

Diverse structural assemblies of silver-thiophene-2, 5-dicarboxylate coordination complexes contribute to different proton-conducting performances

Xiao-Feng Zheng*, Wen-Qiang Li, Jun Du, Xian-Zhu Luo, Miao-Miao Liu, Yang Yu and Lai-Jin Tian

School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, PR China

* To whom correspondence should be addressed. E-mail:

xiaofengzheng004@163.com.

Table S1. The corresponding physical quantities of complexes **1 - 3** and the polymer **1 / 2-PVDF**.

	L / cm	S / cm ²	R / Ω	σ / S·cm ⁻¹
Complex 1	0.15	0.25	30.15	1.99 × 10 ⁻²
Complex 2	0.097	0.5	45.55	4.25 × 10 ⁻³
Complex 3	0.06	0.5	64.43	1.98 × 10 ⁻³
Polymer 1 -PVDF	0.025	1.045	11.00	2.17 × 10 ⁻³
Polymer 2 -PVDF	0.025	1.045	26.60	8.99 × 10 ⁻⁴

Table S2. Selected Bond Lengths (Å) and Angles (deg) for Complex **1-3^a**

Complex 1			
Ag1-O3	2.4150(18)	Ag1-P1	2.4328(7)
Ag1-P2	2.4496(7)	Ag1-O1	2.4743(18)
O3-Ag1-P1	106.37(5)	O3-Ag1-P2	103.13(5)
P1-Ag1-P2	143.83(2)	O3-Ag1-O1	93.18(7)
P1-Ag1-O1	105.71(5)	P2-Ag1-O1	92.96(5)
Complex 2			
Ag1-N1	2.155(3)	Ag2-O3	2.240(4)
Ag1-O1	2.168(3)	Ag2-N3	2.345(4)
Ag1-O1 ⁱ	2.482(3)	Ag2-O4 ⁱⁱ	2.189(4)
Ag2-Ag2 ⁱⁱ	2.8923(12)		
N1-Ag1-O1	155.43(12)	N1-Ag1-O1 ⁱ	97.56(12)
O1-Ag1-O1 ⁱ	104.76(6)	O4 ⁱⁱ -Ag2-O3	159.76(16)
O4 ⁱⁱ -Ag2-N3	104.83(16)	O3-Ag2-N3	95.27(15)
O4 ⁱⁱ -Ag2- Ag2 ⁱⁱ	81.44(13)	O3-Ag2- Ag2 ⁱⁱ	80.78(12)
N3-Ag2- Ag2 ⁱⁱ	157.87(11)	Ag1-O1-Ag1 ⁱ	117.91(12)
Complex 3			
Ag1-N4	2.356(2)	Ag1-N2	2.485(3)

Ag1-O1	2.471(3)	Ag1-N1	2.504(3)
Ag2-O4	2.326(3)	Ag2-N8	2.355(3)
Ag2-N5	2.363(3)	Ag2-O3	2.495(3)
Ag2-Ag2 ⁱⁱ	3.4145(5)		
N4-Ag1-O1	129.72(8)	N4-Ag1-N2	111.95(9)
O1-Ag1-N2	79.61(8)	N4-Ag1-N1	117.26(9)
O1-Ag1-N1	83.55(8)	N2-Ag1-N1	127.13(8)
O4-Ag2-N8	108.62(13)	O4-Ag2-N5	112.00(11)
N8-Ag2-N5	115.38(10)	O4-Ag2-O3	111.95(11)
N8-Ag2-O3	90.96(12)	N5-Ag2-O3	116.14(11)

^a Symmetry codes for **2**: i, 1-x, -1/2+y, 2-z; ii, 1-x, 1/2+y, 2-z; iii, 1-x, 2-y, 2-z; **3**: i, 1-x, -1/2+y, 2-z; ii, 1-x, 1/2+y, 2-z; iii, 1-x, 2-y, 2-z.

Table S3. H-Bonding Geometry Parameters (Å and deg) for Complex **2**^a

D-H...O	D-H	H...O	D...A	D-H...A
Complex 2				
N2-H2B...O2 ⁱ	0.89	2.37	2.964(4)	124
Complex 3				
O(5)-H(5A)...O(7)	0.85	2.17	2.995(5)	166
O(5)-H(5B)...O(3) ⁱ	0.85	2.15	2.939(5)	155
O(6)-H(6A)...O(1)	0.85	1.90	2.735(3)	168
O(6)-H(6B)...N(7) ⁱⁱ	0.85	2.06	2.910(4)	177
O(7)-H(7A)...O(2) ⁱ	0.85	2.07	2.885(3)	161
O(7)-H(7B)...O(6) ⁱⁱⁱ	0.85	1.95	2.794(3)	173

^a Symmetry codes for **2**: i, -1+x, y, z; ii, 3/2-x, 1/2+y, z; iii, 1/2-x, 1/2+y, z; **3**: i, 2-x, -1/2+y, 1/2-z.

