Ordering of hydroxylated fullerenes in aqueous solutions

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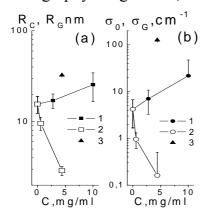
Water-soluble derivatives of fullerenes $C_{60}(OH)_X$ have been studied in aqueous solutions (25°C, pH = 5-8, addition of sodium citrate or phosphate) to examine molecular self-organization via van-der-Waals forces and hydrogen bonds by small-angle neutron scattering. There were used the solutions of $C_{60}(OH)_X$ (X ~ 20, concentration $C_F = 0.5$ mg/ml in H_2O , pH=5), the systems containing also sodium citrate (c = 2.8 mg/ml, pH = 6; c = 10 mg/ml, pH = 7). Salt addition caused a stronger clustering and the increase of scattering cross sections

$$dy/dIII = y(q) = y_0/[1 + (R_C q)^2]^{D/2},$$
(1)

at momentum transfers $q=0.08\text{-}4.4~\text{nm}^{\text{-}1}$. Here y_o is forward cross section, $R_C\sim 16\text{-}25~\text{nm}$ is the size of cluster. The exponent D =4 indicates globular clusters. The system with the amount of sodium phosphate c=0.6~mg/ml has demonstrated the scattering described by the function (1), but at the content of sodium phosphate c=4.4~mg/ml the scattering became stronger by 2 orders in magnitude

$$y(q) = y_o/[1 + (R_C q)^2]^{D/2} + y_G \exp[-(R_G q)^2/3].$$
 (2)

The 1st component does not differ from the function (1), the 2nd one depends on forward cross section y_G and the gyration radius R_G of large structures. The parameters of functions (1), (2) for solutions with different salts are displayed in Fig. The association of fullerenes in aqueous solutions can be varied using additives to regulate the interactions of fullerenes. The evaluation of peculiarities of fullerenes association is important for medical applications: contraSt agents for Nuclear Magnetic Tomography Diagnostics, carriers of medicine etc.



Parameters of scattering functions (1) and (2): forward cross sections (a) and radii (b). Notations: 1 – data for solutions with sodium citrate; 2 and 3 – data for solutions with sodium phosphate (parameters of the 1St and the 2nd components of scattering function (2).