

## **Inversion twinning in troilite**

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### **ABSTRACT**

The crystal structure of troilite from chondrites Etter and Georgetown and a troilite analog synthesized by sulfurization of an iron wire was refined using single-crystal X-ray data. Troilite is known to be hexagonal, with space group  $P\bar{6}2c$ , which is non-centrosymmetric, allowing two non-identical inversely related spatial arrangements of atoms within the unit cell. All three samples represent the so-called inversion twins. They contain both inversely related atomic orientations instead of a single atomic arrangement. The inversion twinning may have developed as a result of a phase transition from the ideal centrosymmetric NiAs-type structure to troilite-type structure during cooling. In addition, all samples were found to be cation-deficient. The departure from ideal stoichiometry—up to almost 3.5 rel% of metal atoms are missing—is also possibly related to atomic ordering when the crystals cooled.

**Keywords:** Troilite, crystal structure, absolute structure, inversion twin, meteorite, chondrite, Etter, Georgetown