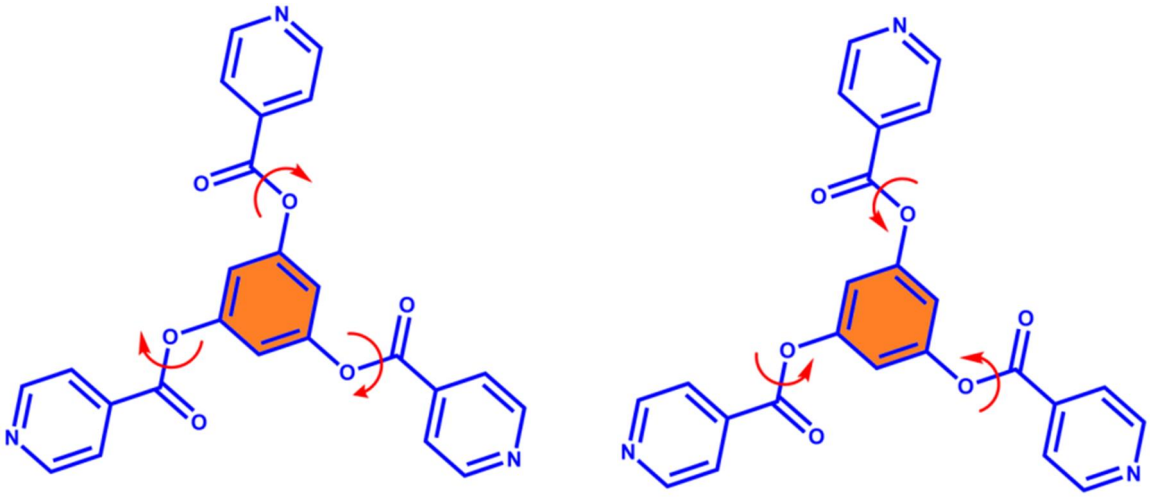
Electronic Supplementary Information

Assembly of Ag(I) coordination polymers from a tripyridyl-ester: Effects of counter anion, ligand conformation and π - π interaction on non-interpenetrating 2D→3D dimension increase

Ying Xiong,[a] Rui Yang,[a] Sha Chen,[a] Ji-Jun Jiang*[ab] and Cheng-Yong Su*[ab]

[a] MOE Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional materials, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China.
b State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China.
E-mail address:cesscy@mail.sysu.edu.cn . Tel: +86 020 84115178, Fax: +86 020 84115178.
E-mail address: jiangjij@mail.sysu.edu.cn . Tel: +86 020 84113990, Fax: +86 020 84113994.



Scheme 1. Various plausible conformation of the free ligands BTTP4 dominated by the rotation of C-O single bond.

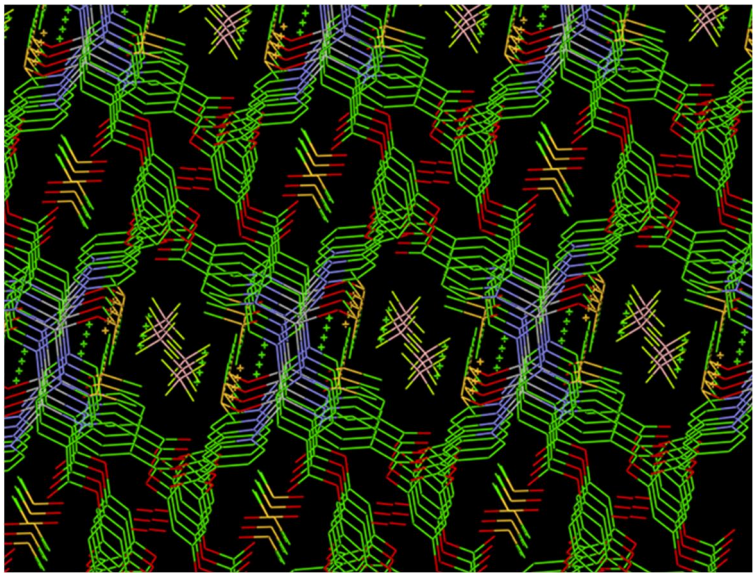


Fig. S1. Counter anions and solvent molecules locate between the (6, 3) layers in Complex **1**

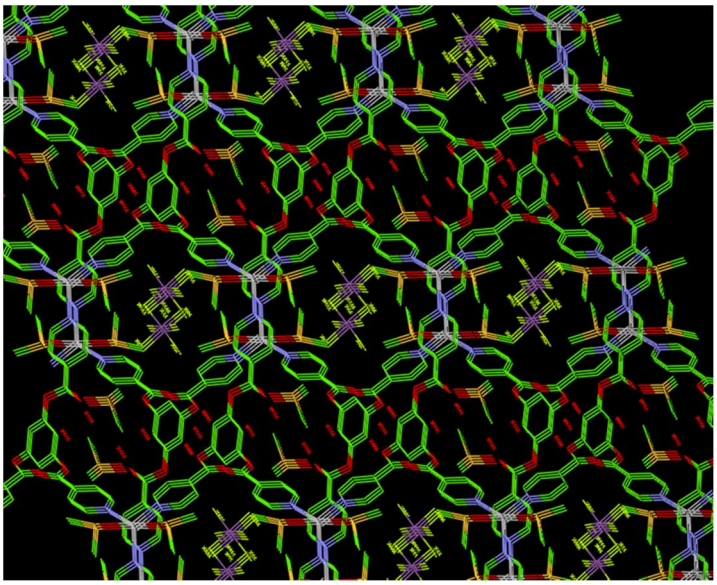


Fig. S2. Counter anions and solvent molecules locate between the (6, 3) layers in Complex **2**, view from *c* axis

