Fullerene Clusters in the Systems C60 - Polar Solvents

N.V. Avramenko [C, S], M.V. Korobov, N.I. Ivanova, A.M. Parfenova and O.I. Kiseleva
Department of Chemistry, Moscow State University, Moscow, Russia
natali@td.chem.msu.su

M.V. Avdeev
Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Moscow, Russia

Solutions of fullerenes in nitrogen-containing solvent as well as in their mixtures with water constitute a specific class characterized by the formation of fullerene clusters. The specific feature of this class of solvents is the interaction with fullerenes. C60 may form charge-transfer complexes in these solvents, which facilitates its dissolution comparatively strong polarity of the solvent molecules hinders the dissolution. A competition between the two factors together with the complex dissolution kinetics of C60 molecules can be a reason for solvatochromatic effects observed in these systems.

Formation of the clusters is substantial for medical applications of the fullerenes to develop the new ways to transfer fullerenes into aqueous media.

In the present work we demonstrate the aggregation of C60 in the neat N-methylpyrrolidone (NMP) and in the binary solvents NMP – H2O. NMP is completely miscible in water. NMP with the dielectric constant 32 is a powerful solvent for C60. Strong evidences of the non-equilibrium behavior were found in all systems studied. The aggregation process was followed in time with the UV-visible spectroscopy, dynamic light scattering (DLS), small angle neutron scattering (SANS). The solutions of C60 in NMP (up to 1000 μM) were prepared by gentle stirring during four days at room temperature. Ternary solutions C60/NMP/H2O (up to 500 μM of C60) were prepared by water dilution of C60/NMP system. Changes in the UV-vis spectra of C60/NMP solution showed changes during one month after the preparation (slow solvatochromic effect) reflecting the formation of the clusters in the system. DLS revealed clusters with a characteristic size of 500 nm.

SANS study shows that large stable clusters (size > 100 nm in the C60 – NMP solution partially dissociate into smaller ones (size < 100 nm) on addition of water. The effect has a sharp character when the water content in the system approaches 40 vol %. The contrast variation indicates that these clusters are close to fullerene crystals or highly packed amorphous structures of fullerene molecules.

Solid solvate crystals were not detected in the C60 – NMP system by means of DSC.

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