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Pressure-induced phase transition and high-pressure response of hydrogen bonds in portlandite

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$Ca(OH)_2$, portlandite, belongs to brucite-type layered hydroxides, which is considered to be a model structure of hydrous minerals. This has hydrogen bonds within the interlayer of CaO_6 octahedral sheets. According to previous neutron diffraction studies of $Ca(OD)_2$, repulsive D...D interaction and hydrogen bonds in portlandite becomes much stronger under high pressure up to 4.5 GPa. Recently, it is said that portlandite undergoes a phase transition to a high-pressure phase at 6-8 GPa, at room temperature. However, the crystal structure of the high-pressure phase and the role of hydrogen bonds are still unknown. In the present study, the crystal structure of the high-pressure phase was clarified for the first time from powder and single crystal X-ray diffraction measurements. The crystal structure was determined to be monoclinic. In the structure, octahedral layers shift close each other, and some of the oxygen atoms become close enough to form the bondings with two neighboring Ca atoms. Based on the clarified structure of high-pressure phase accompanying the displacements of CaO_6 layers and Ca atoms, it is suggested that hydrogen bonds are closely related to the phase transition. In addition, several plausible positions of the hydrogen atoms in the structure are estimated in the high-pressure phase. Preliminary neutron diffraction experiments were also carried out using the new high-pressure cell. The high-pressure phase of $Ca(OD)_2$ was observed for the first time by the neutron diffraction. Further advanced experiments using much stronger neutron flux will allow us to acquire structural information of hydrogen bonds and the hydrogen positions in portlandite.

Keywords: Paris-Edinburgh cell, high pressure, neutron diffraction, hydrous minerals, phase transition, hydrogen bond