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Building the equation of state of TATB from ab initio simulations and DAC experiments NICOLAS PINEAU, THOMAS PLISSON, ARNAUD SOLLIER, CEA DAM DIF — Modelling equations of state for energetic molecular crystals in the full thermodynamic range of inert compression, prior to detonation, is a challenging issue. Indeed the unreacted regime under high pressure is difficult to explore experimentally, and although first principle calculations allow filling that gap (T.R. Shan et al., J. Phys. Chem B, 117 (2013), 928; E. Stavrou et al. J. Chem. Phys., 143 (2015), 144506), the need for experimental support is crucial in order to validate the chosen methodological approach, and *in fine* the simulation results. In this study we present our methodology for building *ab initio* based EOSs for molecular crystals, using van der Waals corrected DFT (J.P. Perdew et al., Phys. Rev. Lett. 77 (1996), 3865; S. Grimme, J. Comput. Chem. 27 (2006), 1787) and Path Integral Molecular Dynamics (PIMD). Then we present recent experimental results on the isotropic compression of TATB using diamond anvil cells (DAC) and synchrotron radiation to reach pressures up to 65 GPa, beyond the current estimations for the von Neumann spike. The close agreement between the experimental and simulation data validates the methodology employed to obtain the cold curve of the explosive. The shock properties of inert TATB obtained with this EOS compare well to recent laser-driven shock compression experiments.

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