Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

Thermal and Pressure – Induced Spin Crossover in a Novel Three-Dimensional Hoffman-like Chathrate Complex

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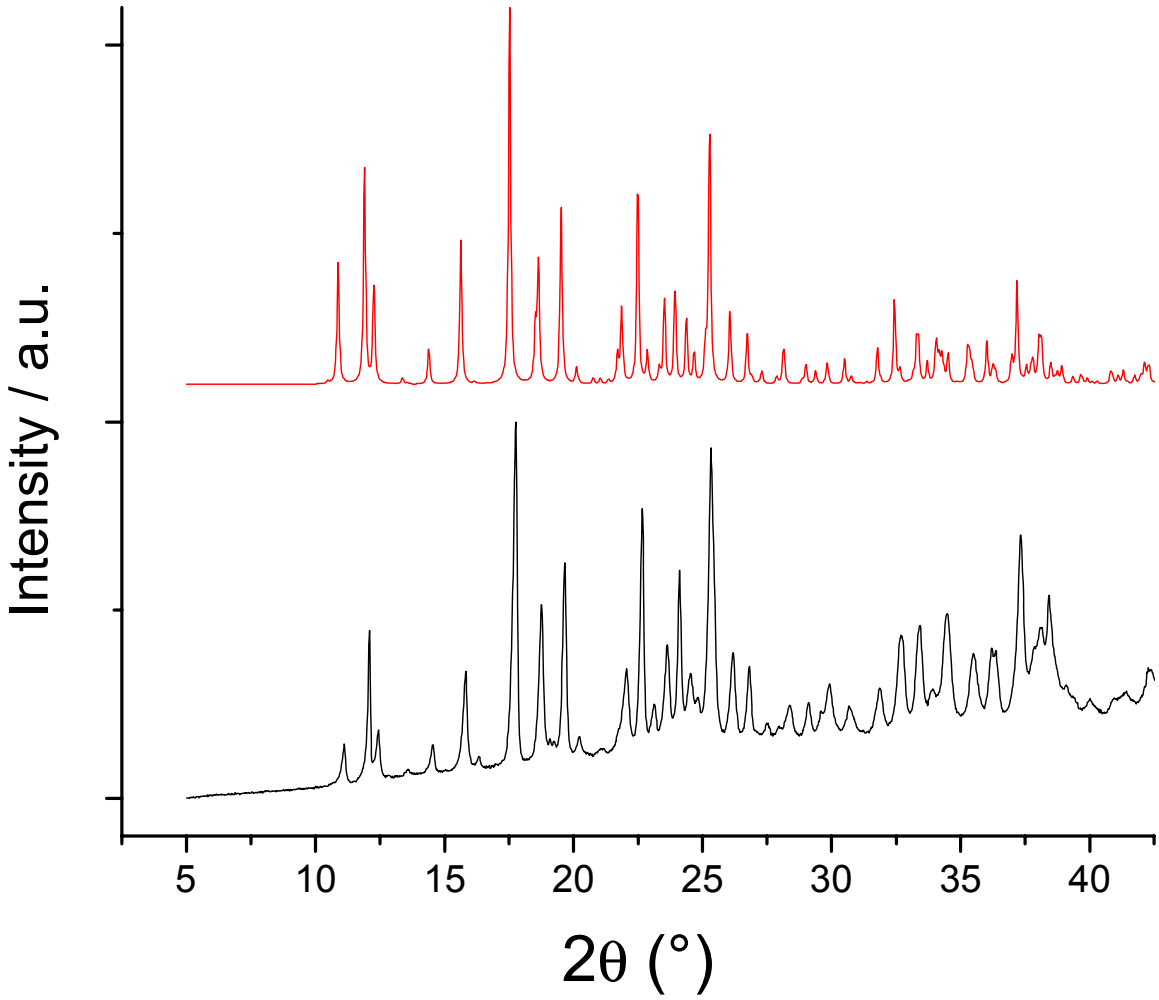
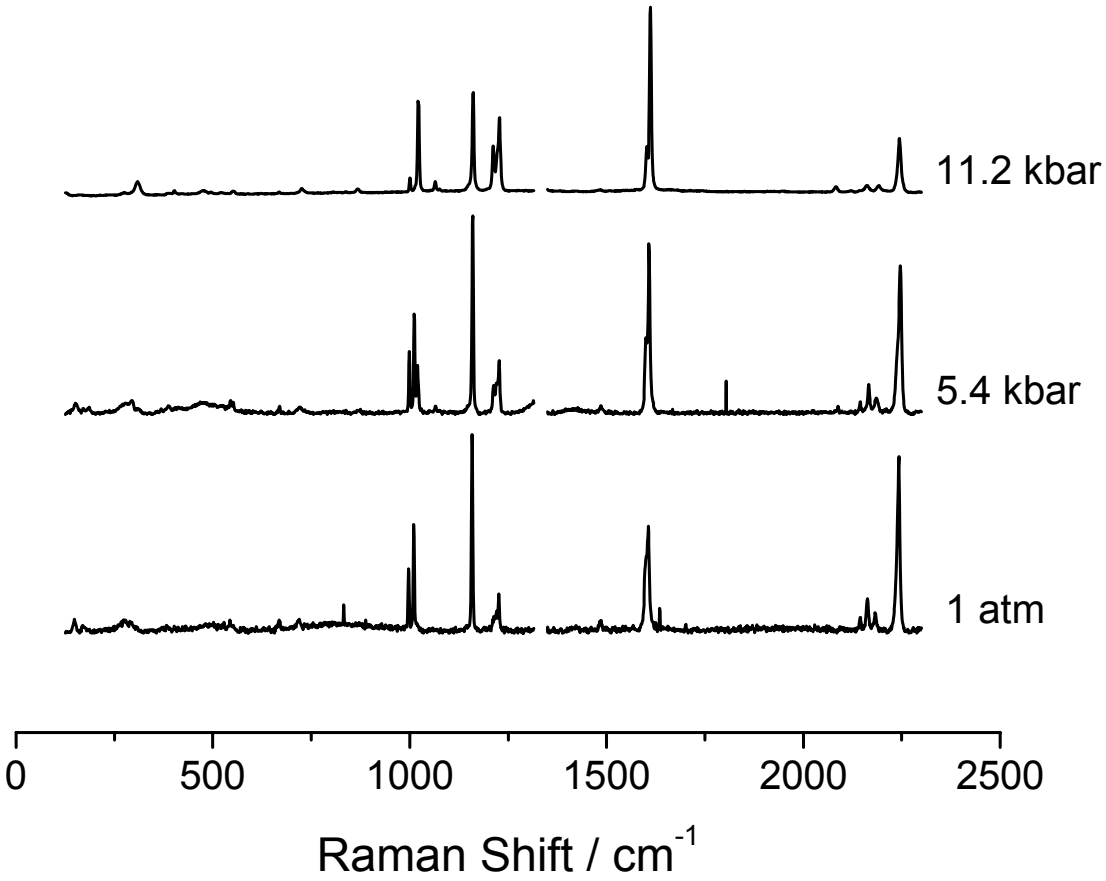
The X-ray diffraction pattern of the powder sample is shown in (ESI Figure 1), along with that calculated from the single crystal pattern. One can conclude that the crystal structure obtained from single crystal methods is representative of the powder sample that was used for all other characterisation techniques.

