

Electronic Supplementary Material for CrystEngComm
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Electronic Supplementary Information for MS:

Mercury(II) coordination polymers with pyrazine derivatives

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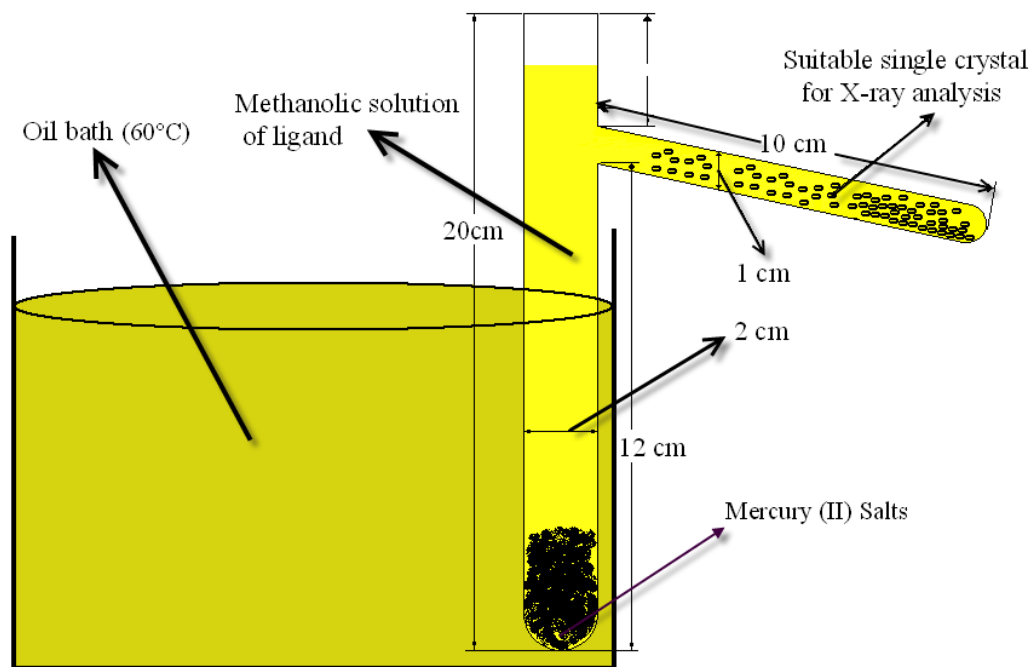


Fig. S1. Depiction of the branched tube for syntheses and isolation of single crystals of compounds **1-8**.

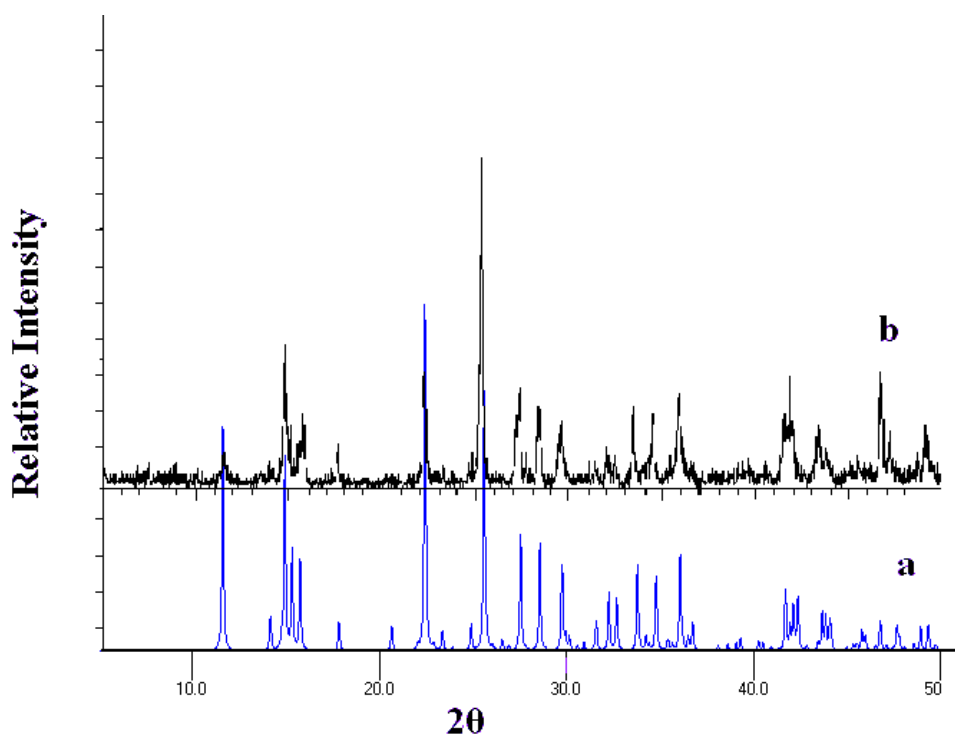


Fig. S2. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}_2(\mu\text{-pyr})(\mu\text{-I})_2\text{I}_2]_n$ (**2**) at 100 K, **b)** The XRD pattern of $[\text{Hg}_2(\mu\text{-pyr})(\mu\text{-I})_2\text{I}_2]_n$ (**2**) at room temperature (both based on Cu K_α radiation).