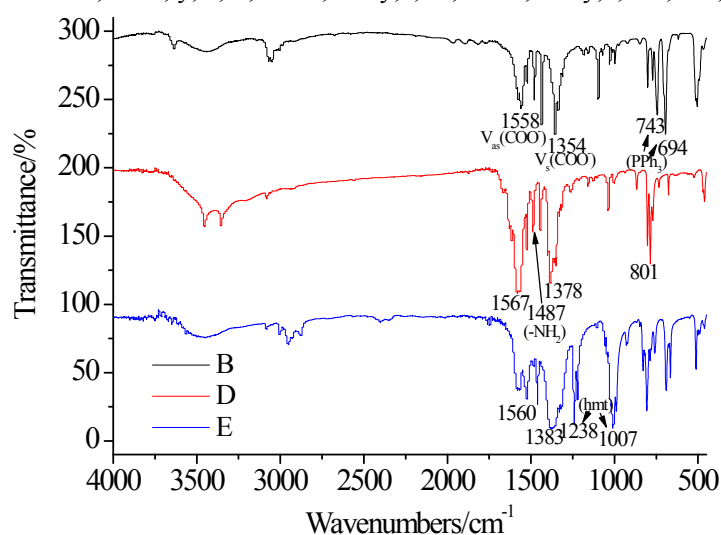


Figure S1, FT-IR spectra of **1 - 3** respectively.

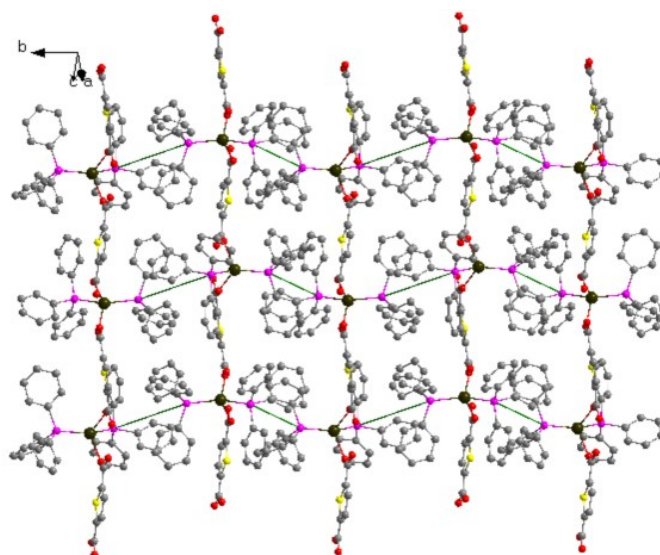


Figure S2, The 2-D layer formed by 4PE (the green rods) motifs between the 1-D chains in **1**. The H atoms are omitted for clarity.

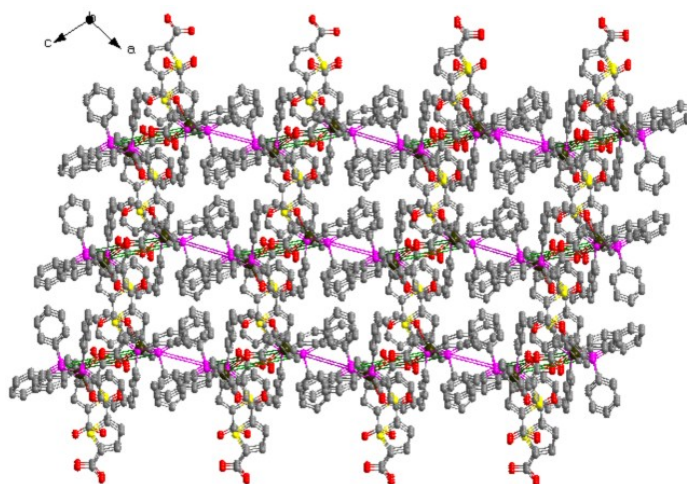


Figure S3, The 3-D network formed by 6PE (the brown rods) and 4PE (the green rods) motifs between the 2-D layers in **1**. The H atoms are omitted for clarity.

