Supporting Information

Influence of Corona Structure on Binding of an Ionic Surfactant in Oppositely Charged Amphiphilic Polyelectrolyte Micelles

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The evaluation of the SAXS curve

The SAXS curve was fitted using the SASfit 0.93.3 software.[1] The following model was used for the fitting:

$$I(q) = NS(q)I_{\mathrm{mic}}(q) + \frac{I_{\mathrm{fluct}}}{1+\xi^2 q^2} \tag{1}$$

where I_{fluct} is the forward scattering intensity and ξ is the correlation length for the short range fluctuations, N is the number of the micelles in the unit volume $I_{\mathrm{mic}}(q)$ is the scattering function of the single micelle and $S(q)$ is the structure factor of the micellar solution.

The scattering from the micelle is approximated by the form factor of homogeneous spherical shell with the Gaussian distribution of the core radii:

$$I_{\mathrm{mic}}(q) = \int_0^\infty \sqrt{\frac{\pi}{2}}\sigma\left[1+\mathrm{erf}\left(\frac{R}{\sqrt{2}\sigma}\right)\right]^{-1} \mathrm{e}^{-\frac{(R-R_0)^2}{2\sigma^2}} \left[F(q,R+\Delta R,\Delta\eta_2) - F(q,R,\Delta\eta_2-\Delta\eta_1)\right]^2 \mathrm{d}R \tag{2}$$

Here R_0 is the mean core radius and σ is the FWHM of the distribution, ΔR is the shell thickness, $\Delta\eta_1$ and $\Delta\eta_2$, respectively, are the excess scattering length densities for the core and the shell, and the $F(q, R, \Delta\eta)$ function is given by the relationship:

$$F(q,R,\Delta\eta) = 4\pi R^3 \Delta\eta \frac{\sin(qR) - qr\cos(qR)}{q^3 R^3} \tag{3}$$

The structure factor of the micelles was approximated as the structure factor of hard spheres,

$$S(q) = \left[1 + 12\varphi \frac{G(\varphi, r)}{qr}\right]^{-1} \tag{4}$$

where r is the interaction radius, φ is the volume fraction of the spheres and the $G(\varphi,r)$ function has the form

$$\begin{aligned} G(\varphi,r) = {} & \left[\frac{1+2\varphi}{(1-\varphi)^2}\right]^2 \frac{\sin(2qr) - 2qr\cos(2qr)}{(2qr)^2} - \\ & - 6\varphi\left[\frac{1+\varphi/2}{(1-\varphi)^2}\right]^2 \frac{2qr + (2-4q^2R^2)\cos(2qr) - 2}{(2qr)^3} + \\ & + \frac{\varphi}{2}\left[\frac{1+2\varphi}{(1-\varphi)^2}\right]^2 \frac{4\left[(12q^2r^2 - 6)\cos(2qr) + (8q^3r^3 - 12qr)\sin(2qr) + 6\right] - (2qr)^4\cos(2qr)}{(2qr)^5} \end{aligned} \tag{5}$$

(1) Software package SASfit for fitting small-angle scattering curves.
https://kur.web.psi.ch/sans1/SANSSoft/sasfit.html