

Supporting Information

Comparison of Small Angle Scattering Methods for the Structure Analysis of Octyl- β -maltopyranoside Micelles

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Section 1s -Volumetric Properties of OM

Table 1s summarizes the apparent molar volume of OM in water at different temperatures. The data obtained with D₂O were given in Table 2s for comparison. It was found that the apparent molar volume in D₂O is close to that in H₂O. By fitting the data in Table 1s, the parameters V_{ϕ}^0 , a and b in eq 3 were obtained, which are summarized in Table 3s. Using these parameters, the partial molar volume of OM, \bar{V} , were calculated by eq 4.

The Tanford method gives the volume of hydrocarbon chain at 25 °C (see eq 5). To get the value at a different temperature, a correlation procedure was carried out by combining the Gunn et al. method¹ with the Chueh et al method.¹ It is known that these two methods were proposed for bulk liquid hydrocarbon. However, since the state of liquid hydrocarbon in the micelle core is close to that in bulk liquid hydrocarbon,² this procedure is reasonable. For a given temperature, the ratio of the saturated molar liquid volume to that at 25 °C was calculated using the Gunn et al. method. Then, this ratio was used in the Chueh et al. method to get the liquid density at the pressure of 1 atm using the density value at 25 °C as the reference. From the liquid density data, the volume of a hydrocarbon chain at the desired temperature was obtained. The vapor pressure needed in the Chueh et al. method was

obtained by the Antoine vapor-pressure equation, and all other parameters were obtained from the reference 1.

As the molecular volume and hydrocarbon chain volume are known, the head group volume can be calculated via

$$v_h = v_{mol} - v_c \quad (1s)$$

The molecular volume, hydrocarbon chain volume and the head group volume at different temperatures were summarized in Table 4s.

Section 2s- SAXS data

Figure 1s. Effect of temperature on SAXS scattering curves. $c = 96.5$ mM, solvent: H₂O.

Figure 2s. Effect of temperature on SAXS scattering curves. $c = 97.4$ mM, solvent: D₂O.

Figure 3s. Comparison of $p(r)$ function from SAXS data in H₂O and D₂O at 25 °C. In H₂O, $c = 96.5$ mM; In D₂O, $c = 97.4$ mM.

Figure 4s. Comparison of $p(r)$ function from SAXS data in H₂O and D₂O at 50 °C. In H₂O, $c = 96.5$ mM; In D₂O, $c = 97.4$ mM.

References in Supporting Information

- 1) Reid, R.; Prausnitz, J. M.; Sherwood, T.K. *The Properties of Gas and Liquids*; 3rd Edition; McGraw-Hill Book Company: New York, 1977
- 2) Tanford, C. *The Hydrophobic Effect: Formation of Micelle and Biological Membranes*; John Wiley & Sons: New York, 1980

