Behavior of the solvate molecules in solid solvate of C_{60} and C_{70} fullerenes under heating

Aksenova V.V.*, Nikonova R.M., Lad'yanov V.I.

Physical-Technical Institute, Ural Branch, Russian Academy of Sciences, Izhevsk 426000, Russia
**e-mail: las@pti.udm.ru*

One of the priority directions in physics and chemistry of the fullerenes is studying their interaction with solvents. To date values solubility of the fullerenes in different classes of organic solvents as well a structural laws that explain their high solubility in aromatic hydrocarbons were determined. There are many works devoted to mixed crystals or van der Waals crystals - the fullerenes molecular complexes with nonpolar molecules.

In studying thermal stability of the fullerites including the making of the composites modified with fullerenes C_{60} and C_{70} and also their mixes, it is necessary to take into account effect of residual solvent during the oxidation. In this study the deformation of the molecules of the solvent ($C_5H_6CH_3$ and CCl_4) in the crystal solvates of the fullerenes C_{60} and C_{70} that form from the solutions have been studied by methods of FT-IR-spectroscopy, the differential scanning calorimetry and X-ray diffraction. Herewith the thermal stability of crystalline solvate depends on the strain of molecules of solvent that was detected due to the shift of the vibrational absorption bands.

It was shown that under the low-temperature annealing (up to 500°C) crystal solvates are destroyed, which leads to the removal of deformation of the solvent molecules and “loosening” a crystal lattice of the fullerenes when the solvent was evacuated from the fullerites. As the result – the presence of the solvent in fullerites facilitates both the diffusion of the oxygen during heating in the air and the oxidation of the fullerite.

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