

In-situ vibrational spectroscopy to study the phase relations in the system CaCO_3 at high P and T

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To study the stability of the CaCO_3 -polymorphs, experiments were performed in conventional diamond anvil cells (DAC) at ambient temperatures as a function of pressure up to 30 GPa as well as in internally heated diamond anvil cells (DAC-HT) in the pressure range 2 to 22 GPa and temperatures up to 800 K. As probe for the structural changes we used conventional and synchrotron mid-infrared-, synchrotron far-infrared- and Raman-spectroscopy. Complementary first-principles calculations were performed to support the interpretation of the experimental spectra. Within the cc-III stability field (2 to 15 GPa at room temperature, e.g. [1]) we observed in all types of experiments consistently three different spectral patterns: one at lower P < 3.3 GPa another between 3.3 and about 6 GPa, which has been assigned to cc-IIIb and cc-III, respectively, [2] and the third one from 6 GPa until the transition into cc-VI at about 15 GPa, which has not been observed yet and which we tentatively assigned to a new modification cc-IIIc. We studied the transition from cc-IIIc to cc-VI in-situ at high P and T. The reaction has a negative slope of about $-7.0 \times 10^{-3} \text{ GPa K}^{-1}$. Thus, under the P, T- conditions of the Earth's mantle cc-VI may be stabilized towards lower pressure replacing aragonite in some parts of the mantle.

[1] Catalli & Williams (2005) *Am Mineral*, **90**, 1679. [2] Pippinger *et al.* (2015) *Phys Chem Min*, **42**, 29.