

Supplementary Information

Room-temperature barocaloric effect in [Fe(pap-5NO₂)₂] spin-crossover material

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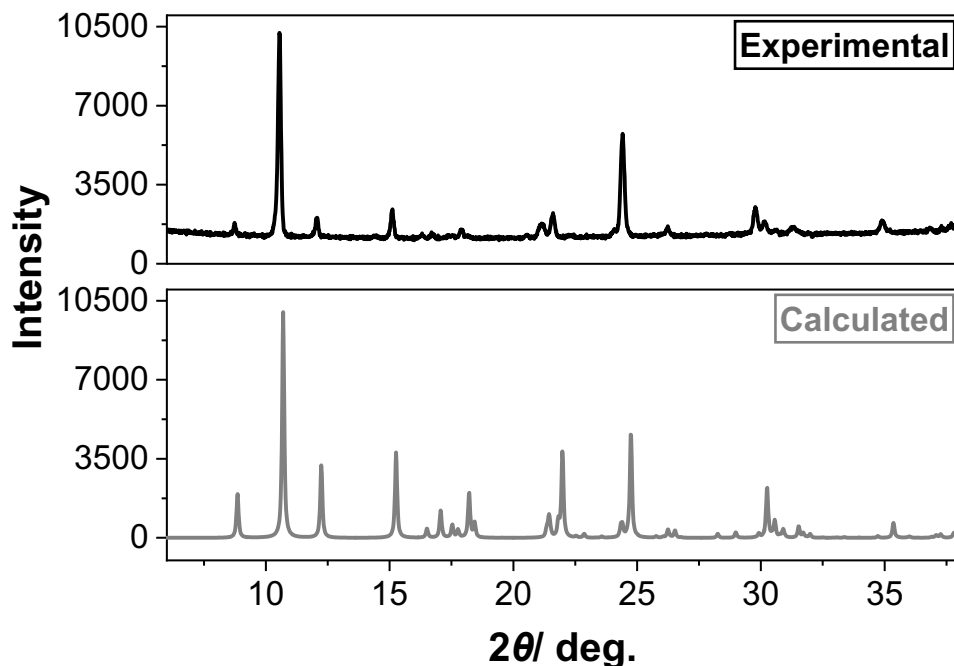


FIG. S1. Experimental (top-black line) and calculated (bottom-grey line) X-ray powder diffraction patterns for $[\text{Fe}(\text{pap-5NO}_2)_2]$. The calculated diffractogram was obtained from single-crystal X-ray diffraction data collected at 100 K.

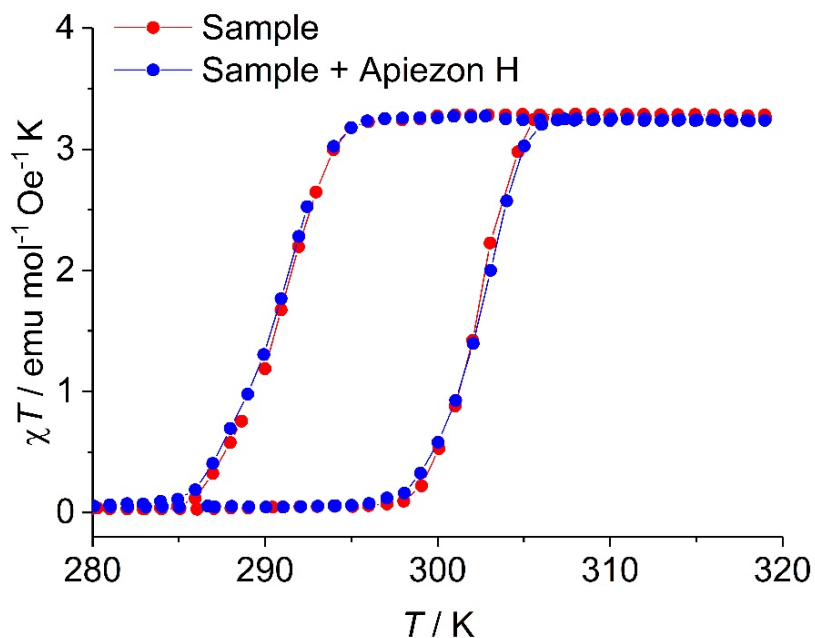


FIG. S2. Magnetic susceptibility-temperature product, χT , for $[\text{Fe}(\text{pap-5NO}_2)_2]$, collected for $B = 1$ T. The sample was prepared in two forms: as bare crystallites and embedded in Apiezon H, i.e., replicating the experimental conditions of the high-pressure calorimetry measurements. The reproducibility indicates that the presence of the thermal grease does not affect the properties of $[\text{Fe}(\text{pap-5NO}_2)_2]$.

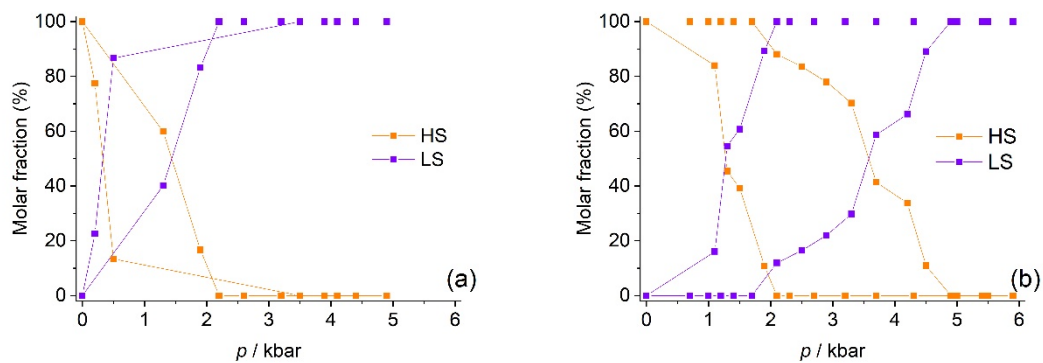


FIG. S3. Pressure dependence of each molar fraction in $[\text{Fe}(\text{pap-5NO}_2)_2]$, collected at 310 K (a) and 330 K (b).

