Structural, vibrational and thermodynamic properties of $(NH_4)_2SO_4$ and NH_4NO_3: Ab initio study

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Abstract. Structural, vibrational and thermodynamic properties of inorganic aerosols, including ammonium sulfate $(NH_4)_2SO_4$ and ammonium nitrate NH_4NO_3 have been investigated at the periodic ab initio quantum mechanical level with the CRYSTAL code, which is based on Gaussian basis sets. Local density (LDA), gradient-corrected (PW91), and hybrid (B3LYP) density functionals have been used and the results are compared with experiment. All three functionals reproduce the equilibrium geometry of these crystals to a high level of accuracy. The calculations of frequencies and thermodynamic properties gave a mean absolute deviation from experiment of few percent for B3LYP, clearly showing that this functional performs extremely well in this case.

Keywords: Ab initio, Ammonium sulfate, Ammonium nitrate, Structural, Vibrational modes, Thermodynamic properties.