327. Title:Application of London-type dispersion corrections in solid-state density functional theory for predicting the temperature-dependence of crystal structures and terahertz spectra
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Abstract:Solid-state density functional theory (DFT) has been shown to be a valuable tool for the simulation of low-frequency vibrational motions in molecular crystals. While it is typically required that an experimentally known crystal structure be used as the initial input for these types of calculations, it is sometimes found that suitable crystallographic data are not easily obtainable. In this study, the low-temperature unit cell structure of the β polymorph of deuterated oxalic acid dihydrate, for which a structure has only been reported at room temperature, was predicted using solid-state DFT augmented with a modified empirical correction for weak long-range dispersive interactions. The dispersion correction parameters were optimized against the known 100 K crystal structure of the α polymorph, and then used for full-geometry optimization of the β crystal structure. Using this predicted structure for the β polymorph, the observed cryogenic THz spectrum of a mixture of deuterated oxalic acid dihydrate polymorphs was simulated.