Single step site-selective reaction to construct a Ag_2Au_2 ← Ag4 supramolecular assembly from hybrid- *N*-heterocyclic carbene (NHC); Synthesis, structures and optoelectronic properties

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Electronic Supplementary Information (ESI)

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Table S1 Summary of key crystallographic data of **2**and **3**.

Empirical formula	'C30 H28 Ag2 F12 N8 P2'	'C30 H28 Ag Au F12 N8 P2'
Formula weight	1006.28	1095.38
Crystal system	Triclinic	Triclinic
Space group	'P-1'	'P-1'
T (K)	273.15	273(2)
Cell dimensions		
a (Å)	12.1446(5)	12.2152(9)
b (Å)	12.9632(5)	12.9415(10)
c (Å)	13.8516(6)	13.7513(11)
α(°)	68.2040(10)	68.601(2)
β(°)	82.8810(10)	82.896(2)
γ(°)	66.6170(10)	66.589(2)
V(Å^3)	1857.81(13)	1856.8(3)
Z	2	2
D_{calc} (Mg m^{-3})	1.799	1.959
Absorption coefficient	1.236	4.655
F(000)	992	1056
Crystal size (mm)	0.2×0.1×0.1	0.1×0.1×0.2
Theta range for data collection	2.386- 27.511	0.725-0.755
Index ranges	-15<=h<=15,-16<=k<=15,-17<=l<=18	-15<=h<=15,-16<=k<=16,-17<=l<=17
Reflections collected	6270	6902
Independent reflections	8443	8503
Goodness-of-fit on (GOF)	1.059	1.031
Final R indices [I > 2r(I)]	R1= 0.0447, wR2= 0.1012	R1=0.0356, wR2=0.0743
R indices (all data),Rw	R1= 0.0702, wR2= 0.1223	R1=0.0523, wR2=0.0830

Table S2 Summary of selected bond distances (Å) of complex **2** and complex **3**.

2		**3**	
Ag(1)-Ag(1)	3.2490(6)	Au(1)-Au(1)	3.2991(4)
Ag(2)-Ag(2)	3.3461(11)	Ag(1)-Ag(1)	3.3205(13)
Ag(1)-C(1)	2.096(4)	Au(1)-C(1)	2.020(5)
Ag(1)-C(14)	2.096(4)	Au(1)-C(14)	2.021(4)
Ag(2)-N(3)	2.149(4)	Ag(1)-N(3)	2.146(5)
Ag(2)-N(6)	2.149(4)	Ag(1)-N(6)	2.137(4)
C(1)-N(1)	1.360(5)	N(1)-C(1)	1.361(6)
C(1)-N(2)	1.350(5)	N(2)-C(1)	1.365(5)
C(14)-N(4)	1.362(5)	N(4)-C(14)	1.368(5)
C(14)-N(5)	1.357(4)	N(5)-C(14)	1.350(5)
N(3)-C(12)	1.330(6)	N(3)-C(12)	1.321(8)
N(3)-C(13)	1.341(5)	N(3)-C(13)	1.346(6)
N(6)-C(25)	1.331(6)	N(6)-C(25)	1.336(7)
N(6)-C(26)	1.337(5)	N(6)-C(26)	1.339(6)

Table S3 Summary of selected bond angles (°)of complex **2** and complex **3**.

2		**3**	
C(1)-Ag(1)-C(14)	171.11(14)	C(1)-Au(1)-C(14)	173.45(16)
N(3)-Ag(2)-N(6)	167.90(15)	N(6)-Ag(1)-N(3)	167.66(18)
C(12)-N(3)-C(13)	117.2(4)	C(12)-N(3)-C(13)	116.5(5)
C(25)-N(6)-C(26)	117.2(4)	C(25)-N(6)-C(26)	116.4(5)
N(1)-C(1)-N(2)	103.2(3)	N(1)-C(1)-N(2)	103.4(4)
N(4)-C(14)-N(5)	103.4(3)	N(4)-C(14)-N(5)	102.9(4)

Table S4 Lifetime (in ns) of complexes **2** and **3** in DMSO at an excitation wavelength of 273 nm.

Name	τ_1	β_1	τ_2	β_2	τ_{avg} **(ns)**
Complex 2	3.56	1	-	-	3.56
Complex 3	0.75	0.34	3.17	0.65	2.31