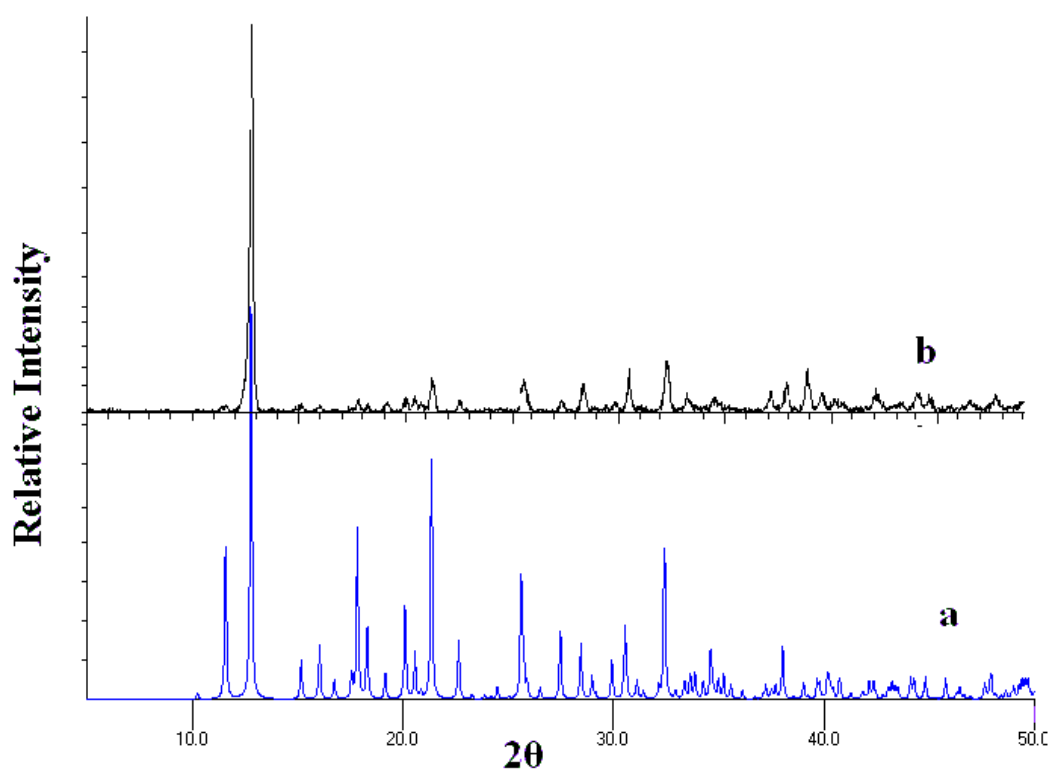


Fig. S3. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}(\mu\text{-pyr})(\mu\text{-SCN})_2]_n$ (**3**) at 100 K, **b)** The XRD pattern of $[\text{Hg}(\mu\text{-pyr})(\mu\text{-SCN})_2]_n$ (**3**) at room temperature (both based on Cu K_α radiation).

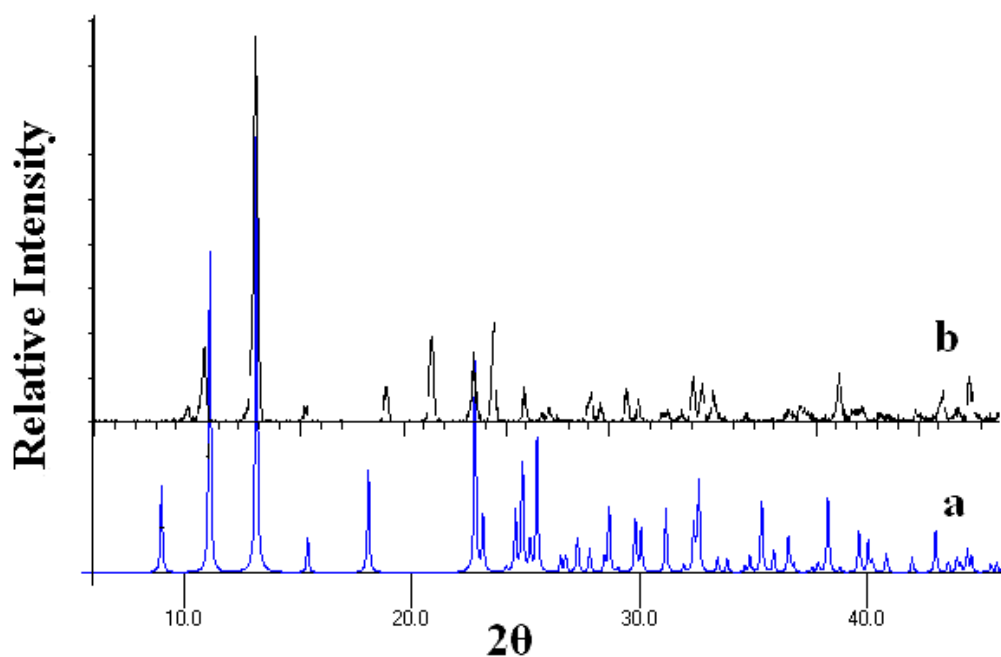


Fig. S4. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-Cl})_4]_n$ (**4**) at 100 K, **b)** The XRD pattern of $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-Cl})_4]_n$ (**4**) at room temperature (both based on $\text{Cu K}\alpha$ radiation).

