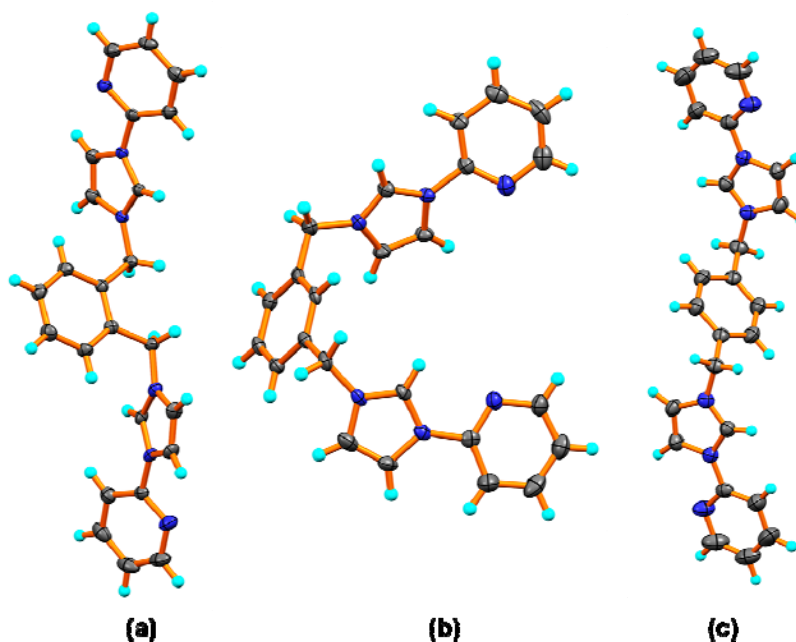


Figure 17S. Molecular structure of H₂L₁(PF₆)₂ in 40% ellipsoids. C-H...F interactions between cationic and anionic parts of the ligand are shown. Selected bond lengths [Å] and angles [°] with estimated standard deviations are tabulated in Table S1.

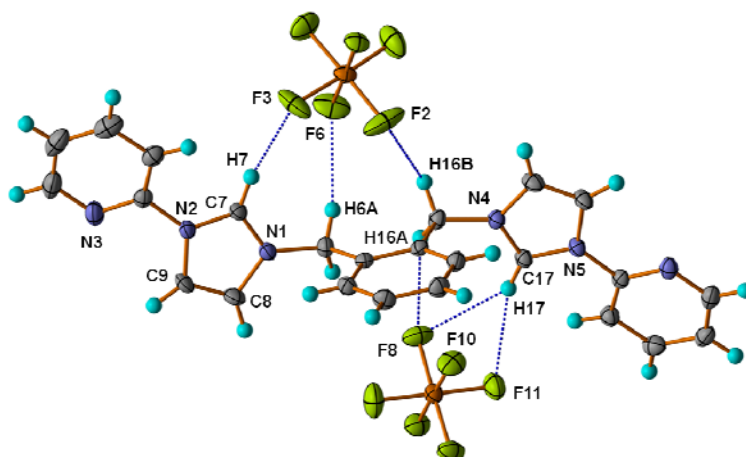


Figure 18S. ESI-MS (+ve) of **1**

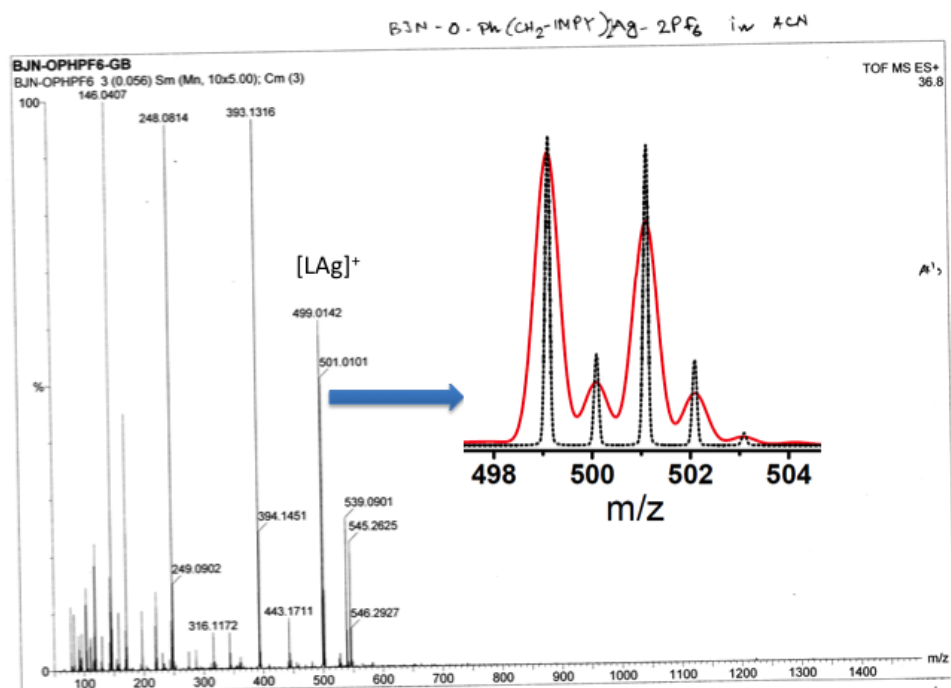


Figure 19S. ^1H -NMR spectrum of **1** in CD_3CN at 25°C (300 MHz)

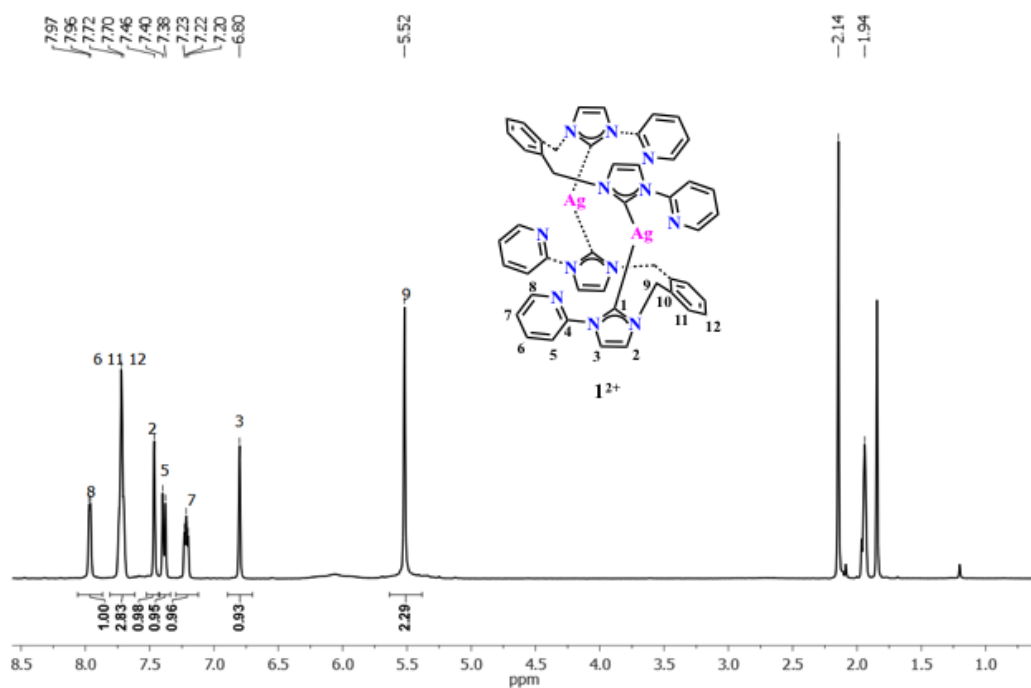


Figure 20S. ¹³C-NMR spectrum of **1** in CD₃CN at 25°C (75 MHz)