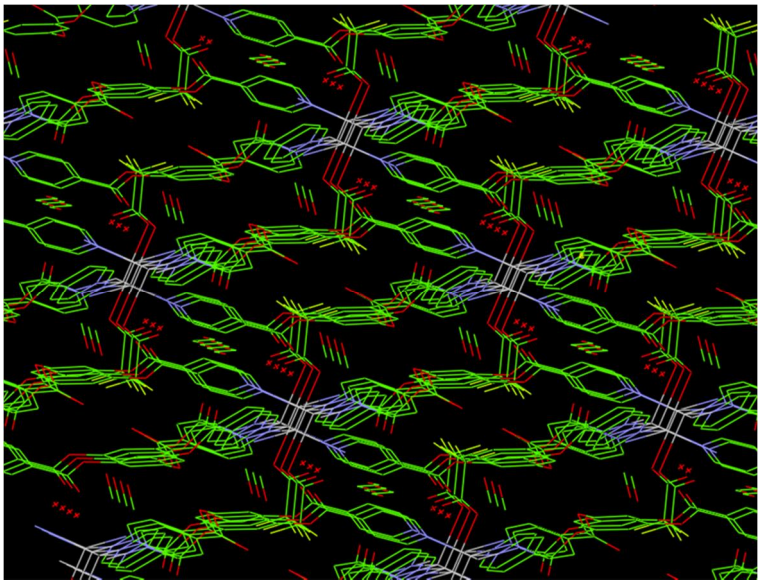


Fig. S3. Counter anions and solvent molecules locate between the (6, 3) layers in Complex **3**

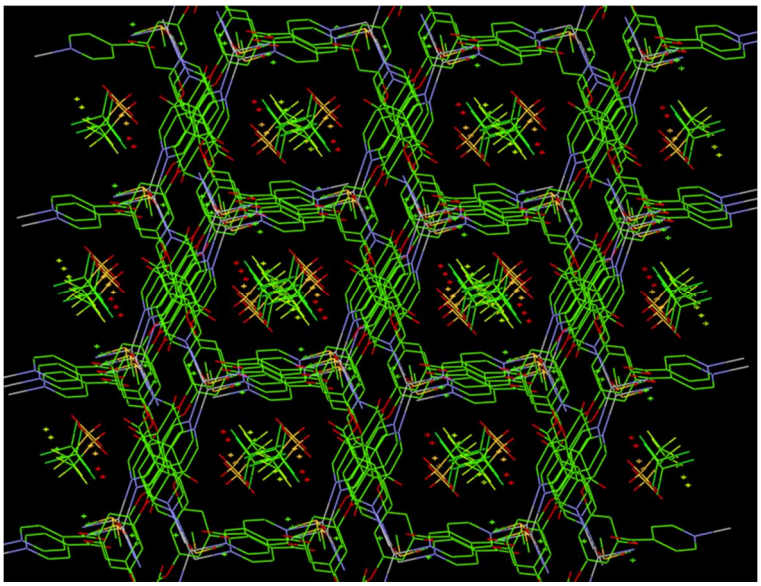


Fig. S4. Counter anions and solvent molecules locate between the (6, 3) layers in Complex **4**

Measurements of dihedral angles

Plane 1 is the central benzene ring which consists of C1, C2,C3,C4,C5 and C6; Plane 2-4 are generated through three terminal pyridine rings which are consist of atoms of C10, C11, C12,C13,C14 N1, and

C15, C16, C17,C18,C19, N2, and C20, C21, C22, C23, C24.

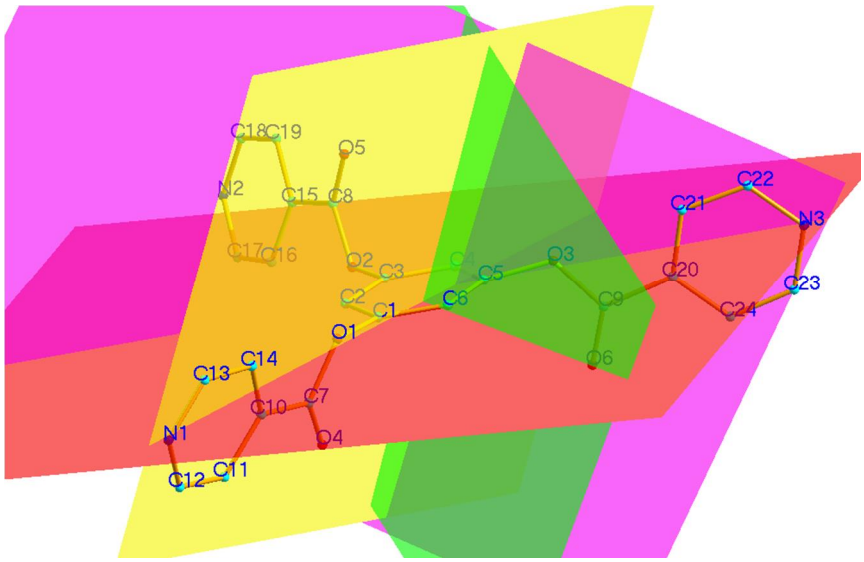


Fig. S5. In complex **1**, Angle between planes1 to plane 2 is 68.438^{o} , planes1 to plane 3 is 69.731^{o} , planes1 to plane 4 is 89.544^{o} .

