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pH-Dependent Ag(I) coordination architectures constructed from 4-cyanopyridine and phthalic acid: from discrete structure to 2D sheet

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(1) Table S1 The hydrogen bond geometries for **1-4**.

Complex **1**				
D—H···A	D—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4A···O2^{ii}	0.85	1.76	2.5926(19)	164
Symmetry code: (ii) −*x*+1, −*y*, −*z*+1.				
Complex **2**				
O7—H7B···O5	0.84	1.57	2.406(8)	179
O2—H2B···O8^{ii}	0.84	1.83	2.661(8)	172
Symmetry code: (ii) −*x*+2, −*y*+2, −*z*+1				
Complex **3**				
O1W—H1WA···O3	0.85	1.93	2.771(3)	173
O1W—H1WB···O5^{i}	0.85	2.04	2.746(3)	141
Symmetry codes: (i) *x*, *y*+1, *z*.				
Complex **4**				
N3—H3A···O5	0.88	1.99	2.869(5)	173
N4—H4C···O6^{iii}	0.88	2.07	2.884(5)	153
O1W—H1WA···O3	0.85	1.89	2.734(4)	171
O1W—H1WB···O6^{iv}	0.85	1.92	2.754(4)	168
O3W—H3WA···O4	0.85	1.92	2.757(4)	167
O2W—H2WB···O3W^{v}	0.85	2.16	3.003(5)	169
O2W—H2WA···O1W^{vi}	0.85	1.96	2.757(5)	156
O3W—H3WB···O1W	0.85	2.07	2.859(5)	153
Symmetry codes: (iii) *x*+1, *y*−1, *z*−1; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*+1, *y*, *z*−1.				

(2) Table S2 π···π interactions in **1**-**4**

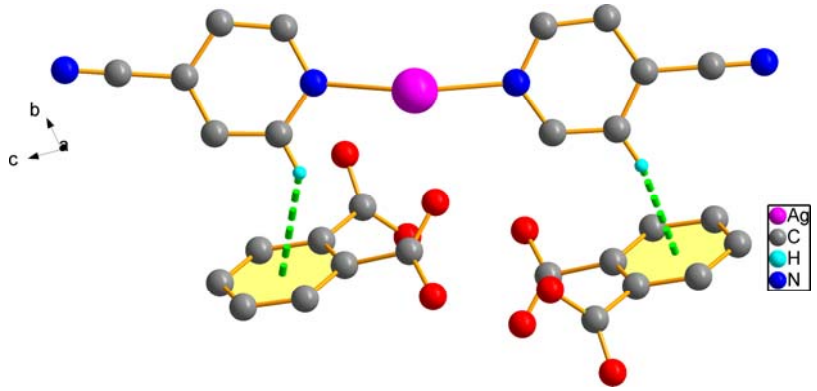
ring (i)→ring (j)	*Cg*···*Cg*	Dihedral angle (i,j) [°]	*Cg*(i) → ring (j) (Å)	*Cg*(j) → ring (i) (Å)	β[°][a]
Complex **1**					
*Cg*1···*Cg*2^{iv}	3.6925(14)	3.62(9)	3.3422(8)	3.2367(8)	28.77
*Cg*1···*Cg*2^{i}	3.7740(14)	3.62(9)	3.2839(8)	3.3942(8)	25.93
*Cg*1: N1/C1-C5; *Cg*2: N3/C7-C11;					
Symmetry codes: (i) −*x*, −*y*+1, −*z*+1, (iv) −*x*−1, −*y*+1, −*z*+1.					
Complex **2**					
*Cg*1···*Cg*2^{i}	3.911(5)	1.6(4)	3.416(4)	3.435(4)	28.58
*Cg*1···*Cg*2^{iii}	3.893(5)	1.6(4)	3.431(4)	3.451(4)	27.53
*Cg*3···*Cg*4	3.903(5)	2.0(4)	3.488(4)	3.446(4)	27.98
*Cg*3···*Cg*4^{iv}	3.943(6)	2.0(4)	3.607(4)	3.594(4)	24.29
*Cg*1: N1/C1-C5; *Cg*2: N3/C7-C11; *Cg*3: C14-C19; *Cg*4: C22-C27					
Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1, (iii) −*x*+2, −*y*+1, −*z*+1, (iv) −*x*+1, *y*, *z*					
Complex **3**					
*Cg*1···*Cg*2^{v}	3.674(2)	3.96(19)	3.4093(16)	3.3535(16)	24.13
*Cg*3···*Cg*4^{vi}	3.681(2)	3.60(19)	3.3760(16)	3.4132(16)	22.00
*Cg*1: N1/C1-C5; *Cg*2: C22-C27; *Cg*3: N3/C15-C19; *Cg*4: C8-C13					
Symmetry code: (v) *x*, −*y*+2, *z*−1/2, (vi) *x*, −*y*, *z*+1/2					
Complex **4**					
*Cg*1···*Cg*1^{vii}	3.472(3)	0	3.1950(17)	3.1951(17)	23.06
*Cg*1···*Cg*2^{viii}	3.483(3)	4.6(2)	3.2678(17)	3.2726(17)	20.02
*Cg*1: N1/C1-C5; *Cg*2: N2/C7-C11					
Symmetry code: (vii) −*x*+1, −*y*+1, −z, (viii) −*x*+1, −*y*, −z,					

