

m36.p06

On the Compression Mechanism of FeF₃J.-E. Jørgensen,^a R.I. Smith^b^aDepartment of Chemistry, University of Aarhus, DK-8000 Aarhus C, Denmark, ^bISIS Neutron Facility, Rutherford Appleton Laboratory Chilton, Didcot, Oxon OX11 0QX, United Kingdom. E-mail: jenserik@chem.au.dk**Keywords:** neutron powder diffraction, high pressure, Rietveld analysis

The structure of FeF₃ 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 the volume reduction is achieved through rotation of the FeF₆ 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 hypothetical 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 FeF₆ 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 FeF₃ is discussed in terms of the deformation of a 8/3/c2 sphere packing model of the fluorine atoms [1] and the results obtained for FeF₃ are compared with previously obtained results for CrF₃ [2].

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

m36.p07

Structural and electronic properties of ferropericlase at high pressures

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Keywords: ferropericlase, high pressure, diamond anvil cell

Ferropericlase (Mg,Fe)O is the second after (Mg,Fe)SiO₃ perovskite abundant mineral in the Earth's 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 Fe²⁺ 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.

[1] Kantor I., Dubrovinsky L., McCammon C., Kantor A., Pascarelli S., Aquilanti G., Crichton W., Mattesini M., Ahuja R., Almeida J., Urusov V., *Phys. Chem. Miner.*, 2006, DOI: 10.1007/s00269-005-0052-z.[2] Kantor I.Yu., Dubrovinsky L.S., McCammon C.A., *Phys. Rev. B*, in press, 2006.