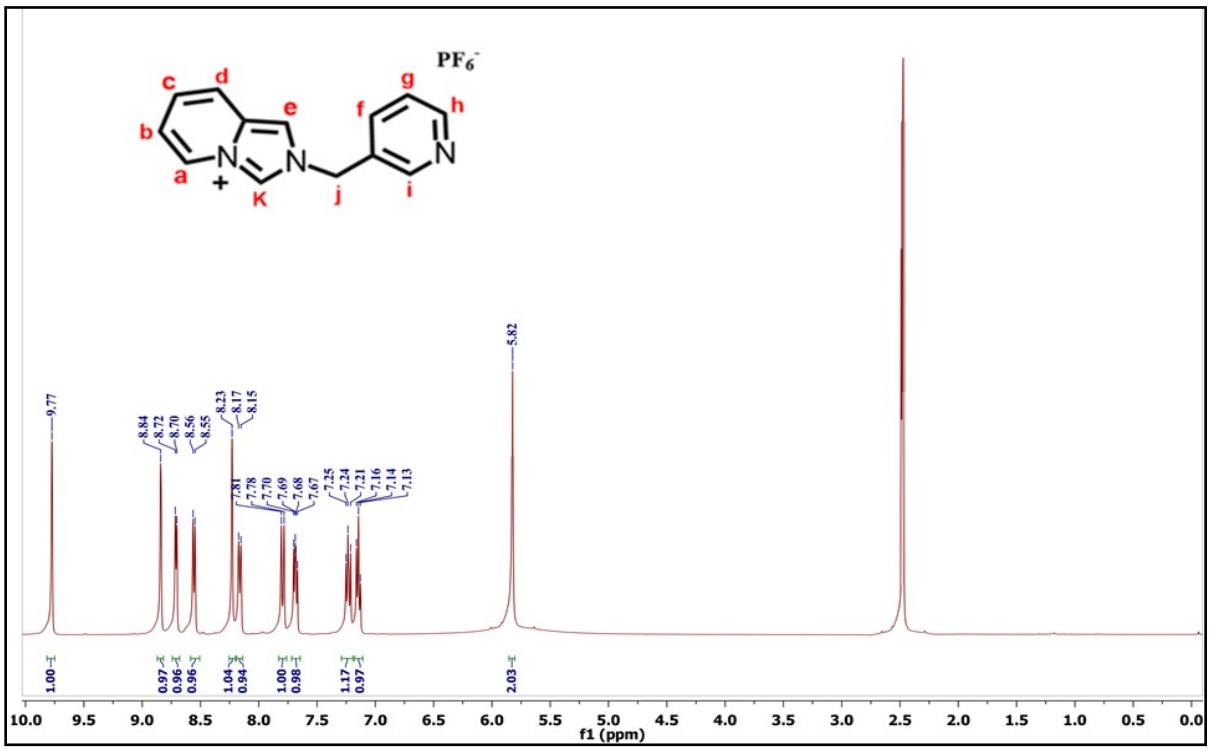

Fig. S1. ^{1}HNMR spectra of **1**.HPF_6(DMSO-d6).

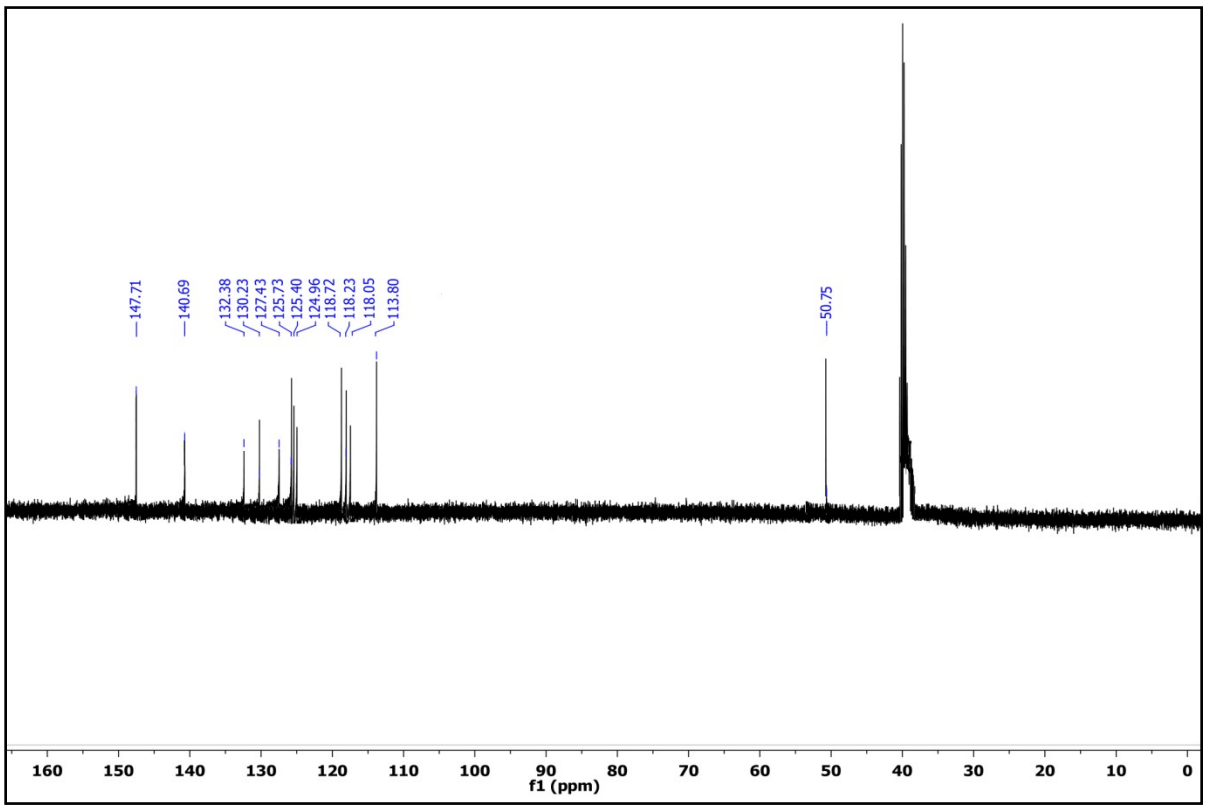

Fig. S2. ^{13}CNMR spectra of **1**.HPF_6(DMSO-d6).