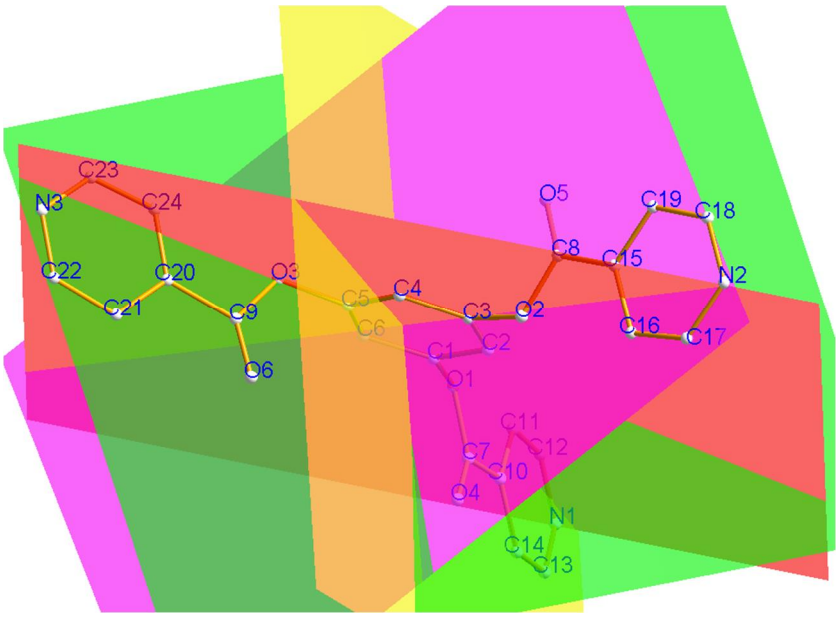


Fig. S6. In complex **2**, Angle between planes1 to plane 2 is 77.912^{o} , planes1 to plane 3 is 71.605^{o} , planes1 to plane 4 is 85.252^{o} .

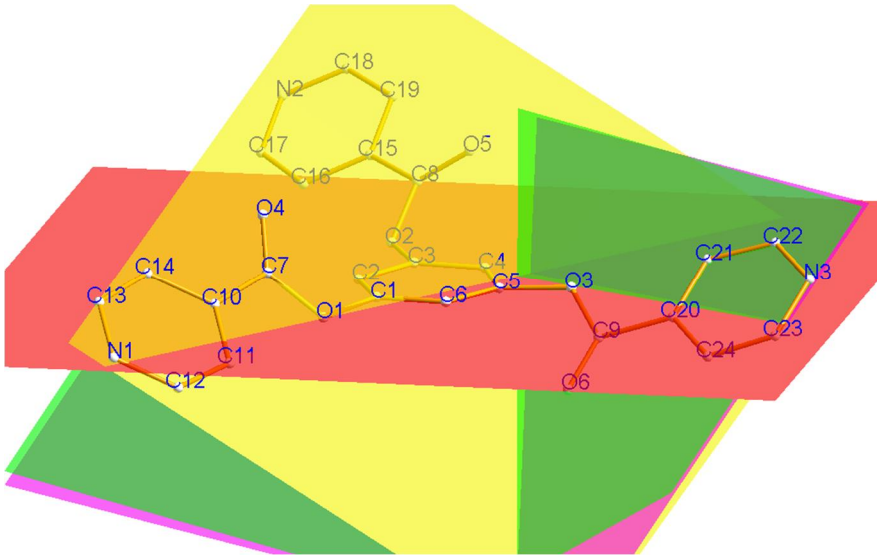


Fig. S7. In complex **3**, Angle between planes1 to plane 2 is 39.347^{o} , planes1 to plane 3 is 38.009^{o} , planes1 to plane 4 is 38.938^{o} .

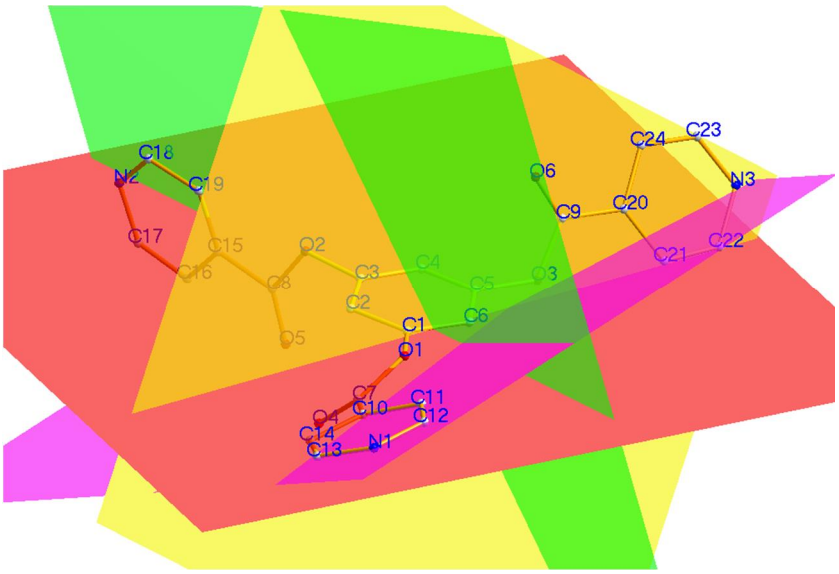


Fig. S8. In complex **4**, Angle between planes1 to plane 2 is 24.731^{o} , planes1 to plane 3 is 82.122^{o} , planes1 to plane 4 is 57.809^{o} .