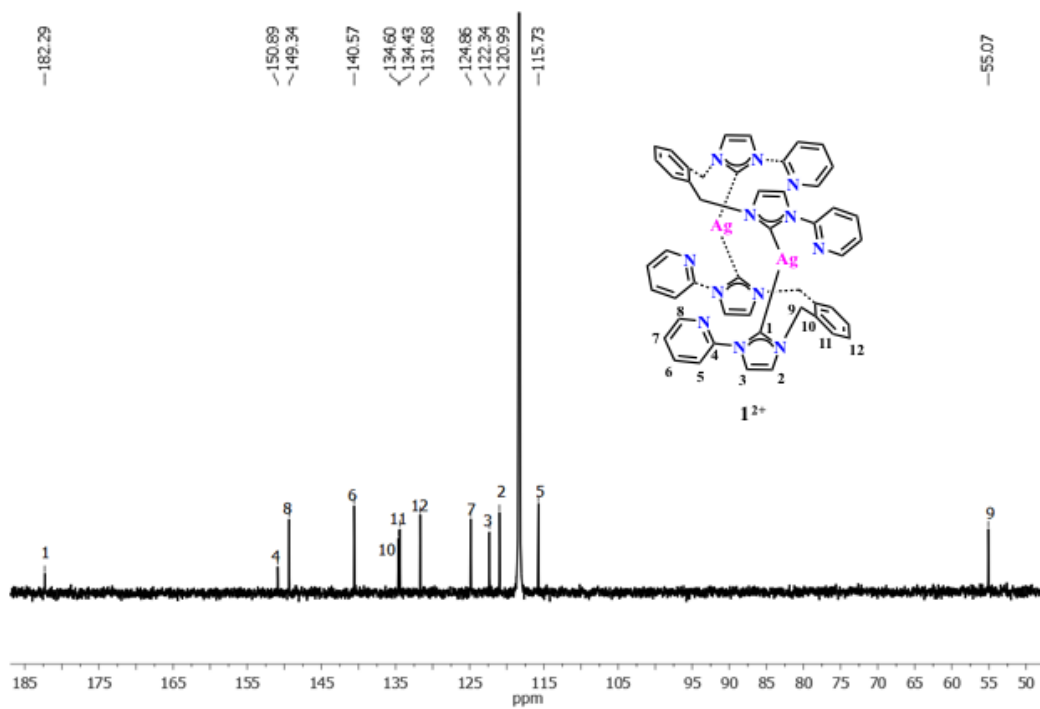


Figure 21S. DEPT-135 spectrum of **1** in CD₃CN at 25°C (75 MHz)

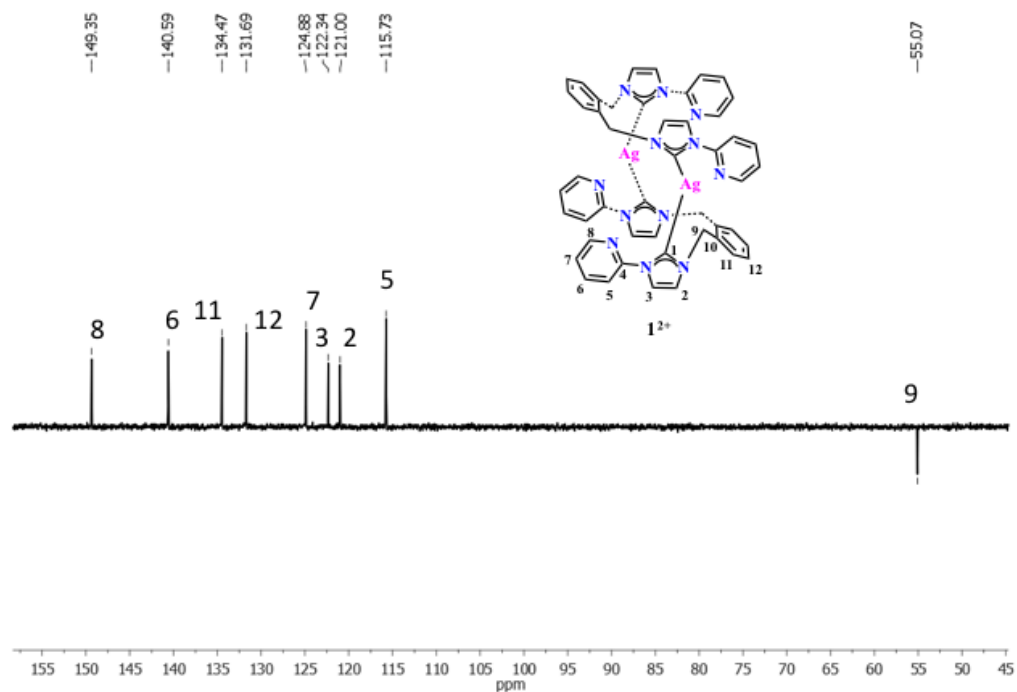


Figure 22S. ^1H - ^1H COSY spectrum of **1** in CD_3CN at 25°C (400 MHz)