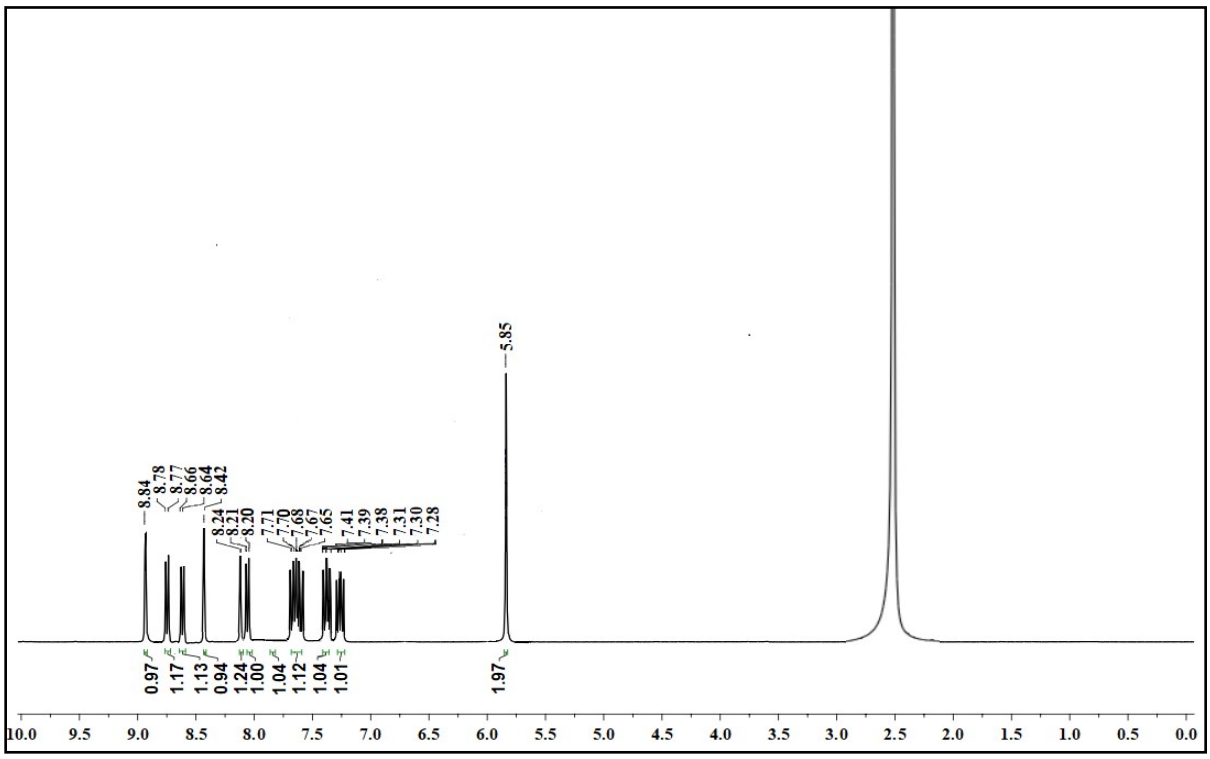

Fig.S3. [1]HNMR spectra of complex **2**(DMSO-d6).

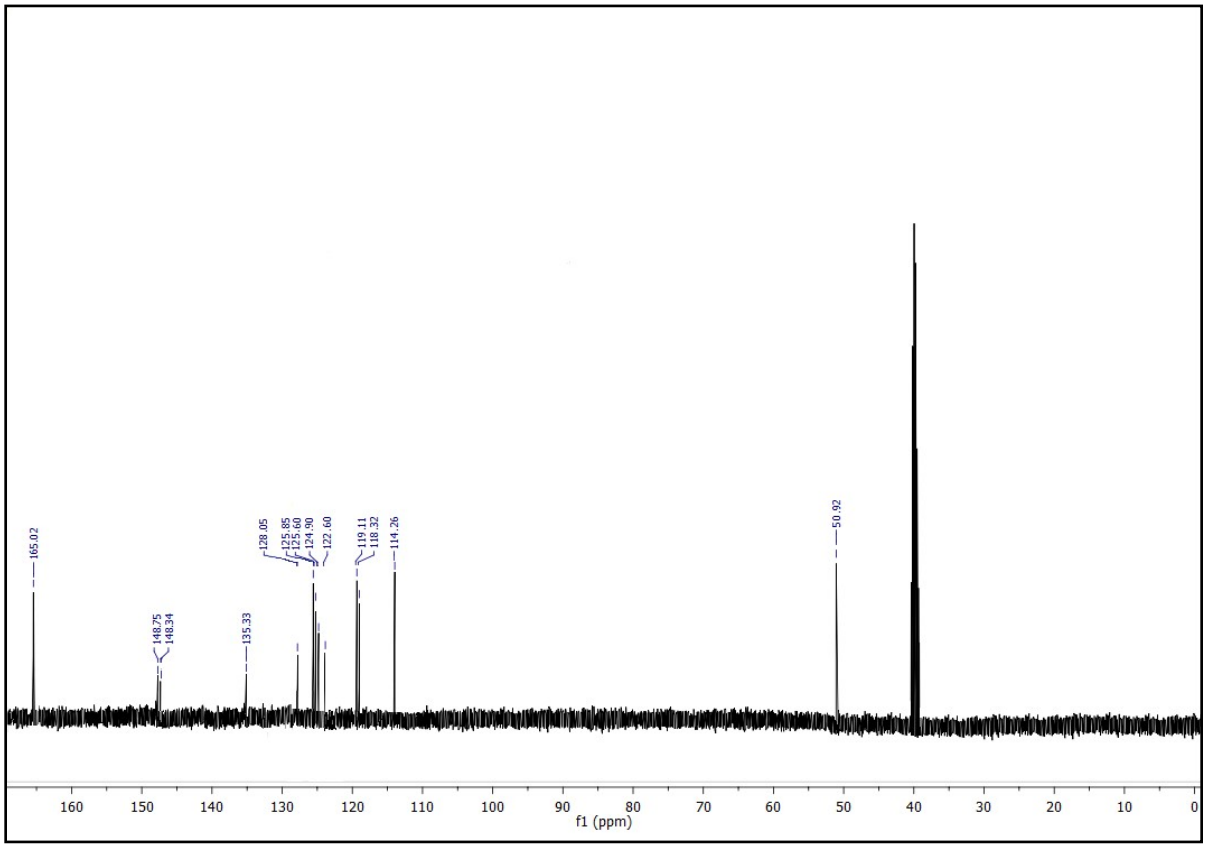

Fig. S4. [13]CNMR spectra of complex **2**(DMSO-d6).