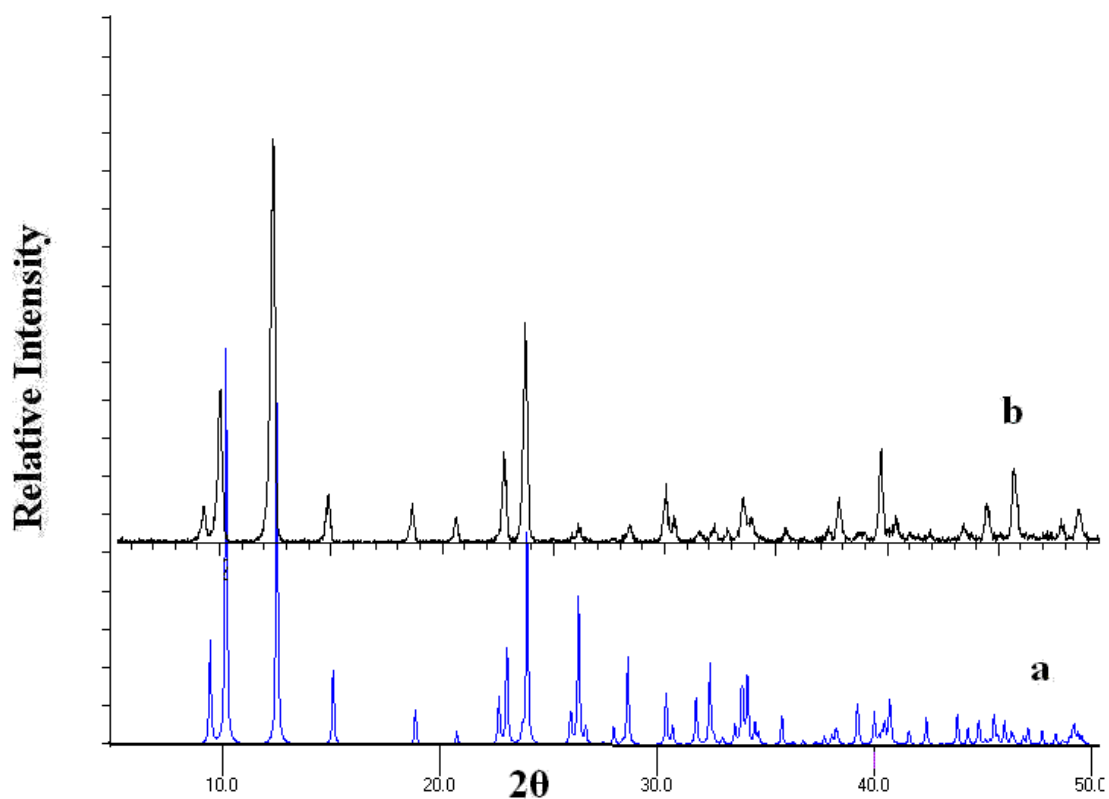


Fig. S5. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-Br})_4]_n$ (**5**) at 100 K, **b)** The XRD pattern of $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-Br})_4]_n$ (**5**) at room temperature (both based on Cu K_α radiation).

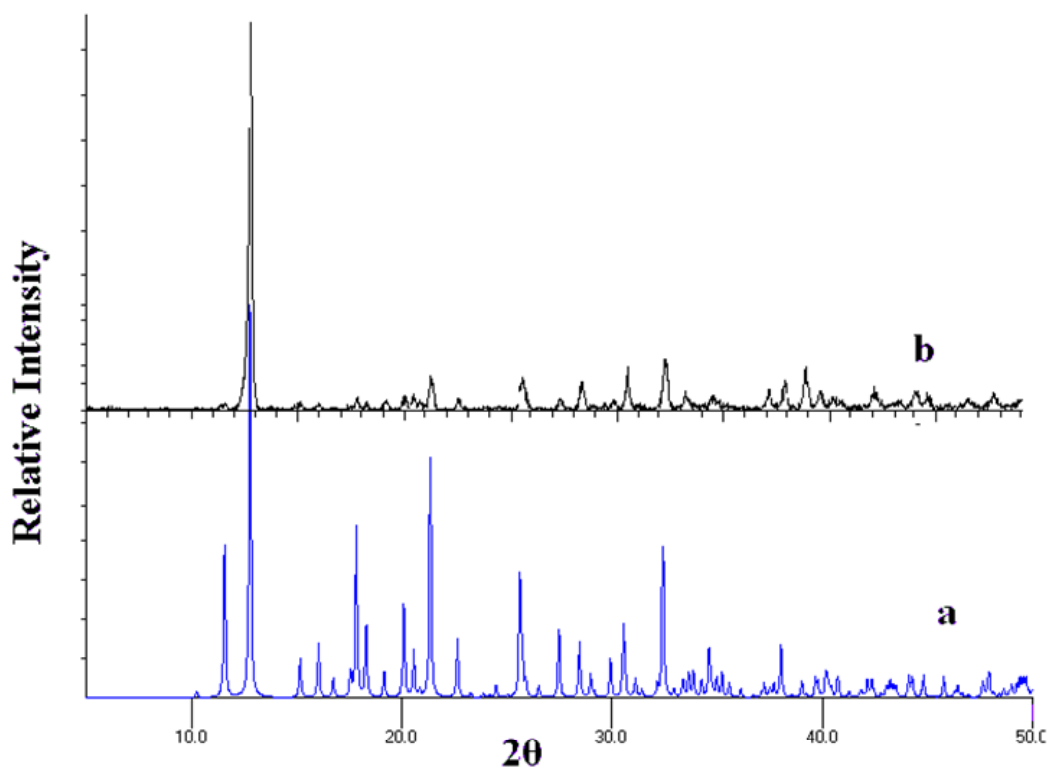


Fig. S6. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-SCN})_2(\text{SCN})_2]_n$ (**6**) at 100K, **b)** The XRD pattern of $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-SCN})_2(\text{SCN})_2]_n$ (**6**) at room temperature (both based on Cu K_α radiation).

