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Small angle scattering: scaling cross-sections and widening the q-window to answer scientific questions

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We will recap published and unpublished work initiated on D11, D17 and D1B with J.B. Hayter: what happens at low-q and high-q for common and uncommon ionic micelles made from self-assembled amphiphiles in a given solvent?

In the standard SAS range, the Hayter-Penfold decoupling procedure work well for all ionic micelles investigated as long as the chain length is not too short or too long.

As suggested by Luzzati, the absolute scale was crucial to go beyond wild shape fitting of a broad peak with unphysical parameters: from then, the micellar growth controlled by the area per molecule in the lateral equation of state was understood.

But there are still fully open questions, even after 50 years of active X-ray/neutron work on "simple" systems that were not fully understood last century, even for systems where an apparent implicit consensus on unproven facts are favored by the absence of absolute scale and comparison of the results with models.

We will give three examples:

- At high-q, in the range 0.4 $Å^{-1}$ to 0.6 $Å^{-1}$, there is only very few published work about localization of methyl end-groups and this only for saturated aliphatic chains.[1]
- At low-q, there is sometimes an elusive intensity upturn following q^{-1} or q^{-2}:[2] this may be related to flexible necklaces of "flocculated" micelles with threadlike images in electron microscopy, common in the case of magnetic nanoparticles, as suggested by J.B. Hayter and R. Pynn.[3] Their domain of existence as a function of ionic strength is not yet identified.
- there are several observation of non-spherical micelles close to cmc. Theoreticians don't believe experimentalists observations because it is contradictory with elastic theory. We suggest that taking the chain packing as well as the head elastic contributions with one parameter, and not only one with two unphysical bending constants of a molecular film, may solve this long-standing scientific problem.

As always, a broad q window and comparing data on absolute scaled with different predictive models lead to solid scientific progress beyond multiparametric fitting with or without Fourier transforming the data.

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2. B. Hammouda, J Res Natl Inst Stand Technol. 2013; 118: 151–167, DOI: 10.6028/jres.118.008
3. W. A. Hamilton, P. D. Butler, S. M. Baker, G. S. Smith, John B. Hayter, L. J. Magid, and R. Pynn, Phys. Rev. Lett. 74, 335 (1995), DOI: 10.1103/PhysRevLett.72.2219

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