

SUPPLEMENTARY INFORMATION

Thermal expansion and rattling behavior of Gd-filled Co₄Sb₁₂ skutterudite determined by high-resolution synchrotron X-ray diffraction

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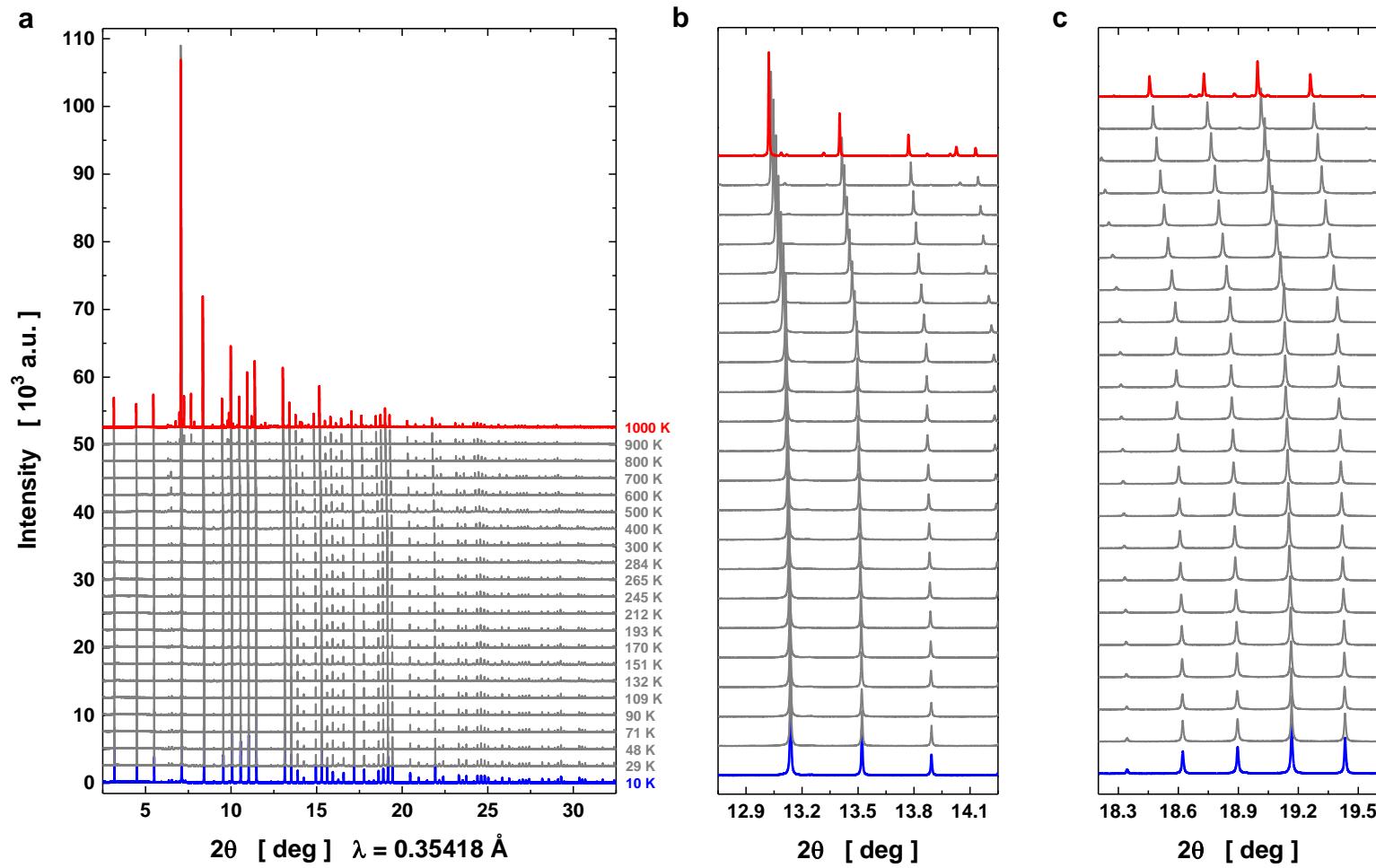


Figure S1. (a) Temperature-dependent SXRD patterns of $\text{Gd}_x\text{Co}_4\text{Sb}_{12}$ skutterudite recorded in the temperature range 10–1000 K. An unidentified minor phase is segregated at 900 and 1000 K, as observed in the $7\text{--}8^\circ$ angular region. Selected 2θ ranges are shown, namely: 2θ $12.9^\circ\text{--}14.1^\circ$ (b) and 2θ $18.3^\circ\text{--}19.5^\circ$ (c) to elucidate the lattice thermal expansion.

