Linear extension of bithiophene compounds by the combination of C–N covalent bond cross-coupling and N–Ag coordinative bond formation

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Electronic Supporting Information

Table 1 Selected bond distances (Å) and bond angles (°) in ligand L and three silver(I) complexes **1**-**3**.

L					
C1–N1	1.406(8)	C4–S1	1.739(6)	C6–N2	1.359(9)
C1–S1	1.733(6)	C5–N2	1.300(9)	C7–N1	1.375(8)
C4–C4[a]	1.450(11)	C5–N1	1.354(8)		
C5–N1–C7	105.6(5)	C7–N1–C1	128.1(5)	C1–S1–C4	90.6(3)
C5–N1–C1	126.3(5)	C5–N2–C6	104.9(6)		
[a] -*x*, 1-*y*, 1-*z*.					
1					
Ag1–N2[a]	2.172(5)	C1–N1	1.412(8)	C5–N1	1.380(9)
Ag1–N2	2.172(5)	C1–S1	1.717(6)	C6–N2	1.376(9)
Ag1–O1[a]	2.745(8)	C4–S1	1.730(7)	C7–N1	1.377(8)
Ag1–O1	2.745(8)	O1[a]–Ag1–O1	46.0(3)		
N2[a]–Ag1–N2	152.1(3)	C5–N2	1.303(8)	O2–N3–O1[a]	119.0(6)
N2[a]–Ag1–O1[a]	81.4(2)	C7–N1–C5	106.9(6)	O2–N3–O1	119.0(6)
N2–Ag1–O1[a]	126.4(2)	C7–N1–C1	127.2(6)	O1[a]–N3–O1	122.0(11)
N2[a]–Ag1–O1	126.4(2)	C5–N1–C1	125.8(6)	C1–S1–C4	90.9(3)
N2–Ag1–O1	81.4(2)	C5–N2–C6	106.4(6)		
[a] 3-*x*, *y*, 0.5-*z*.					
2					
Ag1–N4	2.140(6)	C8–N3	1.405(9)	C6–N2	1.374(10)
Ag1–N2	2.134(6)	C8–S2	1.727(7)	C7–N1	1.376(9)
Ag1–O2[a]	2.843(6)	C11–C11[b]	1.425(14)	C1–N1	1.404(9)
C12–N4	1.317(9)	C11–S2	1.739(7)	C1–S1	1.730(7)
C12–N3	1.335(9)	C5–N2	1.319(9)	C4–C4[c]	1.464(14)
C13–N4	1.357(10)	C5–N1	1.329(9)	C4–S1	1.736(6)
C14–N3	1.389(9)	C5–N2–C6	105.4(6)	C5–N1–C1	125.2(6)
C12–N4–Ag1	120.7(5)	N4–Ag1–N2	159.1(2)	C7–N1–C1	127.5(6)
C13–N4–Ag1	132.6(5)	C12–N3–C14	106.5(6)	C1–S1–C4	90.2(4)

C12–N3–C8	124.9(6)	C12–N4–C13	106.1(6)	C8–S2–C11	90.9(4)
C14–N3–C8	128.4(6)	C5–N1–C7	107.1(6)		
[a] 1+*x*, 1+*y*, *z*; [b] 1-*x*, 1-*y*, -*z*; [c] 3-*x*, 1-*y*, 1-*z*.					
3					
Ag1–N4[a]	2.126(5)	C10–N2	1.349(8)	C12–N4	1.316(6)
Ag1–N2	2.126(4)	C1–N1	1.416(6)	C12–N3	1.352(6)
Ag1–O2[b]	2.738(9)	C1–S1	1.721(5)	C13–N4	1.364(8)
Ag1–Ag1[c]	3.0084(9)	C4–S1	1.726(4)	C14–N3	1.365(7)
C9–N2	1.310(6)	C5–S2	1.723(5)	C15–O2	1.156(11)
C9–N1	1.336(6)	C8–N3	1.418(6)	C15–O1	1.191(9)
C11–N1	1.358(7)	C8–S2	1.711(5)	C14–N3–C8	127.4(4)
N4[a]–Ag1–N2	169.0(2)	C9–N1–C11	106.2(5)	C12–N4–C13	106.1(5)
N4[a]–Ag1–O2[b]	91.3(3)	C9–N1–C1	126.1(4)	C1–S1–C4	91.4(2)
N2–Ag1–O2[b]	93.4(3)	C11–N1–C1	127.6(5)	C8–S2–C5	91.1(2)
N4[a]–Ag1–Ag1[c]	96.4(1)	C12–N3–C14	106.8(4)	O2[b]–Ag1–Ag1[c]	88.8(3)
N2–Ag1–Ag1[c]	93. 7(1)	C12–N3–C8	125.8(4)	C9–N2–C10	105.2(5)
[a] 1+*x*, 1+*y*, -1+*z*; [b] 2-*x*, 1-*y*, -*z*; [c] 3-*x*, 1-*y*, -*z*; [d] -1+*x*, -1+*y*, 1+*z*.					

