

## New High-pressure Phase of Calcite at Room Temperature

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A new high-pressure phase of calcite ( $\text{CaCO}_3$ ) has been found by single-crystal X-ray analyses. Recently we determined the crystal data of calcite III (monoclinic *C*-centered lattice,  $Z=8$ ) using single-crystal X-ray diffraction methods at 300K and pressures between 2.3 and 4.1 GPa [1]. The present studies have been carried out to determine the crystal data of calcite at room temperature and higher pressures.

The samples are single crystals of natural calcite from Creel, Chihuahua, Mexico. For high-pressure experiments, the Merrill-Bassett type diamond-anvil-cells were used. Pressures were estimated based on the ruby-fluorescence method. X-ray diffraction measurements were performed using an Enraf-Nonius CAD-4 diffractometer with  $\text{MoK}\alpha$  radiation monochromatized by graphite. A film cassette for a flat imaging plate was attached on the diffractometer.

On the oscillation photographs taken at 2.5GPa, all the reflections could be assigned as calcite III being composed two twinned individuals. By increasing the sample pressure to 4.5GPa, several reflections disappeared. Then remained reflections were re-indexed and the cell parameters were determined with the angular data of 25 reflections. The triclinic unit-cell are  $a=3.855(3)$ ,  $b=4.815(2)$ ,  $c=6.165(5)\text{\AA}$ ,  $\alpha=84.10(4)$ ,  $\beta=72.15(5)$ ,  $\gamma=88.73(5)$ ,  $Z=2$  at 300K and 4.5GPa. The cell parameters were determined at pressures between 4.3 and 5.6GPa. Thus the phase transition from calcite III to the new phase may occur at 4.1-4.3GPa.

[1] Hagiya K., Matsui M., Kimura Y., Akahama Y., *J. Mineralogical and Petrological Sciences*, 2005, **100**, 31.

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