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Title: Terahertz Spectroscopy of the Explosive Taggant 2,3-Dimethyl-2,3-Dinitrobutane
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Abstract:The terahertz spectrum of the crystalline explosive taggant 2,3-dimethyl-2,3-dinitrobutane (C6H12N2O4) has been investigated as an alternative means of detecting solid-state explosives. The room-temperature spectrum exhibits two broad absorption features centered at 38.3 and 49.2 cm(-1). Once the sample is cooled to liquid-nitrogen temperatures, the resolution of three additional peaks occurs, with absorption maxima now appearing at 40.1, 47.5, 56.6, 63.9, and 73.6 cm(-1). Solid-state density functional theory simulations, both with and without London force dispersion corrections, have been used for the assignment of the experimental cryogenic THz spectrum to specific molecular motions in the crystalline solid. The B3LYP hybrid density functional paired with the 6-311G(2d,2p) basis set provides an excellent reproduction of the experimental data revealing that the THz spectrum arises from a mixture of intramolecular torsional vibrations localized primarily in the nitro groups and intermolecular lattice vibrations composed of rigid molecular rotations.
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