Table 2. Hydrogen–bonding parameters (Å, °) in ligand L and three silver(I) complexes **1**-**3**

D–H···A	D–H	H···A	D···A	∠DHA	Sym. Trans.
L					
C2–H2···N2	0.93	2.52	3.446(8)	175	-*x*, 1/2+*y*, 1/2-*z*
1					
C2–H2···O1	0.93	2.42	3.247(10)	148	-1+*x*, -1+*y*, *z*
C5–H5···O2	0.93	2.33	3.163(9)	149	*x*, -1+*y*, *z*
C6–H6···O1	0.93	2.44	3.067(10)	125	
2					
C5–H5···O3	0.93	2.58	3.438(16)	153	1+*x*, *y*, *z*
C10–H10···O4	0.93	2.56	3.430(11)	155	1/2-*x*, -1/2+*y*, 1/2-*z*
C12–H12···O4	0.93	2.44	3.220(11)	142	1+*x*, *y*, *z*
C13–H13···O1	0.93	2.51	3.232(12)	134	1+*x*, 1+*y*, *z*
3					
C2– H2···O1	0.93	2.54	3.427(10)	160	1+*x*, -1+*y*, *z*
C13–H13···O1	0.93	2.58	3.337(10)	138	*x*, -1+*y*, 1+*z*

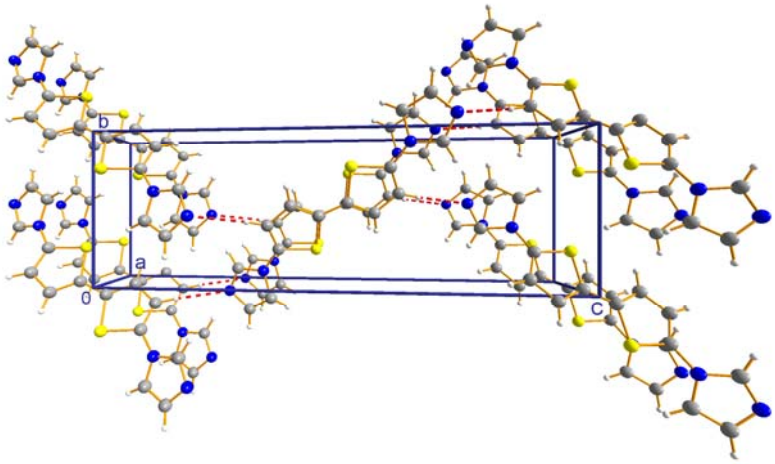


Fig. SI1. View of the hydrogen bonding and π-π stacking interactions in L.

