

Spectroscopic study of β -Ni(OH)₂ under pressure

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Abstract. Infrared absorption and Raman study of β -Ni(OH)₂ has been carried out up to 25 GPa and 33 GPa, respectively. The frequency of A_{2u} internal antisymmetric stretching O–H mode decreases linearly with pressure at a rate of $-0.7 \text{ cm}^{-1}/\text{GPa}$. The FWHM of this mode increases continuously with pressure and reaches a value of $\sim 120 \text{ cm}^{-1}$ around 25 GPa. There was no discernible change observed in the frequency and width of the symmetric stretching A_{1g} O–H Raman mode up to 33 GPa. The constancy of the Raman mode is taken as a signature of the repulsion produced by H–H contacts in this material under pressure. Lack of any discontinuity in these modes suggests that there is no phase transition in this material in the measured pressure range.

Keywords. β -Ni(OH)₂; phase transition; infrared absorption; Raman study; high pressure.

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1. Introduction

High pressure study of mineral dihydroxides $M(\text{OH})_2$ (where $M = \text{Mg, Ca, Co, Ni, etc.}$) is of importance for understanding the nature of hydrous minerals under compression in the earth's interior. These hydroxides crystallize in trigonal CdI_2 structure with space group $P\bar{3}m1$ [1]. β -Ni(OH)₂ belongs to this family of compounds. It is widely used in nickel batteries because of the unusually high level of activity of hydrogen atoms in this material. It is therefore of interest to understand the high pressure behaviour of hydrogen sublattice in this material. As hydrogen atoms are insensitive to x-ray diffraction techniques, neutron diffraction study of hydroxide compounds is an effective tool for understanding the behaviour of hydrogen sublattice of these compounds under different thermodynamic conditions. However, a simpler technique is the vibrational spectroscopic technique. In this method the reduction in the frequency of O–H mode with pressure is correlated with the enhancement of hydrogen bonding under pressure. This technique also throws light on the pressure induced phase transitions. High pressure studies reported in recent years have revealed pressure induced hydrogen disordering of $\text{Ca}(\text{OH})_2$, $\text{Mg}(\text{OH})_2$ and $\text{Co}(\text{OH})_2$. In polycrystalline samples of $\text{Ca}(\text{OH})_2$ pressure induced amorphization is reported around 12 GPa [2] whereas the single crystal samples of this compound exhibit a crystal–crystal transition around 6 GPa followed by amorphization