THERMODYNAMICS OF FULLERENE NANOSTRUCTURES

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Abstract

In this research the heat capacity in the temperature range from 6 to 600 K for functional derivatives of C60 and C70 fullerenes were determined by precision Adiabatic Vacuum Calorimetry (AC) and Differential Scanning Calorimetry (DSC). The phase transitions and in some case chemical transformations were detected for compounds rank under study. The thermodynamic characteristics of these transformations were determined and analyzed with literature results about composition and structure of objects.

Thus, covalent bounded fullerene contained polymers was investigated. The influence of C60 and C70 fullerenes on thermodynamic characteristics and parameters of devitrification and glassy state was revealed. The dependence of temperature of destruction onset for polymers from fullerene content was established.

The heat capacity, characteristics of phase transitions and standard thermodynamic properties of C60 and C70 fullerides with organoelement fragments were studied for the temperature range from 6 to 350 K. On the based of our thermodynamic data, information about the structure and the composition of these and the respective data for the neutral dimer (C60)2 the some conclusion about the bound nature between fullerene fragments in the complex was made.

The standard thermodynamic properties of crystalline polymeric nanostructures of C60 fullerene and amorphous graphite-liked and diamond-liked nanostructures were studied. The dependences of thermodynamics properties vs composition and structure of compounds were analyzed. The rank of relative thermodynamic stability of crystalline phases of C60 at T = 298.15 K and standard pressure was determined. Thus, standard thermodynamic properties of indicated nanostructures, C60 and C70 fullerites, graphite and diamond were compared.

The results of AC were used to calculate the thermodynamic functions: the heat capacity, enthalpy, entropy, residual entropy and Gibbs energy over the range from 0 to 350 K.

Keywords: Fullerene, calorimetry, nanostructure, thermodynamics

Author did not supply full text of the paper.