Supporting information

for the manuscript

Immersion Depth of Surfactants at the Free Water Surface. A computer Simulation and ITIM Analysis Study

by

Nóra Abrankó-Rideg, Mária Darvas, George Horvai, and Pál Jedlovszky

Table S1. Bond Lengths and Bond Angle Bending Parameters of the Potential Model Used for the Surfactant Molecules.

bond	b_0/Å	angle	ϕ_0/deg	k_ϕ/kJ mol^{-1} rad^{-2}
C-C	1.53			
C-O(H)	1.43			
O-H	1.00			
C-O(S)	1.42			
S-O(C)	1.58			
S=O	1.46			
N-C	1.47			
		CH_3-CH_2-CH_2	111.0	520.4
		CH_2-CH_2-CH_2	109.5	520.4
		C-C-O(H)	109.5	520.4
		C-O-H	108.5	443.0
		C-C-O(S)	109.5	520.4
		C-O-S	112.6	520.4
		O(C)-S=O	102.6	427.1
		O=S=O	115.4	427.1
		C-C-N	111.0	530.0
		C-N-C	109.5	425.0

Table S2. Dihedral Angle Rotation Parameters of the Potential Model Used for the Surfactant Molecules.

dihedral	f	ϕ_0/deg	k_ϕ/kJ mol^{-1}	n
C-C-C-C	1	0.0	5.900	3
C-C-C-O	1	0.0	4.187	3
C-C-O-C	1	0.0	5.900	3
C-C-O-S	1	0.0	3.035	3
C-O-S=O	1	0.0	1.407	3
C-C-C-N	1	0.0	5.900	3
C-C-N-C	1	0.0	5.900	3