Density Functional Theory Study on Equation of State and Vibration Properties of TATB Crystal

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Abstract: The equation of state and vibration properties of TATB crystal were investigated by using the density functional theory (DFT) and combining with van der Walls force correction (vdW-DF2). The partial vibration modes of TATB crystal were reassigned. Vibration mode coupling and the intermolecular interaction process were studied under pressure process up 8.5 GPa. Results show that the NO_2 and NH_2 vibrations were strongly coupled in TATB crystal. The vibration in the wave number range of 1100 cm^{-1} to 1500 cm^{-1} is particularly complex because of the coupling of NH_2 with NO_2 and benzene ring vibrations. With increasing pressure, TATB molecules from neighboring layers bend and close to each other, causing a coupling of NH_2 plane twist vibration or wag with NO_2 shear vibration, indicating a strengthening of intermolecular hydrogen bonding.

Key words: TATB; equation of state; vibration properties; density functional theory (DFT)
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