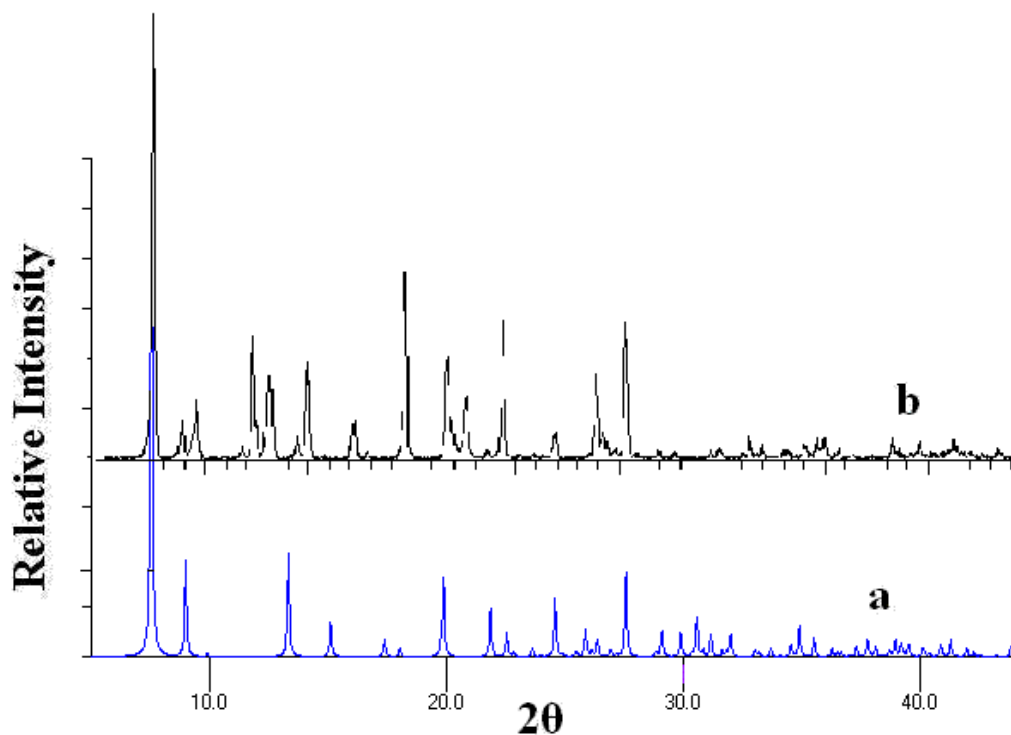


Fig. S7. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}(2,6\text{-dmpyr})(\mu\text{-Br})_2]_n$ (**7**) at 100 K, **b)** The XRD pattern of $[\text{Hg}(2,6\text{-dmpyr})(\mu\text{-Br})_2]_n$ (**7**) at room temperature (both based on $\text{Cu K}\alpha$ radiation).

