

## **In situ structure determination of the high-pressure phase of Fe<sub>3</sub>O<sub>4</sub>**

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### **ABSTRACT**

The crystal structure of a high-pressure Fe<sub>3</sub>O<sub>4</sub> phase was determined by in situ X-ray diffraction measurements at high pressure and temperature, using an imaging plate detector and monochromatic synchrotron X-radiation. The high-pressure phase has the *Pbcm* space group (CaMn<sub>2</sub>O<sub>4</sub>-type structure) with cell parameters  $a = 2.7992(3)$  Å,  $b = 9.4097(15)$  Å, and  $c = 9.4832(9)$  Å at 23.96 GPa and 823 K. Fe<sup>3+</sup> occupies an octahedral site and Fe<sup>2+</sup> is in an eightfold-coordinated site described as a bicapped trigonal prism. The high-pressure CaMn<sub>2</sub>O<sub>4</sub>-type Fe<sub>3</sub>O<sub>4</sub> phase is about 6.5% more dense than the spinel form at 24 GPa.