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Fundamental functional form of thermic equation of state

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Abstract

An electrically neutral system consisting of a finite number of electrons that are fermions and nuclei that are fermions or bosons is considered. The subsystem of nuclei can consist of identical nuclei, which corresponds to a system consisting of atoms of one chemical element, the subsystem can also contain different types of nuclei, which corresponds to a system consisting of identical molecules, mixtures (solution, alloy, etc.) of various substances, plasma of various degrees of ionization, chemically reacting system. The motion of electrons and nuclei is described in the framework of nonrelativistic quantum mechanics, taking into account the spins of electrons and nuclei. Only the Coulomb interaction of electrons with electrons and nuclei and nuclei with each other is taken into account. The influence of relativistic effects on the interaction of electrons with electrons and nuclei and nuclei with each other is neglected. Using the virial theorem, a fundamental functional form of the thermal equation of state of real substances, their mixtures, solutions and alloys has been obtained. It is shown that: the equation of state consists of the sum of non-negative and non-positive functions of thermodynamic parameters; the nonnegative function is determined by averaging over the quantum states of the energy of the Coulomb attraction between electrons and nuclei, and the positive function by averaging the sum of the kinetic energies of electrons and nuclei, the repulsion energy of electrons from each other, and the energy of repulsion of the nuclei from each other; in each quantum state it is impossible to separate the Coulomb attraction from the Coulomb repulsion, so it is in principle impossible to separate the Coulomb attraction from the Coulomb repulsion in the thermal equation of state; the last statement is also true if the motion of the nuclei is described by the laws of classical mechanics.

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