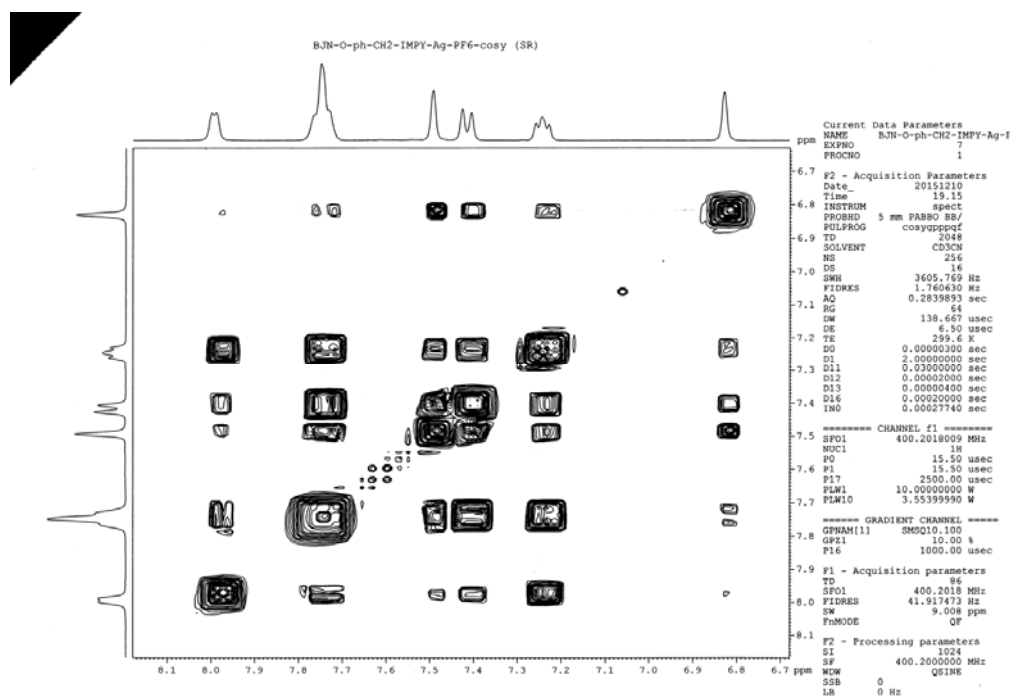


Figure 23S. ^1H - ^1H HSQC spectrum of **1** in CD_3CN at 25°C (500 MHz)

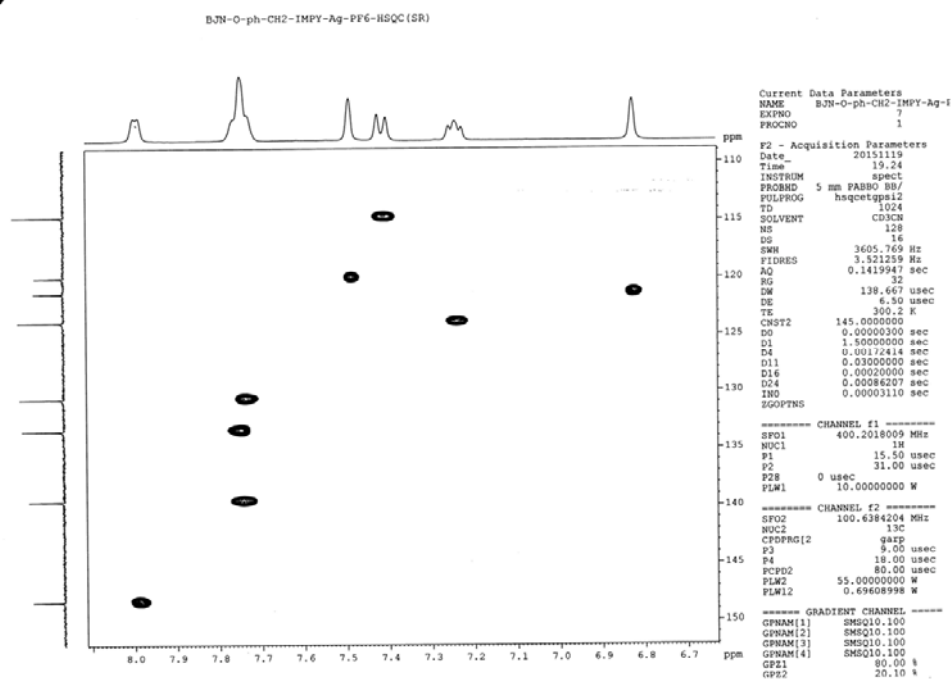


Figure 24S. ^1H - ^{13}C HMBC spectrum of **1** in CD_3CN at 25°C (500 MHz)

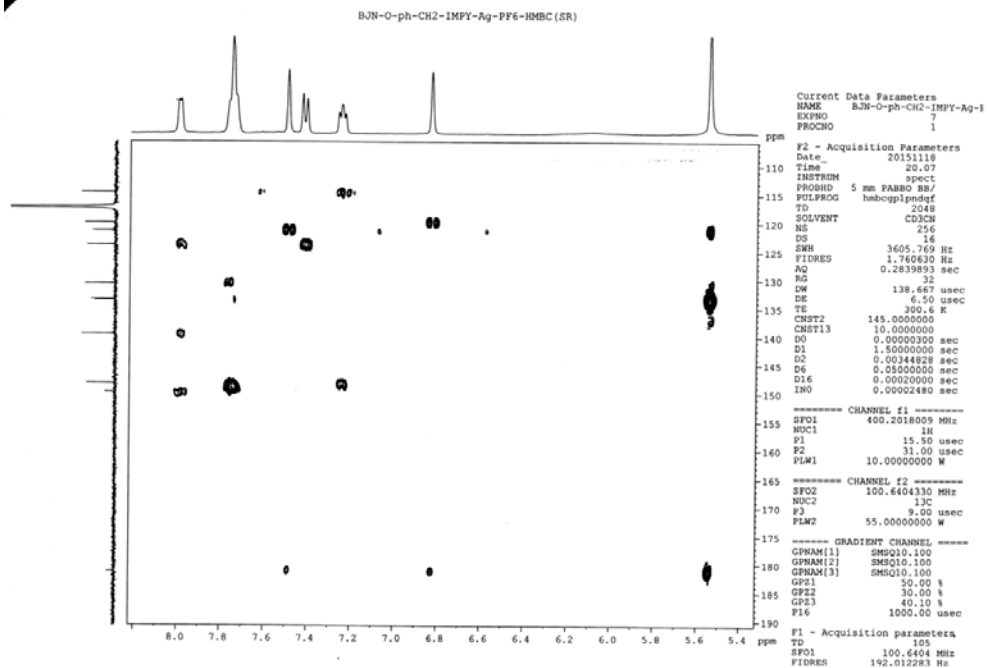


Figure 25S. ESI-MS (+ve) of **2**

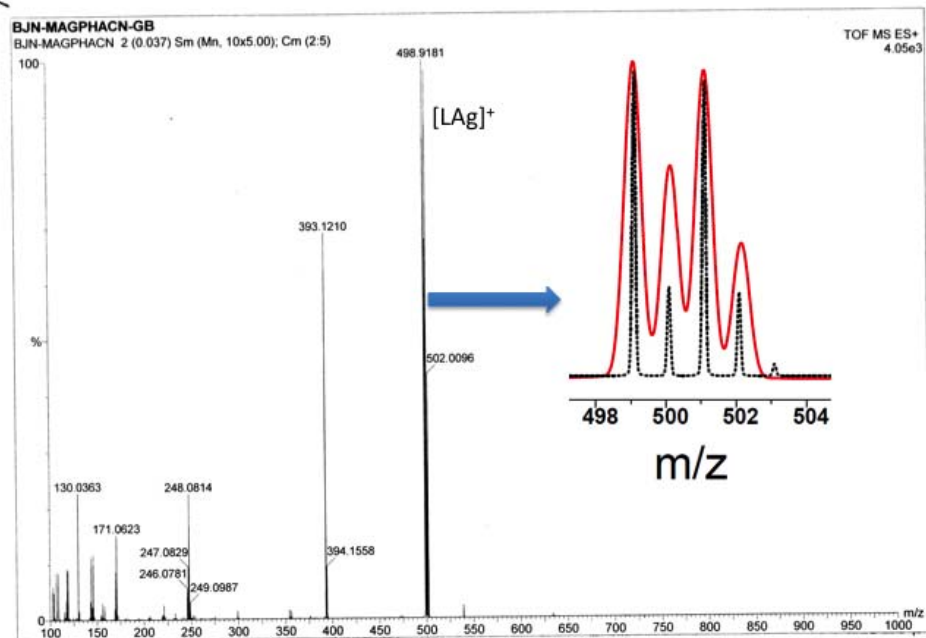


Figure 26S. ^1H -NMR spectrum of **2** in CD_3CN at 25°C (500 MHz)

