Appendix 4: Shape of Self-Assembled Amphiphilic Structures

Shape of Self-Assembled Amphiphilic Structures

In the classical description, the factor determining the shape of self-assembled amphiphilic structures is the size of the hydrophobic moiety relative to the hydrophilic part. It determines the curvature of the hydrophobic-hydrophilic interface as described by its mean curvature $H$ and its Gaussian curvature $K$, which are given by the two radii of the curvature $R_1$ and $R_2$, as shown in Figure 1. The curvature is related to the surfactant packing parameter by

$$\frac{\nu}{al} = 1 + Hl + \frac{(Kl^2)}{3}$$  \hspace{1cm} (1)

where $\nu$ is the hydrophobic volume of the amphiphile, $a$ the interfacial area and $l$ the chain length normal to the interface (Figure 1).

![Figure 1. Description of amphiphile shape in terms of the surfactant parameter $\nu(al)$ and its relation to the interfacial mean curvature ($H$) and Gaussian curvature ($K$).](image)

The simplest shapes are spheres, cylinders and bilayers, which are characterized by certain values of the packing parameter and curvature as shown in Table 1.
Appendix 4: Shape of Self-Assembled Amphiphilic Structures

Table 1. Packing parameter, mean curvature $H$ and Gaussian curvature $K$ for aggregation structures of different shapes.

<table>
<thead>
<tr>
<th>Shape</th>
<th>$\nu(al)$</th>
<th>$H$</th>
<th>$K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>$1/3$</td>
<td>$1/R$</td>
<td>$1/R^2$</td>
</tr>
<tr>
<td>Cylinder</td>
<td>$1/2$</td>
<td>$1/(2R)$</td>
<td>$0$</td>
</tr>
<tr>
<td>Bilayer</td>
<td>$1$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
</tbody>
</table>

Remarkably, flexible amphiphiles can reconcile molecular demands with curvature and shape of the assembly by “soft” molecular rearrangements.

Reference