Table 1s Apparent molar volume of OM in H₂O, V_{ϕ} , at different temperatures

| C (mol.kg ⁻¹) | V_{ϕ} , (cm ³ .mol ⁻¹) | | | | | | | |
|---------------------------|--|-------|-------|-------|-------|-------|-------|-------|
| | 10 °C | 15 °C | 20 °C | 25 °C | 30 °C | 35 °C | 40 °C | 50 °C |
| 0.01007 | 336.8 | 338.0 | 339.6 | 341.8 | 343.4 | 345.1 | - | - |
| 0.01547 | 335.6 | 337.7 | 339.4 | 341.7 | 343.4 | 344.7 | - | - |
| 0.01818 | 335.5 | 337.8 | 339.9 | 341.3 | 343.4 | 345.1 | - | - |
| 0.02046 | 335.9 | 338.0 | 339.9 | 341.6 | 343.5 | 345.1 | - | - |
| 0.02500 | 336.7 | 338.9 | 340.8 | 342.7 | 344.8 | 346.5 | 348.3 | 351.3 |
| 0.02562 | 336.4 | 338.5 | 340.9 | 342.7 | 344.7 | 346.4 | - | - |
| 0.03077 | 336.6 | 339.1 | 341.4 | 343.6 | 345.7 | 347.5 | - | - |
| 0.03503 | 337.8 | 340.6 | 342.9 | 345.2 | 347.0 | 348.7 | 350.4 | 353.4 |
| 0.04145 | 338.6 | 341.1 | 343.4 | 345.4 | 347.2 | 349.0 | - | - |
| 0.04398 | 339.6 | 342.3 | 344.4 | 346.3 | 348.3 | 350.0 | 351.4 | 354.3 |
| 0.05196 | 340.8 | 343.2 | 345.5 | 347.3 | 349.1 | 350.5 | - | - |
| 0.05769 | 340.7 | 343.1 | 345.2 | 347.0 | 348.7 | 350.4 | 351.8 | 354.6 |
| 0.08218 | 343.3 | 345.5 | 347.3 | 349.0 | 350.6 | 352.2 | 353.6 | 356.3 |
| 0.10022 | 344.6 | 346.6 | 348.4 | 350.1 | 351.6 | 353.1 | 354.4 | 357.1 |
| 0.11678 | 344.8 | 346.8 | 348.5 | 350.1 | 351.6 | 353.0 | 354.4 | 357.0 |
| 0.14732 | 345.5 | 347.3 | 349.0 | 350.5 | 352.0 | 353.4 | 354.7 | 357.4 |
| 0.19952 | 346.5 | 348.2 | 349.8 | 351.3 | 352.7 | 354.1 | 355.5 | 357.9 |

Table 2s Apparent molar volume of 0.0914 mol.kg⁻¹ OM in D₂O at different temperatures

| | 10 °C | 15 °C | 20 °C | 25 °C | 30 °C | 35 °C | 40 °C |
|--|-------|-------|-------|-------|-------|-------|-------|
| V_{ϕ} (cm ³ .mol ⁻¹) | 343.2 | 345.5 | 347.4 | 348.6 | 349.8 | 351.7 | 353.9 |

Table 3s Fitting parameters for calculation of the partial molar volume^a

| | 10 °C | 15 °C | 20 °C | 25 °C | 30 °C | 35 °C | 40 °C | 50 °C |
|---|--------|--------|--------|--------|--------|--------|--------|--------|
| V_{ϕ}^0 (cm ³ .mol ⁻¹) ^b | 328.9 | 329.6 | 330.9 | 333.0 | 334.8 | 336.47 | 338.8 | 342.3 |
| a (cm ³ .mol ^{-1.5} .kg ^{0.5}) | 58.11 | 72.52 | 79.84 | 79.02 | 79.86 | 80.48 | 76.98 | 73.48 |
| b (cm ³ .mol ⁻² .kg) | -38.30 | -66.74 | -82.93 | -84.47 | -89.10 | -92.17 | -89.93 | -87.18 |

^a The application of these parameters should be restricted in the measured concentration region in Table 1s.

^b V_{ϕ}^0 is only a fitting parameter here, and it does not correspond to the partial molar volume at infinite dilute solution.

Table 4s Molecular volumetric properties of OM at different temperatures

| T (°C) | Molecular volume* hydrocarbon chain head group | | |
|--------|--|--------------------------------|--------------------------------|
| | v_{mol} (Å ³) | volume v_c (Å ³) | volume v_h (Å ³) |
| 10 | 579.5 | 238.4 | 341.1 |
| 15 | 582.4 | 239.8 | 342.6 |
| 20 | 585.0 | 241.2 | 343.8 |
| 25 | 587.3 | 242.6 | 344.7 |
| 30 | 589.5 | 244.1 | 345.4 |
| 35 | 591.7 | 245.5 | 346.2 |
| 40 | 593.6 | 247.0 | 346.6 |
| 50 | 597.6 | 250.1 | 347.5 |

* calculated from partial molar volume at 100 mM.

