

Supplemental material to the article

“Anomalies of the Electronic Structure and Physical Properties of Rare Earth Cobaltites in the Vicinity of Spin Crossover”

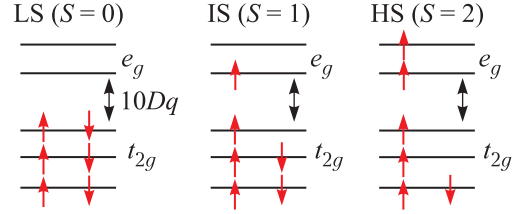


Figure 1: Possible spin states of Co^{3+} ion

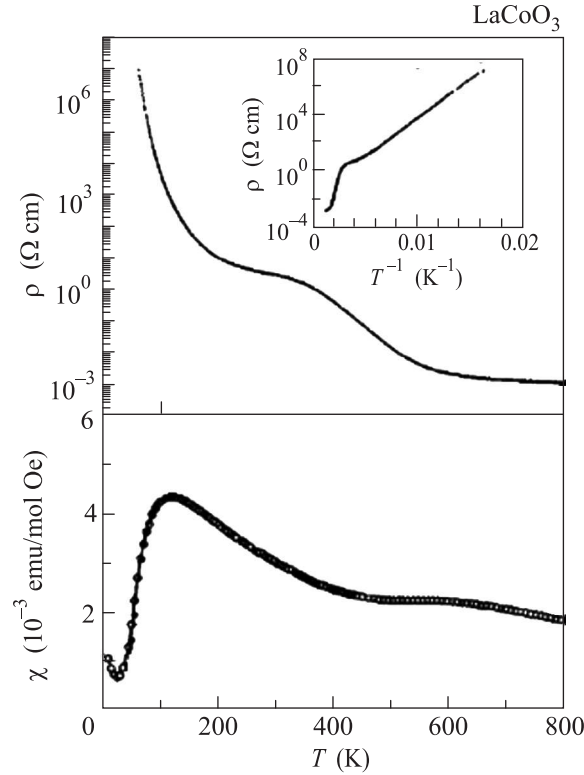


Figure 2: Temperature dependence of the resistivity (upper panel) and magnetic susceptibility (lower panel) of LaCoO_3 [9]

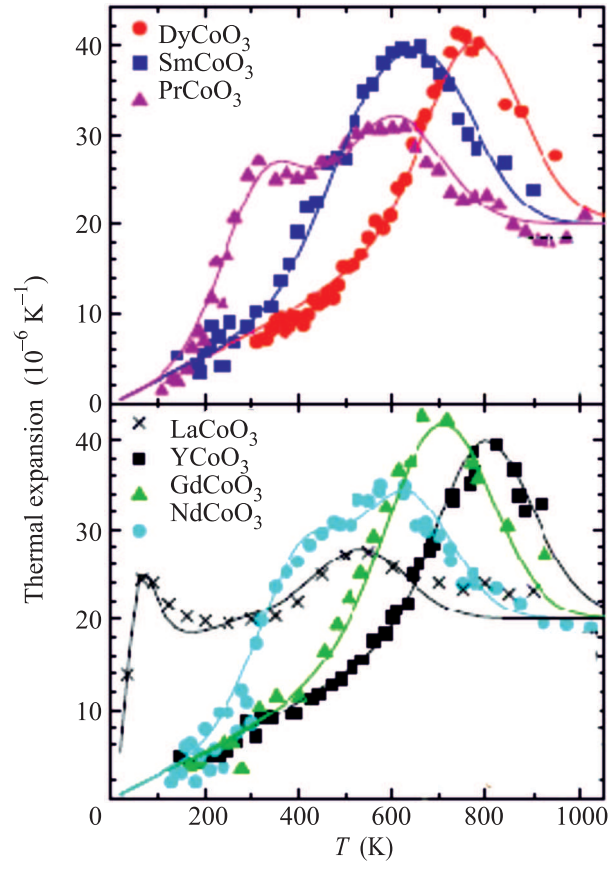


Figure 3: The coefficient of linear thermal expansion α of LnCoO_3 [32]

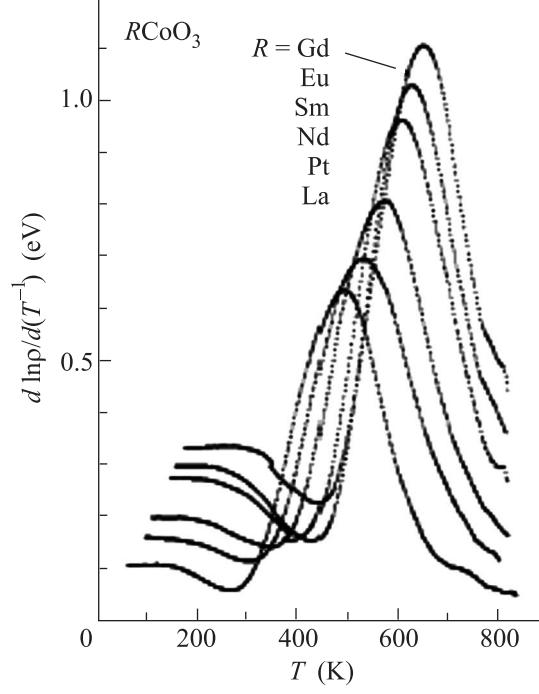


Figure 4: The dependence of $d \ln p / d(T^{-1})$ versus temperature for LnCoO_3 series [31]

