ARRANGEMENT OF SMALL MOLECULES IN AMPHIPHILE AGGREGATION SYSTEM

K. VONGBUPNIMIT, K. NOGUCHI AND K. OKUYAMA

*Faculty of Technology, Tokyo University of Agriculture and Technology, Tokyo
184, Japan*

Structural informations for the complexes between an amphiphile and a small molecule are essential for the study of their chemical and physical properties. Amphiphile molecules were packed in the interdigitated fashion either among themselves or combination with small molecules. The interdigitated conformation seemed to depend on the cross-section balance between the hydrophilic head group and hydrophobic tail part.

In this work, the crystal structure of dodecyltrimethylammonium chloride/hydroquinone (DTAC/HQN; $\text{CH}_3(\text{CH}_2)_{11}\text{N}^+(\text{CH}_3)_3\text{Cl}^-/\text{p-C}_6\text{H}_4\text{O}_2 \cdot 2\text{H}_2\text{O}$) and dodecyltrimethylammonium chloride/catechol (DTAC/CTC; $\text{CH}_3(\text{CH}_2)_{11}\text{N}^+(\text{CH}_3)_3\text{Cl}^-/\text{o-C}_6\text{H}_4\text{O}_2 \cdot 2\text{H}_2\text{O}$), have been determined using a four-circle diffractometer (Rigaku AFC5R) with graphite monochromatized $\text{CuK}\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$). The crystal data are shown in Table 1. Their geometries were found to exhibit normal geometries. The observed density of these complex crystals suggested the existence of two water molecules in each complex molecule. These were also found in the D-Fourier map. The packing structures of these complexes are arranged in the interdigitated fashion. The guest small molecules, i.e., HQN and CTC located between the interdigitated host amphiphile molecules, i.e., DTAC as shown in Fig.1.

Table 1. Crystal data of DTAC/HQN and DTAC/CTC complexes

	DTAC/HQN	DTAC/CTC
Empirical Formula	$\text{C}_{21}\text{H}_{44}\text{O}_4\text{NCl}$	$\text{C}_{21}\text{H}_{44}\text{O}_4\text{NCl}$
Formula Weight	410.04	410.04
Crystal Color	Colorless	Colorless
Crystal System	Monoclinic	Monoclinic
Lattice Parameter	$a = 7.121(2) \text{ \AA}$ $b = 45.099(5) \text{ \AA}$ $c = 8.208(2) \text{ \AA}$ $\beta = 108.96(2)^\circ$ $V = 2492.8(9) \text{ \AA}^3$	$a = 7.084(4) \text{ \AA}$ $b = 44.271(6) \text{ \AA}$ $c = 8.415(2) \text{ \AA}$ $\beta = 108.98(3)^\circ$ $V = 2495(1) \text{ \AA}^3$
Space Group	$P2_1/n$	$P2_1/n$
Z	4	4
D_x	$1.09(2) \text{ g/cm}^3$	$1.09(1) \text{ g/cm}^3$
D_m	1.10 g/cm^3	1.08 g/cm^3
$F(000)$	904.00	904.00

Figure 1. Molecular packings of complexes