

Structure and dynamics of Amphiphiles

We can learn a significant amount about the uses of a compound when we start researching into the atomic structure and dynamics of the compound. Amphiphiles are compounds designed to take advantage of the fact that most compounds are hydrophilic or lipophilic, meaning that they are dissolved in water or oil, by being both. Amphiphiles are also very important in a wide range of applications, such as drug delivery. It follows then quite logically that, to be able to improve on the applications of amphiphiles we must research more into the atomic structure and dynamics of amphiphiles.

To analyze these structures we use diffractometers. When light diffracts between planes in a crystal, we are going to be faced with an interference pattern of that light. By using detectors we can measure what this interference pattern looks like and then use Bragg's Law to find the distance between the planes which we diffracted in. Diffractometers work by this same principle by using X-rays. Until recently this method was not used a significant amount due to the atoms, in the crystals being measured, absorbing a significant proportion of the light which was used to try and form an interference pattern.

With the development of new technology over the past decade, we have now improved on the diffractometers of the past by implementing two sources of light radiation, at different wavelengths, and also implementing a large detection area. These two improvements in the field, combined with the powerful data analysis tools of today, have meant an incredibly smaller amount of time is required to analyze a crystal and the corresponding atomic structure.

2013 saw the Engineering and Physical Sciences Research Council (EPSRC) award University College London (UCL) with money to update equipment, where UCL Chemistry then allocated £1.1M into updating their X-ray diffractometers. Cationic surfactants are a type of amphiphile which a research team at UCL have been studying the atomic structure of at different temperatures. The paper showed data of the changes in the atomic structure of cationic surfactants 10-alkyl trimethylammonium bromide (C10TAB), C12TAB, C14TAB, C16TAB and C18TAB when varying temperature. By using the new equipment, this research team were able to publish a paper where they showed that cationic surfactants such as C12TAB and C10TAB have different solid phases and also have different crystal structures which depend on temperature.

By being able to analyse crystal structures more efficiently and accurately than before we are able to understand more about why these crystals behave the way they do. This has profound implications in fields like medicine where understanding the behaviour of molecules in specific conditions is important. The UCL research team's paper is an example of this and in fact even the results from that paper were already enough to explain a lot of the results in papers previously published on cationic surfactants.

Jeremy K. Cockcroft, André Shamsabadi, Han Wu and Adrian R. Rennie(1996). Understanding the structure and dynamics of cationic surfactants from studies of pure solid phases. *Physical Chemistry Chemical Physics*. DOI: 10.1039/C9CP04486H