THERMODYNAMIC PROPERTIES OF SOLID, LIQUID, AND GASEOUS NITROGEN

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S u m m a r y

A theoretical model of the phonon spectrum, accounting the complete set of acoustic translational and optical translational and orientational modes for description of the themodynamic properties of the phonon subsystem of molecular crystalline nitrogen is proposed. On the basis of experimental values of resonant phonon frequencies, obtained by the methods of neutron and Raman spectroscopy, the phonon density of states, heat capacity, and other thermodynamic functions are calculated without fitting parameters. The statistical mechanical methods of perturbation theory are used for the description of liquid and gaseous states of molecular nitrogen. Advantages of the proposed calculational method for thermodynamic characteristics are the minimum number of the initial data necessary for calculations and the absence of fitting parameters or empirical correlations. The numerical calculations accomplished for the pressure of saturated vapour, head capacity, and sound velocity of molecular nitrogen agree with the available experimental data.