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## On the Compression Mechanism of $FeF_3$

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The structure of $FeF_3$ has been studied in the pressure range from ambient to 8.28 GPa by time-of-flight neutron powder diffraction. No structural phase transitions were found within the investigated pressure range and least squares refinements of the crystal structure were performed in space group $R\bar{3}c$ for all recorded data sets. It was found that thevolume reduction is achieved through rotation of the $FeF_6$ octahedra and the Fe-F-Fe bond angle decreases from 152.5(2) to 134.8(3)° within the investigated pressure range. The fluorine atoms were found to be almost hexagonally close packed at 8.28 GPa. The Fe-F-Fe bond angle is 131.8° in a hypotetical structure with hexagonally close packed fluorine atoms. A small octahedral strain was found to develop during compression. The octahedral strain reflects an elongation of the $FeF_6$ octahedra along the *c*-axis. The zero pressure bulk modulus $B_o$ and its pressure derivative $B_o$' were determined to be $B_o$ = 14(1) GPa and $B_o$' = 12(1). The compression mechanism of $FeF_3$ is discussed in term of the deformation of a 8/3/c2 sphere packing model of the fluorine atoms [1] and the results obtained for $FeF_3$ are compared with previously obtained results for $CrF_3$ [2].

[1] Fisher, W, *Z. Kristalloger*, 1973, 138, 129.
[2] Jørgensen, J.-E., Marshall, W. G., Smith, R. I., *Acta Cryst* 2004, B60, 669.

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## Structural and electronic properties of ferropericlase at high pressures

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Ferropericlase (Mg,Fe)O is the second after $(Mg,Fe)SiO_3$ perovskite abundant mineral in the Earths lower mantle. Crystal structure and physical properties of ferropericlase at high pressures and temperatures are of significant importance for the interpretation of seismological data. Ferropericlase with 20 mol% of Fe (close to the hypothetical mantle composition) was studied in situ using diamond anvil cell technique up to the pressure of the lowermost mantle. Combined X-ray diffraction, X-ray absorption, and Mössbauer effect study was performed. Structural distortion from the cubic to rhombohedral structure was observed at ~35 GPa [1]. Although the distortion is quite small and has minor effect on density, it probably affects elastic properties (bulk and shear modulus) significantly in the vicinity of transition. Transformation from high- to low-spin state of $Fe^{2+}$ was observed in the pressure range 55-105 GPa [2]. Such broadness of the spin transition (corresponding to the major part of the lower mantle) implies no seismic discontinuity associated with spin crossover in ferropericlase. Some possible implications to the Earth sciences are presented.

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