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New silver(I) thiazole-based coordination polymers: structural and photophysical investigation

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General information. Ligands **L1**–**L3** were synthesized according to the described procedures[1]. $AgNO_3$ (99.9 %, Reactiv), EtOH (4% H_2O), CH_3CN (HPLC grade, Cryochrom) were used as purchased. FT-IR spectra were recorded on a Bruker Vertex 80 spectrometer. Thermogravimetric (TGA) and differential thermal analyses (DTA) were carried out under helium flow at 10 deg min^{-1} heating rate using a Netzsch STA 449 F1 Jupiter STA in a closed Al_2O_3 pan. The elemental analyses were performed on a MICRO cube analyzer.

Synthesis and characterization data

CP 1 Silver nitrate (42 mg, 0.25 mmol) and **L1** (39 mg, 0.22 mmol) were dissolved in MeCN (1 ml) upon stirring for 1 min. During the reaction, an orange precipitate and a clear solution were formed. For complete precipitation, Et_2O (10 ml) was added. The deposited product was filtered and dried in air. Orange powder. Yield: 56 mg (74%). Anal. Calcd: $C_9H_8AgN_3O_3S$ (346.11) C, 31.2; H, 2.3; N, 12.1; S, 9.3. Found: C, 31.3; H, 2.5; N, 12.0; S, 9.4. FT-IR (KBr, cm^{-1}): 401 (vw), 424 (w), 446 (w), 501 (m), 509 (m), 557 (m), 664 (w), 696 (s), 745 (s), 783 (w), 839 (vs), 995 (m), 1015 (m), 1094 (m), 1115 (w), 1161 (w), 1231 (w), 1271 (m), 1312 (w), 1335 (m), 1391 (w), 1435 (m), 1450 (m), 1483 (m), 1504 (m), 1564 (w), 1587 (w), 1609 (w), 2872 (w), 2926 (m), 2951 (w), 3055 (w).

CP 2 Silver nitrate (44 mg, 0.26 mmol) and **L2** (67 mg, 0.27 mmol) were dissolved in MeCN (1 ml). After 1 min of stirring, a pale-yellow solution and a colorless by-product precipitate were obtained. The precipitate was removed, and the product was obtained as yellow crystals by precipitation with Et_2O (10 ml). Since this CP has not been obtained in a phase-pure form, it has been characterized by single crystal X-ray diffraction analysis only.

CP 3 Silver nitrate (39 mg, 0.23 mmol) and **L3** (64.7 mg, 0.23 mmol) were dissolved in MeCN (1 ml), and the mixture was stirred for 1 min. A turquoise solution and a colorless precipitate were formed. The mixture was filtered, and the clear solution was then precipitated with Et_2O (8-10 ml) to obtain solid CP **3**. After that, the mother liquor was removed, and the product was dried in air. Orange powder. Yield: 75 mg (73%). Anal. Calcd: $C_{12}H_{13}AgN_4O_4S_2$ (447.94) C, 32.1; H, 2.9; N, 12.5; S, 14.3. Found: C, 32.3; H, 3.1; N, 12.6; S, 14.3. FT-IR (KBr, cm^{-1}): 503 (m), 650 (m), 692 (s), 754 (s), 826 (m), 907 (s), 947 (s), 970 (s), 1036 (s), 1072 (s), 1099 (s), 1161 (s), 1182 (s), 1240 (vs), 1290 (vs), 1385 (m), 1423 (s), 1447 (vs), 1497 (s), 1528 (vs), 1553 (s), 1603 (m), 1668 (s), 1734 (w), 3119 (w).

X-Ray crystallography

(***a***)

(***b***)

(***c***)

