

**THERMODYNAMIC INVESTIGATION
OF NEW ORGANIC AND POLYMERIC MATERIALS**

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Knowledge of the thermodynamic properties of chemical compounds and materials allows us to determine the best options for the processes involving them. The introduction of new materials in various fields of science and technology requires the study of the physico-chemical properties of compounds to optimize their production processes and rational use. Precision calorimetry is a powerful tool for studying the fundamental physico-chemical characteristics (heat capacity, enthalpy, entropy, thermodynamic potentials) of substances and materials. The most important aspect of this study is the determination of the thermodynamic characteristics of phase transitions.

In this work, the phase transitions of macromolecular nanoobjects (organosilicon and liquid crystal dendrimers of various natures, polypeptides, active pharmaceutical substances, bistable transition metal complexes with complex organic ligands, and organic derivatives of fullerene C₆₀ and C₇₀) were studied over a wide temperature range (6–650 K). Using low-temperature adiabatic calorimetry, the temperature dependences of their heat capacities were studied, the thermodynamic characteristics of phase transitions were determined, including the values of configuration and zero (residual) entropy; their physico-chemical interpretation was carried out taking into account the composition and structure of compounds. For the first time, using precision calorimetry methods, structural effects in dendrimers were revealed: a low-temperature anomaly caused by subtle vibrations of fragments of the inner sphere and the surface layer of macromolecules (G₁–G₄), as well as a high-temperature relaxation transition ("nanoscale effect") for G₅–G₆ dendrimers; a hypothesis of the occurrence of transformations was proposed and discussed; their thermodynamic properties were determined and analyzed. characteristics for several representatives of a number of dendrimers. Along with the peculiarities of the molecular structure, the identified effects open up new possibilities for using dendrimers for medical purposes, namely for targeted drug delivery to affected cells of the body. Polymorphic transitions have been identified for pharmaceutical substances in the crystalline state; their thermodynamic characteristics (temperature, enthalpy, entropy) have been determined and analyzed. In the case of some substances, thermodynamically metastable (supercooled) states were obtained.

A complex of standard thermodynamic functions has been defined for all the studied objects, which is necessary for modeling various processes involving promising materials and constructing phase diagrams. The revealed «structure – property» relationships are of interest for predicting the properties of compounds and functional materials based on them that have not yet been studied.

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