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摘要: The role of London dispersion forces in crystalline magnesium nitrate hexahydrate [Mg(NO3)(2)center dot 6H(2)O] has been investigated using terahertz spectroscopy and solid-state density functional theory modeling. The solid-state simulations were augmented with semi-empirical London dispersion corrections and revealed that such corrections are of negligible importance in this ionic solid. The comparison of the simulated and experimental crystal structures indicated a London force correction magnitude of less than 10% of that required in organic molecular solids of similar size and complexity. While London forces are certainly present in magnesium nitrate hexahydrate, electrostatic forces clearly dominate the intermolecular interactions governing its crystalline structure and dynamics. (C) 2012 Elsevier B.V. All rights reserved.
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