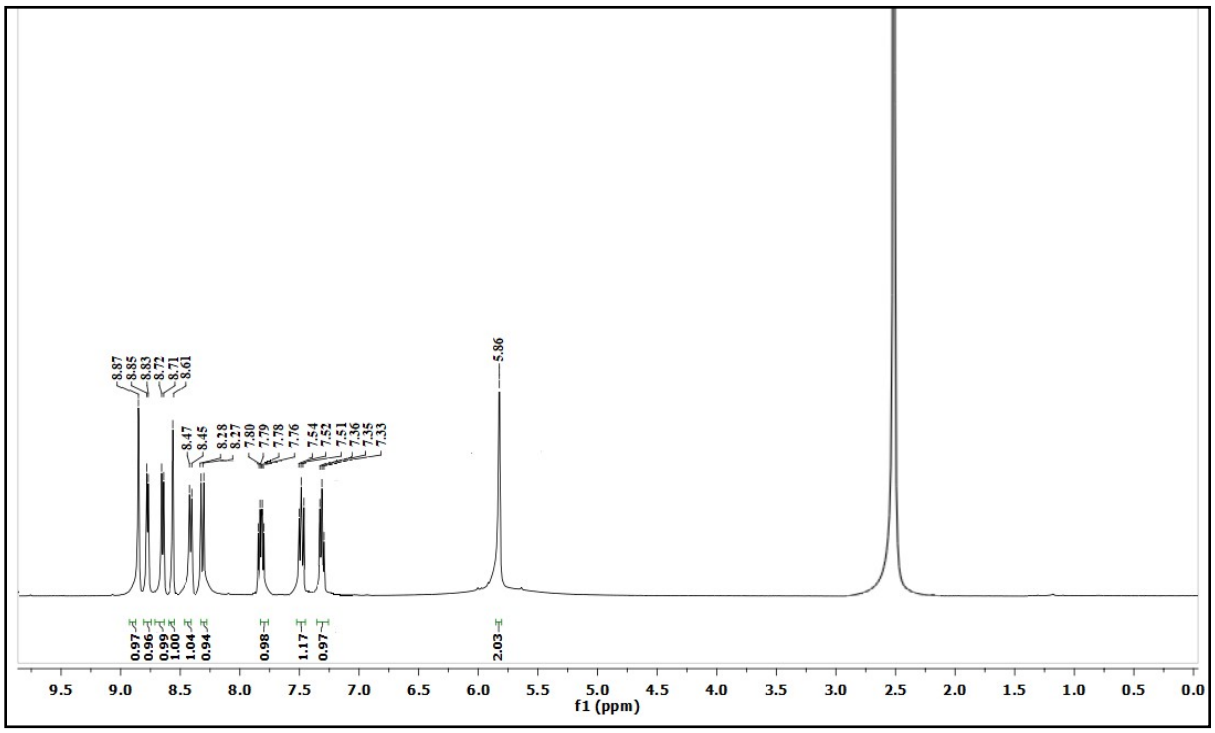

Fig. S5. [1]HNMR spectra of complex **3**(DMSO-d6).

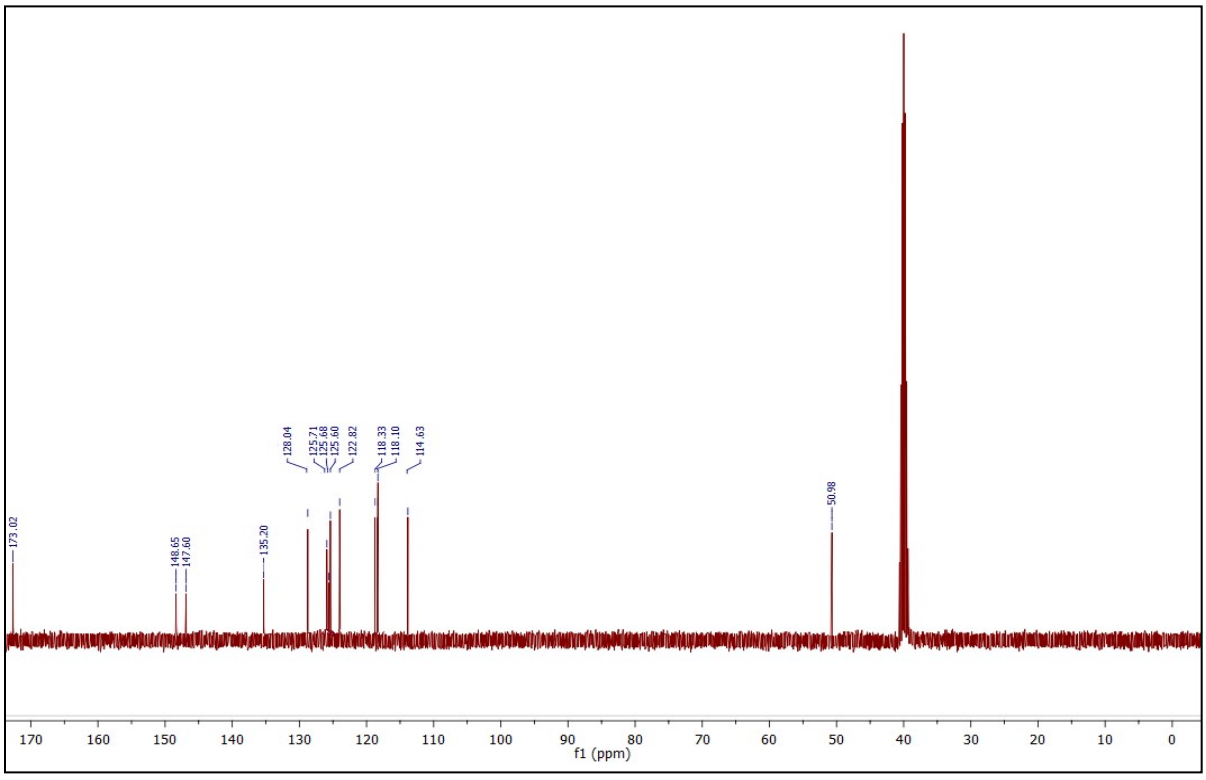

Fig.S6.[13]CNMR spectra of complex **3**(DMSO-d6).

