The study of portlandite, Ca(OH)2, under high pressure by FT-IR observation and single crystal X-ray diffraction

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The study of portlandite, $Ca(OH)_2$, under high pressure at ambient temperature was carried out by FT-IR observation and single crystal X-ray diffraction. Single crystals of portlandite were synthesized by the reaction of 2NaOH aq and $CaCl_2$ aq. IR spectra of the portlandite up to 8.8 GPa were measured by FT-IR microspectrometer. The unit cell parameters and the data sets of X-ray diffraction intensity of portlandite up to 5.7 GPa were measured with an auto-mated four-circle X-ray diffractometer (Rigaku,AFC-7S). The X-ray oscillation photographs were taken at 5.5, 8.3 and 3.0 GPa using synchrotron radiation with a four-circle diffractometer at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization, Tsukuba, Japan.

The IR absorption peak of OH stretching motion was observed at 3638cm^{-1} at 0.4 GPa. As increasing pressure, this peak shifted to the lower wavenumber at the rate of -3.56(9) $cm^{-1}GPa^{-1}$. This result indicates enhancement of hydrogen bonding between layers. The isothermal bulk modulus of portlandite, calculated using the Birch-Murnaghan equation of state, was K_0=34.2(9) GPa assuming K_0'=4. The linear compressibility of c axis ($12.63(2)*10^{-3}$ GPa^{-1}) is approximately 2.7 times as large as that of a axis ($4.71(3)*10^{-3}$ GPa^{-1}). Crystal structure of portlandite at 0.0001, 0.3, 1.7, 3.1, 3.5, 4.5, 5.0, 5.1, 5.3, 5.5, 5.7 GPa were refined, yielding R=3.8, 3.8, 3.7, 3.5, 5.0, 8.6, 3.9, 5.7, 8.2, 4.7, 8.1 respectively. Calcium atom vibrates anisotropically, but oxygen atom isotropically at all the pressure points in this X-ray diffraction study. Pressure dependence of temperature factor of Calcium and oxygen atom was confirmed. X-ray diffraction intensity data set of portlandite were collected at 5.7GPa, but no diffraction spots of sample were observed over 6.2 GPa. On reducing pressure, diffraction spots of portlandite were recovered. This phenomenon means that portlandite shows a reversible transformation from crystal to a glass state around 6 GPa.