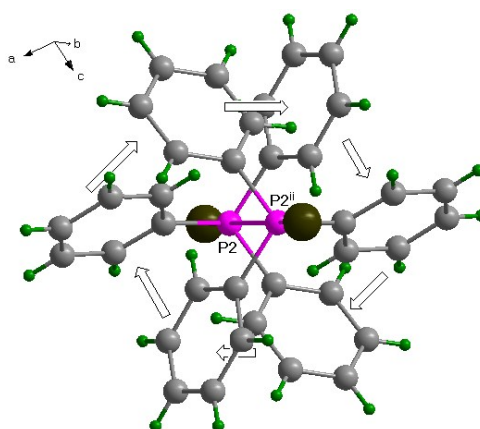


Figure S4, The pseudo-ideal weak 6PE motif between two PPh_3 at P2: the torsion angles for the rings involved are 30, 33 and 57°(and -30, -33 and -57°). The 6PE is

centrosymmetric [at centres of inversion of type (0.5, 0, 0.5 – site 2c)], with a P...P distance of 7.13 Å; Symmetry codes: ii, 1-x, -y, 1-z.

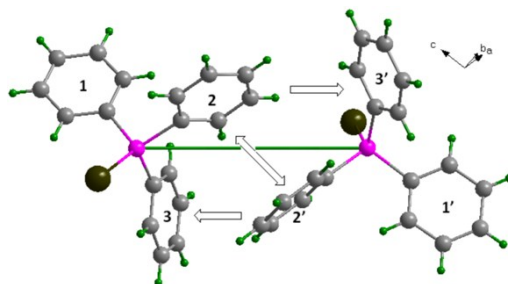


Figure S5, The pseudo weak 4PE motif: the torsion angles for the rings involved are 16 and -68° (84 and -63°), which is non-centrosymmetric with a P...P distance of 7.72 Å. The **off** interaction occurs between rings 2 and 2', while the interactions from 2→3' and 2'→3 are intermediate between **vf** and **ef**.

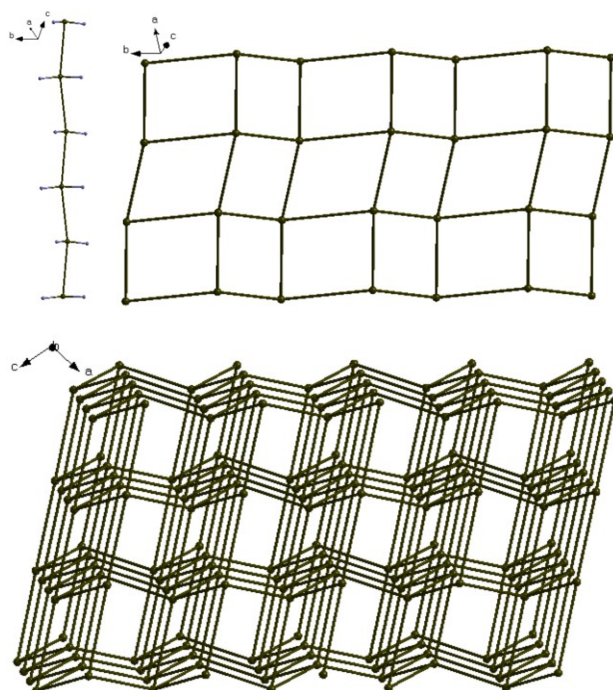


Figure S6, The schematic topological presentation for the structure of **1**.

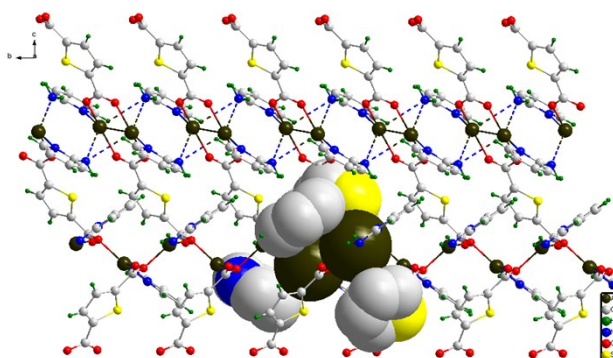


Figure S7, The Ag- π interactions and long Ag...N interactions in **2**. Parts of Ag- π interactions are pictured in space-filling modes.