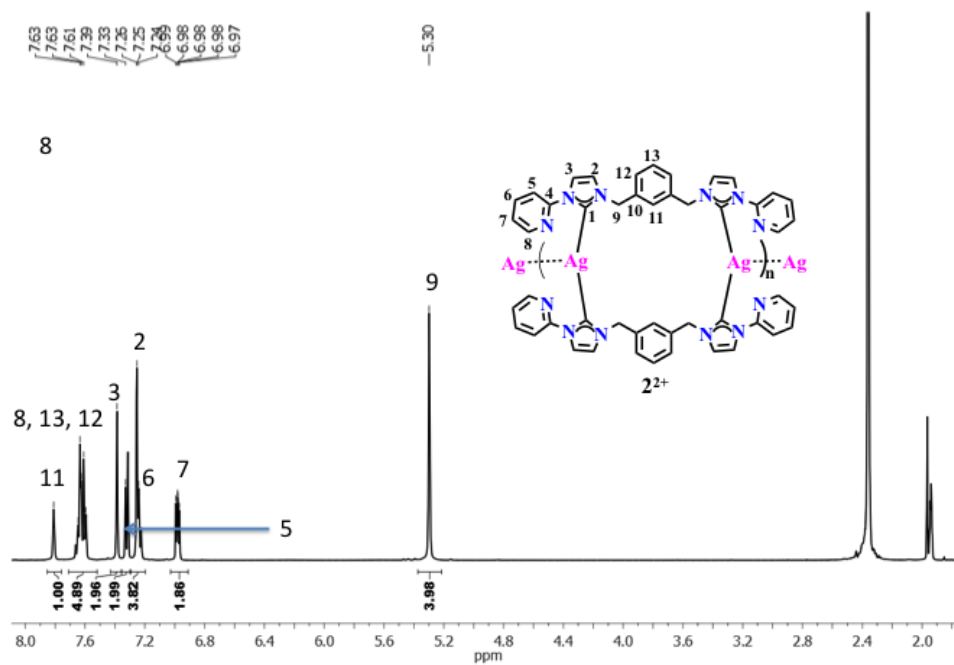


Figure 27S. ^{13}C -NMR spectrum of **2** in CD_3CN at 25°C (75 MHz)

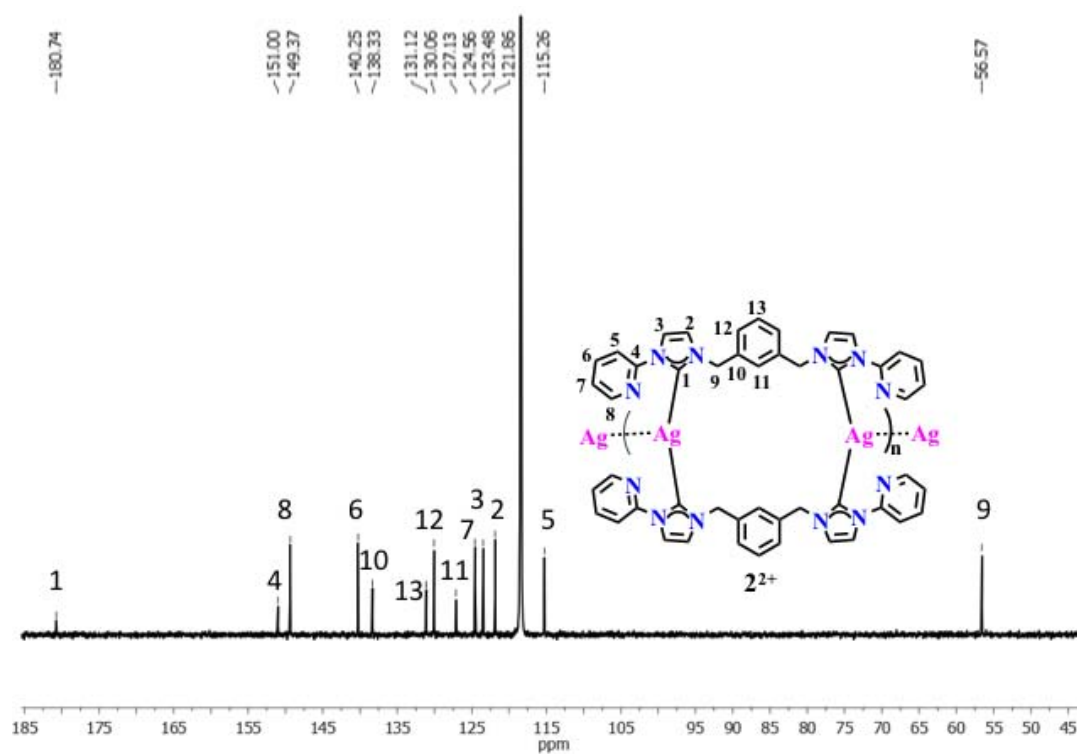


Figure 28S. DEPT-135 spectrum of **2** in CD₃CN at 25°C (500 MHz)

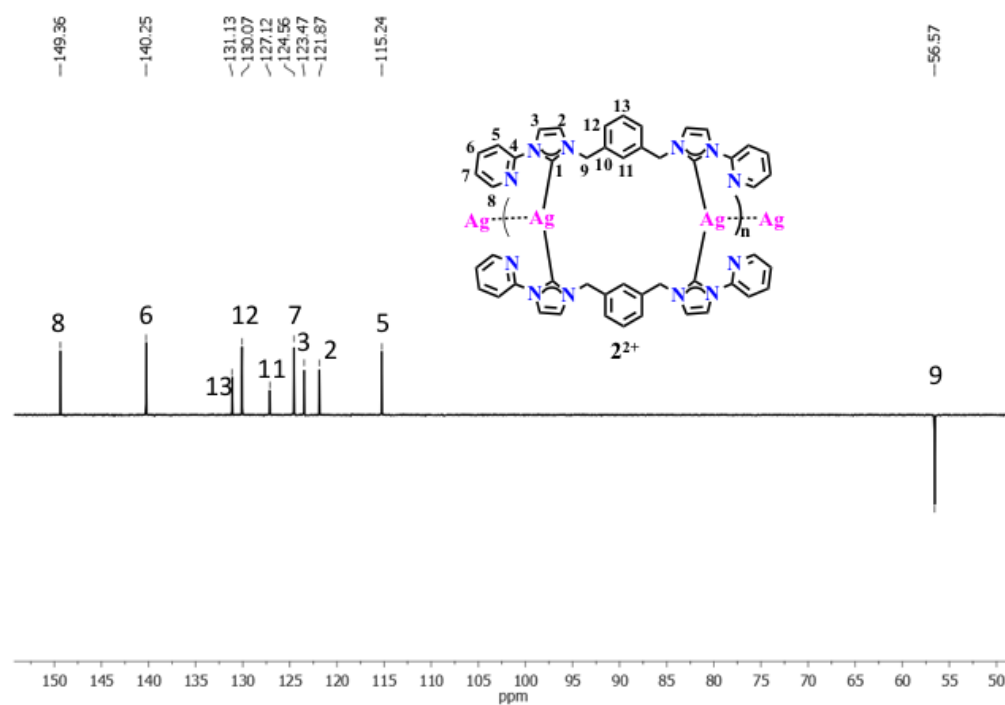


Figure 29S. ¹H-¹H COSY spectrum of **2** in CD₃CN at 25°C (500 MHz)