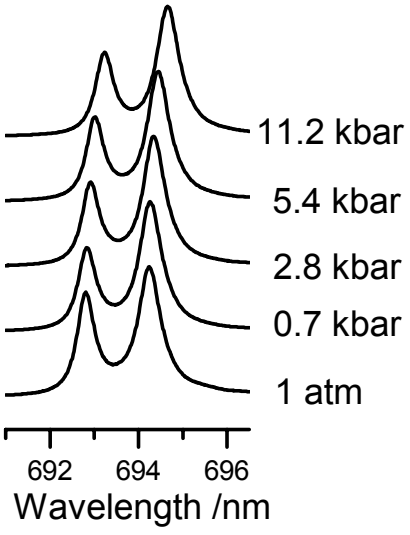


ESI Figure 1. Powder diffraction patterns of $Fe(bpac)_2[Ag(CN)_2]_2$. red - calculated from single crystal data, and black - obtained from the bulk sample

Room temperature Raman spectra as a function of pressure are shown in ESI Figure 2. The luminescence spectra of ruby used for pressure determination are given in ESI Figure 3.



ESI Figure 2. Room temperature Raman spectra of $Fe(bpac)_2[Ag(CN)_2]_2$ as a function of pressure



ESI Figure 3. Ruby fluorescence on increasing pressure.

The thermogravimetric analysis is shown in ESI Figure 4.

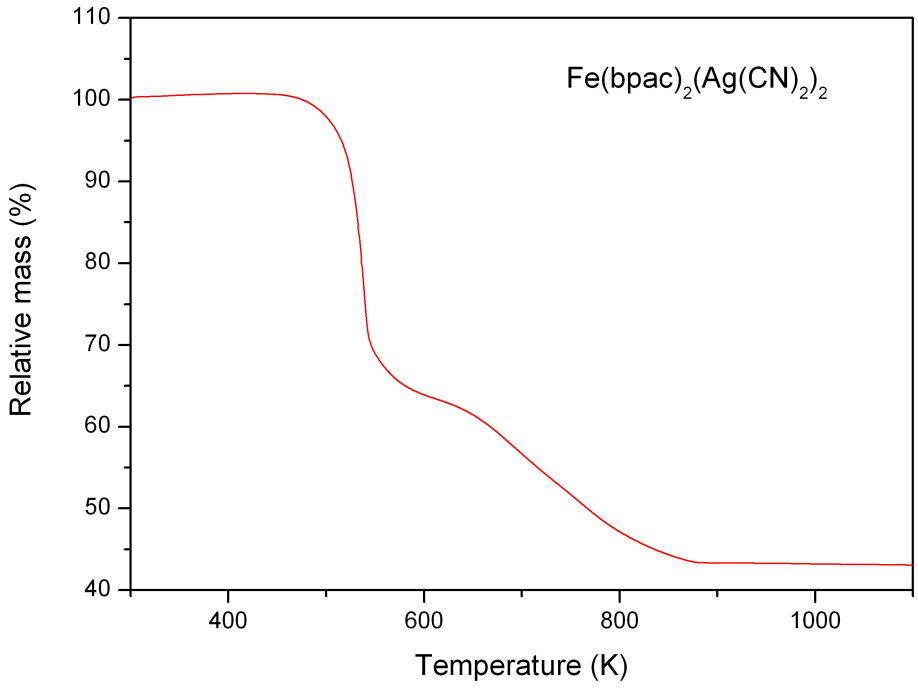


Figure 4. Thermogravimetric analysis of $Fe(bpac)_2[Ag(CN)_2]_2$

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