

Detonation performance of high energy compounds determined by quantum mechanics

Introduction

Important material characteristics of high energy compounds are detonation pressure (and velocity) and impact sensitivity (ignition kinetic energy of impact). We establish these material characteristics for novel high energy compounds by theoretical considerations using quantum mechanics (QM). Four well-known compounds (RDX, TNT, NTO and ANTA) are used as bench mark explosive molecules together with new explosives based on nitrated derivatives of NTO and ANTA. Most calculations are density functional theory (DFT) calculations performed by the GAUSSIAN09 program package with the B3LYP functional and the 6 31G(d) basis set. Density is calculated by using the molecular isosurface volume (ISO) (defined by the volume within a surface with an electron density of 0.001 electrons per Bohr³) alone or together with the variance of the electrostatic potential (ESP).

Optimized molecular structures computed by DFT are also input to the Materials Studio 7.1 Polymorph predictor to calculate the densities by using force fields between molecules and exploring all possible packing arrangement in all reasonable space groups to search for the density among the low-lying minima in total energy. For calculation of detonation pressure the density and enthalpy of the compounds are input into a thermodynamic computer code (EXPLO5). Impact sensitivity is calculated by the correlation with least bond energy of the molecule to detonation temperature.

Conclusion

Density, impact sensitivity and detonation performance for new explosives are calculated by QM. Use of isosurface volume or electrostatic potential is a good alternative for the Polymorph predictor. The B3LYP and M06-2X functionals, both with the 6-31G(d) basis set, show significantly different bond dissociation energies in the nitrimino functional group.

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