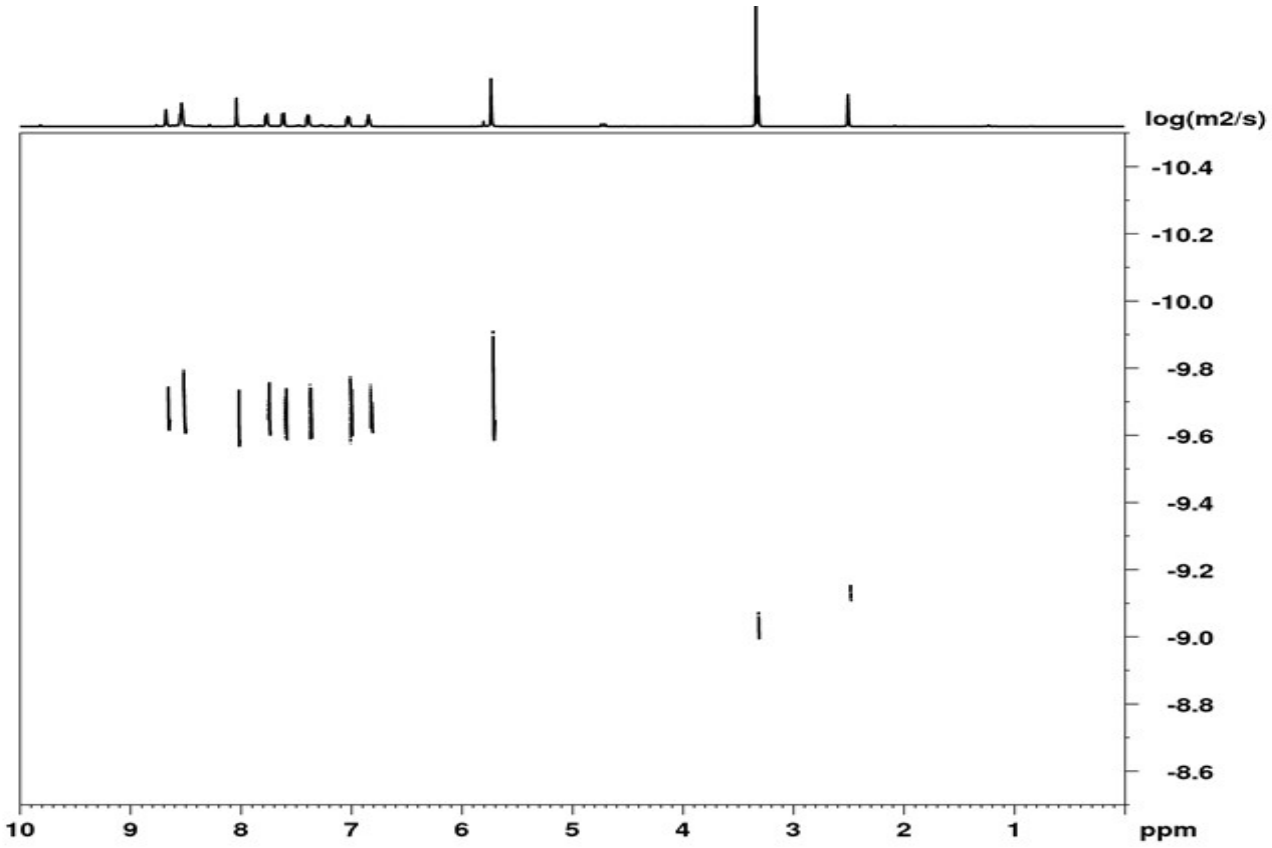

Fig. S7. DOSY NMR of complex **2** (DMSO-d6, 298K).

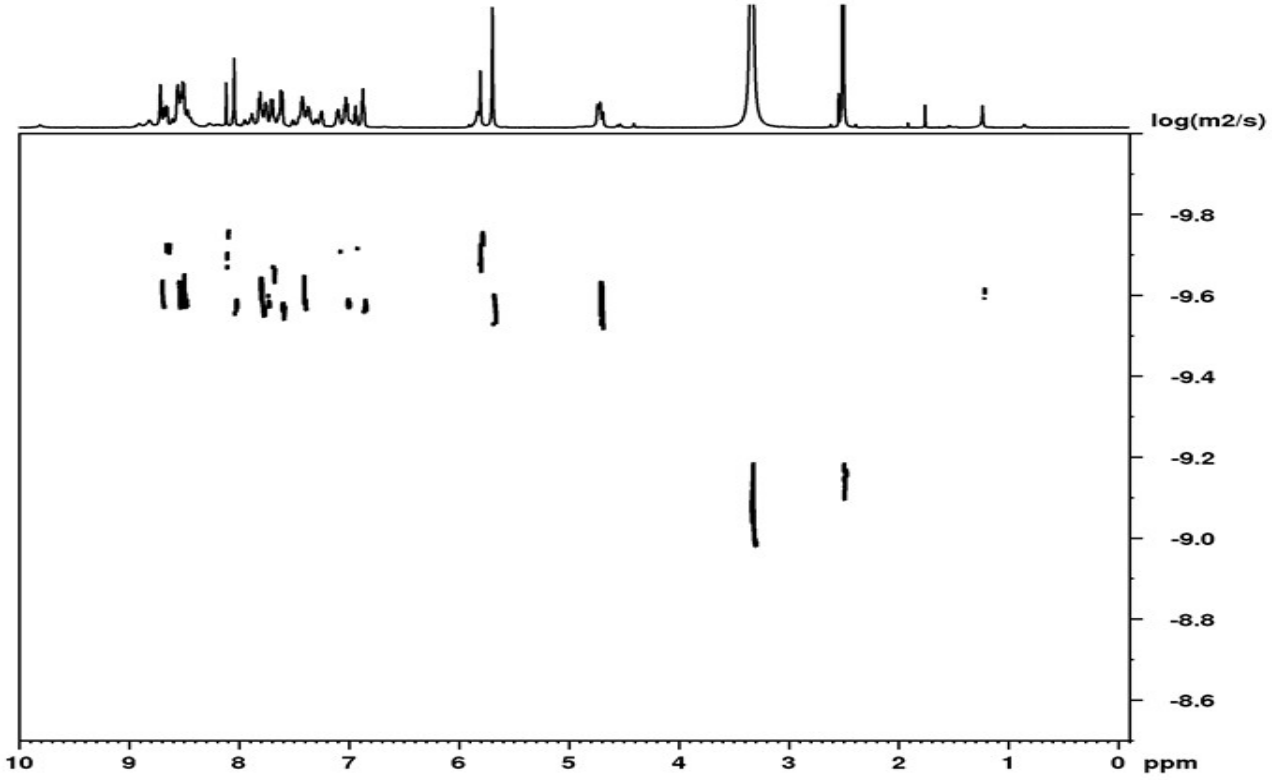

Fig. S8. DOSY NMR of complex **3** (DMSO-d6, 298K).

