

Nanocomposites and nanomaterials

The experimental heat capacity of fullerite C₆₀

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The heat capacity of the fullerite C₆₀ has been investigated in the temperature interval 1 – 120 K using an adiabatic calorimeter. The fullerite is 99.99% pure. The sample mass is equal to about 0.6 g. Analysis of the obtained results and literature data [1-3] in the temperature range 1 – 300 K was carried out assuming that the translational, rotational, and intramolecular degrees of freedom make additive contributions to the heat capacity of fullerite. It was found that the temperature dependence of the heat capacity can be expressed as sum of linear and cubic terms below 3 K. The linear term can be explained by the existence of low energy tunneling levels in the fullerite orientational glass. The calculated Debye temperature is equal to 53 K. The contributions of optical translational and librational vibrations of molecules C₆₀ are noticeable with temperature increasing above 3 K. The contributions of lattice and intramolecular vibrations to the heat capacity of fullerite were determined. The experimental heat capacity, associated to the translational and rotational vibrations, agrees well with the theory of lattice dynamics of the orientational ordered crystal C₆₀ [3] in the temperature range 1 - 25 K. The contribution of the intramolecular vibrations becomes significant above 50 K. The lattice specific heat is almost independent of temperature in the range of 50 – 140 K. The contribution of processes of orientational phase disordering to the heat capacity of C₆₀ is increased with temperature increasing above 140 K. The peak observed in the heat capacity near the temperature of 260 K is associated with the orientational phase transition. In the high-temperature orientation-disordered phase of fullerite the heat capacity equaled to near 4.5R, it corresponds to a case in which the rotation of molecules C₆₀ is close to free.

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