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Mechanism of Bio IOS's Surface Activity and Water Solubility Elucidated, Paving the Way for Broader Applications of Sustainable Surfactants

Kao Corporation's Material Science Research Laboratory has succeeded in identifying the mechanism by which Bio IOS – Kao's independently developed surfactant – manifests its highly surface-active and water-soluble properties. As key functions, "sustainable surfactants" require excellent cleansing ability in addition to being made from sustainable materials. Kao is conducting research on expanding the application of sustainable surfactants while improving their efficacy.

The findings from this research project were published in *RSC Advances*^{*1}, the scientific journal of the U.K.'s Royal Society of Chemistry, and were presented at the IACIS 2022 conference (June 26 to 30, 2022 in Brisbane, Australia) as well as at the 2nd World Congress on Oleo Science (WCOS) 2022 (August 23 to September 3 in Kushiro, Hokkaido, Japan). The study also received the 2021 Highest Award for Academic Paper on Fats and Oils from the Oil & Fat Industry Kaikan Foundation.

*1: Thermodynamically stable structure of hydroxy alkane sulfonate surfactant monomers in water achieving high water solubility and a low CMC, *RSC Advances*, 2021, 11, 19836-19843

■ Background

To continuously support people's enriched life, it is essential to secure sustainable sources of surfactants, which are the main ingredients of detergents. While surfactants are known to have a molecular structure consisting of a lipophilic group (alkyl chain), which has a strong affinity for oil, and a hydrophilic group, which has a strong affinity for water, surfactants in general use today typically have an alkyl chain length of 12 to 14 (C12 to C14) and are made from only 5% of all vegetable oil, so their long-term supply has become a pressing issue.

In 2019, Kao developed Bio IOS (Figure 1), a novel surfactant with a longer alkyl chain (C16 to C18) that has a hydrophilic group located at the middle of the chain^{*2}. Bio IOS is considered to be a sustainable compound because it is made from the solid fraction of palm oil that is not consumed as food so much and has limited applications.

Regarding the basic properties of surfactants, it is important that they possess both high surface activity (affinity for both water and oil) and high water solubility (easy to dissolve in water). If a surfactant has high surface activity, only a small amount is needed to perform a given cleansing task, so its total usage can be reduced. In addition, if

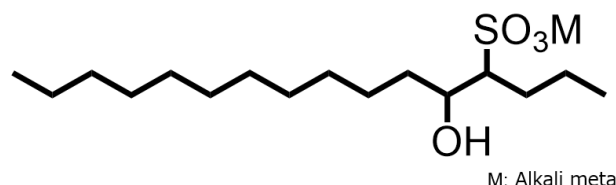


Figure 1: Typical molecular structure of Bio IOS

it is highly soluble in cold and hard water, it can be used virtually anywhere around the world.

Kao believes that demand will continue to rise in the future for this type of sustainable surfactant that not only uses sustainable materials and is less harmful to the natural environment but also possesses both high surface activity that allows consumers to enjoy the same level of cleansing performances as well as high water solubility so that it can be used anywhere in the world. This is why Kao has been conducting research on the essential workings of surfactants while harnessing the full potential of its proprietary Bio IOS, with the ultimate goal of broadening the application of sustainable surfactants and improving their utility.

*2: January 23, 2019 Kao News Release “Kao Develops Bio IOS, to Completely Transform the Concept of Conventional Detergent Bases” <https://www.kao.com/global/en/news/rd/2019/20190123-001/>

■ Bio IOS’s actual stereostructure in water was observed to elucidate how it maintains both excellent surface activity and water solubility

Generally, as the alkyl chain length of a surfactant increases, its surface activity rises but water solubility declines. Conversely, as its alkyl chain length decreases, its water solubility improves but surface activity decreases. Due to this tradeoff, it has been difficult to develop a surfactant that maintains both high surface activity and water solubility. However, Bio IOS has been proven to possess high water solubility as well as excellent surface activity due to its long alkyl chain (Figure 2).

To investigate the mechanism of these characteristics, Kao’s researchers analyzed Bio IOS’s conformation in water^{*3} to test the hypothesis that its spatial molecular structure in water, where detergents are normally used, might differ from that of conventional surfactants.