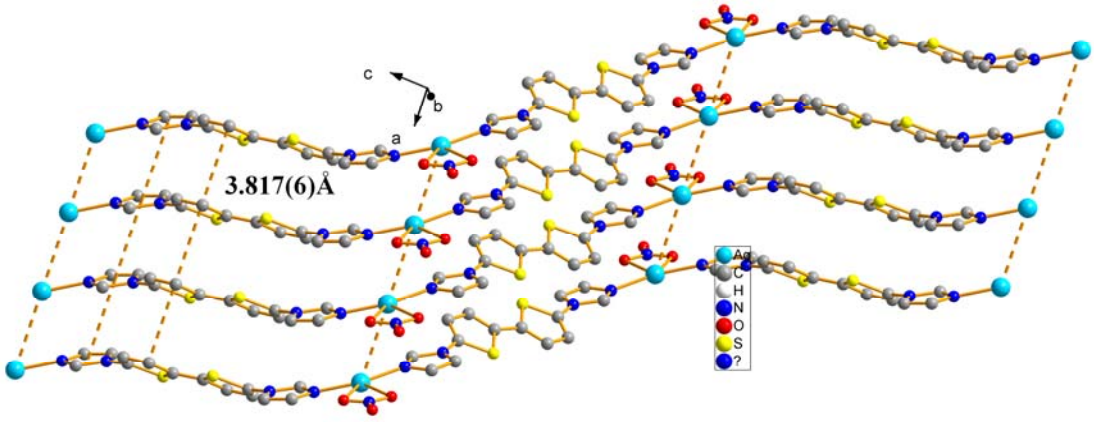
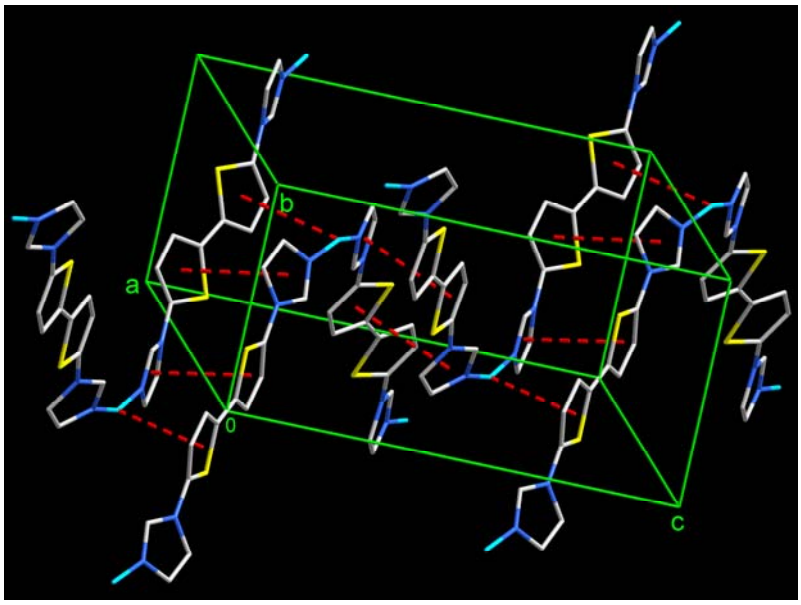


Fig. SI2. View of the undulating chains in $[Ag(L)NO_3]_n$ (**1**).