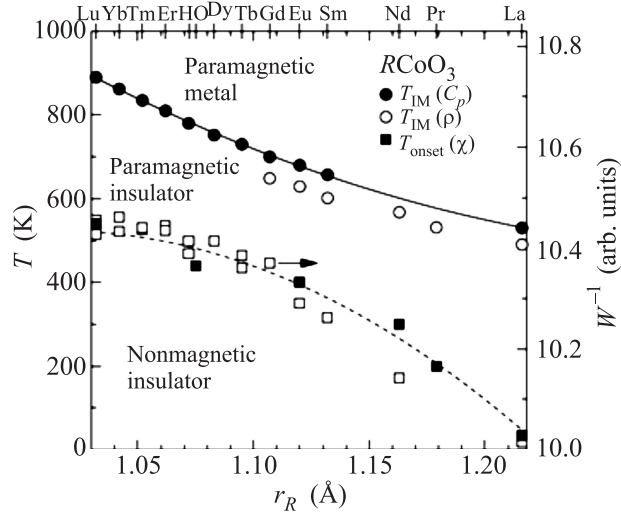


Figure 5: Electronic phase diagram for LnCoO_3 as a function of the ionic radius [34]

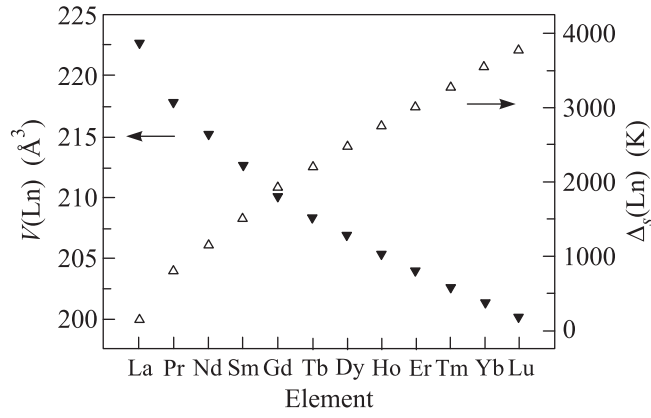


Figure 6: The unit cell volume (black triangles) and the magnitude of the spin gap (white triangles) for a number of rare earth elements [5]

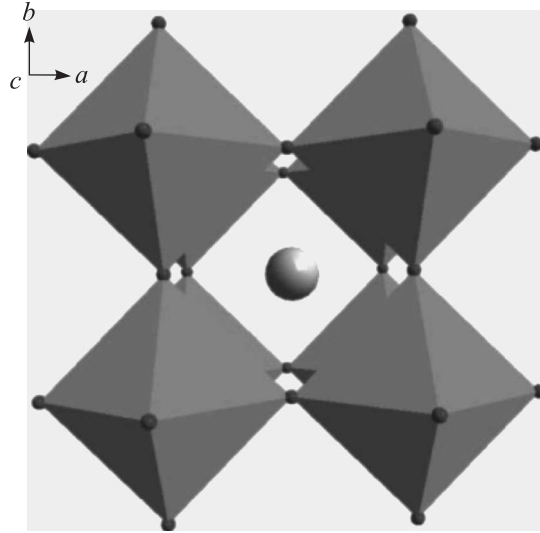


Figure 7: The ideal cubic perovskite structure LnCoO_3 [8]

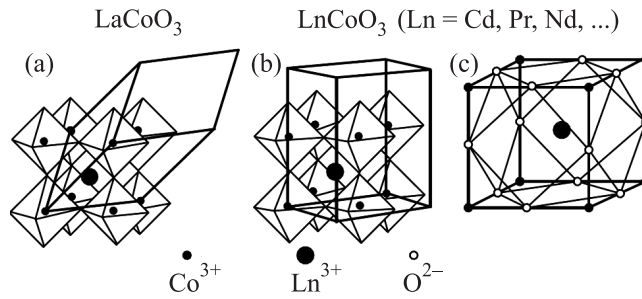


Figure 8: The perovskite crystal structure of LnCoO_3 . (a) – With rhombohedral distortion (group $R\bar{3}c$ for $\text{Ln} = \text{La}$). (b) – With rhombic distortion (group $Pbnm$ for $\text{Ln} \neq \text{La}$). (c) – The environment of the rare earth ion [7]

