THERMOPHYSICAL PROPERTIES OF DENSE MOLECULAR GASES IN QUASICHEMICAL REPRESENTATION

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The interest in the study of the thermodynamic properties of molecular gases at high pressures and temperatures is associated both with their wide distribution in nature and with wide use in various high-energy devices. At pressures of the megabar range, where a high density of matter is accompanied by a strong Coulomb interaction (strongly coupled plasma), the thermophysical properties of gases were theoretically described both in frames of a quasi-chemical approach (free energy model) and by first principles methods using direct numerical simulation of a system of nuclei and electrons. Despite the progress achieved in both experimental and theoretical investigations, further study of the properties of dense gases in these range of parameters is of great importance. The currently available experimental data on the caloric and thermal equation of state overlap the pressure range from kilobars to tens of megabars and high densities. Recently, theoretical results have been obtained, both in frames of the quasi-chemical approach (the chemical model of plasma), and using first-principle methods in a wide range of parameters. This work presents the results of the calculation of hydrogen isochores in a wide range of temperatures, the shock adiabats of deuterium and nitrogen, and deuterium isentropes up to megabar pressures. The results were obtained using codes that implement advanced models of the SAHA family. Calculations have shown that in the considered range of dynamic pressures, compressed molecular gases represent a strongly coupled partially degenerate plasma with densities close to the density of condensed matter. The results of the calculations are presented in comparison with experimental data and the data obtained by the first principle modeling. It is shown that the presented approach allows to obtain an adequate description of the thermophysical properties of molecular gases in a wide range of temperatures and pressures, providing satisfactory agreement with both experiment and other theoretical approaches.