[a]β = Angle *Cg*(i) →*Cg*(j) or *Cg*(i) →Me vector and normal to ring (i)

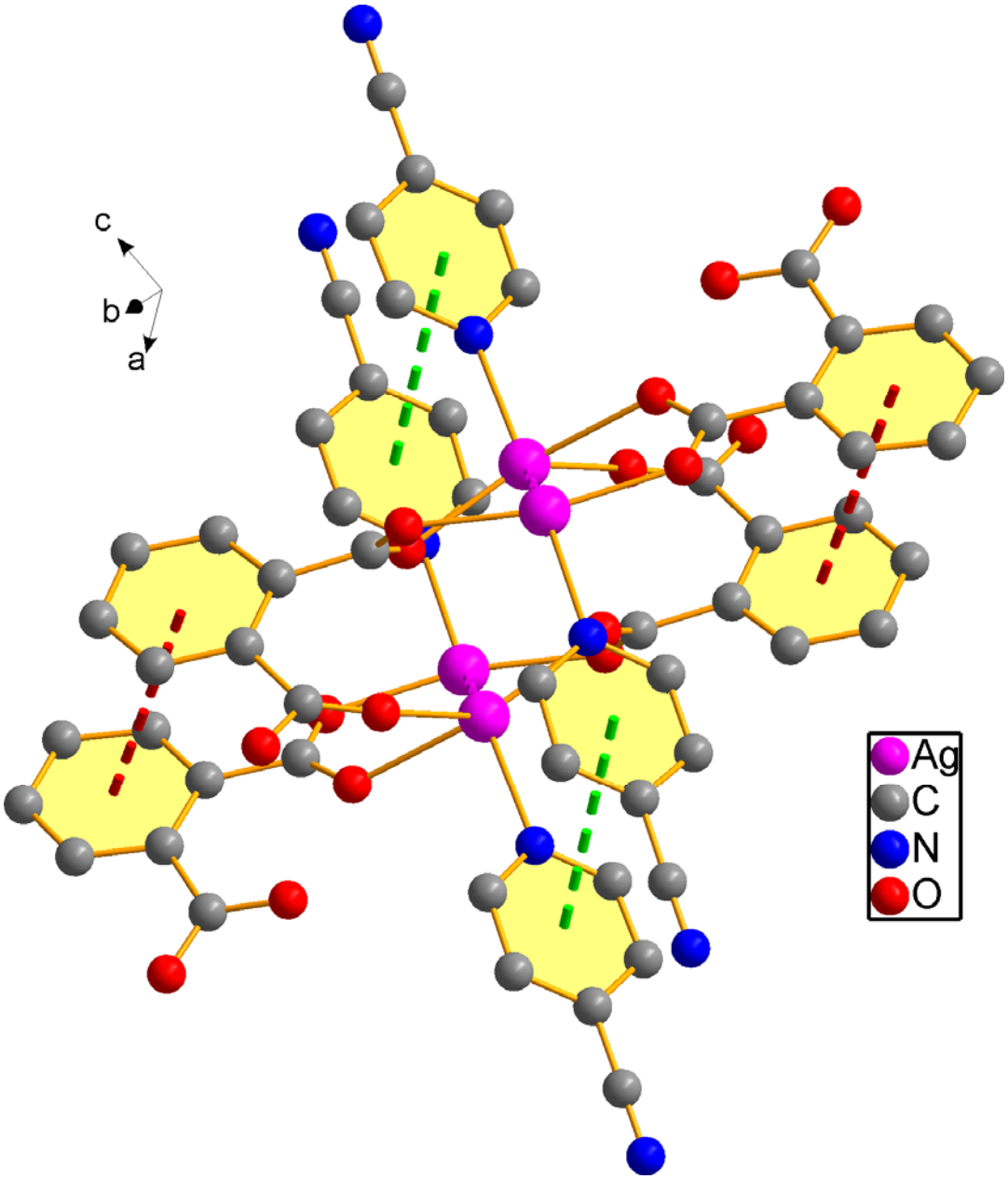
(3) Table S3 C–H···π interactions in **1-4**

