Hydrostatic and shock-wave compression of a molecular crystal

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Thermodynamics of high-molecular organic compounds and especially metastable chemical compounds, both being energy-saturated materials, turns out to be a poorly studied area despite its practical importance. Theoretical determination of relationships characterizing behavior of solid energy-saturated materials runs into difficulties as they belong to molecular crystals and molecules constituting a crystal have great many internal degrees of freedom. The paper analyzes experimental data on the hydrostatic and shock-wave compression of the energy-saturated material. The Mie–Grüneisen–Debye semi-empirical equation of state based on the Helmholtz potential is used to describe thermodynamic properties of metastable molecular crystals without phase transitions taken into account. The equation of state describes experimental data on isothermal compression of a molecular crystal with the above data given by the powder diffraction analysis using diamond anvils. An expression for the Hugoniot curve satisfactorily describes the data on shock compression of the material having different initial porosity. The proposed equation of state is expected to give higher-accuracy description of thermodynamic properties of the energy-saturated material in numerical simulation of shock-wave and detonation processes.