

## Aggregation behavior of dicephalic di-N-oxide surfactants in aqueous solution: experimental and computational approaches.

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A series of dicephalic-type 1,1-bis[[3-(N,N-dimethylamino)ethyl]amido]alkane-di-N-oxide surfactants were synthesized and their aggregation behavior in an aqueous environment was described, both experimentally and theoretically. Surface tension and electron paramagnetic resonance (EPR) spectroscopy were applied to monitor the micellization behavior of the studied dicephalic surfactants in aqueous solutions. In the EPR experiments two nitroxide spin probes (5- and 16-doxylstearic acids) were used whereby not only the critical micelle concentrations could be determined, but also the microenvironment of the formed aggregates could be investigated as a function of temperature and surfactant concentration. Furthermore, the size of the micellar aggregates and the polydispersity indexes of the micellar solutions were established by dynamic light scattering (DLS). The structures of the formed aggregates, defined by the critical packing parameter, were predicted using the QSAR approach. The hydrodynamic radii, micellar volumes and aggregation numbers were computed with the long range corrected B3LYP hybrid functional (CAM-B3LYP). In order to put the results obtained for the dicephalics into perspective the experiments and computations were performed for the standard 2-(dodecanoylamino)ethyl dimethylamine-N-oxide.

### Słowa kluczowe

N-oxides, Micellization, Critical micelle concentration, Electron paramagnetic resonance (EPR), Spin probe, Density functional theory (DFT), Molecular modeling

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