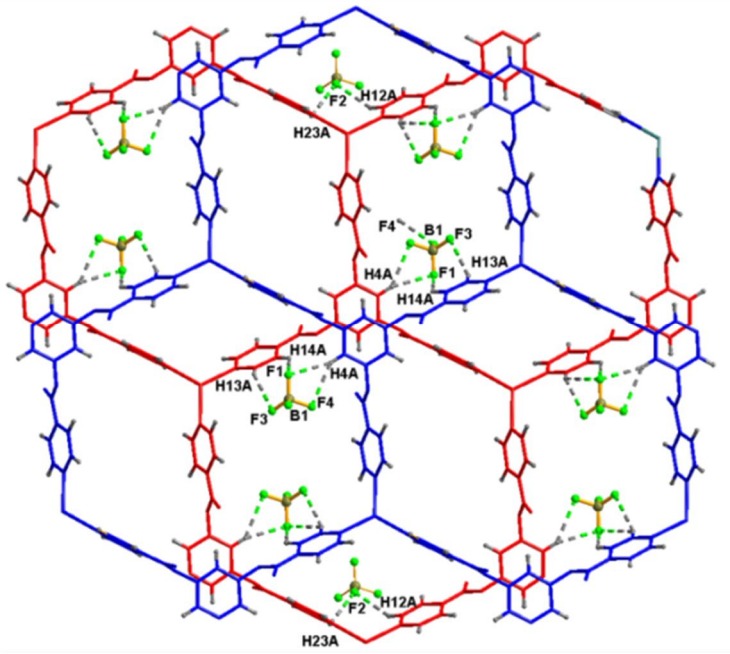


Fig. S9. Hydrogen bonding generated by ligand and BF_4 in the **DLs** and between **DLs** of **1**

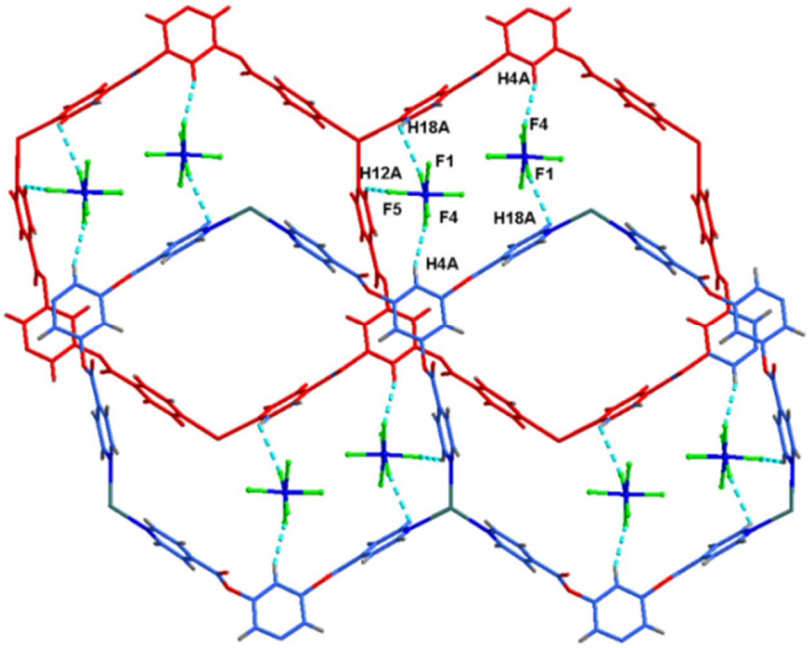


Fig. S10. Hydrogen bonding generated by ligand and SbF_6 in the **DLs** of **2**

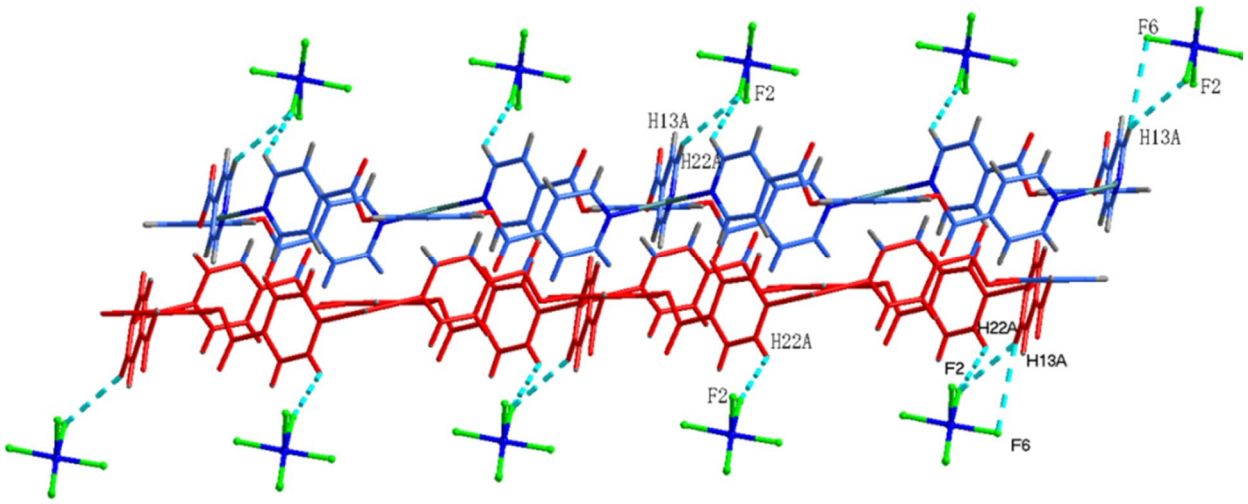


Fig. S11**.** Hydrogen bonding generated by ligand and SbF_6 between **DLs** in **2**.

