Supplementary information

The Conformation Restriction of Non-planar Di-2-pyrimidyl Sulfide with Intramolecular N···C Interaction and Its Supramolecular Silver(I) Complexes

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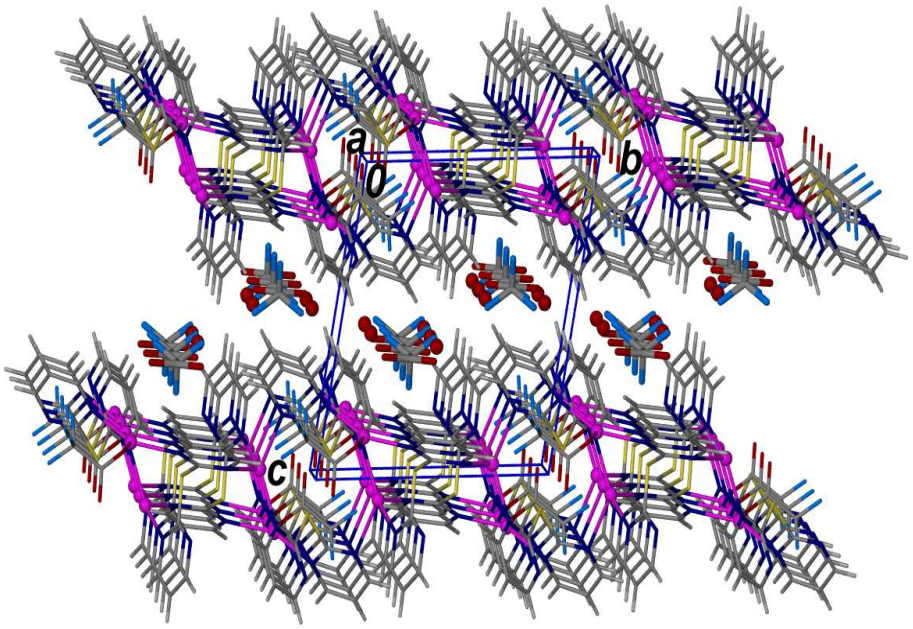


Figure S1 View down the *a* axis of the stacking structure of $\{[Ag_2(DprS)_2(CF_3CO_2)](CF_3CO_2)\cdot 2H_2O\}_\infty$ **(1)**. The purple balls represent Ag(I) ions, while the red balls indicate the lattice water molecules. The trifluoroacetate anions embedded among the interstices are shown as a thick-stick mode.