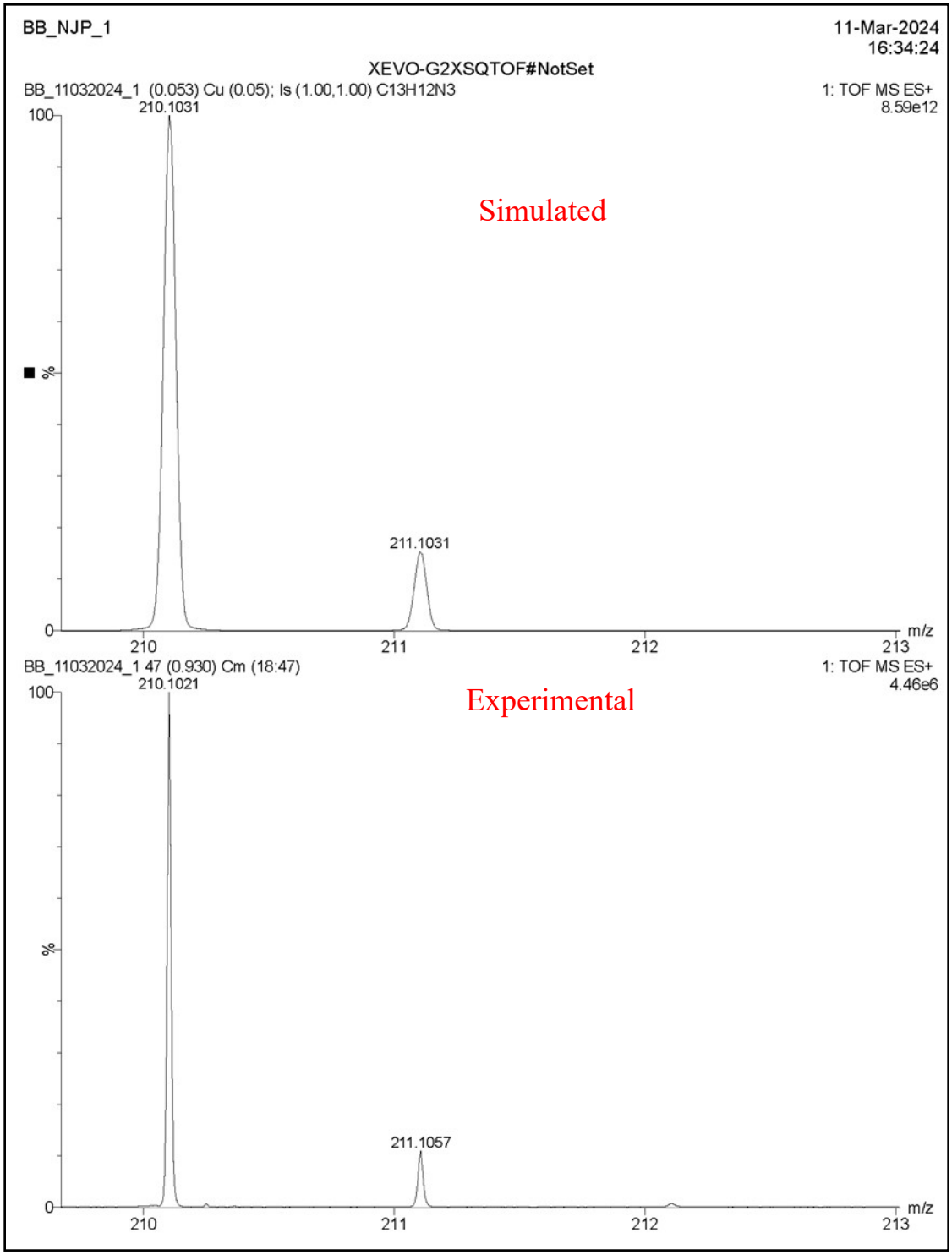

Fig. S9. HR-MS of **1**.HPF_6.

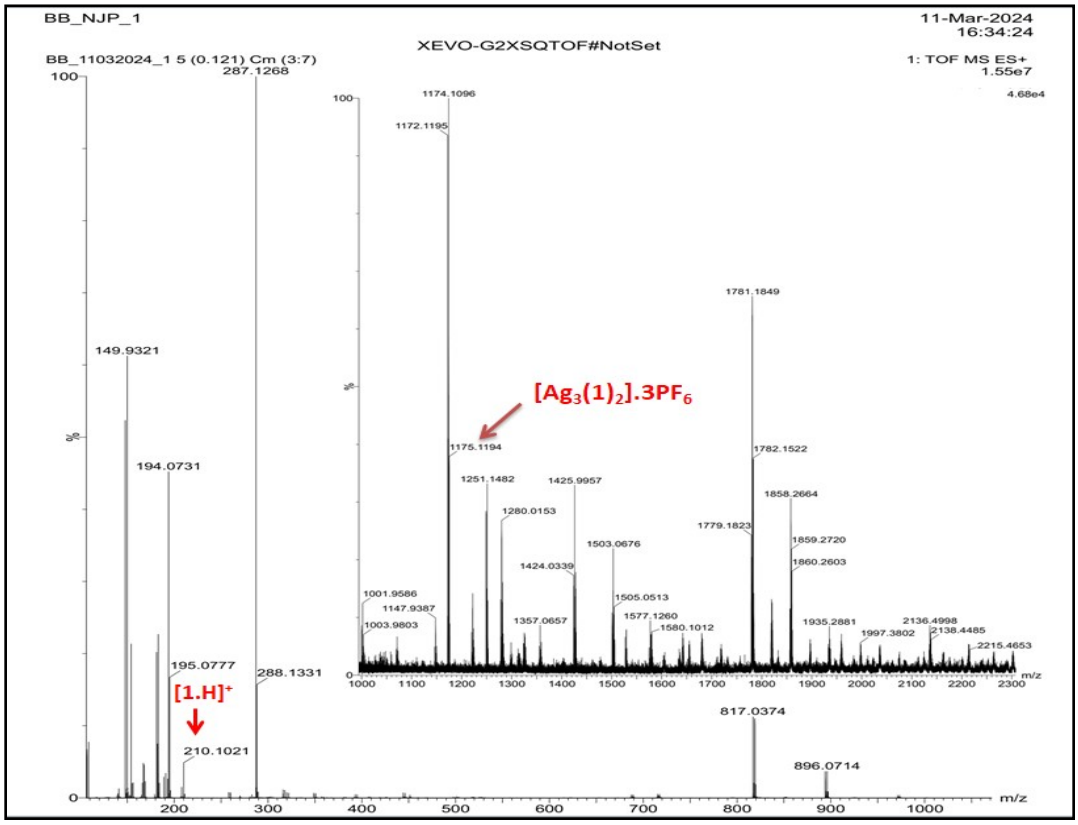

Fig. S10. ESI-MS of complex **2**.