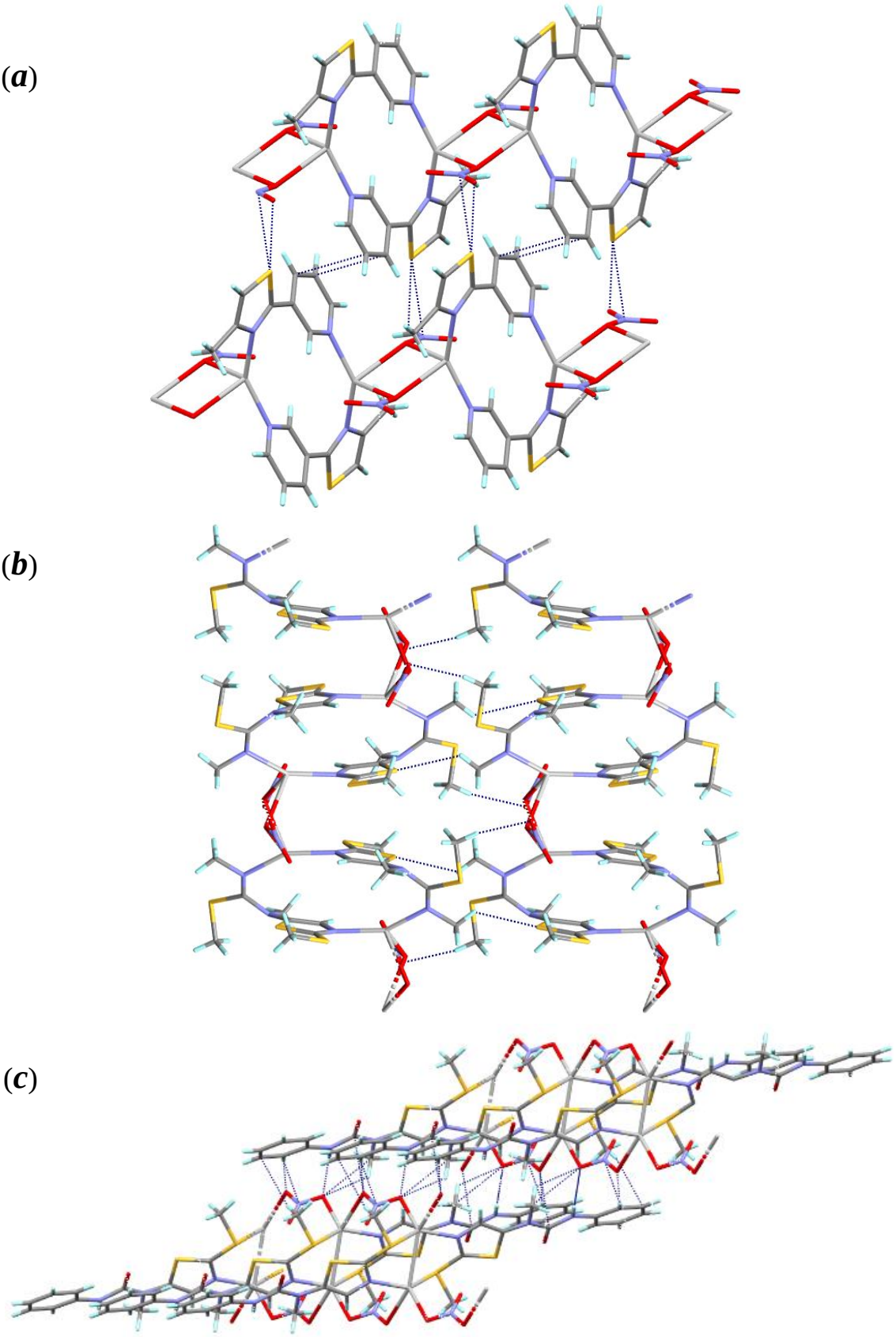

Figure S1. Contacts responsible for interconnection of 1D chains (blue dashed lines): CP **1** (***a***), CP **2** (***b***) and CP **3** (***c***).

X-ray powder diffraction data

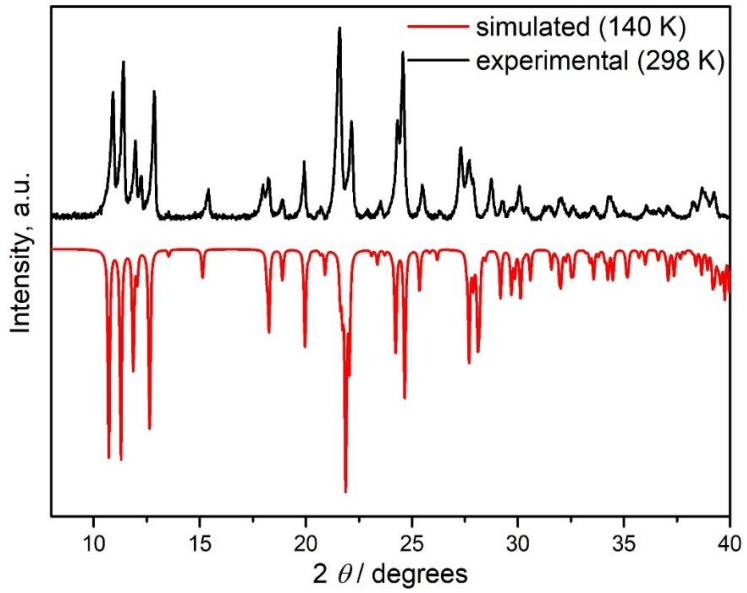

Figure S2. Experimental and simulated PXRD patterns of an as-synthesized sample **1**.

