

The crystal structure of dolomite-IV, a high-pressure polymorph of dolomite, at 115 GPa

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Keywords: high-pressure, single crystal diffraction, dolomite.

We report the crystal structure of dolomite-IV, a high-pressure polymorph of Fe-dolomite stabilized at 115 GPa and 2500 K. It is orthorhombic, space group $Pnma$, $a = 10.091(3)$, $b = 8.090(7)$, $c = 4.533(3)$ Å, $V = 370.1(4)$ Å³ at 115.2 GPa and ambient temperature. The structure is based on the presence of 3-fold C₃O₉ carbonate rings, with carbon in tetrahedral coordination. The structure of dolomite-IV has not been predicted, but it presents similarities with the structural models proposed for the high-pressure polymorphs of magnesite, MgCO₃. A ring-carbonate structure match with spectroscopic analysis of high-pressure forms of magnesite-siderite reported in the literature, and, therefore, is a likely candidate structure for a carbonate at the bottom of the Earth's mantle, at least for magnesian and dolomitic compositions.