Thermogravimetric analysis

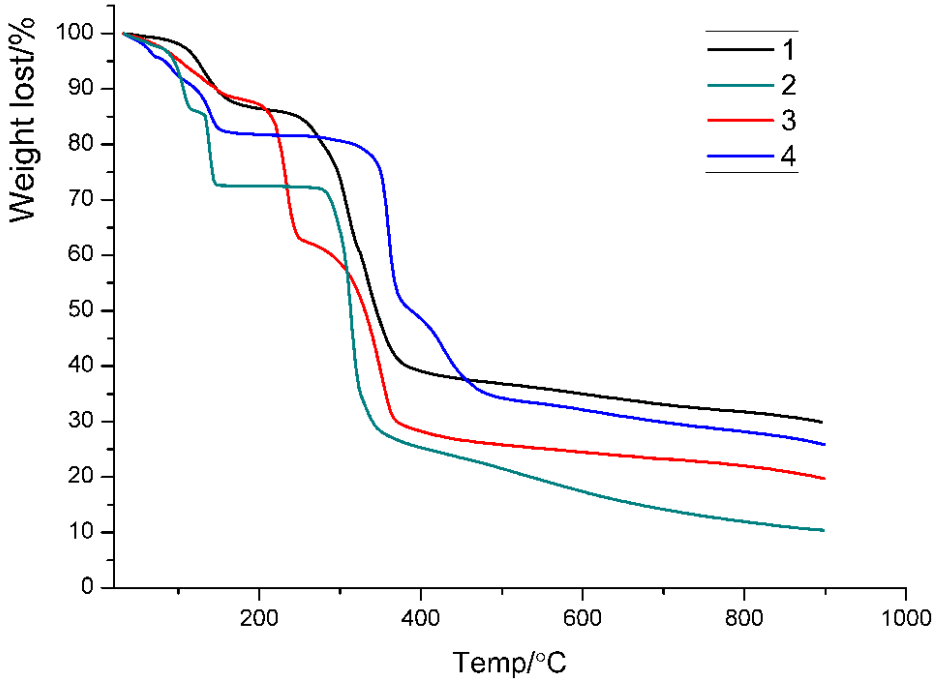
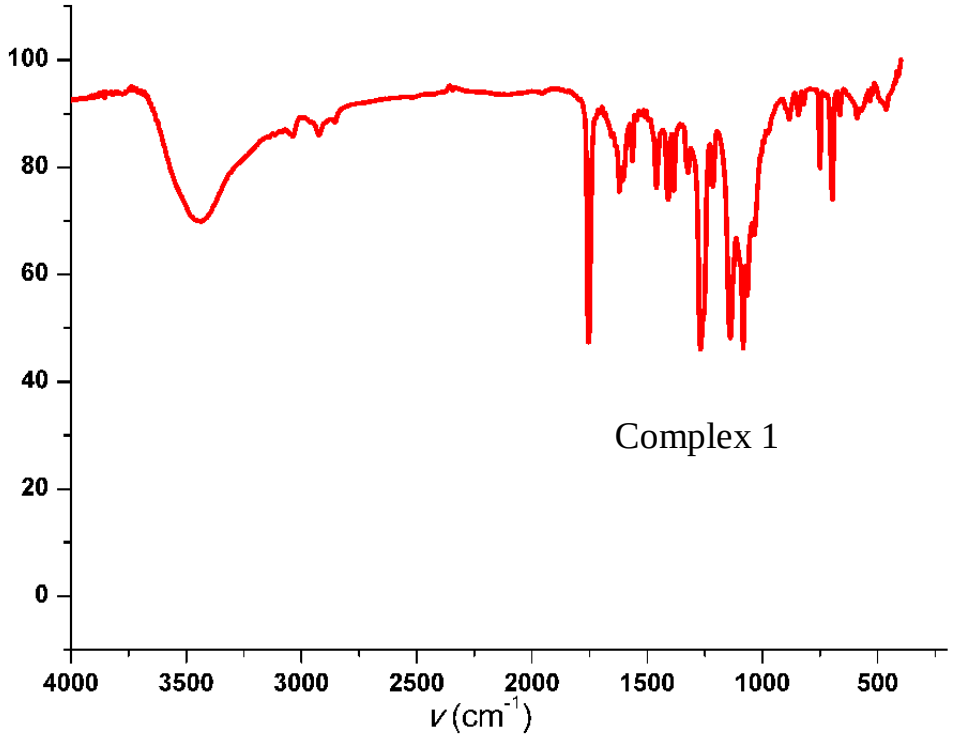
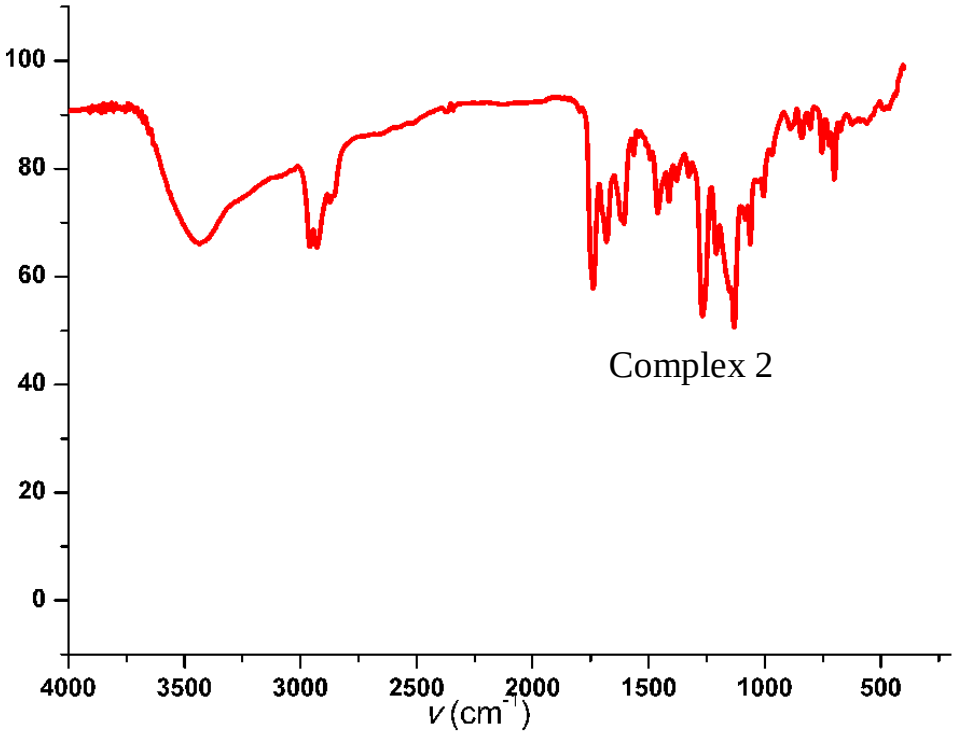


Fig. S12. Thermogravimetric curves of Complexes **1**ï **4**.

