# Density and crystal symmetry of calcite III by high-pressure single-crystal X-ray analysis

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Calcite is reported to transform to calcite II near 1.5 GPa, and to calcite III near 2 GPa(Singh and Kennedy, 1974; Redfern, 2000). Both calcite II and III back-transform to calcite at ambient pressure.   The crystal structure of calcite II has been determined by Merrill and Bassett(1975) using high-pressure single-crystal X-ray analysis.   However, the structure of calcite III is much controversial.   Based on high-pressure powder X-ray data, Davis(1964), Fiquet et al.(1994), and Suito et al.(2001) reported that calcite III is orthorhombic.   On the contrary, Merrill and Bassett(1972) suggested calcite III is monoclinic, and Smyth and Ahrens(1997) proposed another monoclinic structural model for calcite III.   Here, we determine the density and crystal symmetry of calcite III at high pressure, using high-pressure single-crystal X-ray analysis.

A diamond-anvil cell was used for high-pressure experiments at room temperature with a 4:1 methanol-ethanol mixture as the pressure medium, and the ruby fluorescence technique for pressure estimation.   X-ray diffraction measurements with MoKa radiation were made using a four-circle diffractometer and a Weissenberg camera having imaging plate detector.

Starting from a single-crystal of calcite, we increased the pressure gradually to obtain a single-crystal of calcite II at 1.5 GPa, and a single-crystal of calcite III at 2.2 GPa.   High-pressure single-crystal X-ray analyses of calcite III showed the crystal is monoclinic with space group either Cm, C2, or C2/m from systematic absences of reflections.   Unit cell parameters were refined using the four-circle diffractometer, to give the density of calcite III at 2.3 GPa to be 2.94 Mg/m3(Z=8), which is found to be smaller than that of aragonite (3.02 Mg/m3) at 2.3 GPa.   We note the monoclinic crystal lattice of calcite III obtained here is found to be essentially different from the previously proposed monoclinic lattice for calcite III either by Merrill and Bassett(1972) or by Smyth and Ahrens(1997).