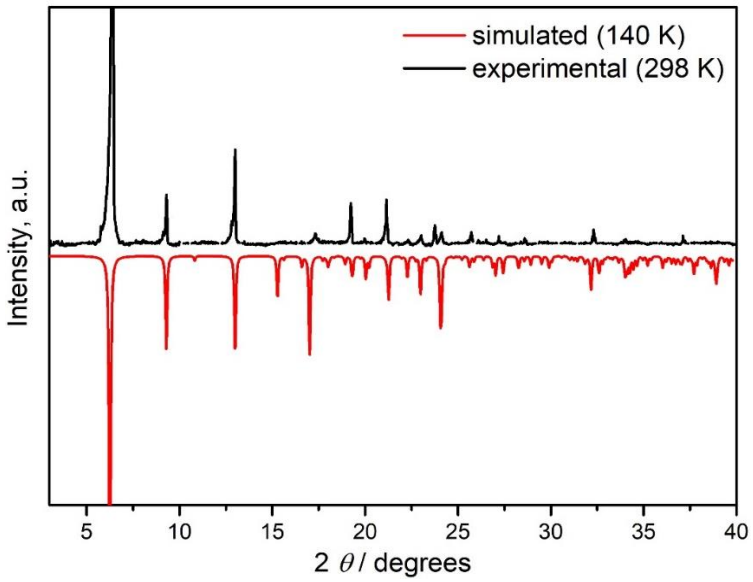

Figure S3. Experimental and simulated PXRD patterns of an as-synthesized sample **3**.

TG profiles

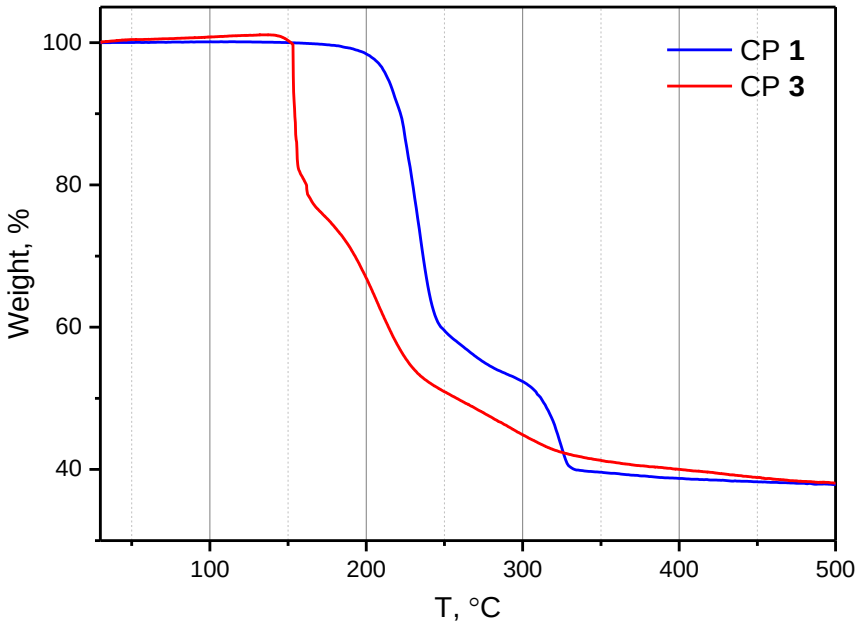

Figure S4. The TGA profiles for **1** and **3**.

IR spectra

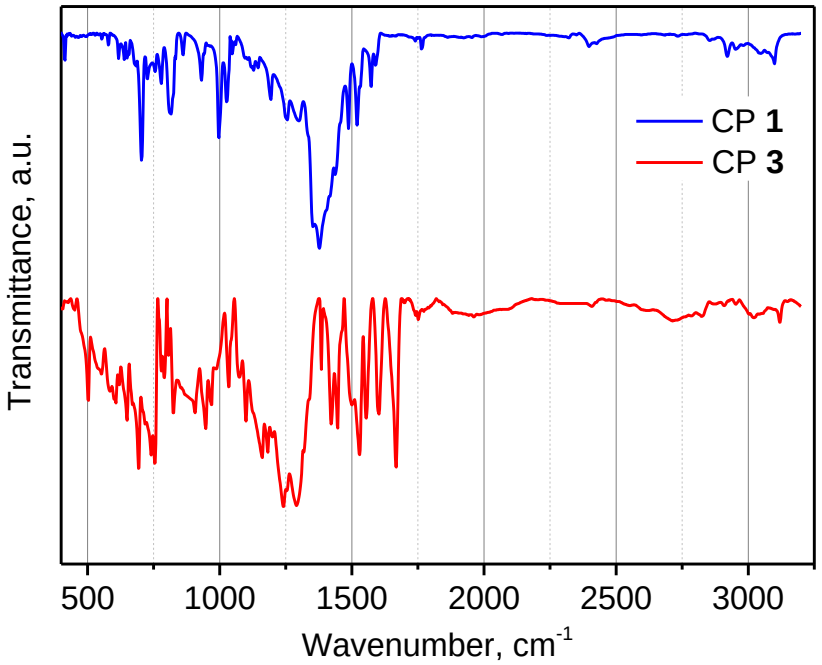

Figure S5. FT-IR spectra for CPs **1** and **3**.