

## **Pressure-induced phase transformation of kalicinite ( $\text{KHCO}_3$ ) at 2.8 GPa and local structural changes around hydrogen atoms**

**HIROYUKI KAGI,<sup>1,\*</sup> TAKAYA NAGAI,<sup>2</sup> JOHN S. LOVEDAY,<sup>3</sup> CHISATO WADA,<sup>1</sup> AND JOHN B. PARISE<sup>4</sup>**

<sup>1</sup>Laboratory for Earthquake Chemistry, University of Tokyo, Tokyo 113-0033, Japan

<sup>2</sup>Department of Earth and Space Science, Osaka University, Osaka 560-0043, Japan

<sup>3</sup>Department of Physics and Astronomy, University of Edinburgh, Edinburgh EH93JZ, U.K.

<sup>4</sup>Department of Geosciences and Chemistry, SUNY at Stony Brook, Stony Brook, New York 11794-21000, U.S.A.

### **ABSTRACT**

The pressure-induced structural phase transition in kalicinite,  $\text{KHCO}_3$ , has been studied by neutron powder diffraction, and infrared (IR) and Raman spectroscopy at high pressure and room temperature. The neutron diffraction study of deuterated kalicinite ( $\text{KDCO}_3$ ) revealed that for the one site for hydrogen (deuterium) found in the low-pressure phase, the O-D $\cdots$ O angle decreases from 176 to 161° and the distance between donor and acceptor O atoms of the O-D $\cdots$ O group decreases from 2.66 to 2.59 Å in the pressure range from 0 to 2.5 GPa. The crystal structure of the high-pressure polymorph was not determined. Infrared spectra were obtained at pressures up to 6.3 GPa using a diamond anvil cell. At ambient pressure, the O-H stretching, O-H $\cdots$ O in-plane bending, and O-H $\cdots$ O out-of-plane bending modes occur at 2620, 1405, and 988  $\text{cm}^{-1}$ , respectively. The frequency of the O-H stretch mode was nearly constant in the pressure range from 0 to 2.8 GPa, while that of O-H $\cdots$ O in-plane bending and out-of-plane modes increased with increasing pressure up to 2.8 GPa and remained constant above the phase transition pressure. The Raman spectra showed a clear phase transition at 2.8 GPa. The three Raman modes observed are assigned to internal vibrational modes of  $\text{HCO}_3^-$  and this suggests that the surrounding environment did change dramatically at the phase transition. These results suggest that the phase transition in kalicinite is triggered by the distortion of C-O-H bond at high pressure.