Analysis using ¹H-NMR^{*4} revealed that Bio IOS’s two alkyl chains of different lengths pointed toward the same direction in water while their roots remained fixed. Analysis using FT-IR^{*5} also revealed that an intramolecular hydrogen bonding was formed between the sulfo group (–SO₃[–]) and the hydroxy group (–OH) within Bio IOS, indicating the formation of this large circular hydrophilic part (Figure 3).

A conventional surfactant with a long alkyl chain tends to become less water soluble as the alkyl chain aggregates. In the case of Bio IOS, however, as the large circular hydrophilic part and the alkyl chains of different lengths become fixed while facing in

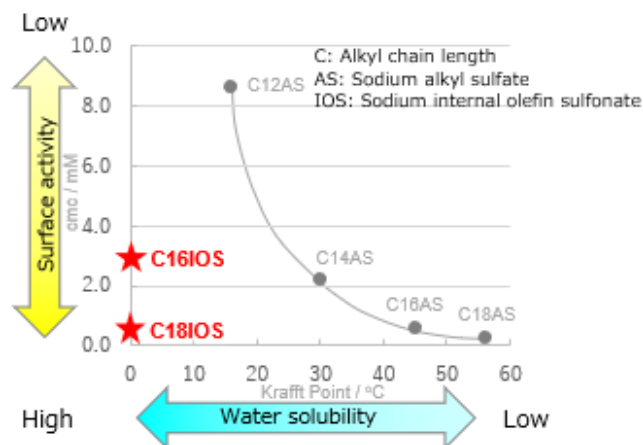


Figure 2: Surface activity and water solubility of conventional surfactants and Bio IOS

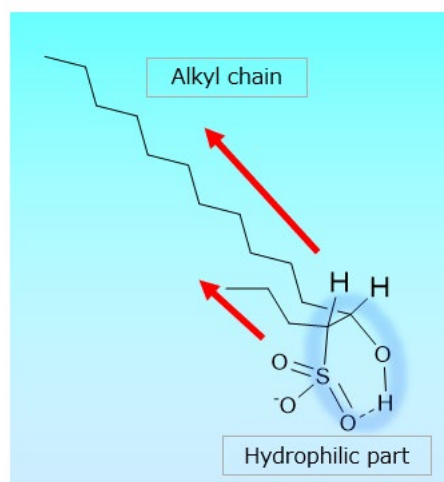


Figure 3: Conformation of Bio IOS in water

the same direction, the alkyl chains' aggregation is interrupted as they act as lipophilic groups, likely allowing Bio IOS to maintain both good surface activity and water solubility.

*3: Spatial arrangement of atoms within molecules and spatial molecular structure

*4: ^1H -Nuclear Magnetic Resonance Spectroscopy is an analytical technique that utilizes the nuclear spin of ^1H (proton) to obtain molecular structure and conformation information based on the environment in which ^1H exists.

*5: Fourier Transform Infrared Spectroscopy is an analytical technique that utilizes the absorption of infrared light induced by the vibration of chemical bonding to obtain information on functional groups.

■ Future outlook

Kao has been marketing its concentrated-liquid laundry detergent Attack ZERO which contains this sustainable surfactant Bio IOS as one of the ingredients. Kao remains committed to conducting research on fundamental technology to continuously build essential knowledge on natural phenomena and to developing products that are truly friendly to both humans and earth, so that people can enrich daily living for generations to come.

About Kao

Kao creates high-value-added products and services that provide care and enrichment for the life of all people and the planet. Through its portfolio of over 20 leading brands such as *Attack*, *Bioré*, *Goldwell*, *Jergens*, *John Frieda*, *Kanebo*, *Laurier*, *Merries*, and *Molton Brown*, Kao is part of the everyday lives of people in Asia, Oceania, North America, and Europe. Combined with its chemical business, which contributes to a wide range of industries, Kao generates about 1,420 billion yen in annual sales. Kao employs about 33,500 people worldwide and has 135 years of history in innovation. Please visit the Kao Group website for updated information.

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