Poly(N-vinyl caprolactam) - C_{60} complexes in aqueous solution

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In aqueous solution Poly(N-vinylcaprolactam) (PVCL) serves for biomolecules encapsulation by coil-globule transition above $T_C \sim 31°C$. It seems reasonable to modify PVCL by fullerenes assuming their antiviral activity. The complex PVCL+C_{60} (1.8 % mas. of C_{60} in dry polymer, mass $M = 2.8 \cdot 10^5$) has been prepared, solved in D_2O (concentration C=0.5 % mas.) and studied around coil-globule transition by neutron scattering. The cross sections $\sigma_P(q) = I_r/[1+(r_L q)^2]$ for pure PVCL and $\sigma_C(q) = I_r/[1+(r_C q)^2] + I_R/[1+(R_C q)^2]^2$ for complexes depend on momentum transfer q = 0.1-4 nm^{-1} and forward cross sections I_r, I_R. The length $r_L \sim 10$ nm defines PVCL-coil gyration radius $r_G = r_L \cdot \sqrt{3}$. Complexes being globular even below T_C indicate the preordering induced by C_{60}. The $\sigma_C(q)$ contains the term attributed to globular core (size $R_C \sim 7$ nm $\geq r_C \sim 3$ nm). Below T_C the size of globules $R_C \sim 7$ nm is smaller than PVCL-coils radius, $r_L \sim 10$ nm. By collapse the globular size comes down, $R_C \rightarrow 5$ nm, but the length $r_C \sim 3$ nm remains at segmental level since it is related to fragments not incorporated into the core. Along with very different scattering at coil scale PVCL and complexes show the exponential law $\sigma(q) \sim 1/q^D$ at $q \geq 1$ nm^{-1}. The exponent D indicates local chains conformation (D=2, D_{EX}=5/3, D=1 for gaussian, excluded volume and strained chain). At 20°C the values of D_{PVCL} and D_{COM} are close to parameter D_{EX} =5/3 for excluded volume chain. The heating, 20°C $\rightarrow$ 31°C ~ T_C, leads to exponents' increase from $D_{PVCL}(T) \sim 1.6$ and $D_{COM}(T) \sim 1.5$ to larger values D ~ 1.7-1.8 that means the approach to θ-conditions (solvent quality becomes worse). On the other hand, above T_C the complexes are shrunken, but their segments get strained conformation, $D(T) \rightarrow 1$, due to strong chains' interactions. Summarizing the neutron scattering results we conclude that fullerenes stabilize collapsed state that reinforces the functional properties of PVCL regarding encapsulation.