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Title:Investigating tautomeric polymorphism in crystalline anthranilic acid using terahertz spectroscopy and solid-state density functional theory
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Abstract:Terahertz spectroscopy is sensitive to the interactions between molecules in the solid-state and recently has emerged as a new analytical tool for investigating polymorphism. Here, this technique is applied for the first time to the phenomenon of tautomeric polymorphism where the crystal structures of anthranilic acid (2-aminobenzoic acid) have been investigated. Three polymorphs of anthranilic acid (denoted Forms I, II and III) were studied using terahertz spectroscopy and the vibrational modes and relative polymorph stabilities analyzed using solid-state density functional theory calculations augmented with London dispersion force corrections. Form I consists of both neutral and zwitterionic molecules and was found to be the most stable polymorph as compared to Forms II and III (both containing only neutral molecules). The simulations suggest that a balance between steric interactions and electrostatic forces is responsible for the favoring of the mixed neutral/zwitterion solid over the all neutral or all zwitterion crystalline arrangements. © 2012 American Chemical Society.
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