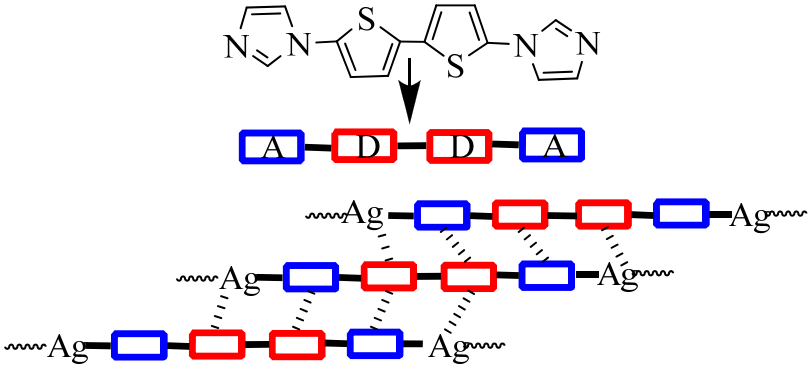


Fig. SI3. View of the π-π stacking and Ag-π interactions in complex **2**

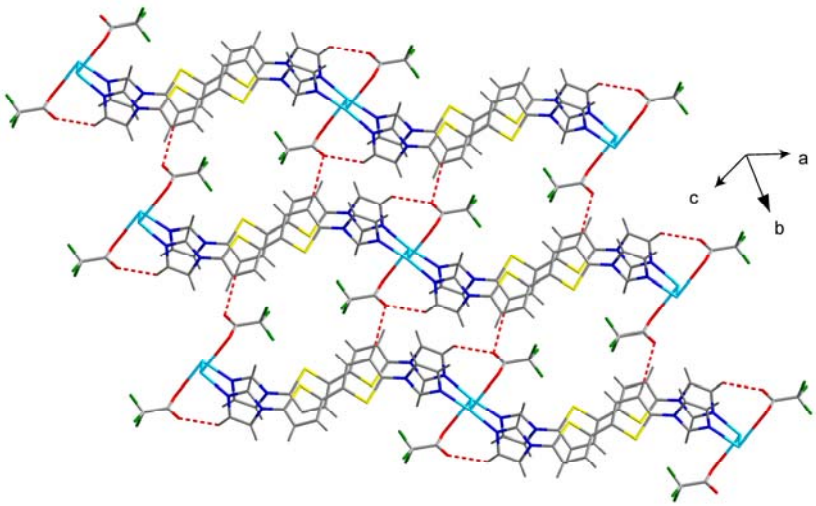


Fig. SI4. View of the π-π stacking and hydrogen bonding interactions in $[Ag(L)(CF_3COO)]_n$ (**3**)

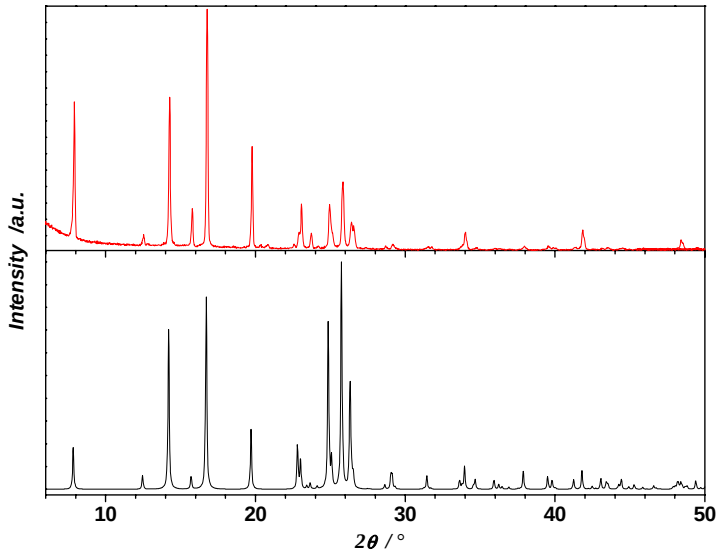


Fig. SI5. The simulative (black line) and experimental (red line) powder X-ray

diffraction patterns for L.

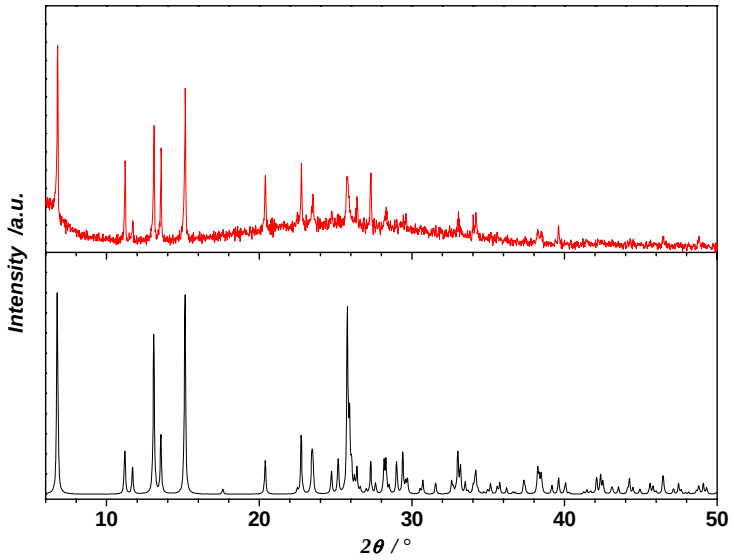


Fig. SI6. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **1**.