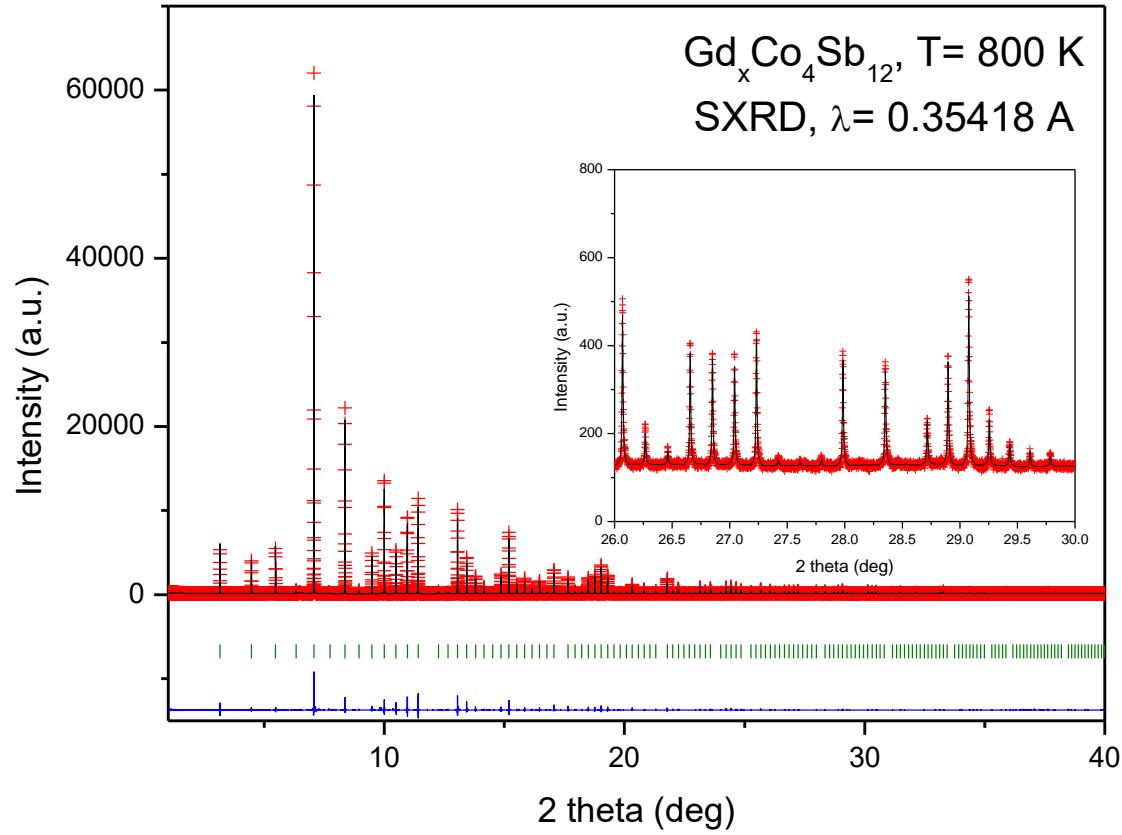


Figure S2. Rietveld plot from synchrotron X-ray diffraction data of Gd-filled $\text{Co}_4\text{Sb}_{12}$ skutterudite at 800 K. Red crosses are the experimental data, the black line denotes the calculated profile, the blue line is the difference between experimental and calculated data, and dark green bars the Bragg reflections. The inset shows the quality of the fit in the high angular region between 26° and 30° .