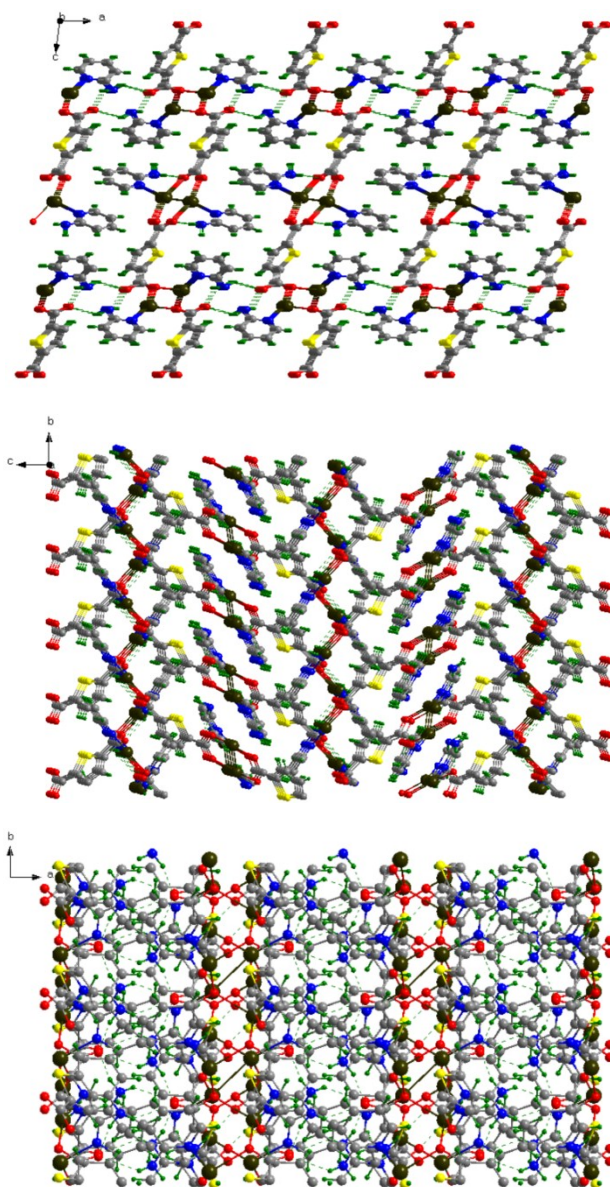


Figure S8, The 3D brick-wall network along b-axis in **2**.

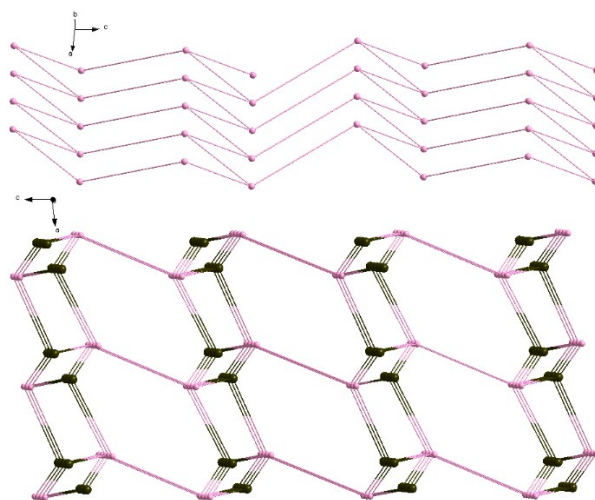


Figure S9, The schematic topological presentation for the structure of **2**.

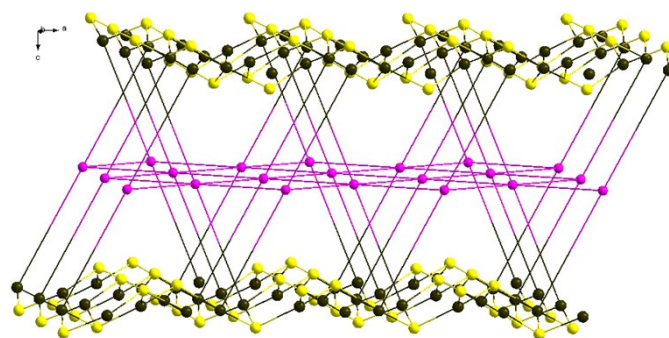


Figure S10, The schematic topological presentation for the structure of **3**.

