

## **A new high-pressure phase transition in natural Fe-bearing orthoenstatite**

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### **ABSTRACT**

Single-crystal X-ray structure refinements have been carried out on natural Fe-bearing orthoenstatite (OEN) at pressures up to 14.53 GPa. We report a new high-pressure phase transition from OEN to a monoclinic phase (HPCEN2) with space group  $P2_1/c$ , with a density change of  $\sim 1.9(3)\%$ . The HPCEN2 phase is crystallographically different from low-pressure clinoenstatite (LPCEN), which also has  $P2_1/c$  symmetry. Upon release of pressure HPCEN2 reverts to OEN, and the transition pressure is bracketed between 9.96 and 14.26 GPa at room temperature. We find no evidence for a  $C2/c$  phase at high pressure. The lattice constants for the new phase at 14.26 GPa are  $a = 17.87(2)$ ,  $b = 8.526(9)$ ,  $c = 4.9485(10)$  Å,  $\beta = 92.88(4)^\circ$  [ $\rho = 3.658(9)$  g/cm<sup>3</sup>]. Refinement of the new structure indicates rotation of tetrahedral chain as the key characteristic of this transition. This experiment points to the possibility of OEN and HPCEN2 as the stable phases in Earth's upper mantle.

**Keywords:** Orthoenstatite, high-pressure clinoenstatite, high-pressure phase transition, upper mantle, synchrotron single-crystal X-ray diffraction