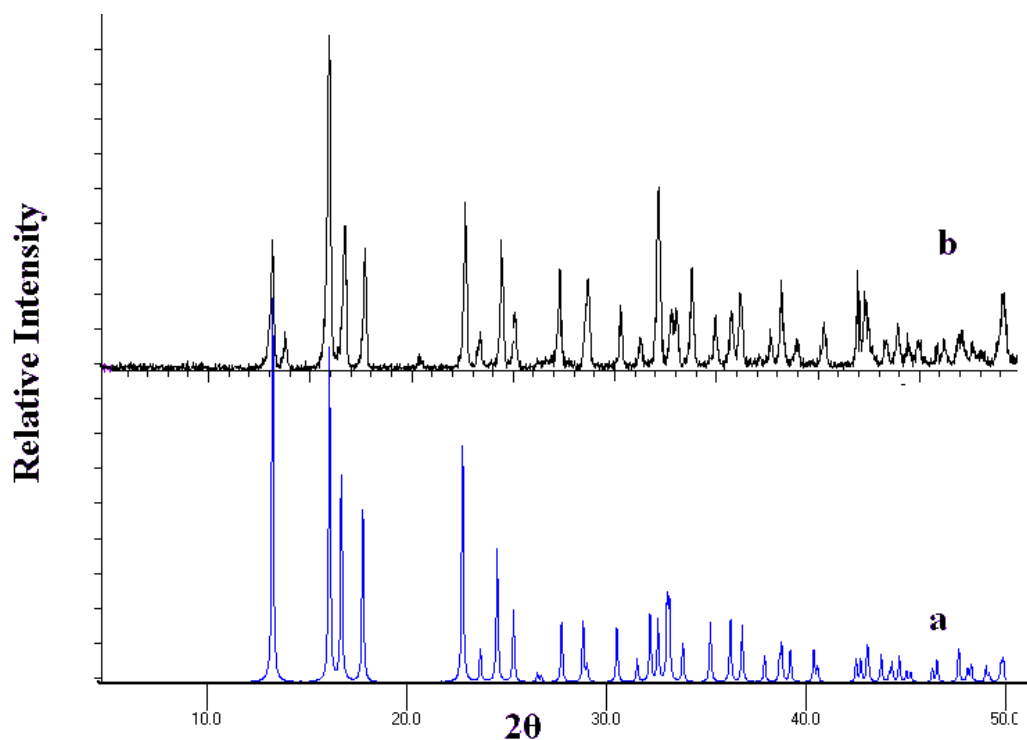


Fig. S8. **a)** The simulated XRD pattern from single crystal X-ray data of the compound $[\text{Hg}(\mu\text{-2,6-dmpyr})(\mu\text{-SCN})_2]_n$ (**8**) at 100 K, **b)** The XRD pattern of $[\text{Hg}(\mu\text{-2,6-dmpyr})(\mu\text{-SCN})_2]_n$ (**8**) at room temperature (both based on Cu K_α radiation).

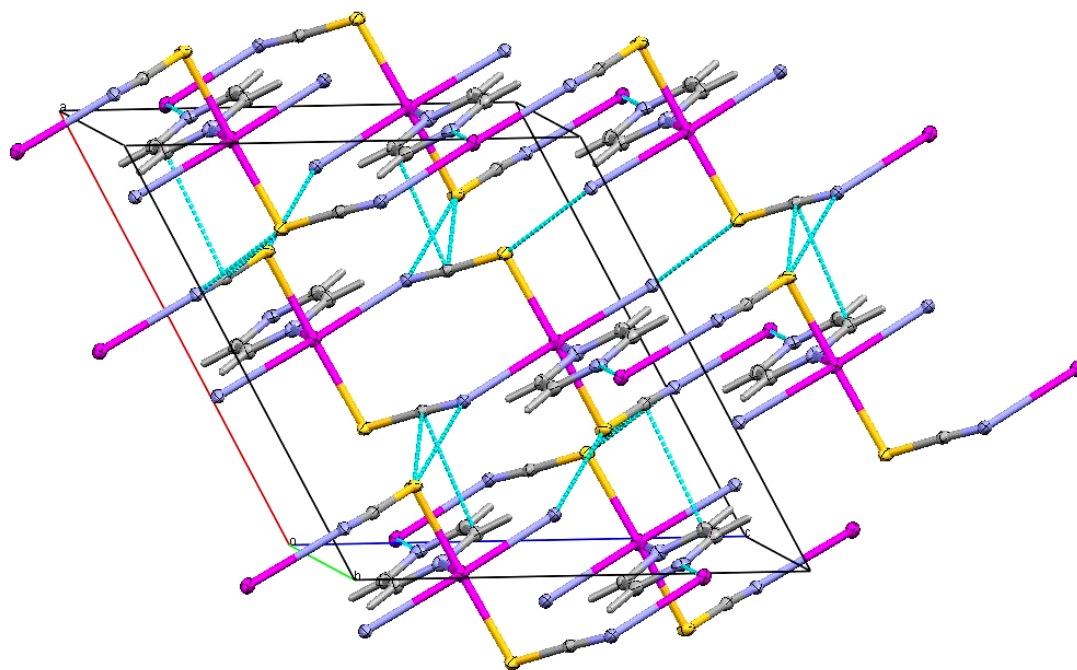


Fig. S9. Thermal ellipsoid plot of $[\text{Hg}(\mu\text{-pyr})(\mu\text{-SCN})_2]_n$ (**3**) showing the S...C and S...N interactions.

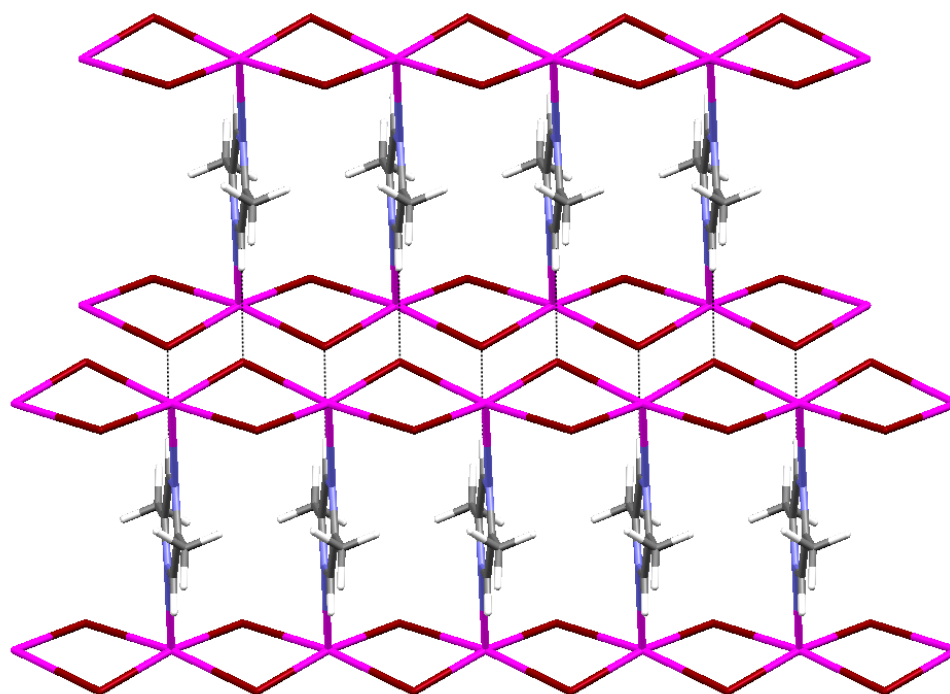


Fig. S10. Thermal ellipsoid plot of $[\text{Hg}_2(\mu\text{-2,5-dmpyr})(\mu\text{-Br})_4]_n$ (**5**) showing the two-dimensional network generated via $\text{Br}\cdots\text{HC}$ hydrogen bonds.

