

## **The crystal structure of Fe<sub>2</sub>S at 90 GPa based on single-crystal X-ray diffraction techniques**

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### **ABSTRACT**

The Fe-S system was explored in a laser-heated diamond-anvil cell at 89(2) GPa and 2380(120) K to better understand the phase stability of Fe<sub>2</sub>S. Upon temperature quenching, crystallites of Fe<sub>2</sub>S were identified, and their structure was investigated using single-crystal X-ray diffraction techniques. At these conditions, Fe<sub>2</sub>S adopts the *C23* structure (anti-PbCl<sub>2</sub>, Co<sub>2</sub>P) with space group *Pnma* (*Z* = 4). This structure consists of columns of corner-sharing, FeS<sub>4</sub> tetrahedra, and columns of edge-sharing FeS<sub>5</sub> square pyramids linked along edges in the *b* direction. Sulfur is in ninefold coordination with Fe. This study marks the first high-pressure structural solution and refinement of Fe<sub>2</sub>S synthesized in a multigrain Fe+FeS sample at 90 GPa and 2400 K and establishes the stability of *C23* Fe<sub>2</sub>S at these conditions. A previous powder diffraction study reports an orthorhombic Fe<sub>2</sub>S phase with a *C37*, Co<sub>2</sub>Si-like unit cell above 190 GPa. A *C23*–*C37* structural transition is inferred to explain the previously observed unit-cell parameters at higher pressures and temperatures. These results highlight the utility of applying single-crystal X-ray diffraction techniques to high *P-T* multigrain samples to explore the structural properties of iron-rich phases in Earth and planetary cores.

**Keywords:** Crystal structure, iron sulfides, Earth's core, diamond anvil cell, single crystal, high pressure, high temperature, iron alloys