Complex 1			
C—H···Cg	H···*C*g	∠C···H···*C*g	C···*C*g
C1—H1A···*C*g3^{iii}	2.92	126	3.544(2)
C10—H10A···*C*g3^{v}	2.86	136	3.594(2)
*C*g3 is the centroid of aromatic ring C14-C19			
Symmetry codes: (iii) −1+*x*, *y*, *z*, (v) −*x*, −*y*, −*z*+1			
Complex 2			
No C–H···π interaction was found in complex 2			
Complex 3			
C4—H4A···*C*g2	2.77	124	3.403(4)
C12—H12A···*C*g3^{ii}	2.72	144	3.537(4)
C16—H16A···*C*g4	2.77	130	3.462(4)
C26—H26A···*C*g1^{i}	2.90	139	3.665(4)
Cg1: N1/C1-C5; Cg2: C22-C27; Cg3: N3/C15-C19; Cg4: C8-C13			
Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, *y*−1, *z*;			
Complex 4			
C10—H10A···*C*g3^{ix}	2.84	150	3.696(5)
*C*g3: C14-C19			
Symmetry code: (ix) *x*, *y*−1, *z*−1			

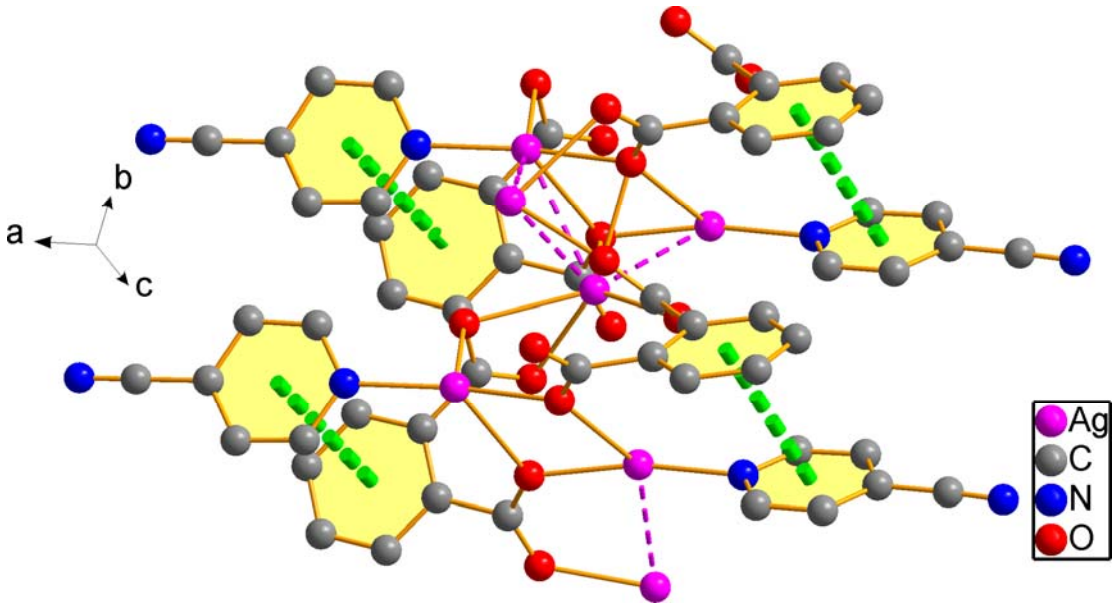
(4) Fig. S1: The C—H···π interaction in 1