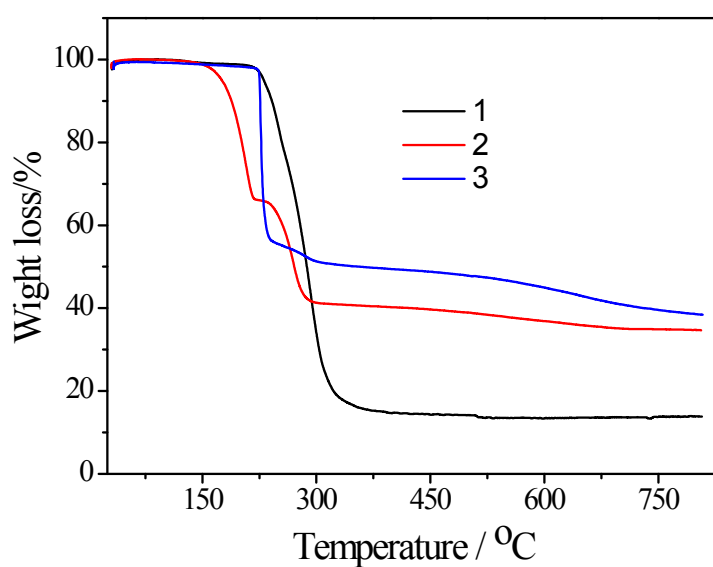


Figure S11, Thermogravimetric analysis (TGA) data for **1-3**.

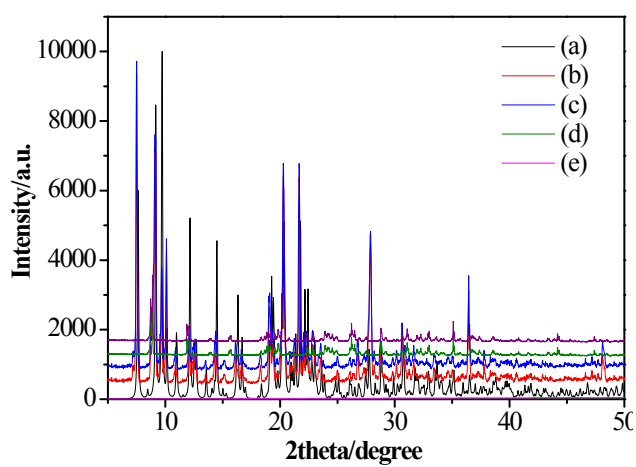


Figure S12, PXRD patterns showing the structural integrity in water of compound **1**. (a) Simulated PXRD patterns, (b) as-prepared of **1**, and after soaked in H₂O at r.t. for (c) 1 d, (d) 3 d, (e) 7 d.

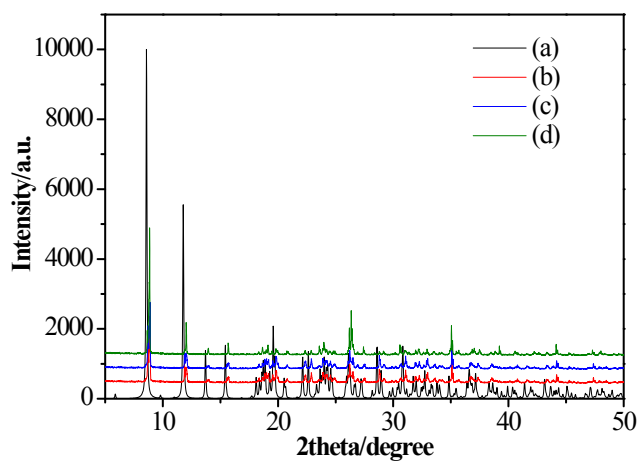


Figure S13, PXRD patterns showing the structural integrity in water of compound **2**. (a) Simulated PXRD patterns, (b) as-prepared of **2**, and after soaked in H₂O at r.t. for (c) 1 d, (d) 7 d.

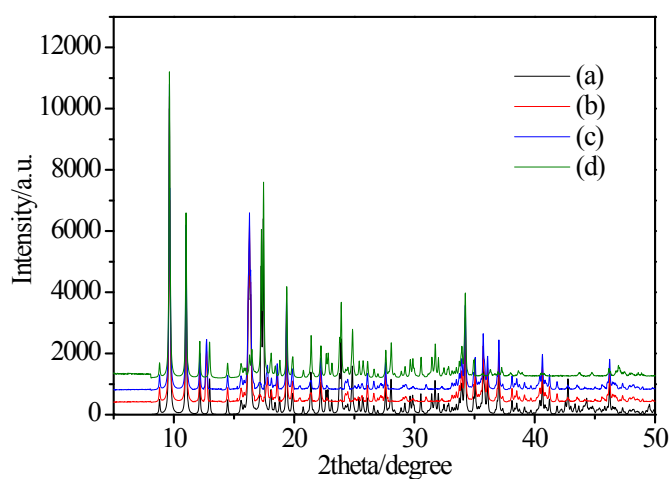


Figure S14, PXRD patterns showing the structural integrity in water of compound **3**. (a) Simulated PXRD patterns, (b) as-prepared of **3**, and after soaked in H₂O at r.t. for (c) 1 d, (d) 7 d.