Infrared Spectroscopy





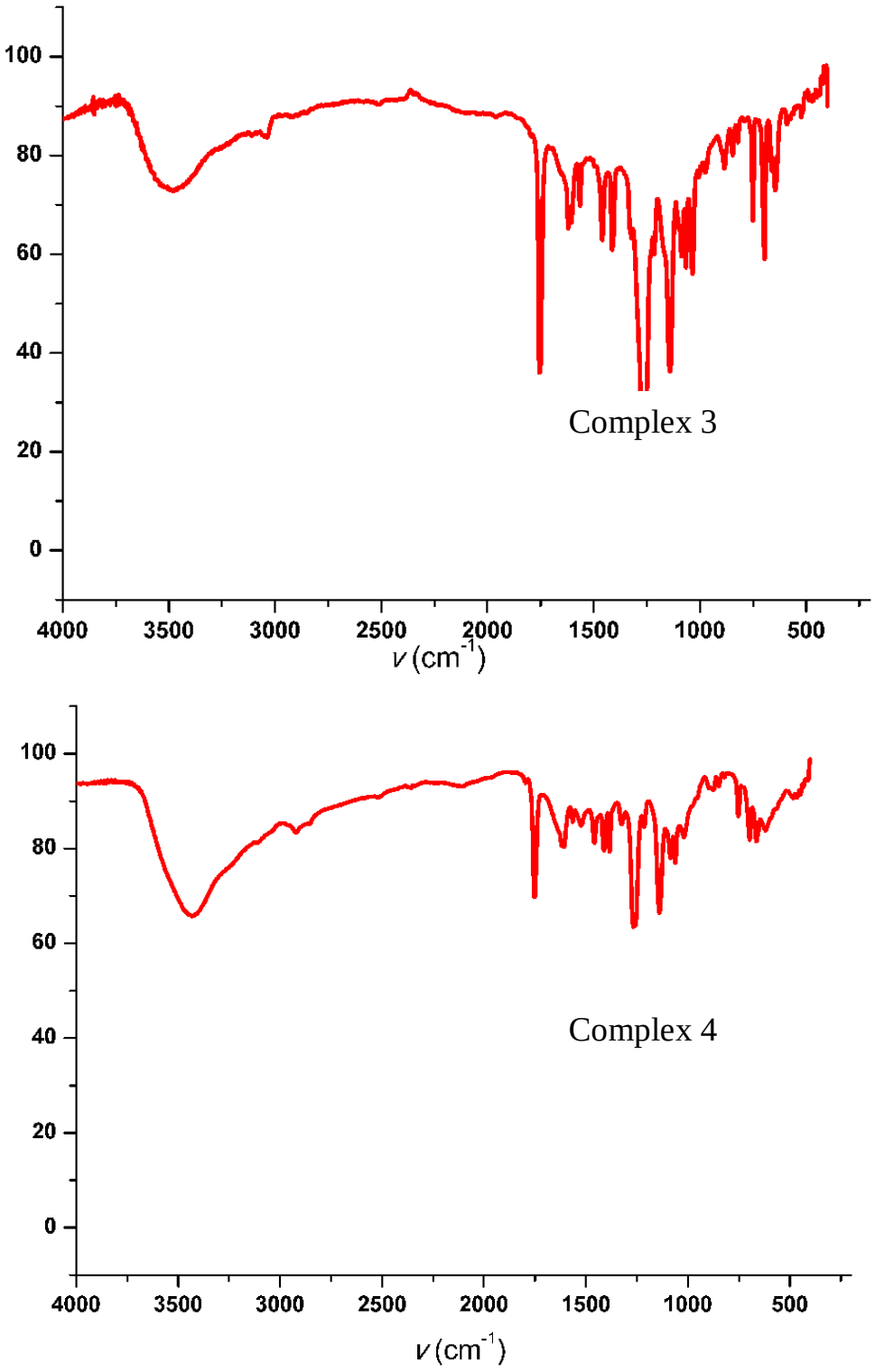
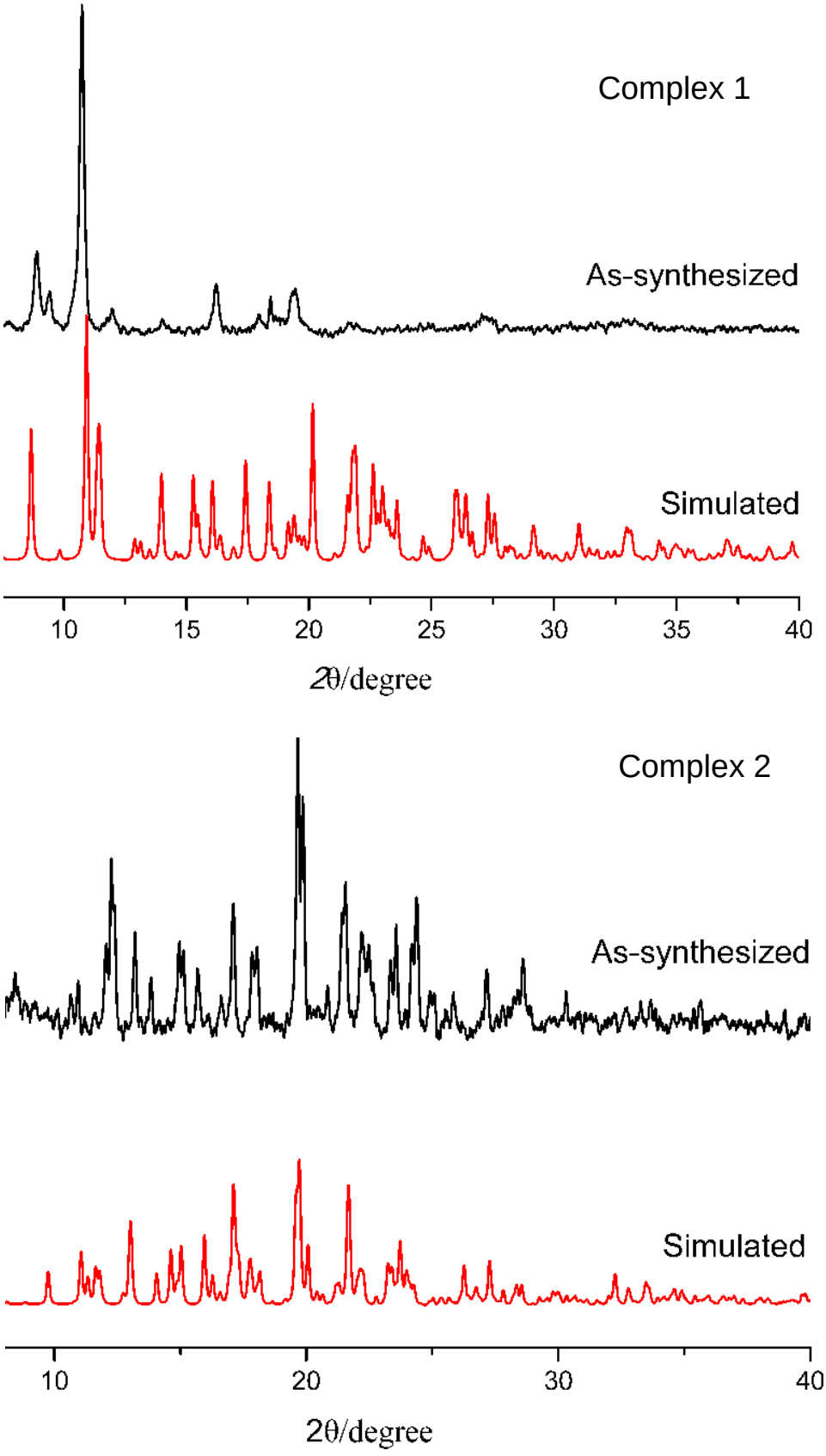


