	Experiment title: Crystallographic symmetry of antiferromagnetic CoO	**Experiment number**: 1-01-243
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Report:

The crystallographic symmetry of antiferromagnetic CoO was studied using high-resolution synchrotron powder diffraction in the temperature range 10 – 300 K. The high-quality powder patterns unambiguously revealed a monoclinic symmetry (space group *C*2/*m*) and allowed the extraction of accurate values for the lattice constants. The temperature dependence of the monoclinic deformation scales with the much stronger tetragonal distortion as determined from laboratory x-ray diffraction. Magnetic ordering is associated with a cubic-to-monoclinic transition which is thus of first-order type. Neutron powder diffraction data are compatible with a collinear magnetic structure with the moments ordered in the monoclinic *ac*-plane.

The high-resolution powder diffractometer on BM1B (Swiss-Norwegian beam-line) at ESRF was used with λ = 0.50084 $\Rightarrow$ in a further effort to clarify the true symmetry of CoO. The sample was filled in a 0.5 mm diameter capillary. Complete powder patterns with a 2θ range between 1 and 62° were collected at 10 and 293 K. The sample was cooled by means of a liquid helium cryostat with a temperature stability of ±0.1 K. At the temperatures between 30 to 200 K only partial patterns were recorded. Further data between 150 and 300 K were collected on BM16 with λ = 0.40578 $\Rightarrow$ using a cryostream nitrogen cooling system with a poorer stability of ±5 K. The presence of a monoclinic lattice is clearly manifested by a splitting of the reflections. Rietveld refinements on each powder pattern were performed making use of FULLPROF.9 All peaks were indexed in the space group *C*2/*m* with Co at position 2*a*(0, 0, 0) and O at 2*d*$(0, \frac{1}{2}, \frac{1}{2})$. Additional peaks revealed that the impurity Co3O4 was still present at a concentration of 5%, and it was included in joint refinements. The monoclinic angle may be written as 125.2644° + δ, with δ referring to the deviation from orthogonality of the conventional face-centered cell. It is apparent that the temperature dependence of the monoclinic deformation scales with the much stronger tetragonal distortion. The antiferromagnetic transition is thus accompanied by a cubic-to-monoclinic crystallographic distortion. At 293 K, the lattice constant of the cubic phase is a = 4.26077(2) $\Rightarrow$. At 10 K, the monoclinic lattice constants are: a = 5.18190(6), b = 3.01761(3), c = 3.01860(3) $\Rightarrow$, β=125.5792(9)°. In the face-centered setting, this corresponds to an angle of 89.962° between the two edges of different length.

Futher details can be found in the publication :

Jauch W., Reehuis M., Bleif H. J., Kubanek F., Pattison P.,
Crystallographic symmetry and magnetic structure of CoO,
Physical Review B - Condensed Matter and Materials Physics 64, pp. 052102/1-052102/3, 2001.