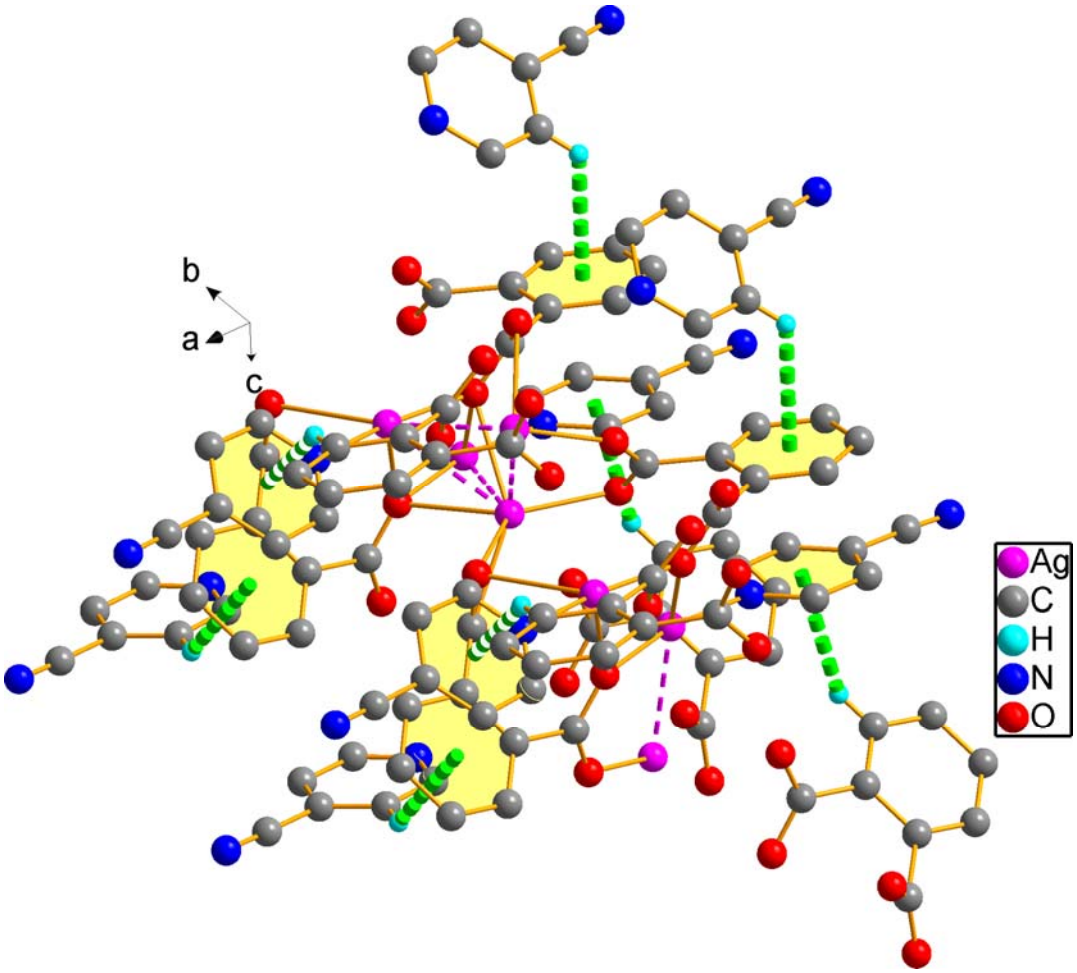
(5) Fig. S2: π···π interaction in 2



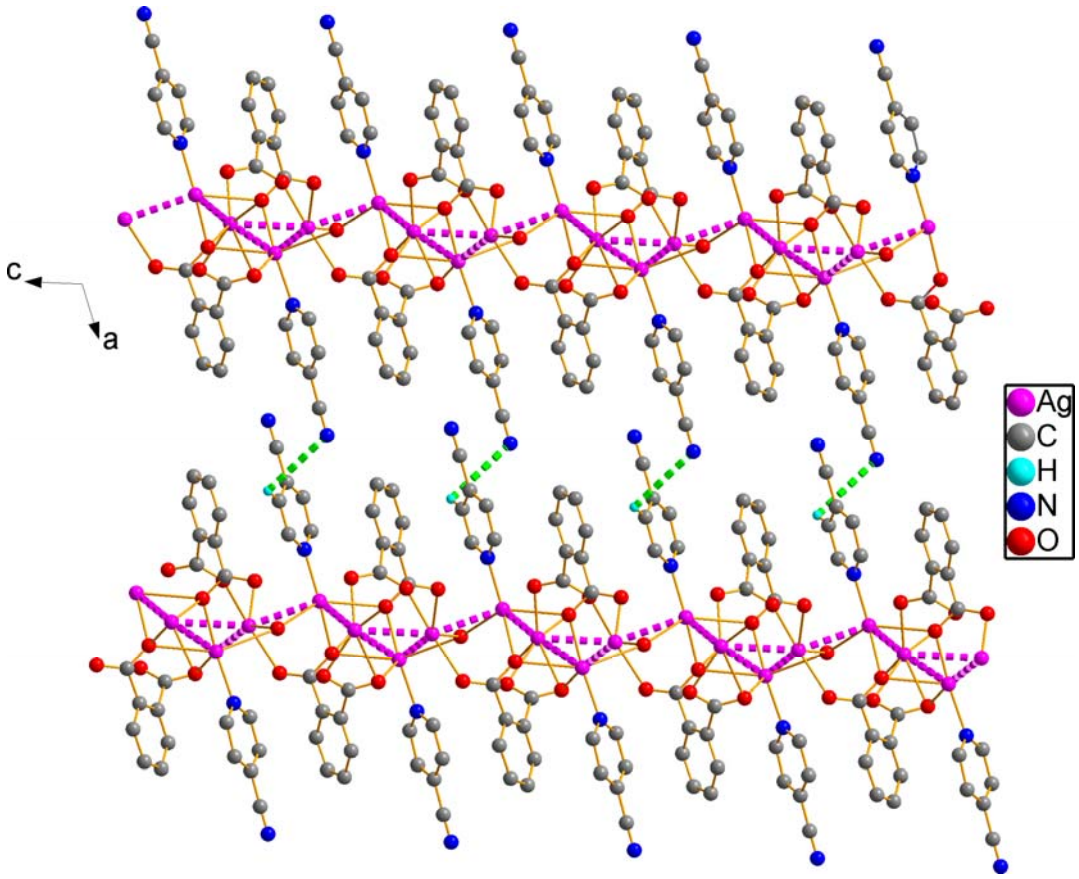
(6) Fig. S3: π···π interaction in 3



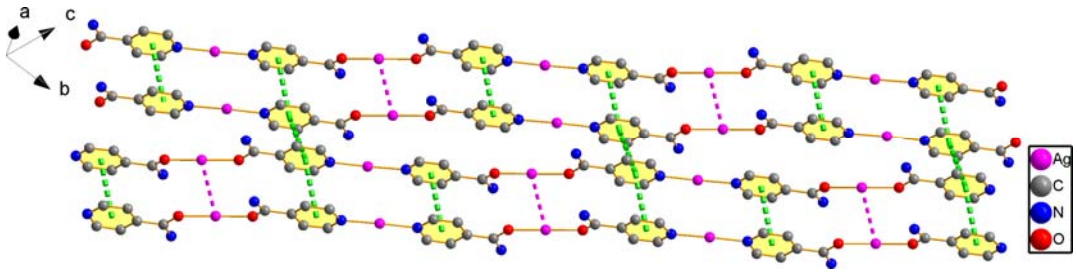
(7) Fig. S4: The C—H···π interaction in 3



