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LETTER

The crystal structures of $Mg_2Fe_2C_4O_{13}$, with tetrahedrally coordinated carbon, and $Fe_{13}O_{19}$, synthesized at deep mantle conditions

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ABSTRACT

We simulated the redox decomposition of magnesium-siderite at pressures and temperatures corresponding to the top of the Earth's D″ layer (135 GPa and 2650 K). It transforms into new phases, with unexpected stoichiometry. We report their crystal structure, based on single-crystal synchrotron radiation diffraction on a multi-grain sample, using a charge-flipping algorithm. $Mg_2Fe_2(C_4O_{13})$ is monoclinic, a = 9.822(3), b = 3.9023(13), c = 13.154(5) Å, β = 108.02(3)°, V = 479.4(3) Å^3 (at 135 GPa). It contains tetrahedrally coordinated carbon units, corner-shared in truncated C_4O_{13} chains. Half of the cations are divalent, and half trivalent. The carbonate coexists with a new iron oxide, $Fe_{13}O_{19}$, monoclinic, a = 19.233(2), b = 2.5820(13), c = 9.550(11) Å, β = 118.39(3)°, V = 417.2(5) Å^3 (at 135 GPa). It has a stoichiometry between hematite, Fe_2O_3, and magnetite, Fe_3O_4. The formation of these unquenchable phases indicates, indirectly, the formation of reduced-carbon species, possibly diamond. These structures suggest the ideas that the mineralogy of the lower mantle and D″ region may be more complex than previously estimated. This is especially significant concerning accessory phases of fundamental geochemical significance and their role in ultra-deep iron-carbon redox coupling processes, as well as the iron-oxygen system, which certainly play an important role in the lower mantle mineral phase equilibria.

Keywords: Carbonate, tetrahedrally coordinated carbon, iron oxide, high pressure, single-crystal