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Neutron diffraction studies on crystal and magnetic structures of BiFeO₃ at high pressures¹ XIAO-JIA CHEN, MALCOLM GUTHRIE, RUS-SELL J. HEMLEY, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, U.S.A., YU-JIE WU, XIAO-KUN CHEN, Department of Physics, South China University of Technology, Guangzhou 510640, China, JAMIE J. MOLAISON, ANTONIO F. MOREIRA DOS SANTOS, CHRISTOPHER A. TULK, Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A. — As one of the most prominent examples of multiferroic materials, bismuth ferrite BiFeO₃ shows both electric polarization below T_C = 1100 K and long-range magnetic ordering below T_N = 640 K. The coexistence of both electric and magnetic order parameters at room temperature is particularly interesting for technological applications. However, the physical and structural properties of BiFeO₃ under pressure are still a matter of debate in the literature. Here we report neutron diffraction data on BiFeO₃ at 294 K up to 10 GPa. The evolution of both the crystal structure and magnetic structure of this material with pressure has been well determined. Our results shed insight on the long standing controversy surrounding the structural transformations at 3 GPa and 7-10 GPa reported by different laboratories.

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