Description of isothermal compression of some molecular crystals

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The introduction of new methods to record fast processes, on the one hand, and development of computer engineering, on the other hand, have made numerical simulation one of the most efficient methods to study and analyze physical processes that allow one to obtain comprehensive and reliable information. All mathematical models of continuum mechanics are closed by equations of state (EOSs). It is shown that at present, despite numerous publications containing the results of experimental and theoretical studies, as well as publications on numerical simulation of thermophysical properties of materials, the challenges related to construction of EOSs still remain one of the central areas of research. When constructing theoretical models of EOSs for molecular crystals, it is assumed that pressure and internal energy can be split into two constituent parts: thermal and "cold" ones. The validity of the constructed EOSs should be checked by independent verification of the thermal and the "cold" constituents of pressure and internal energy using the known experimental data. The object of the present study is verification of the EOS derived by the example of molecular crystals of TATB, PETN, and RDX. The analysis of experimental data of isothermal compression of molecular crystals shows that the experimental and the calculated values are within the experimental error and are in good agreement. The proposed approach allows determining the pressure behavior under isothermal compression before running an experiment.