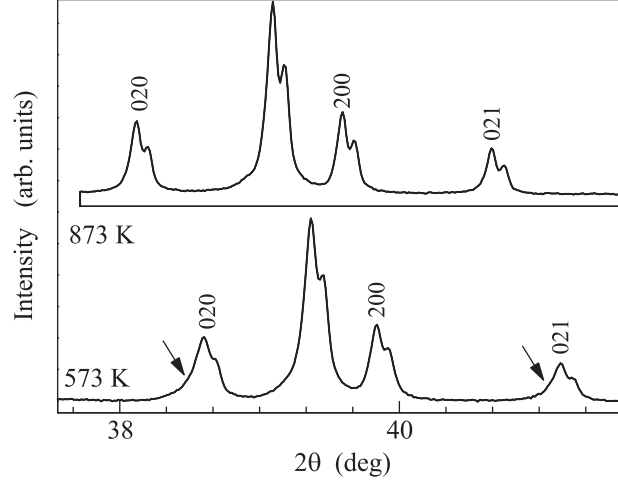


Figure 9: The characteristic fragments of the diffraction patterns at 573 and 873 K. The asymmetric broadening of the peaks for the 573 K is shown by arrows. For a temperature of 873 K asymmetry is absent

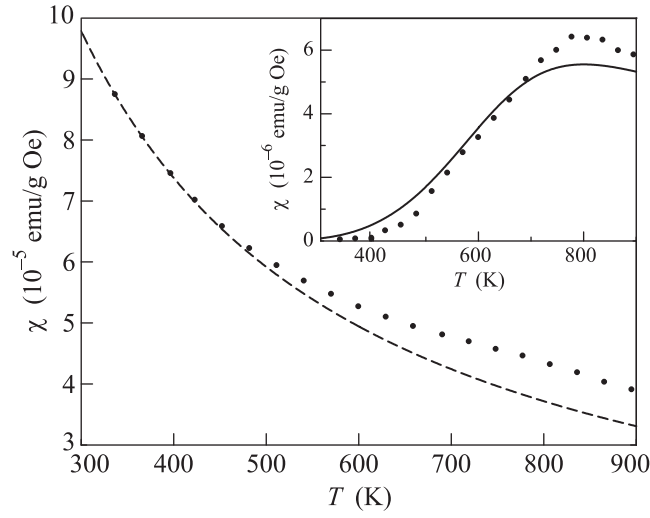


Figure 10: Temperature dependence of the magnetic susceptibility of GdCoO_3 (points) and Gd^{3+} ions contribution, calculated by the Curie–Weiss law. The inset shows Co^{3+} ions contribution (points – the difference between the experimental data and the gadolinium ions contribution, the solid line – the results of the theoretical calculation)

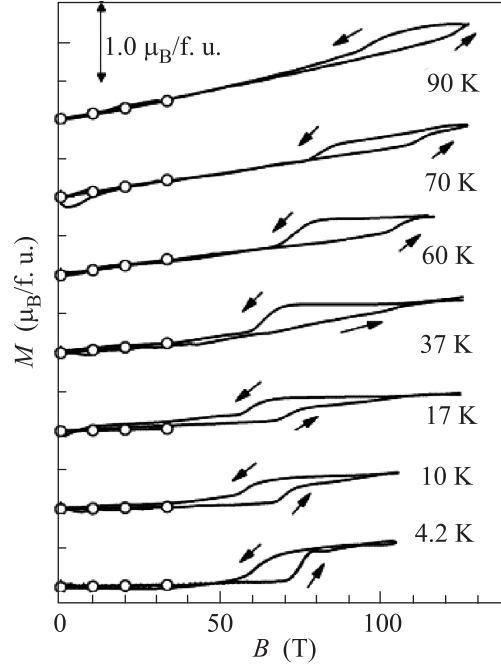


Figure 11: Field dependence of magnetization LaCoO_3 at different temperatures [50]

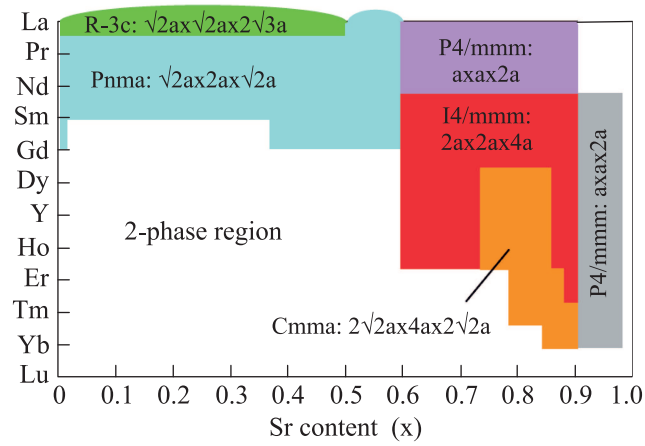


Figure 12: The phase diagram of perovskite structure at 300 K [64]