

Simulation on Aggregation Morphology of Gemini Surfactants for Emulsion Explosive in Aqueous Solution

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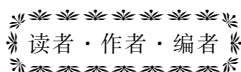
Abstract: Aggregation morphology in aqueous solution on Gemini surfactants usable for emulsion explosive was simulated using the dissipative particles dynamics (DPD) of Material Studio 4.3. Results show that the effect of the structure of spacer group on the aggregation morphology of Gemini surfactants was obvious. The aggregation firstly was transformed from spherical micelles to rod-like micelles, then to lamellar with the increase of the concentration of surfactants. The large and compact micelle was easy to be formed as the increase of the length of hydrophobic carbon chain. When the length of carbon chain was shortened, the trimeric Gemini surfactant was more difficult to form micelles than dimeric Gemini surfactants. When the length of carbon chain was stretched, the trimeric Gemini surfactants was easy to form the rod-like micelles as well as the larger size micelles.

Key words: physical chemistry; dissipative particles dynamics (DPD); Gemini surfactant; aggregation; morphology; simulation

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