On the magnetic and crystal structures of NiO and MnO

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The magnetic and crystal structures of manganese and nickel monoxides have been studied using high-resolution neutron diffraction. The known 1k structures based on the single propagation vector [1/2 1/2 1/2] of the parent paramagnetic space group $Fm\bar{3}m$ are forced to adopt monoclinic magnetic symmetry and are not compatible with rhombohedral symmetry. However, the monoclinic distortions from the rhombohedral crystal metric allowed by symmetry are very small, and explicit monoclinic splittings of the diffraction peaks have not been experimentally observed. We analyse in detail the magnetic crystallographic models that are metrically compatible with our experimental data using the isotropy subgroup representation approach, including rhombohedral solutions based on the propagation-vector star {[1/2 1/2 1/2], [−1/2 1/2 1/2], [1/2 −1/2 1/2], [1/2 1/2 −1/2]}. Although the full-star rhombohedral $R\bar{3}c$ structure can equally well fit our diffraction data for NiO, we conclude that the best solution for the crystal and magnetic structures of NiO and MnO is the 1k monoclinic model with magnetic space group C2/*c* (Belov-Neronova-Smirnova No. 15.90, UNI symbol $C2/c.1'_c[C2/m]$).