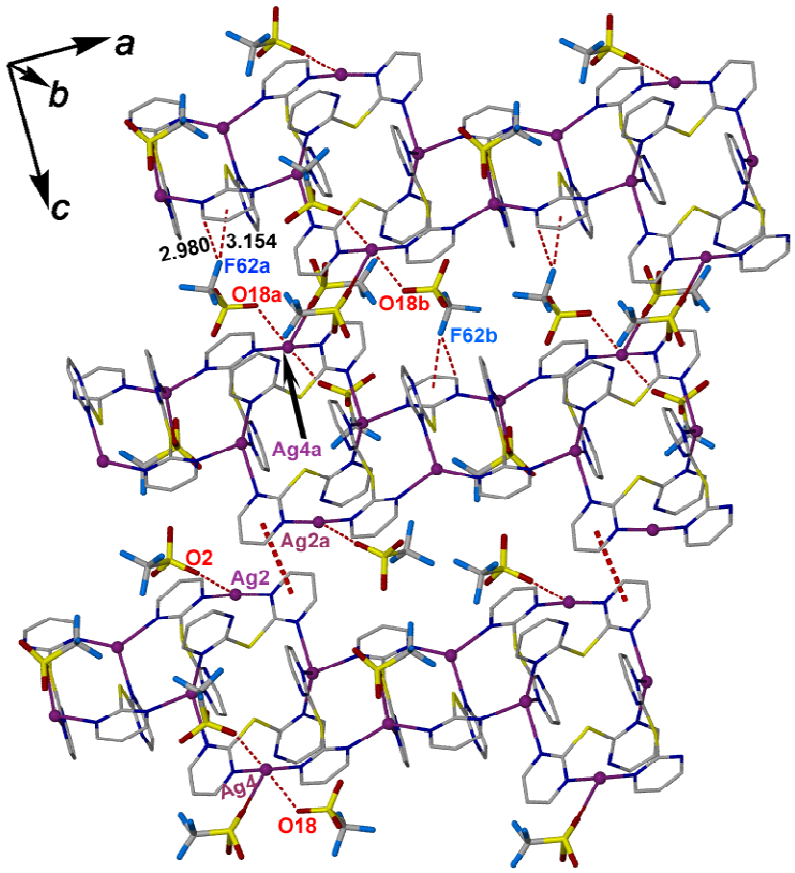


Figure S2 Interaction between adjacent tape-like structures in complex $\{[Ag_6(DprS)_6(CF_3SO_3)_5](CF_3SO_3)\cdot 3.5H_2O\}_\infty$ (**2**). Symmetry codes: a $-x$, $-y + 1$, $-z$; b $x - 1$, y, $z - 1$. All hydrogen atoms and the free triflate are omitted for clarity. Color code: gray C, dark blue N, red O, turquoise F, purple Ag.

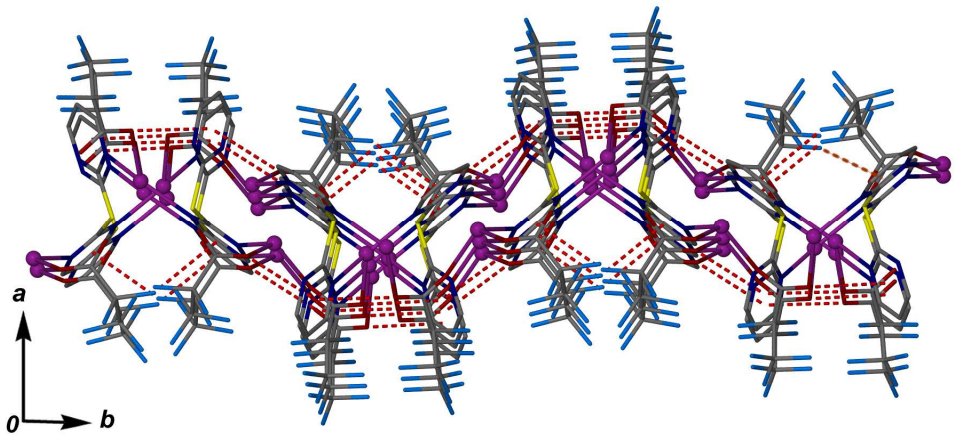
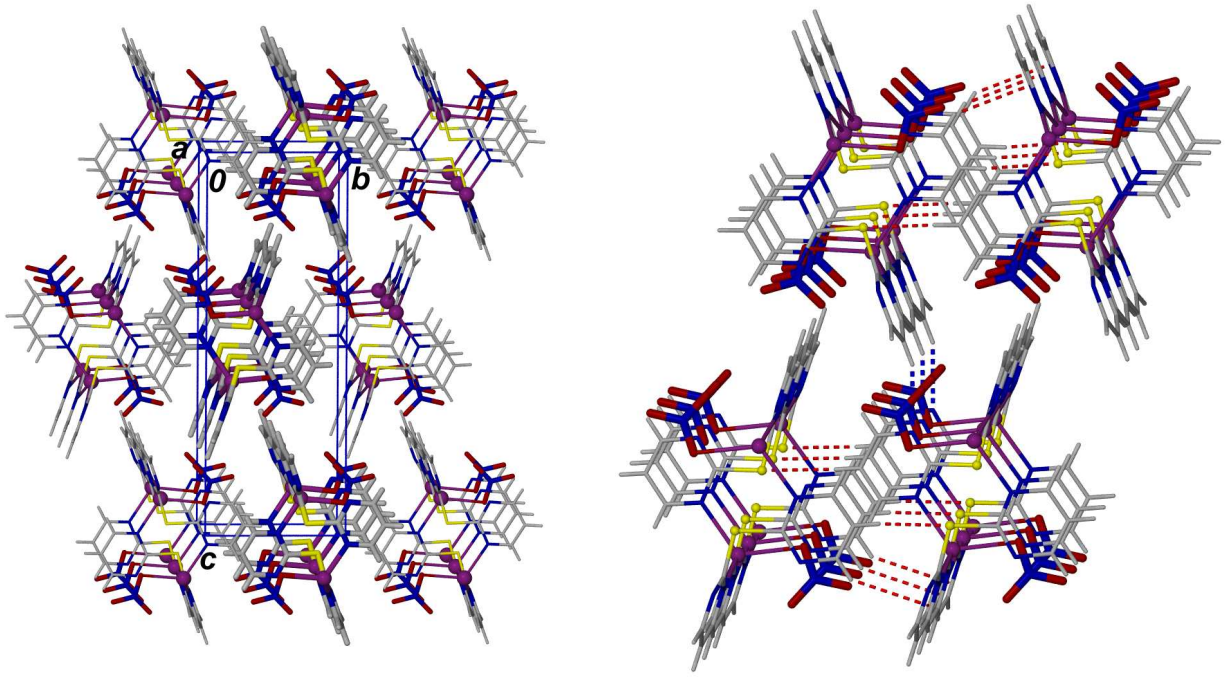