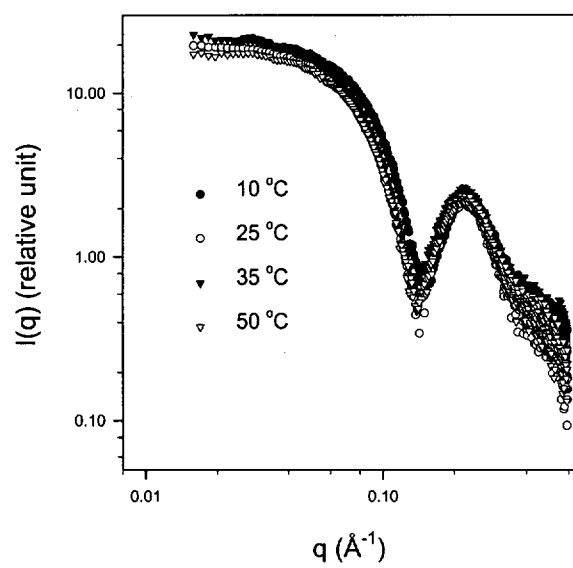


Figure 1s

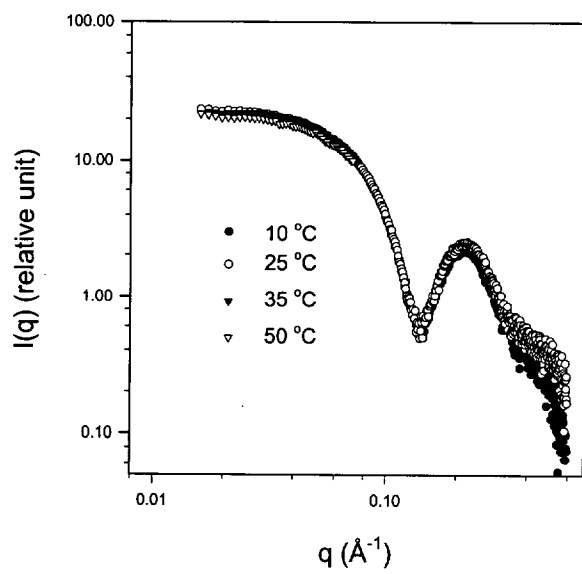


Figure 2s

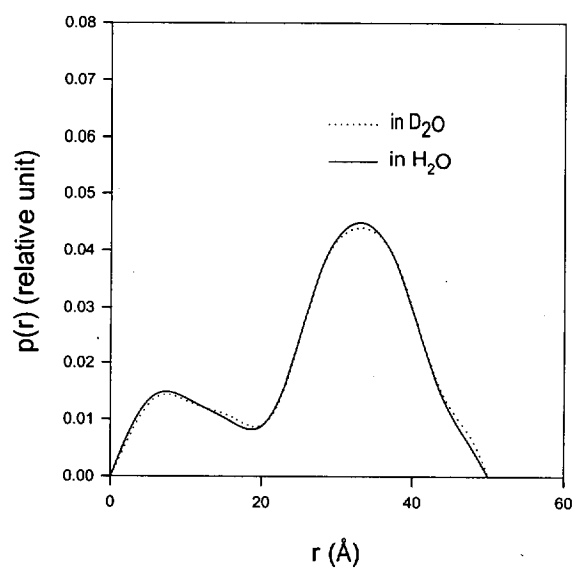


Figure 3s

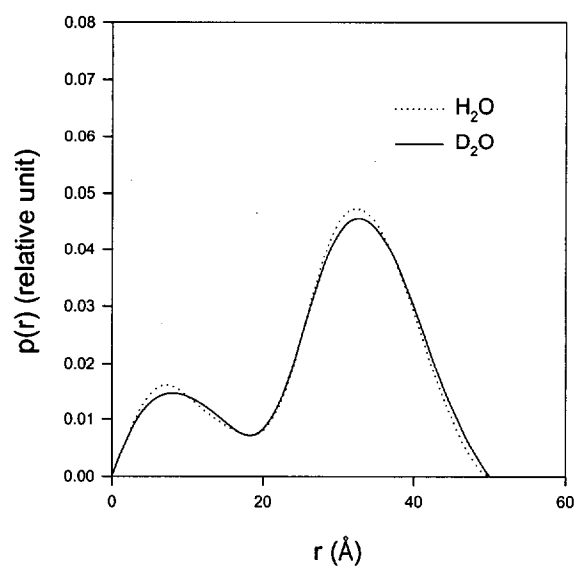


Figure 4s