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标 题 : THE TERAHERTZ INFRARED SPECTRUM OF CYCLOTRIMETHYLENETRINITRAMINE: TARGETING ANHARMONIC MODES FOR THE FINGERPRINTING AND DETECTION OF RDX
作者: Slough, WJ (Slough, William J.); Valenzano, L (Valenzano, Loredana); Perger, WF (Perger, Warren F.)
编者: Elert ML; Buttler WT; Borg JP; Jordan JL; Vogler TJ
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摘要: Recent approaches to the modeling of molecular solids have provided for a dramatic improvement in the prediction of zero Kelvin behavior for some properties of interest. Most notably the vibrational spectrum for these systems can now be calculated robustly via ab initio methods employing density functional theory. This improvement, however, leads to a quandary: the accurate physical modeling of these systems at zero Kelvin in many cases will not provide values and even physical behavior matching experimental values under ambient conditions. We examine this quandary in detail by considering zero Kelvin calculations using the B3LYP-D* functional of the terahertz infrared spectrum of the energetic material cyclotrimethylenetrinitramine (RDX). Most importantly we show what knowing the deviation from the simple harmonic approximation of a given mode at zero Kelvin says about the anharmonicity of the mode near ambient volumes. Finally, we discuss the practical implications for using ab initio calculations to create "finger-prints" for the detection of explosives such as RDX.
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地址: [Slough, William J.; Valenzano, Loredana; Perger, Warren F.] Michigan Technol Univ, Dept Phys, Houghton, MI 49931 USA
通讯作者地址: Slough, WJ (通讯作者),Michigan Technol Univ, Dept Phys, 1400 Townsend Dr, Houghton, MI 49931 USA
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