Single-crystal to single-crystal thermal spin-crossover with a large hysteresis spanning room temperature†

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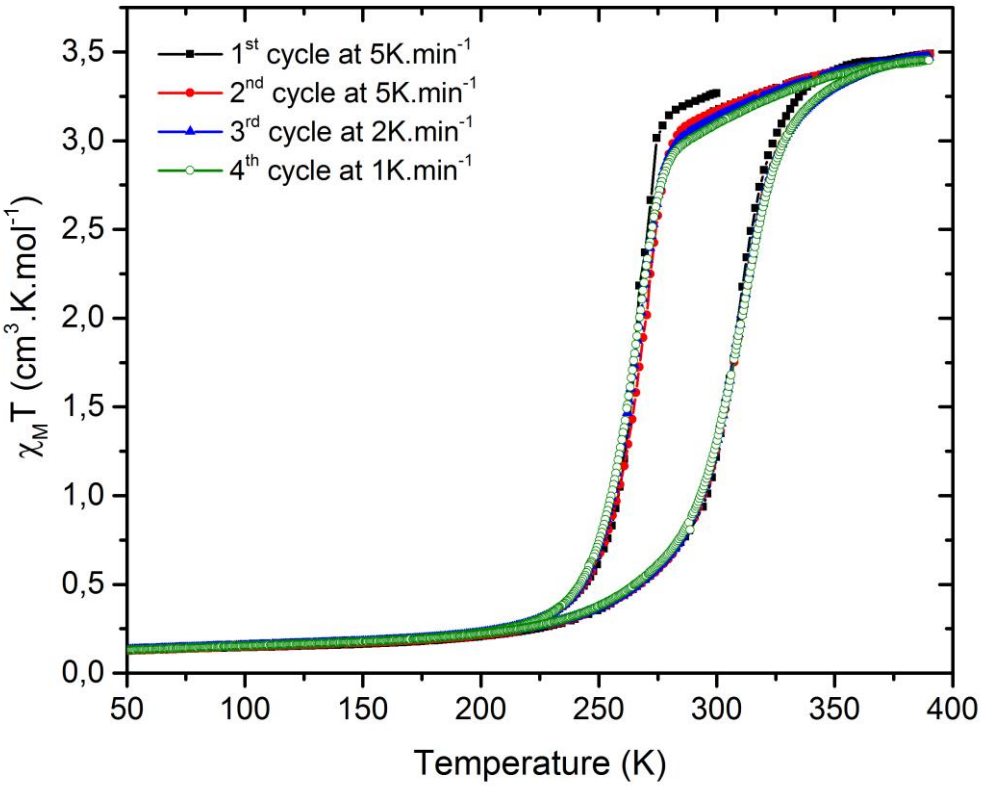
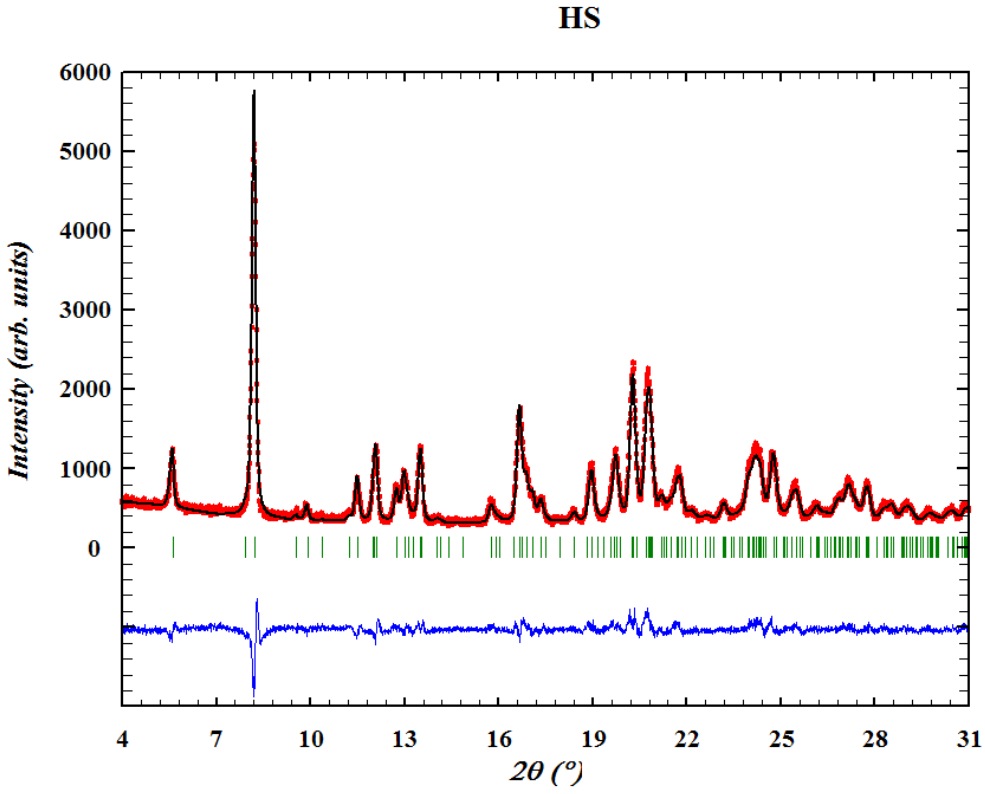
ESI

ESI-1. Squid measurements for a polycrystalline assembly of [Fe(PM-PEA)$_2$(NCSe)$_2$] at various speed and for subsequent thermal cycles. No significant effects is noted.



ESI-2. Figure showing the powder X-Ray diffraction experimental pattern (black) and the simulated diffraction pattern from single-crystal XRD data (red) as well as their difference (blue). Allowed Bragg peaks positions from the single-crystal unit-cell and symmetry (green). This superposition demonstrates that powder and single-crystal are isostructural.



ESI-3. Squid measurements on one single-crystal for $[Fe(PM\text{-}PEA)_2(NCSe)_2]$.