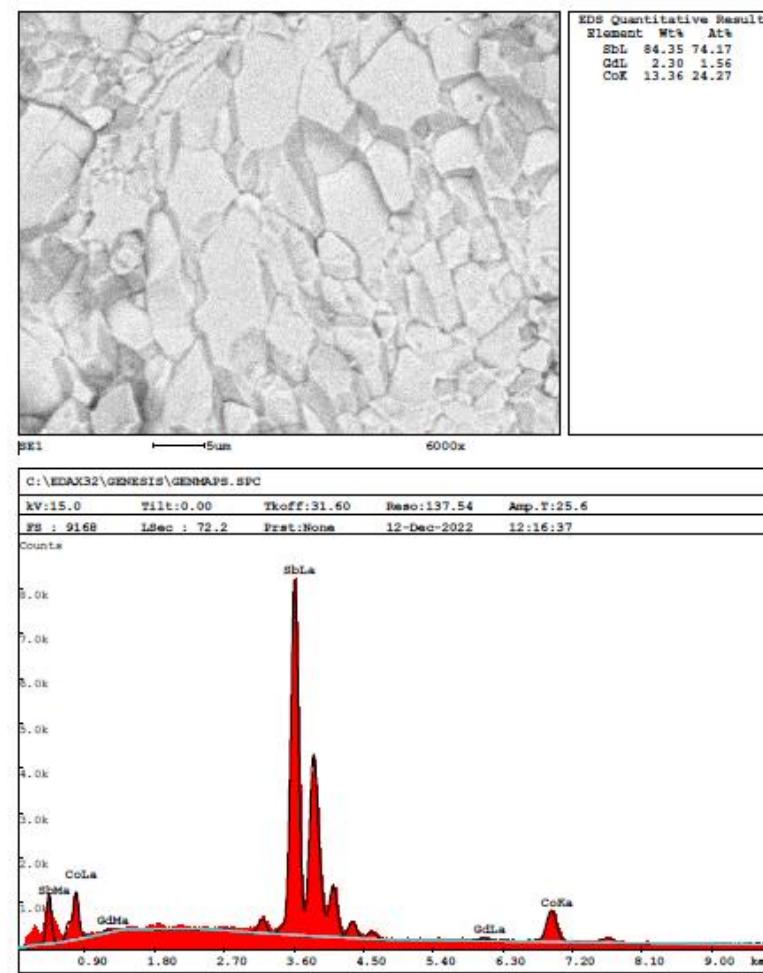


Figure S3. EDX analysis coupled to the FE-SEM images. A typical EDX spectrum, showing the region where it has been collected. The atomic composition is close to 0.033:4:12 for the Gd:Co:Sb ratio.

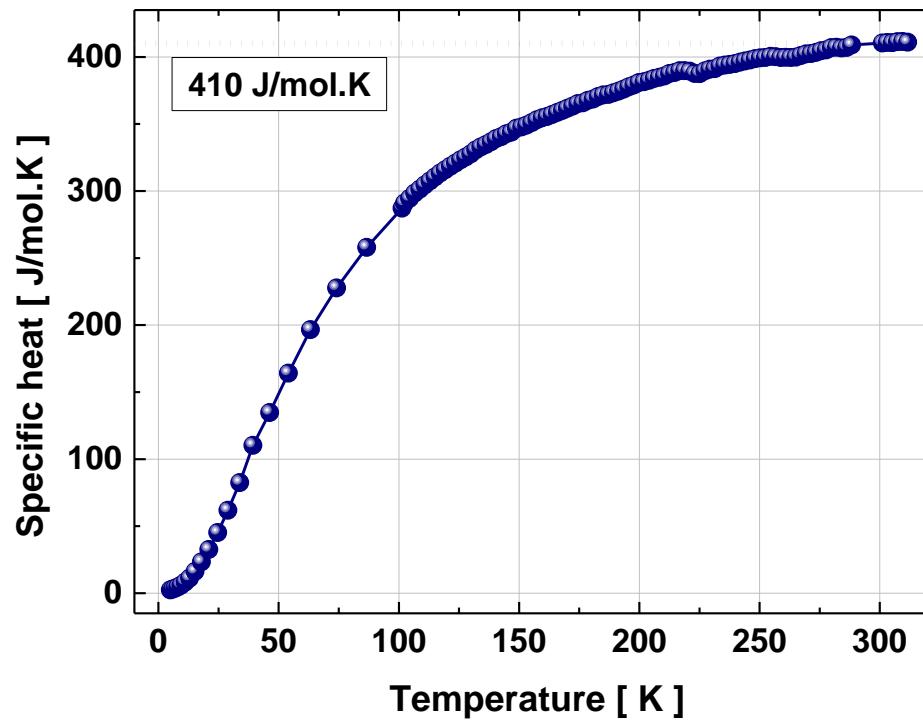


Figure S4. Specific heat of $\text{Gd}_{0.03(2)}\text{Co}_4\text{Sb}_{12}$ composition in the temperature range 5–310 K.