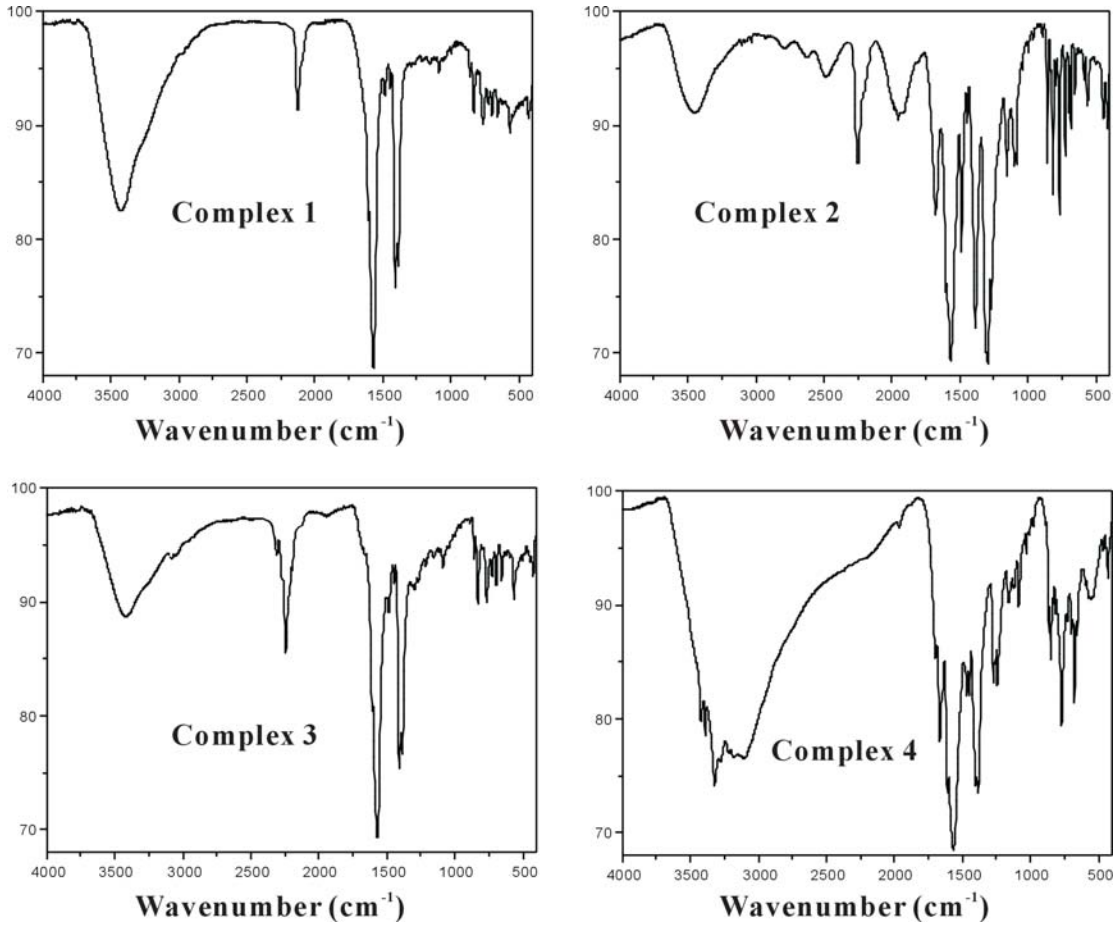
(8) Fig. S5: The intersheet C—H···N interaction in 3



(8) Fig. S6: The interchain π···π and Ag···Ag interaction in 4



(9) Fig. S7 IR of complex 1-4



(10) Fig. S8 The powder XRD patterns and the simulated one from the single-crystal diffraction data for complex 1-4