Figure S3 View down along the *c* axis of the pleated-sheet structure formed in *bc* plane of complex $\{[Ag_2(DprS)(C_2F_5CO_2)_2]_\infty$ (**3**). The red arrows indicate the goffering forces of anion-π interactions.



a b

Figure S4 Viewed down the *a* direction of the packing structure of $\{[Ag(DprS)NO_3]\}_\infty$ (**4**) (a) and the special show of the non-covalent interactions between the tape moieties (b), in which the red dashed lines indicate C–H···π, C–H···N and C–H···S interactions, while the C–H···O(NO_3^-) are not shown for clarity. C–H···O(NO_3^-) interactions: C8a–H···O1 D···A 3.330(2) Å, <DHA 136.9°; C8a–H···O3 D···A 3.442(2) Å, <DHA 171.7°; C3b–H···O2 D···A 3.281(1) Å, <DHA 154.7°; C1c–H···O1 D···A 3.250(2) Å, <DHA 143.7°. Symmetry codes: a *x*, *y* – 1, *z*; b –*x* + 1/2, –*y*, *z* – 1/2; c –*x* + 3/2, –*y*, *z* – 1/2. Color code: Purple Ag, Yellow S, Blue N, Gray C and H, Red O.

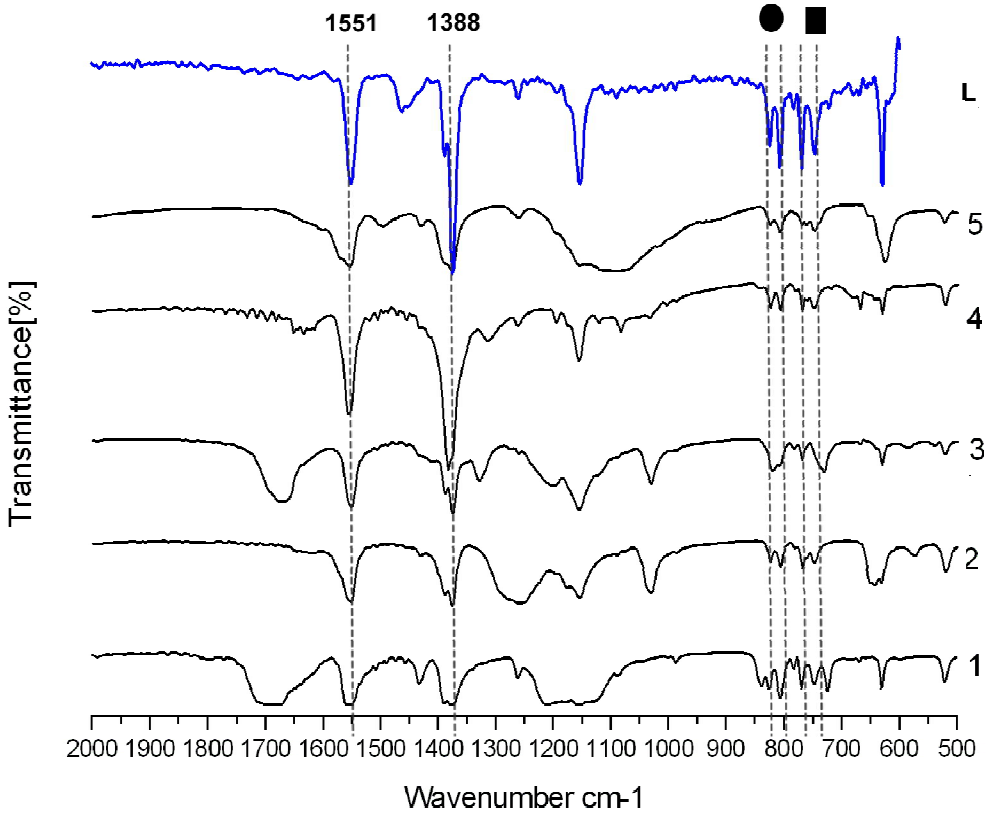


Figure S5 FTIR spectra of DprS and complexes **1-5**. ● and ■ denote double bands around 806~824 cm^{-1} and 748~770 cm^{-1}, respectively.

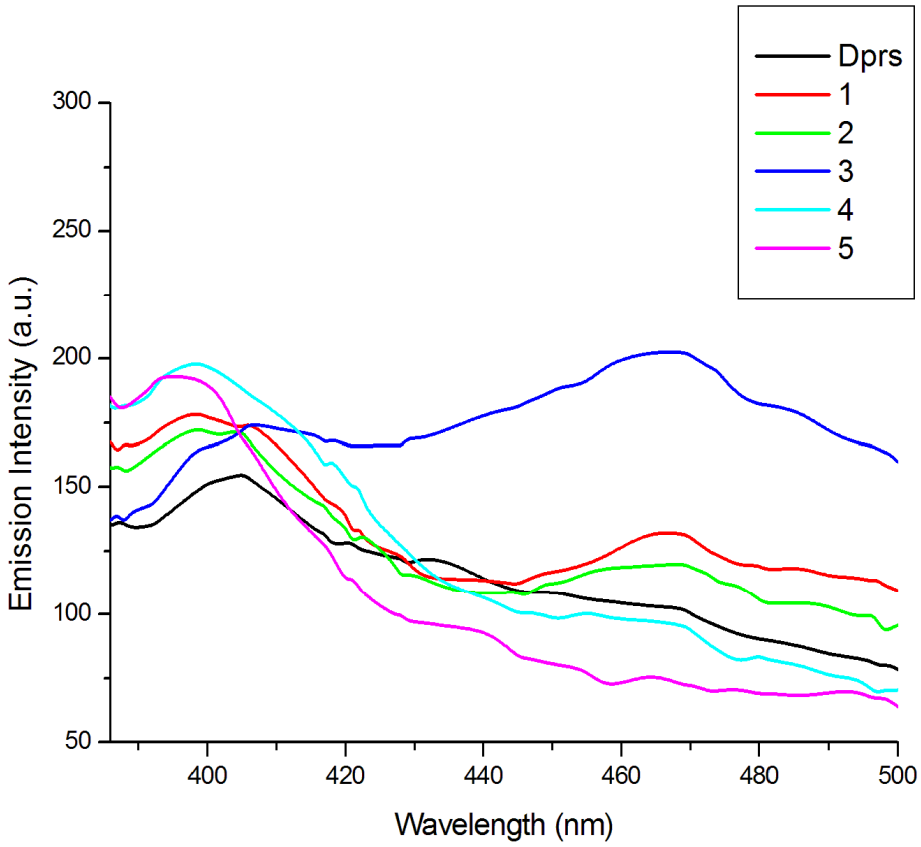


Figure S6 Photoluminescent emissions of complexes **1-5** and DprS upon excitation at 341 nm.