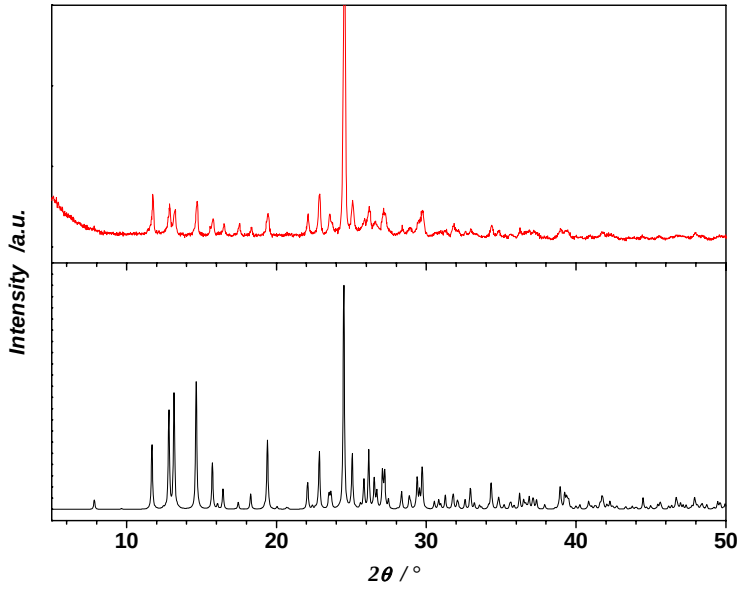


Fig. SI7. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **2**.

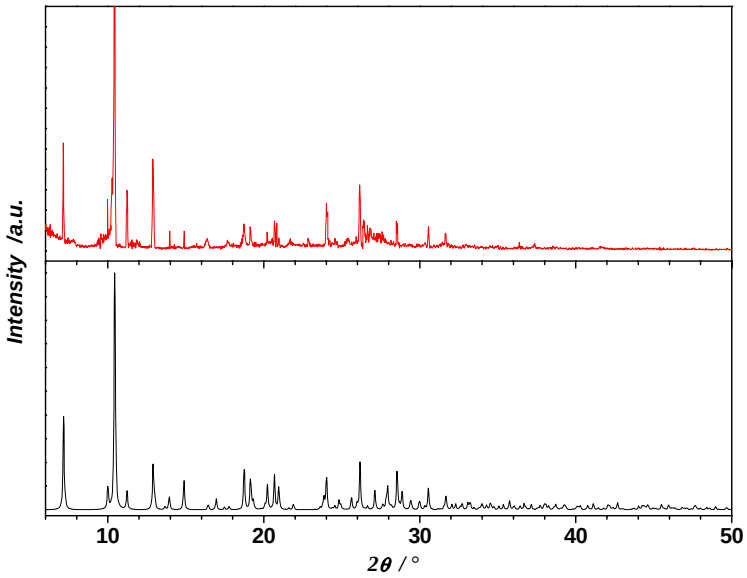


Fig. SI8. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for **3**.

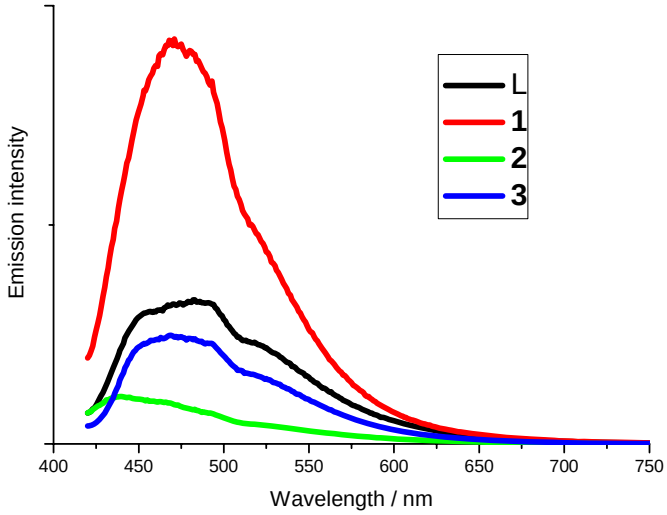


Fig. SI9. Solid-state fluorescence emission spectra of L, **1**, **2** and **3** at room temperature.