Molecular correlations in bulk star-shaped polystyrene with fullerene C_{60} center

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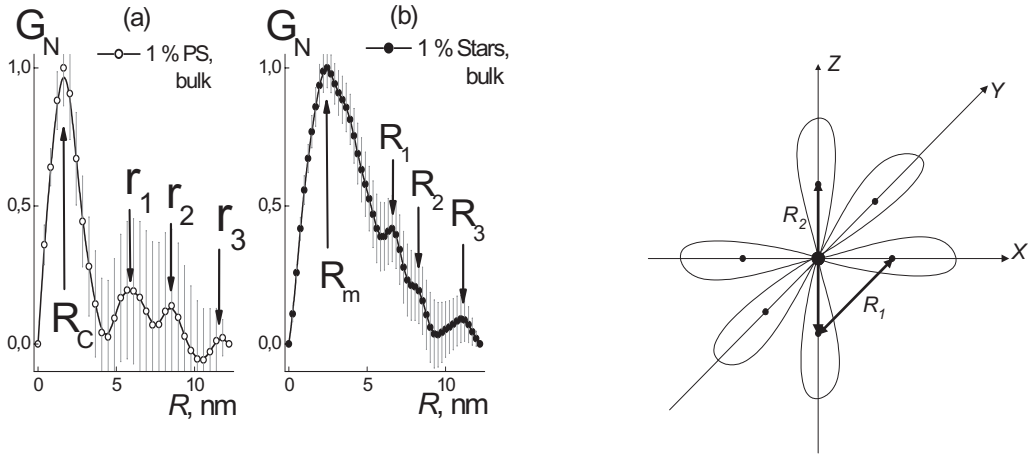
Deuterated Star-shaped Polystyrenes [1], $(PS)_6C_{60}$, dissolved in protonated analogs (1; 10%), have been studied (20°C) by small-angle neutron scattering as well as linear chains with arm's mass $M_A \sim 5\cdot10^3$. Using spatial correlation functions of chain units $G_N(R)$ in "stars" regarding to linear PS (Figures b and a) we have developed a model of "star" where the arms' centers lay at the orthogonal axes (X,Y,Z) with origin attached to fullerene and the distances between neighboring arms' centers obey the condition $R_2/R_1 = \sqrt{2}$ confirmed experimentally, $R_2/R_1 \approx 1.3$. The labeled "stars" contact in matrix when their centers are at the distance close to diameter $R_3 \approx 11$ nm. Meanwhile, the association of labeled linear PS (Figure a) is described by the model of hard spheres dense package confirmed by correlation maxima positions (r_1,r_2,r_3) corresponding to distances h, $\sqrt{3}\cdot$h, 2h … where $h = \sqrt{18}\cdot R_C$ is the coil diameter defined by its correlation radius $R_C \approx 1.6$ nm. This allows us to conclude that synthesis creates via covalent bonding a compact "star" (correlation radius $R_C \approx$ 2.4 nm) which neighboring arms interact like PS-coils in solution by centers separation $R_1 \sim r_1$, while the distance between the centers of opposite arms (along X,Y,Z axes) is rather large, $R_2 \approx 8.3$ nm $> r_1$. It indicates a stretched arms' conformation in "stars".



[1] V.T. Lebedev, L.V. Vinogradova, Gy.Török. *Polymer Sci. Ser. A.* **50**, 1089 (2008).