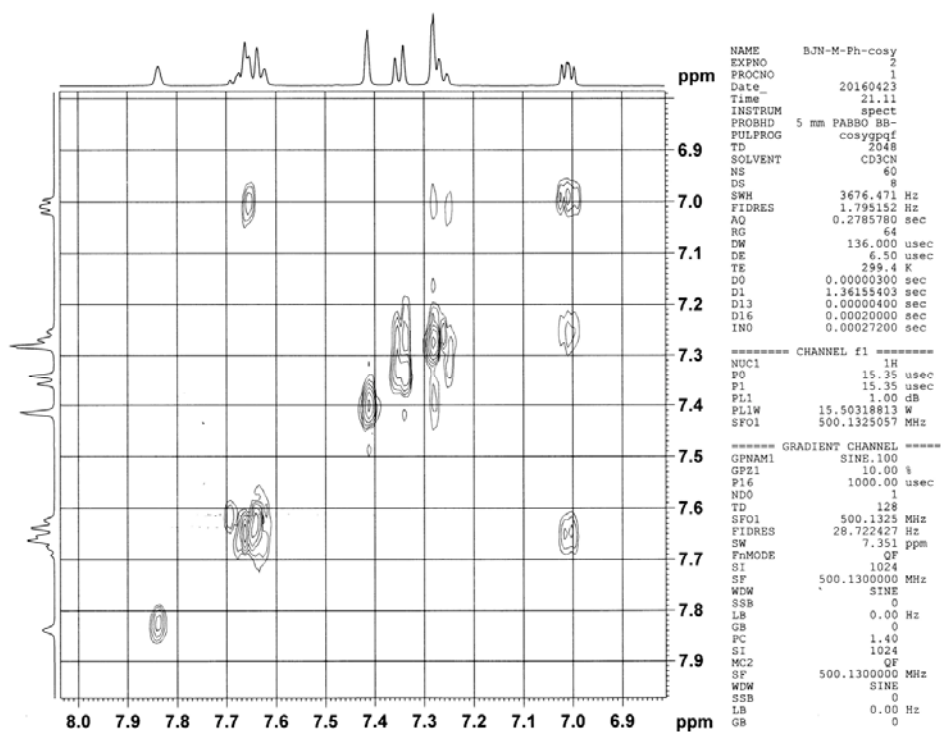


Figure 30S. ^1H - ^{13}C HSQC spectrum of **2** in CD_3CN at 25°C (500 MHz)

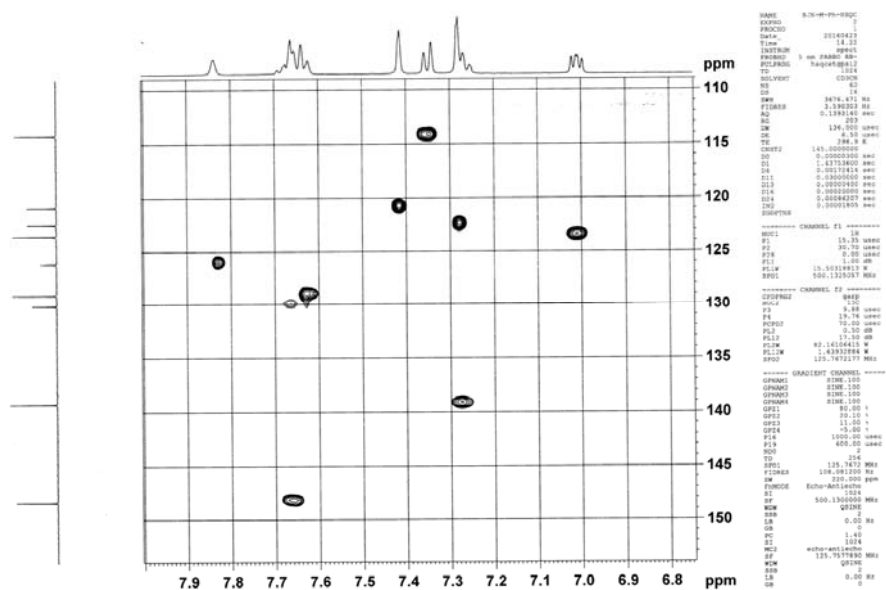


Figure 31S. ^1H - ^{13}C HMBC spectrum of **2** in CD_3CN at 25°C (500 MHz)

