

## **Anharmonic OH vibrations in brucite: Small pressure-induced redshift in the range 0–22 GPa**

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### **ABSTRACT**

The uncoupled anharmonic OH-stretching vibrational frequency for the layered mineral  $\text{Mg}(\text{OH})_2$  (brucite) has been calculated in the pressure range 0–22 GPa. Quantum-mechanical electronic structure (DFT) calculations were performed, followed by quantum-mechanical vibrational energy calculations. The following findings emerged: (1) The calculated  $\text{d}\nu(\text{OH})/\text{d}P$  slope is  $-4 \text{ cm}^{-1}/\text{GPa}$ , in agreement with the experimental literature value [taken as the average between the Raman and IR-measured slopes for  $\text{Mg}(\text{OH})_2$ ]. (2) The calculated  $\nu(\text{OH})$  vs.  $R(\text{O}\cdots\text{O})$  correlation is linear and the slope is much smaller than that of traditional H-bond correlation curves in the literature. (3) The main origin of the small  $\text{d}\nu/\text{d}P$  and  $\text{d}\nu/\text{d}R(\text{O}\cdots\text{O})$  slopes is the small electric field variation as the mineral layers are pressed toward each other. (4) At high pressure, the  $\text{OH}^-$  ions show some tendency to be tilted with respect to the  $c$  axis, and a larger tilt angle leads to a larger  $\nu(\text{OH})$  downshift. (5) The pressure variation of the D quadrupole coupling constant is approximately  $-1 \text{ kHz/GPa}$ .

**Keywords:** Brucite, anharmonic OH frequencies, high pressure, electric field, hydrogen bonding, correlation curve, hydrous mineral