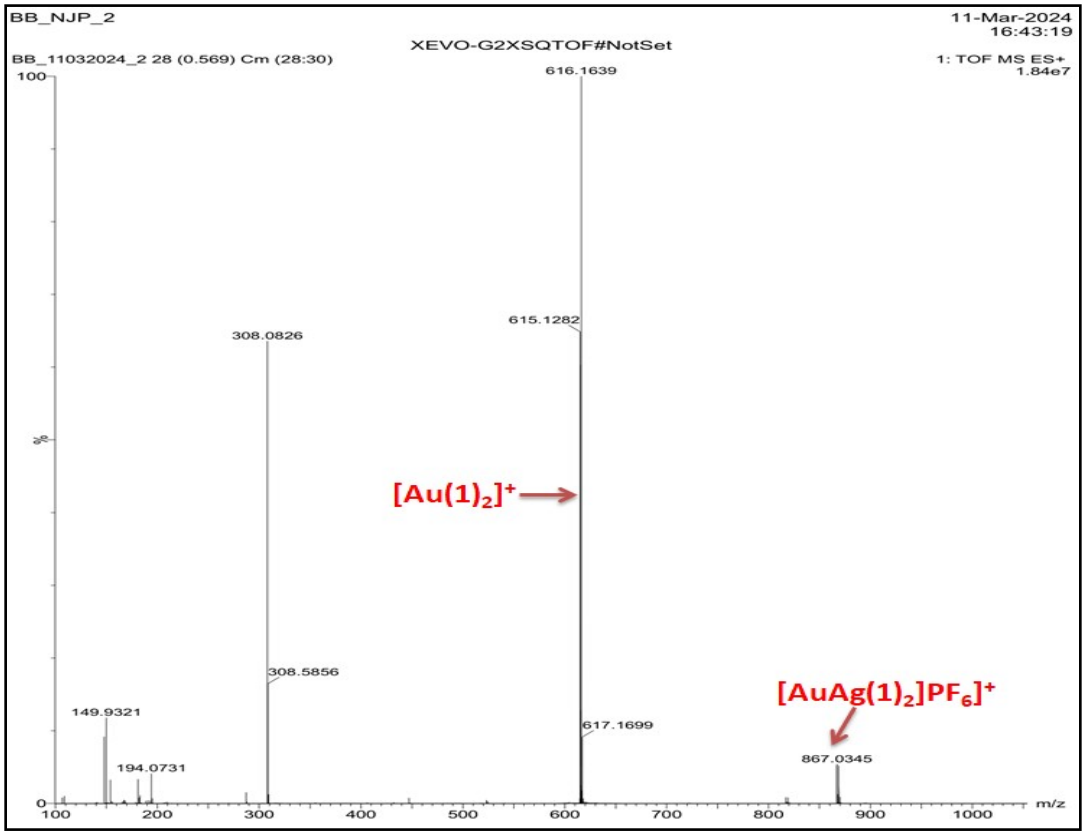

Fig. S11. ESI-MS of complex **3**.