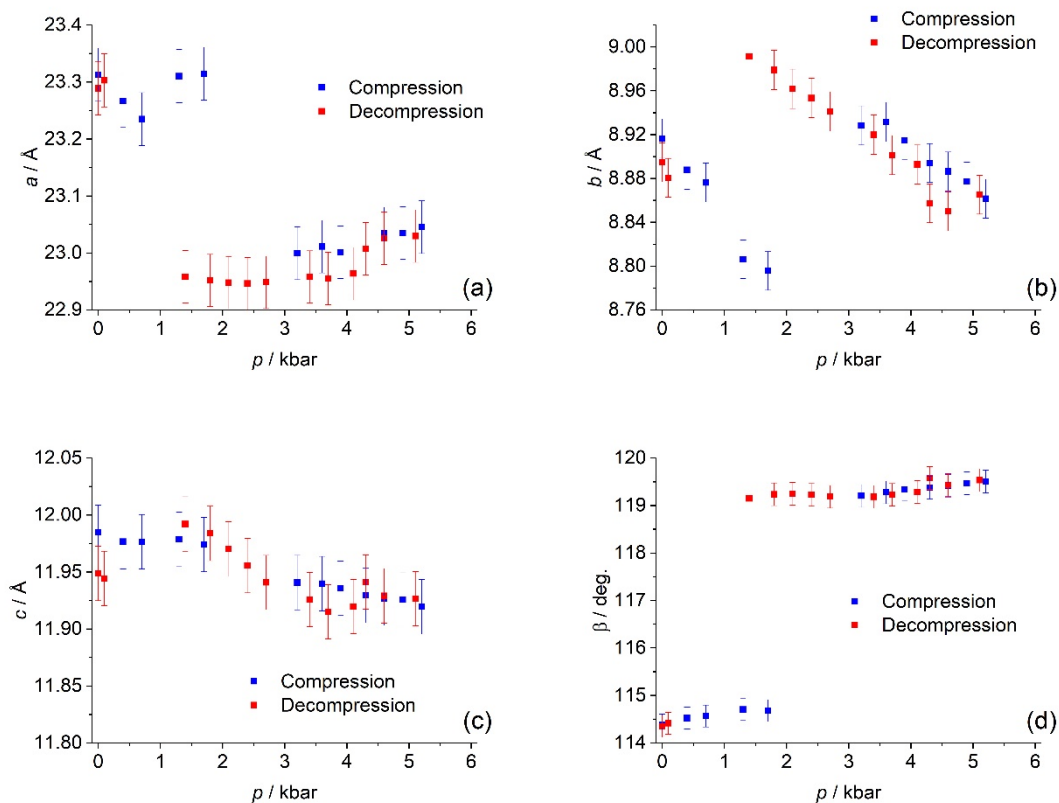


FIG. S4. Monoclinic unit-cell parameters a (a), b (b), c (c), and β (d) of $[\text{Fe}(\text{pap-5NO}_2)_2]$, as a function of pressure, for 320 K.

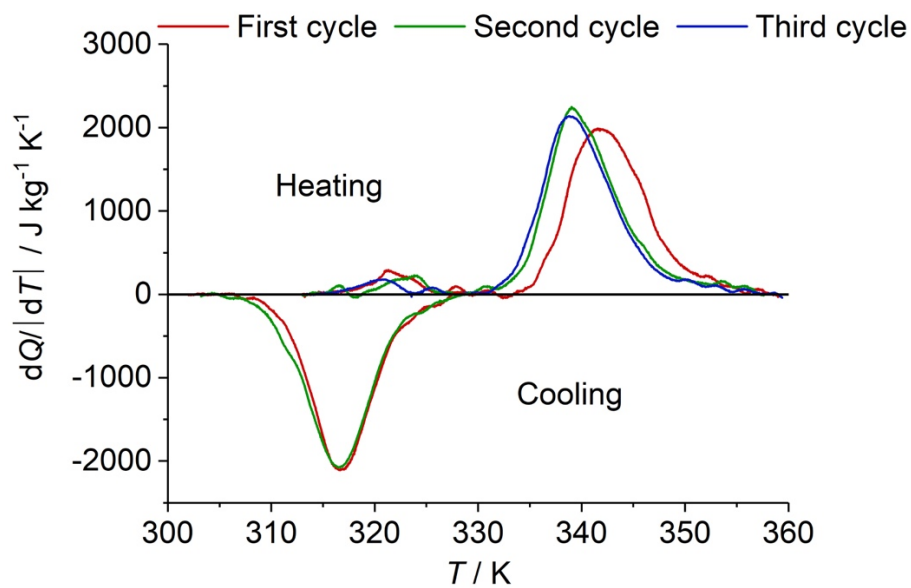


FIG. S5. Representative isobaric thermograms at a pressure of $p = 1.4$ kbar, upon baseline subtraction, for $[\text{Fe}(\text{pap-5NO}_2)_2]$, for the first, second and third thermal cycles.