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Vibrational properties of δ-AlOOH under pressure

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Abstract

We have performed first-principles calculations to investigate the behavior of the hydrogen bond in δ-AlOOH under pressure. The highest OH-stretching A_1 and B_2 mode frequencies decrease under pressure leading to hydrogen bond symmetrization. After hydrogen bond symmetrization, the corresponding frequencies gradually increase. This softening and subsequent hardening of the OH bonds is a good spectroscopic indicator of hydrogen bond symmetrization and is observed in our GGA static calculations at ~30 GPa without considering tunneling effects. We have also carried out calculations of Raman peak intensities in several supercells with various hydrogen orderings to investigate the potential effect of H-disorder on the Raman spectrum of δ-AlOOH. Our results suggest that the four broad Raman bands observed experimentally in the range of OH-stretching mode frequencies could originate in H-disorder in this phase.

Keywords: Hydrogen bond, hydrous mineral, first-principles calculation, vibrational property, high pressure