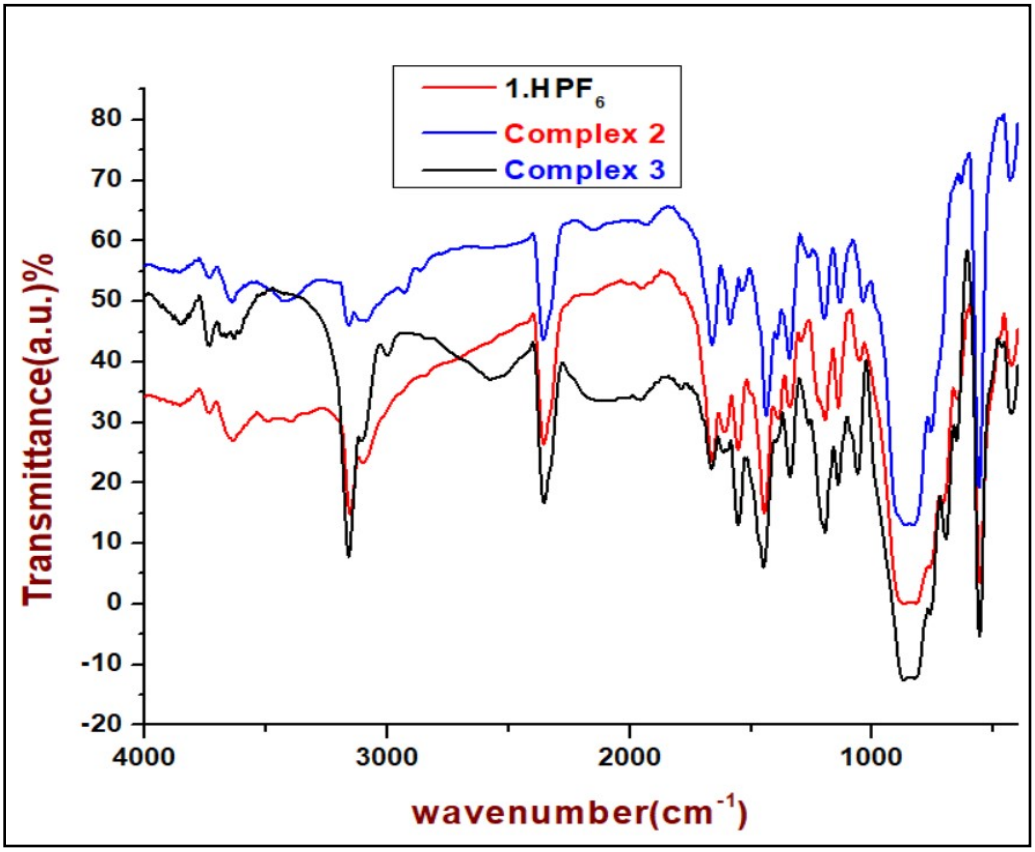

Fig. 12: IR spectra of **1**.HPF_6 and complexes **2** and **3.**

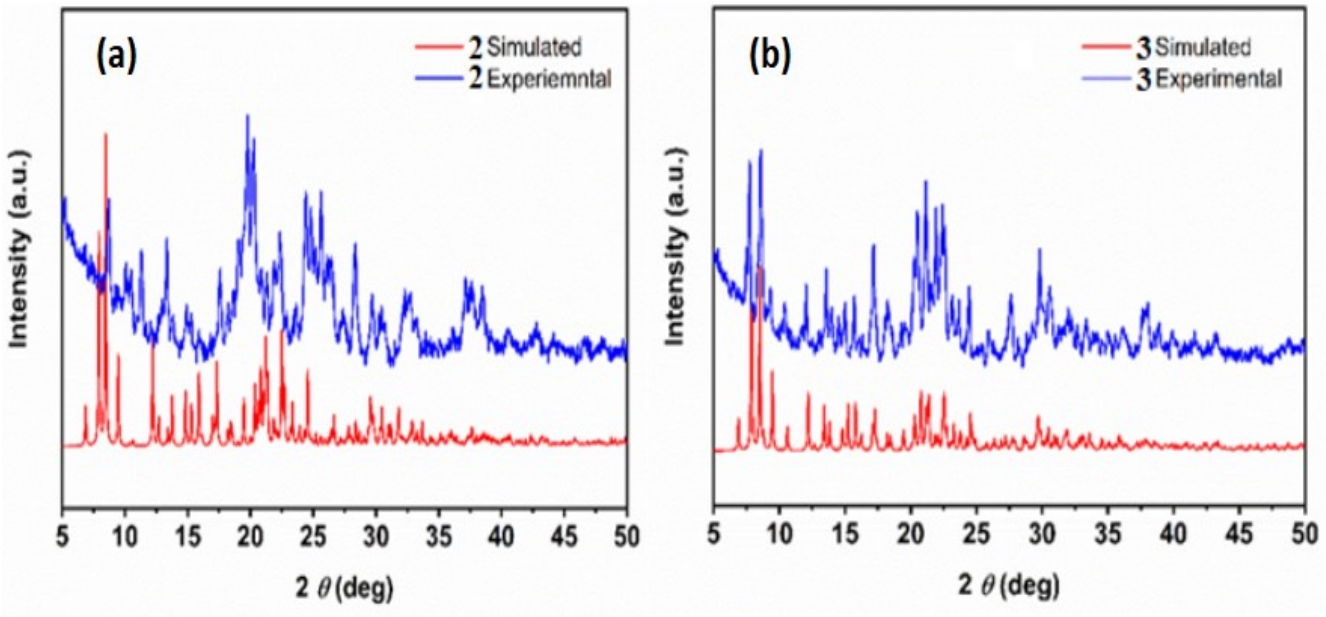

Fig.S13: Comparison of the simulated and experimental powder X-ray diffraction (PXRD) patterns of the complexes **2** and **3**: Complex **2** (a); Complex **3** (b).

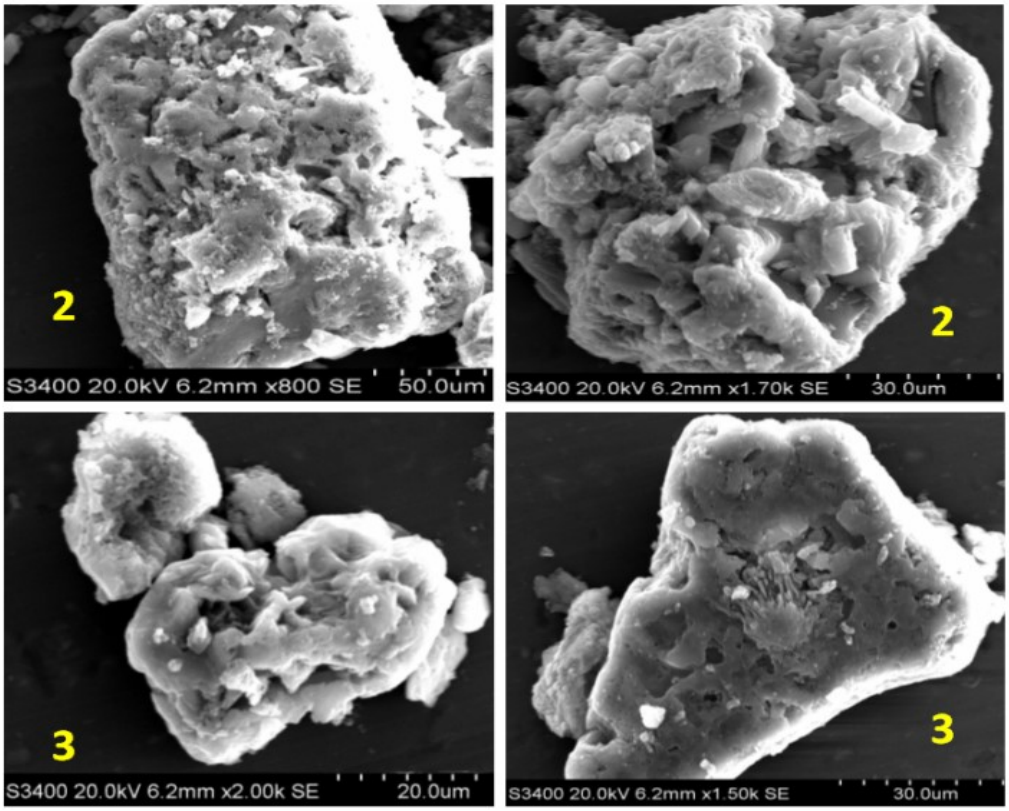

Fig.S14. SEM images of **2** (Top) and **3**(bottom)showing porous nature of the complexes.