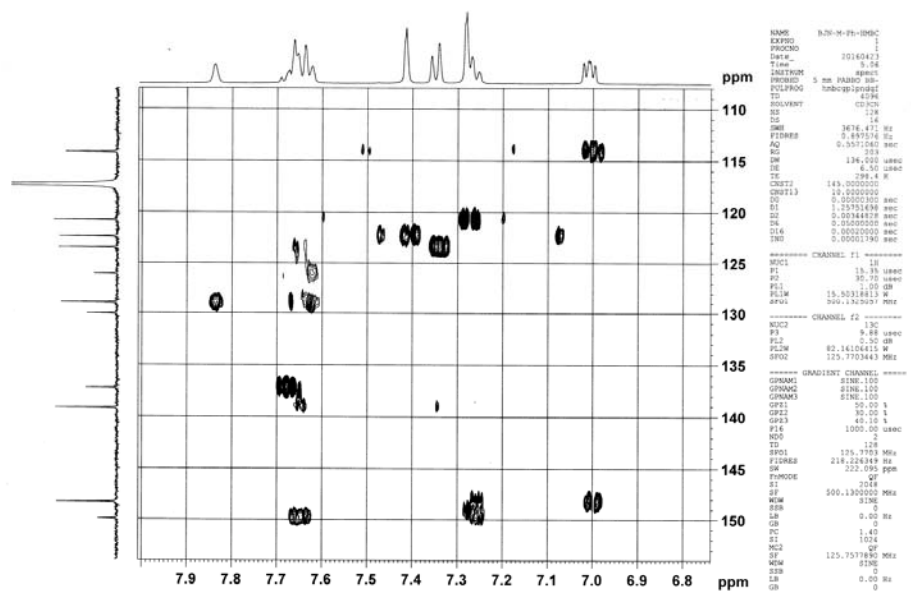


Figure 32S. ESI-FTICR-MS (+ve) of **3**

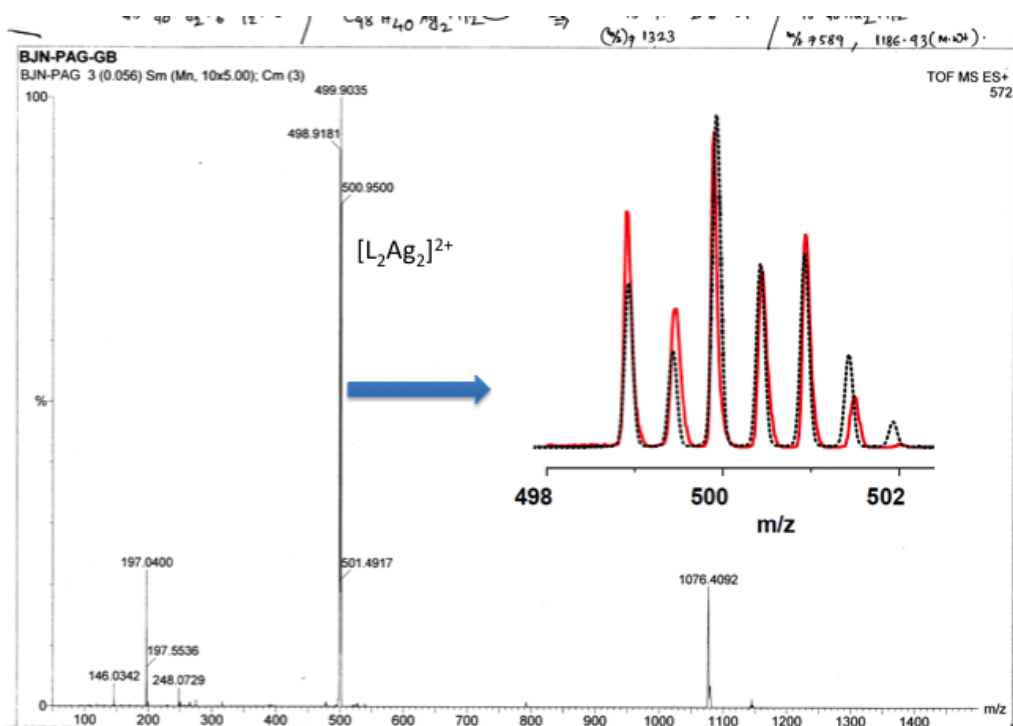


Figure 33S. ¹H-NMR spectrum of **3** in CD₃CN at 25°C (300 MHz)

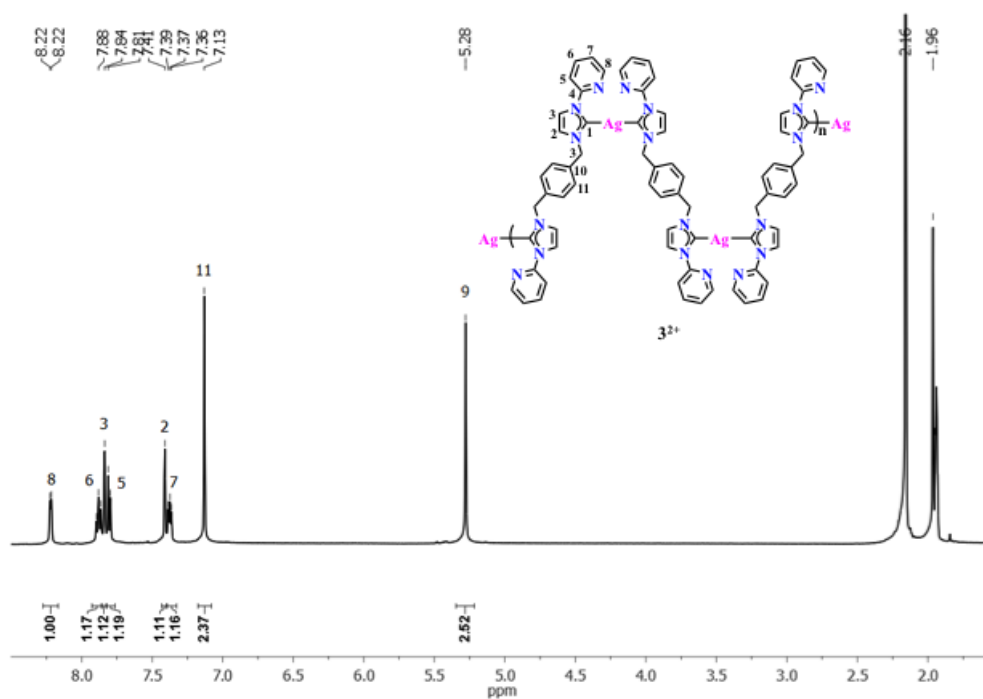


Figure 34S. ¹³C-NMR spectrum of **3** in CD₃CN at 25°C (75 MHz)

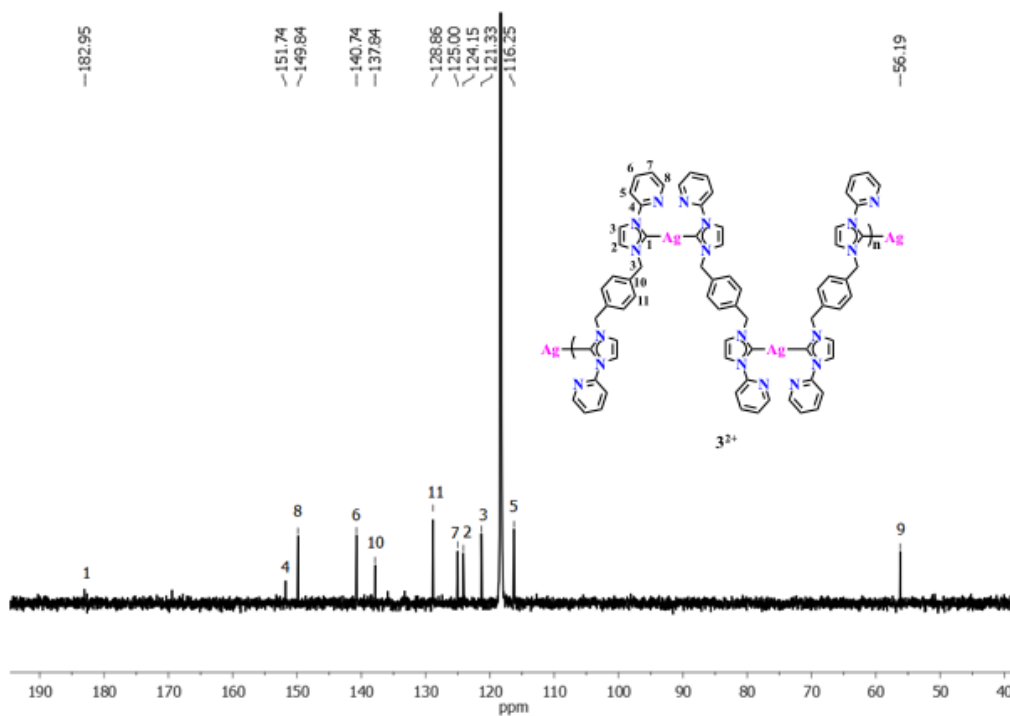


Figure 35S. ¹³C-NMR spectrum of **3** in CD₃CN at 25°C (75 MHz)

