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Synthesis of calcium orthocarbonate, Ca_2CO_4-*Pnma* at *P-T* conditions of Earth's transition zone and lower mantle

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Abstract

We show, by single-crystal diffraction studies in laser-heated diamond-anvil cells, that Ca_2CO_4 orthocarbonate, which contains CO_4^{4-} tetrahedra, can be formed already at ~20 GPa at ~1830 K, i.e., at much lower pressures than other carbonates with sp^3-hybridized carbon. Ca_2CO_4 can also be formed at ~89 GPa and ~2500 K. This very broad *P-T* range suggests the possible existence of Ca_2CO_4 in the Earth's transition zone and in most of the lower mantle. Raman spectroscopy shows the typical bands associated with tetrahedral CO_4^{4-}-groups. DFT-theory based calculations reproduce the experimental Raman spectra and indicate that at least in the athermal limit the phase assemblage of $Ca_2CO_4 + 2SiO_2$ is more stable than $2CaSiO_3 + CO_2$ at high pressures.

Keywords: Carbonate, Ca_2CO_4, structure, X-ray diffraction, Raman spectroscopy, density functional theory; Volatile Elements in Differentiated Planetary Interiors