Fig. S13. IR spectrums of Complexes **1**-**4**.

Powder X-ray diffraction study



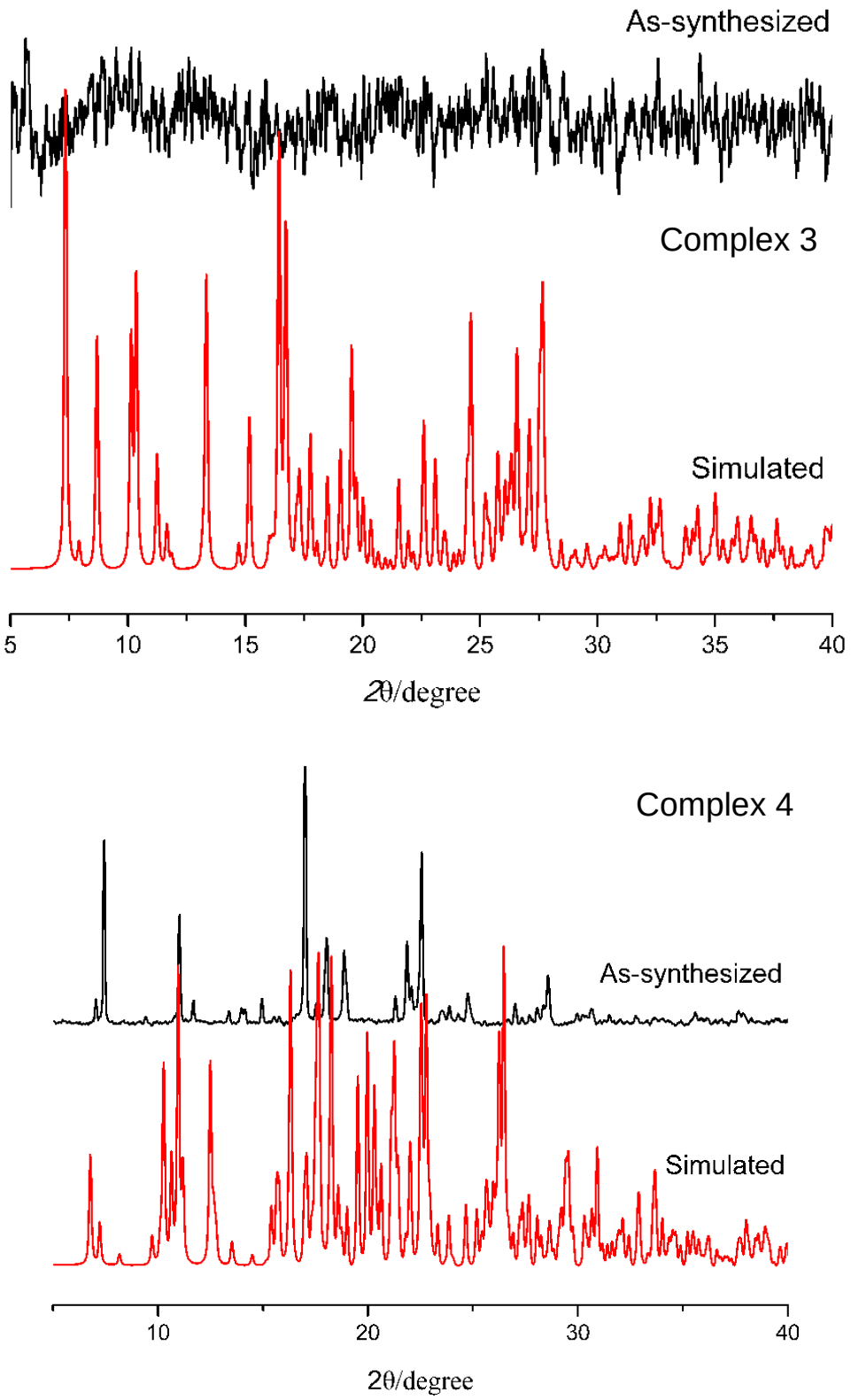


Fig. S14. PXRD patterns of **1**ï **4** compared with a simulated pattern.