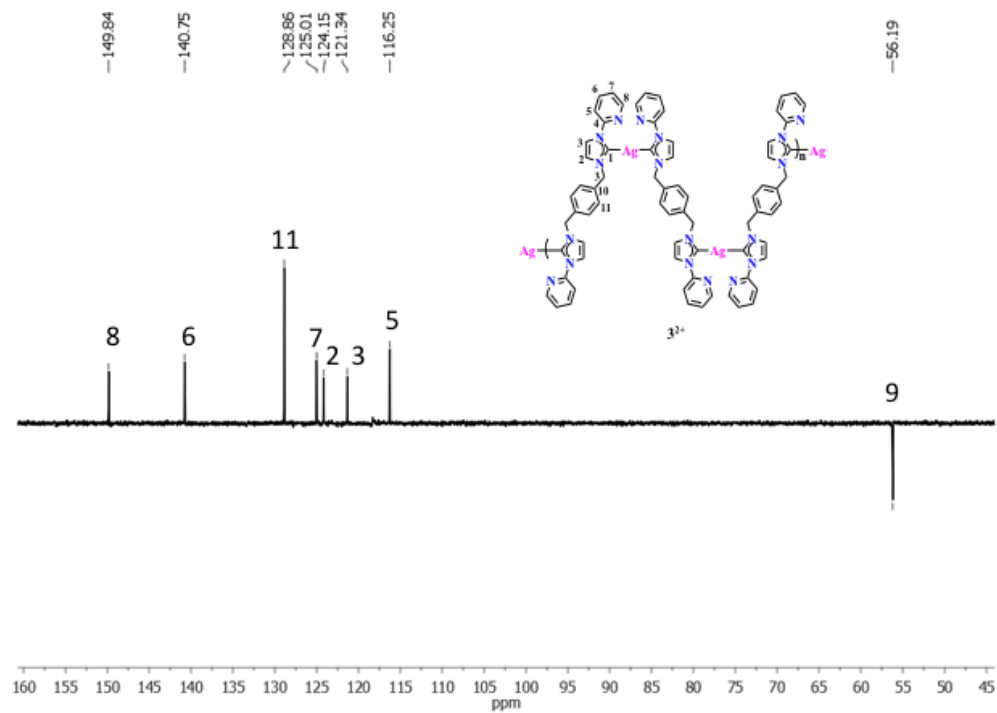


Figure 36S. ^1H - ^1H COSY spectrum of **3** in CD_3CN at 25°C (500 MHz)

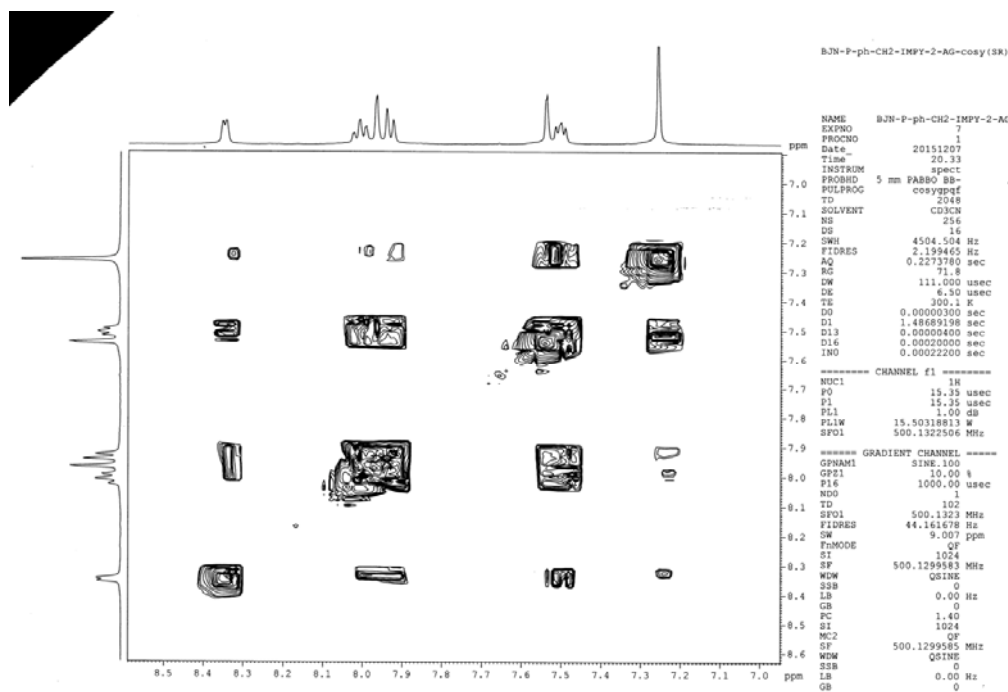


Figure 37S. ^1H - ^{13}C HSQC spectrum of **3** in CD_3CN at 25°C (500 MHz)

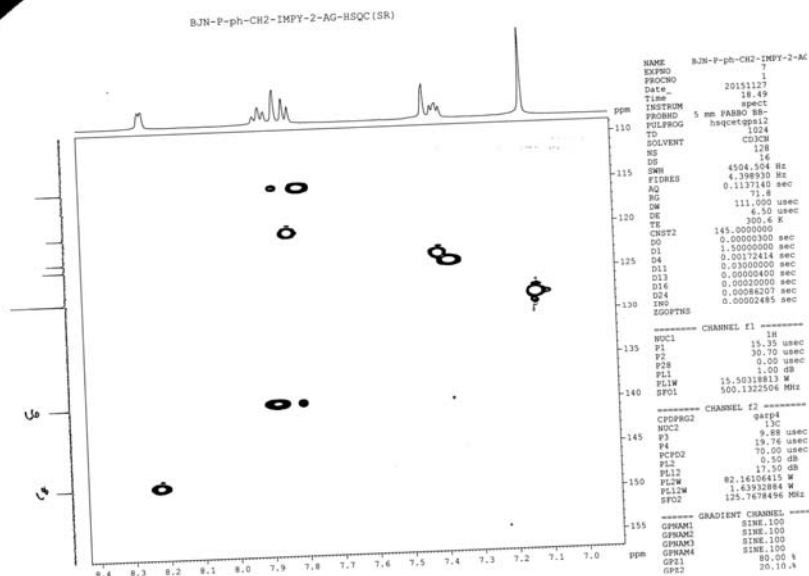


Figure 38S. ^1H - ^{13}C HMBC spectrum of **3** in CD_3CN at 25°C (500 MHz)