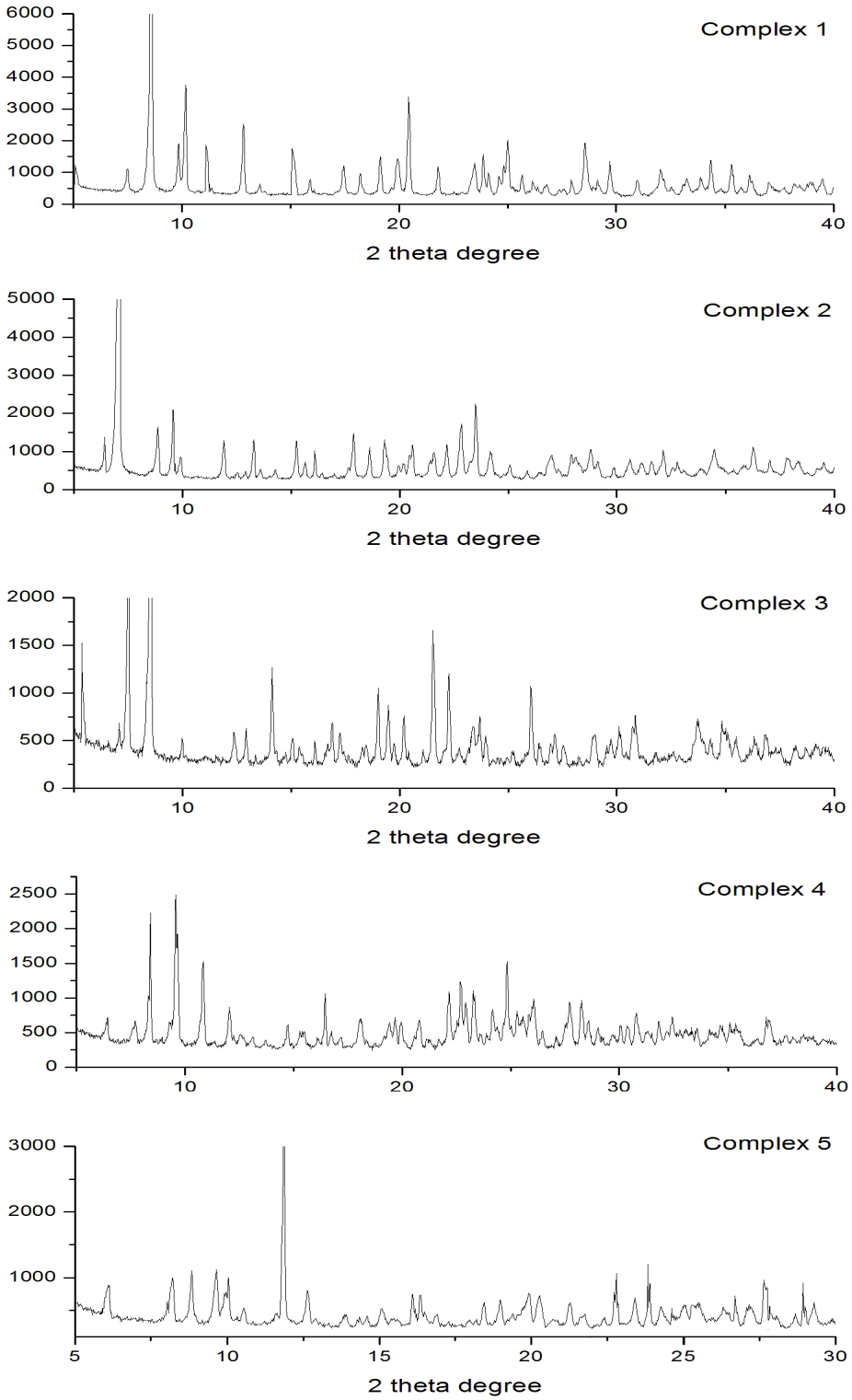


Figure S7 Powder X-ray diffraction patterns of **1-5**. Powder patterns were recorded on a Bruker D8 Advance Powder X-ray diffractometer (Cu Kα, λ = 1.5418 Å) operating

at 40 KV and 40 mA, with a graphite reflected beam monochromator and variable divergence slits.