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标题: gamma PHASE RDX: INITIAL STUDY OF GEOMETRY, SPECTRUM AND EOS

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摘要: We present a full 3D periodic density functional theory study of the geometry and vibrational spectrum of gamma phase nitramine, hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). The B3LYP-D* functional as adjusted for molecular solids from Grimme's semi-empirical approach for molecules is used to better describe the van der Waals interactions in this system. Specifically, the low terahertz portion of the spectrum is computed to determine modes that change substantially in behavior with respect to an alpha phase that is near the transition pressure for the system. These key modes provide possible clues into the nature of the alpha-gamma phase transformation.

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