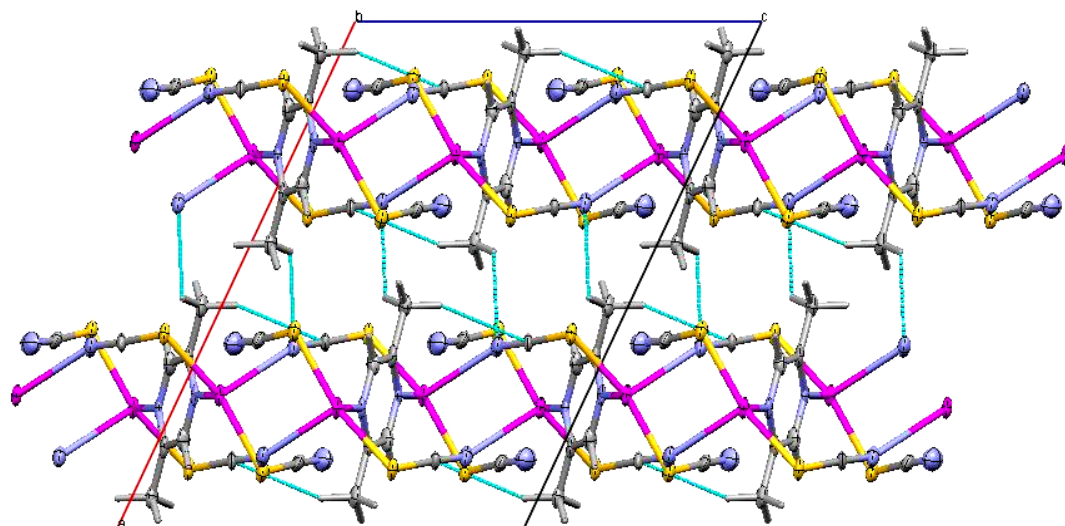


Fig. S11. Thermal ellipsoid plot of $[\text{Hg}_2(\mu\text{-2,5-dmpyr})(\mu\text{-SCN})_2(\text{SCN})_2]_n$ (**6**) showing the S...HC interactions.

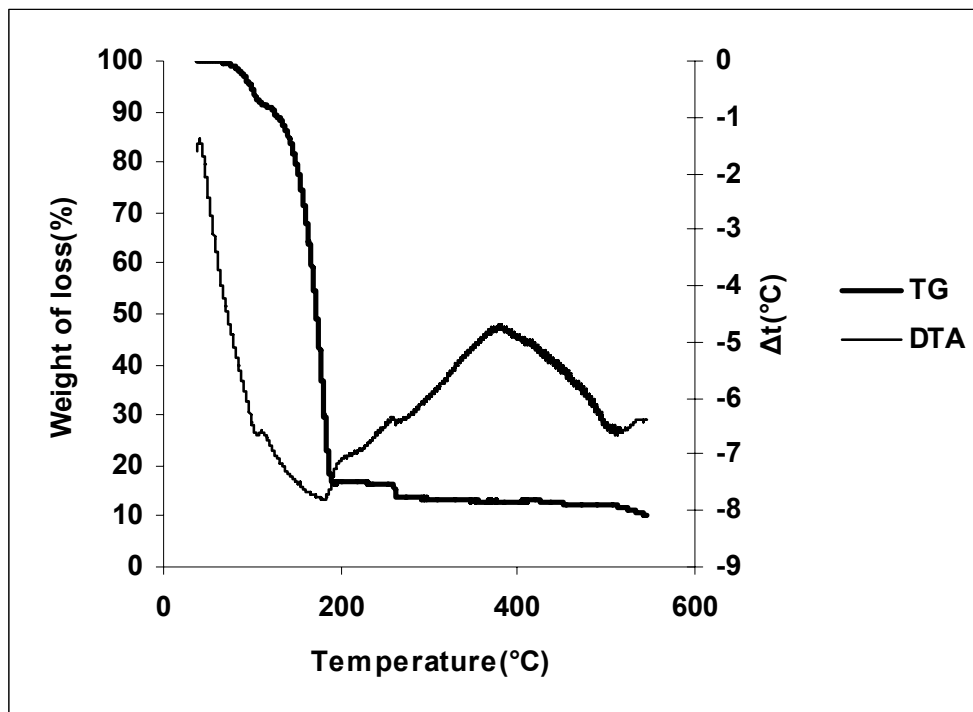


Fig. S12. Thermal behavior of $[\text{Hg}_2(\mu\text{-pyr})(\mu\text{-I})_2\text{I}_2]_n$ (2).

