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LETTER

Dolomite-IV: Candidate structure for a carbonate in the Earth's lower mantle

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ABSTRACT

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) Å^3 at 115.2 GPa and ambient temperature. The structure is based on the presence of threefold C_3O_9 carbonate rings, with carbon in tetrahedral coordination. The starting Fe-dolomite single crystal during compression up to 115 GPa transforms into dolomite-II (at 17 GPa) and dolomite-IIIb (at 36 GPa). The dolomite-IIIb, observed in this study, is rhombohedral, space group *R*3, a = 11.956(3), c = 13.626(5) Å, V = 1686.9(5) Å^3 at 39.4 GPa. It is different from a previously determined dolomite-III structure, but topologically similar. The density increase from dolomite-IIIb to dolomite IV is ca. 3%. 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, $MgCO_3$. 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 magnesitic and dolomitic compositions.

Keywords: Carbonate, high-pressure structure, tetrahedral ring-carbonate, single-crystal X-ray diffraction