Experimental and simulation study of reverse micelles formed by Aerosol-OT and water in non-polar solvents: Electronic Supplementary Information

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(Dated: October 1, 2024)

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OPLS-AA AND CHARGE PARAMETERS FOR AEROSOL-OT

The atom labelling scheme for Aerosol-OT (AOT, $C_{20}H_{37}NaO_7S$) is shown in Fig. S1.

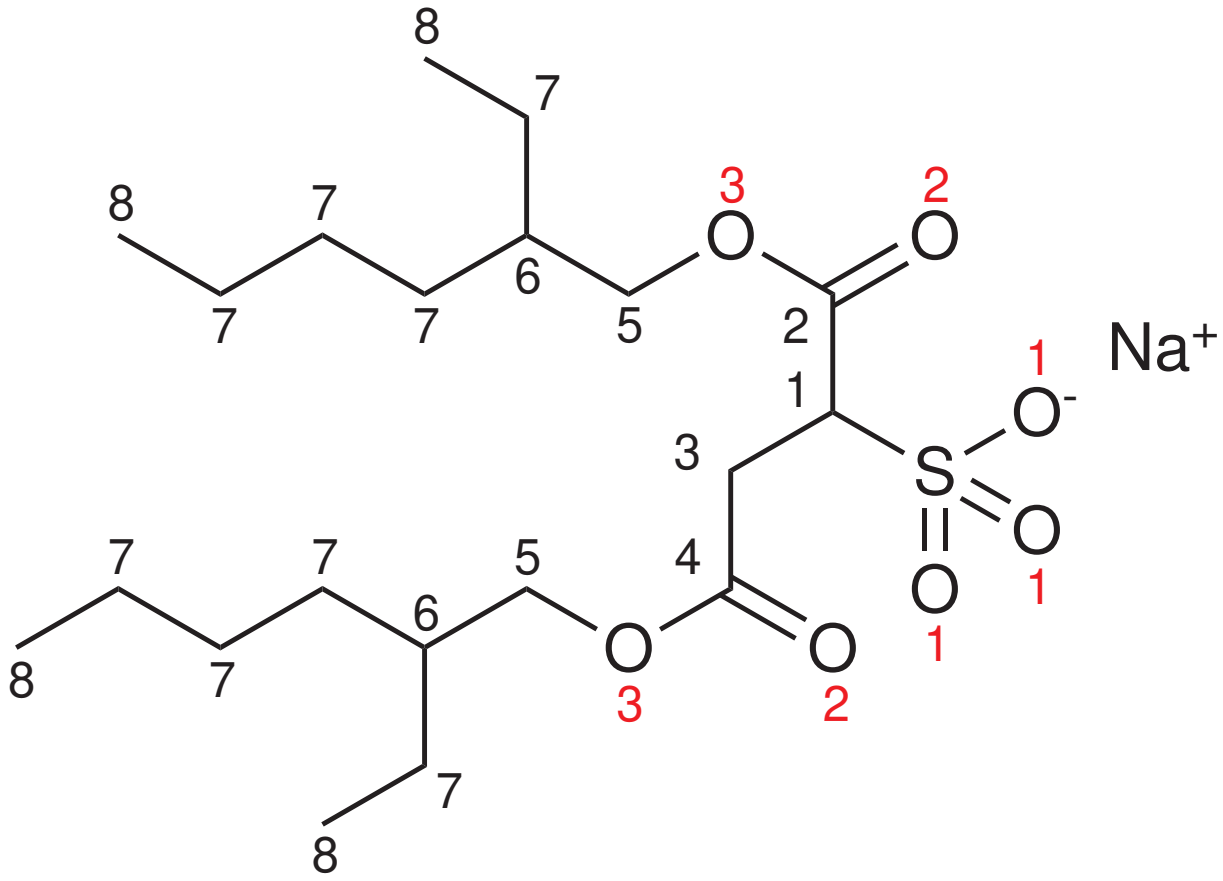

Figure S1. Aerosol-OT molecule with labels used for the purposes of parameterization. Oxygen atom numbers are indicated in red, and carbon and hydrogen atom numbers are in black.

The OPLS-AA Lennard-Jones parameters for the AOT atoms in the sulfonate group were taken from the work by Abdel-Azeim [1]. These are given in Table S1. The partial charges of AOT atoms from C5 and H5 on one side chain to C5 and H5 on the other were determined using DFT calculations as detailed in Section 2.2 of the main article. These are given in Table S2. All other parameters, for AOT and solvents, were taken from the L-OPLS-AA force field [2–6]. Water was described using the TIP3P (Ewald) model [7].

Table S1. Lennard-Jones force field parameters for the sulfonate group, taken from Ref. 1.

label	ϵ [kcal/mol]	σ[Å]
O1	0.17	2.96
O2	0.21	2.96
O3	0.17	3.00
S	0.25	3.55

Table S2. Partial charges for the AOT molecule. Values from C5 and H5 on one side chain to C5 and H5 on the other were calculated from DFT geometry optimization. Values for the tail-group atoms, C6–C8 and H6–H8, were taken from the L-OPLS-AA force field [2–6].

label	charge [e]	index	charge [e]
C1	−0.073	H1	0.07
C2	0.45		
C3	0.416	H3	0.03
C4	−0.148		
C5	0.2305	H5	0.03
C6	−0.06	H6	0.06
C7	−0.12	H7	0.06
C8	−0.18	H8	0.06
Na	1		
O1	−0.66		
O2	−0.423		
O3	−0.345		
S	1.16		

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