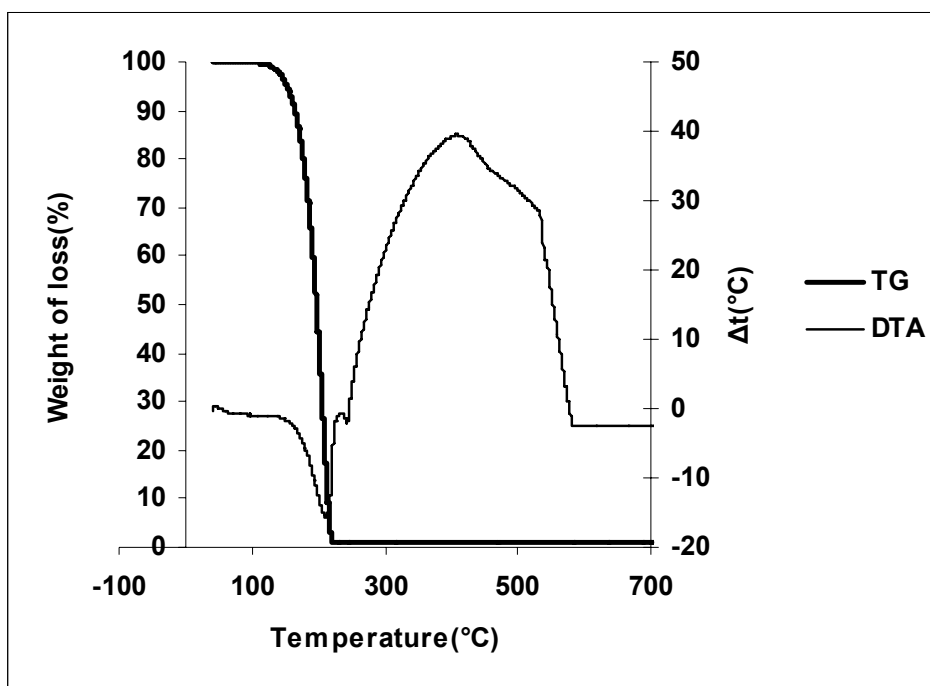


Fig. S13. Thermal behavior of $[\text{Hg}_2(\mu\text{-2,5-dmpyr})(\mu\text{-Cl})_4]_n$ (4).

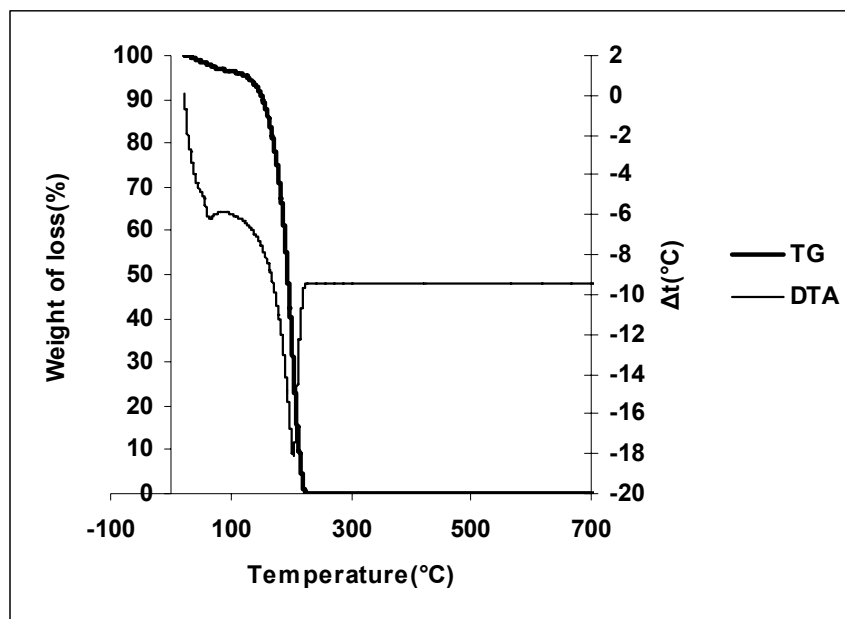


Fig. S14. Thermal behavior of $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-Br})_4]_n$ (**5**).