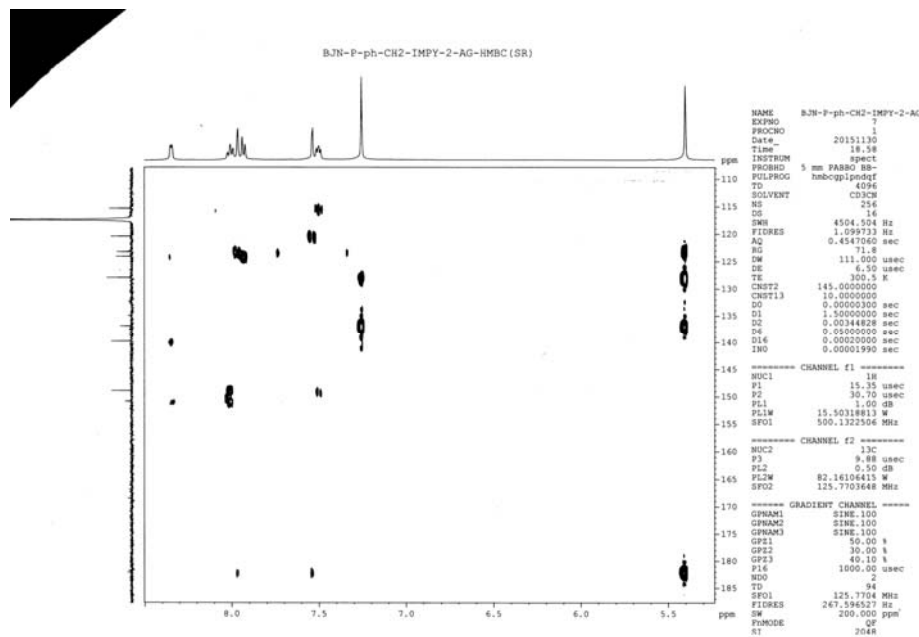


Figure 39S. Molecular structure with numbering scheme of compound **1**

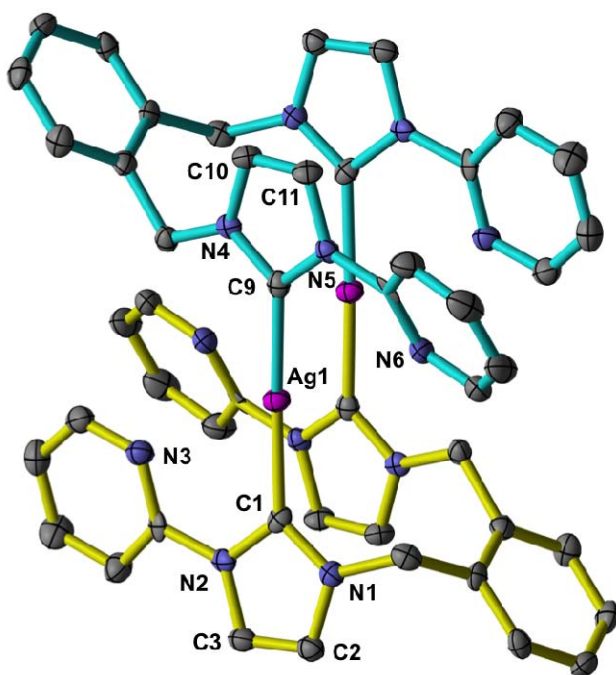


Figure 40S. Molecular structure with numbering scheme of compound **2**

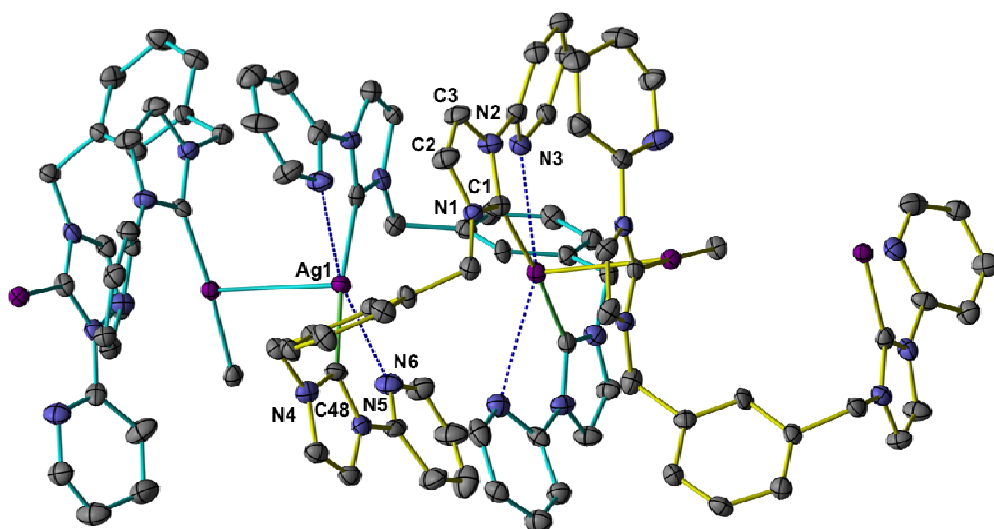


Figure 41S. Molecular structure with numbering scheme of compound **3**

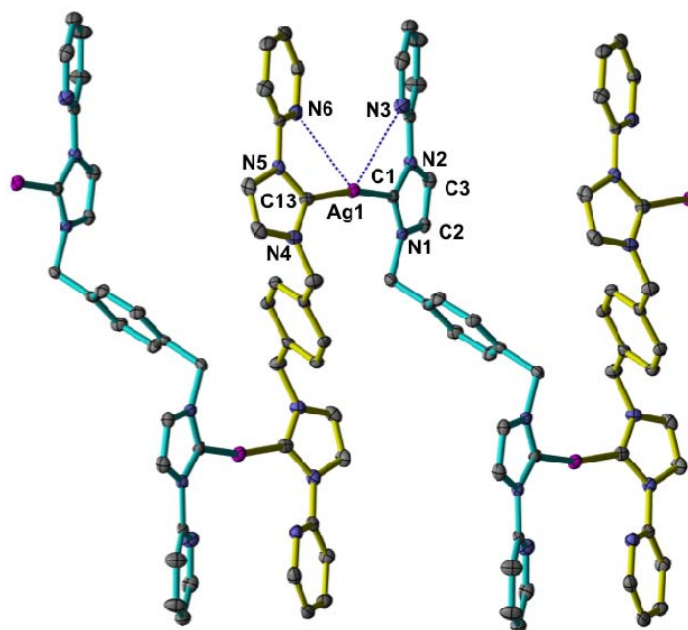


Table 1S. Selected bond lengths [Å] and angles [°] with estimated standard deviation for compounds **1**, **2** and **3**

1		2		3	
Ag1...Ag1(intramolecular)	3.257(9),	Ag2-C1	2.064(3)	Ag1-C1	2.104(2)
Ag1...Ag1(inter-molecular)	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)	$\pi - \pi$ (pyridyl-imidazole)	3.740
Ag1-C9	2.103(6)	Ag1...N6	2.962(4)	$\pi - \pi$ (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)