Table S1. Selected bond lengths (Å) for Complexes **1**-**4**

	Complex **1**	
Ag(1)-N(1) 2.278(6)	Ag(1)-N(3)#1 2.280(6)	Ag(1)-N(2)#2 2.282(6)
B(1)-F(1) 1.376(11)	B(1)-F(2) 1.328(12)	B(1)-F(3) 1.328(11)
B(1)-F(4) 1.420(13)		
N(1)-Ag(1)-N(3)#1 120.0(2)	N(1)-Ag(1)-N(2) #2 119.9(2)	N(3)#1-Ag(1)-N(2)#2 119.1(2)
Symmetry code: #1 x-1,y,z+1,#2 x,y-1,z+1,#3 x,y+1,z-1,#4 x+1,y,z-1		

	Complex **2**	
Ag(1)-N(3)#1 2.256(4)	Ag(1)-N(1) 2.256(4)	Ag(1)-N(2)#2 2.291(4)
Ag(1)-O(7) 2.594(4)		
N(3)#1-Ag(1)-N(1) 121.76(16)	N(3)#1-Ag(1)-N(2)#2 122.45(16)	N(1)-Ag(1)-N(2)#2 115.68(16)
N(3)#1-Ag(1)-O(7) 93.36(15)	N(1)-Ag(1)-O(7) 90.30(16)	N(2)#2-Ag(1)-O(7) 89.56(16)
Symmetry code: #1 x-1,y-1,z-1, #2 x,y,z-1, #3 x,y,z+1, #4 x+1,y+1,z+1		

	Complex **3**	
Ag(1)-N(3)#1 2.271(3)	Ag(1)-N(2)#2 2.310(3)	Ag(1)-N(1) 2.341(3)
Ag(1)-O(8A) 2.453(12)		
N(3)#1-Ag(1)-N(2)#2 123.53(12)	N(3)#1-Ag(1)117.41(12)	N(2)#2-Ag(1)-N(1) 103.46(12)
N(3)#1-Ag(1)-O(8A) 115.0(3)	N(2)#2-Ag(1)-O(8A) 86.1(3)	N(1)-Ag(1)-O(8A) 106.3(3)
Symmetry code: #1 x+1,y,z+1,#2 x,y-1,z+1,#3 x,y+1,z-1,#4 x-1,y,z-1 #5 -x+1,-y+1,-z-1		

	Complex **4**	
Ag(1)-N(1) 2.237(2)	Ag(1)-N(3)#1 2.298(2)	Ag(1)-N(2)#2 2.311(2)
Ag(1)-O(10) 2.577(5)		
N(1)-Ag(1)-N(3)#1 121.70(8)	N(1)-Ag(1)-N(2) #2 136.97(9)	N(3)#1-Ag(1)-N(2)#299.38(8)
N(1)-Ag(1)-O(10) 87.79(13)	N(3)#1-Ag(1)-O(10) 121.00(15)	N(2)#2-Ag(1)-O(10) 80.77(13)
Symmetry code: #1 x-1,y,z+1,#2 x,y+1,z+1,#3 x,y-1,z-1,#4 x+1,y,z-1		

Table S2. Hydrogen bonds lengths (Å) for Complexes **1** and **2** between counteranions

Complex **1**				
D-H-A	D-A (Å)	H-A (Å)	D-H-A (Å)	∠D-H-A (°)
C(4)-H(4A)-F(1)#2	0.93	2.54	3.4372	161
C(17)-H(17A)-O(8)#3	0.93	2.56	3.2230	129
C(29)-H(29C)-O(6)#1	0.96	2.57	3.4476	152
Symmetry code:#1 x,-1+y,1+z, #2 1-x,1-y,1-z, #3 x,y,-1+z,				
Complex **2**				
D-H-A	D-A (Å)	H-A (Å)	D-H-A (Å)	∠D-H-A (°)
C2 --H2A ..O9#1	0.95	2.25	3.1569	160
C4 --H4A ..F4#2	0.95	2.37	3.2558	156
C12 --H12A ..F5'#3	0.95	2.47	3.1553	129
C16 --H16A ..O4#4	0.95	2.55	3.4168	152
C24 --H24A ..O9#5	0.95	2.47	3.1167	125
C25 --H25B ..F5#3	0.98	2.40	3.3184	155
C25 --H25C ..F2#6	0.98	2.54	3.5184	176
C26 --H26B ..F3'#6	0.98	2.50	3.4574	167
C27 --H27B ..F4	0.98	2.37	3.3366	171
C27 --H27C ..F1'	0.98	2.43	3.3000	147
C28 --H28B ..F6	0.98	2.27	3.2069	160
C28 --H28C ..F1#3	0.98	2.48	3.3919	155
C30 --H30A ..F3#3	0.98	2.39	3.0425	123
C30 --H30B ..O6#6	0.98	2.54	3.772	143
Symmetry code: #1 1+x,y,z, #2 x,y,-1+z, #3 1-x,1-y,1-z, #4 2-x,1-y,-z, #5 -x,1-y,-z, #6 x,1+y,z				