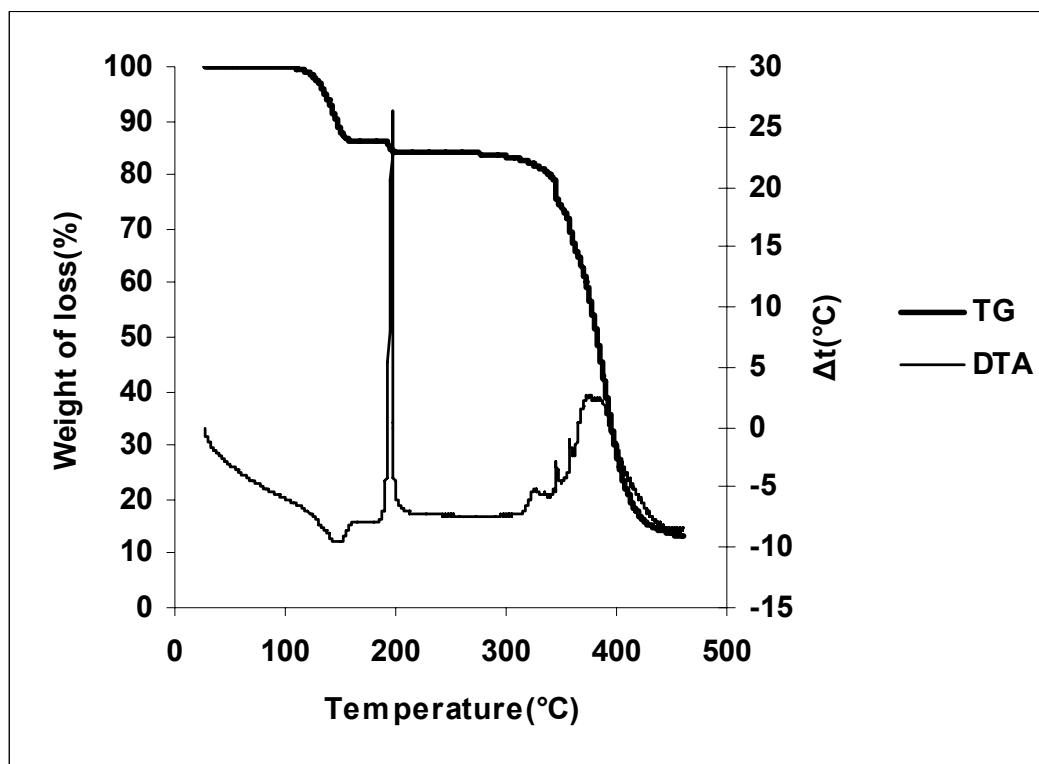


Fig. S15. Thermal behavior of $[\text{Hg}_2(\mu\text{-}2,5\text{-dmpyr})(\mu\text{-SCN})_2(\text{SCN})_2]_n$ (6).

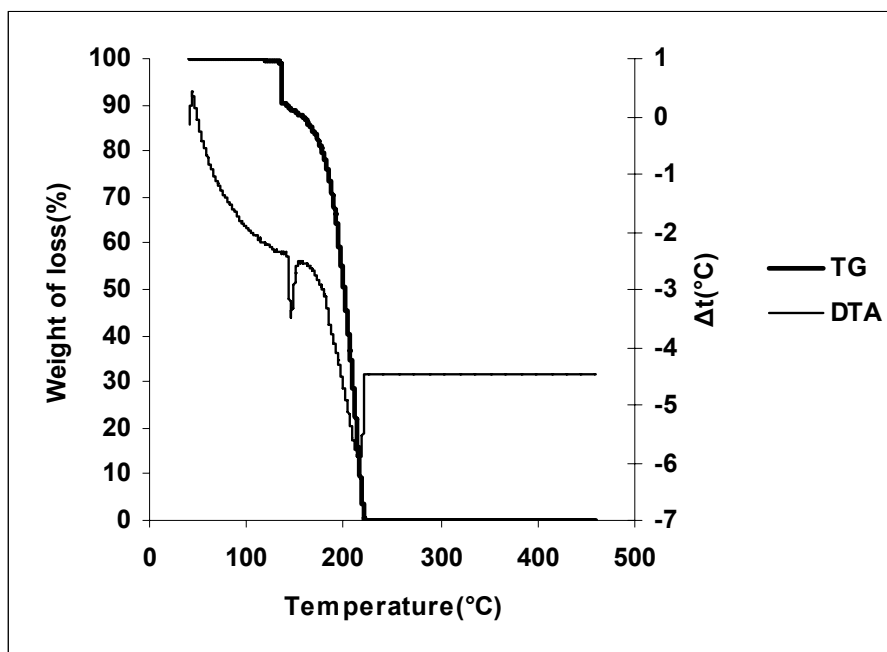


Fig. S16. Thermal behavior of $[\text{Hg}(2,6\text{-dmpyr})(\mu\text{-Br})_2]_n$ (7).

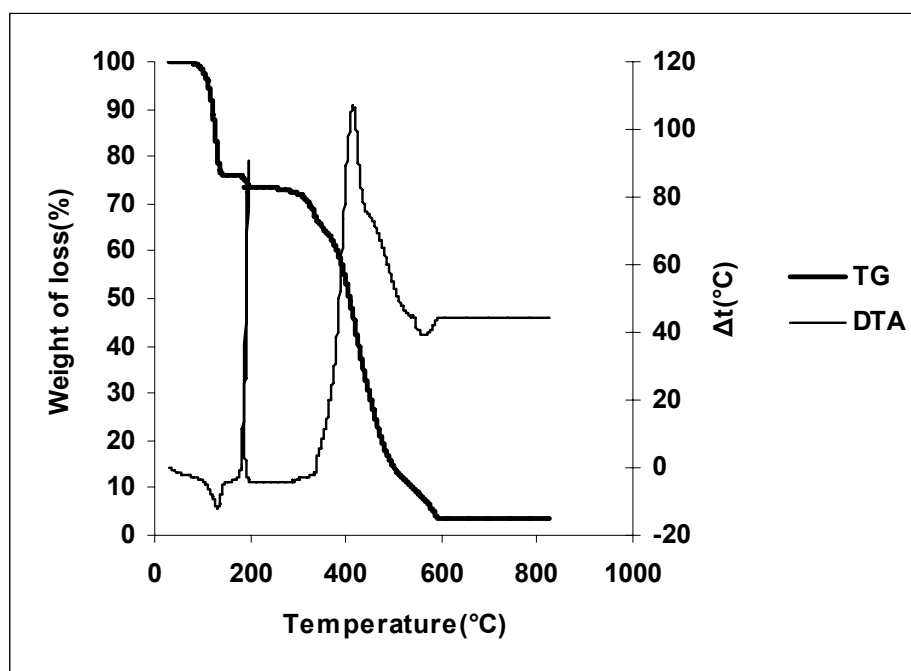


Fig. S17. Thermal behavior of $[\text{Hg}(\mu\text{-}2,6\text{-dmpyr})(\mu\text{-SCN})_2]_n$ (**8**).