

Article

Mix-and-Match Diols: Adjusting Self-Assembly of Micellar Phases in Choline Chloride Eutectics

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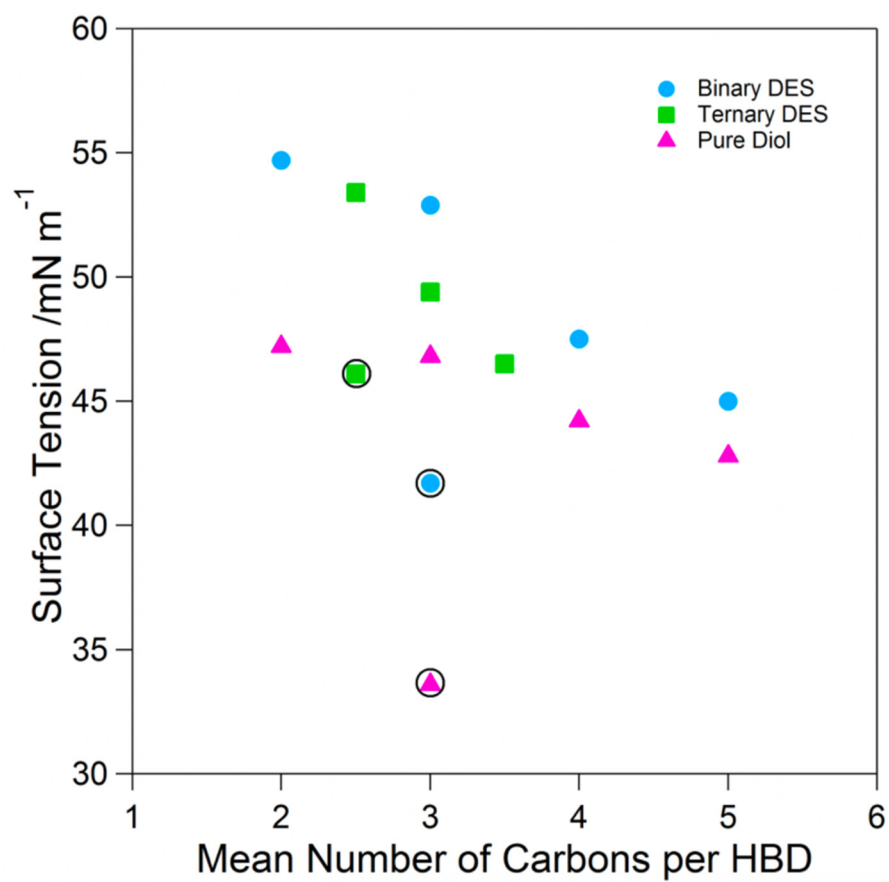


Figure S1. The measured surface tension of ternary and binary DES, and the pure diols, as a function of the mean carbon chain length of the HBD. The encircled datapoints correspond with 1,2-propanediol, to distinguish them from 1,3-propanediol.

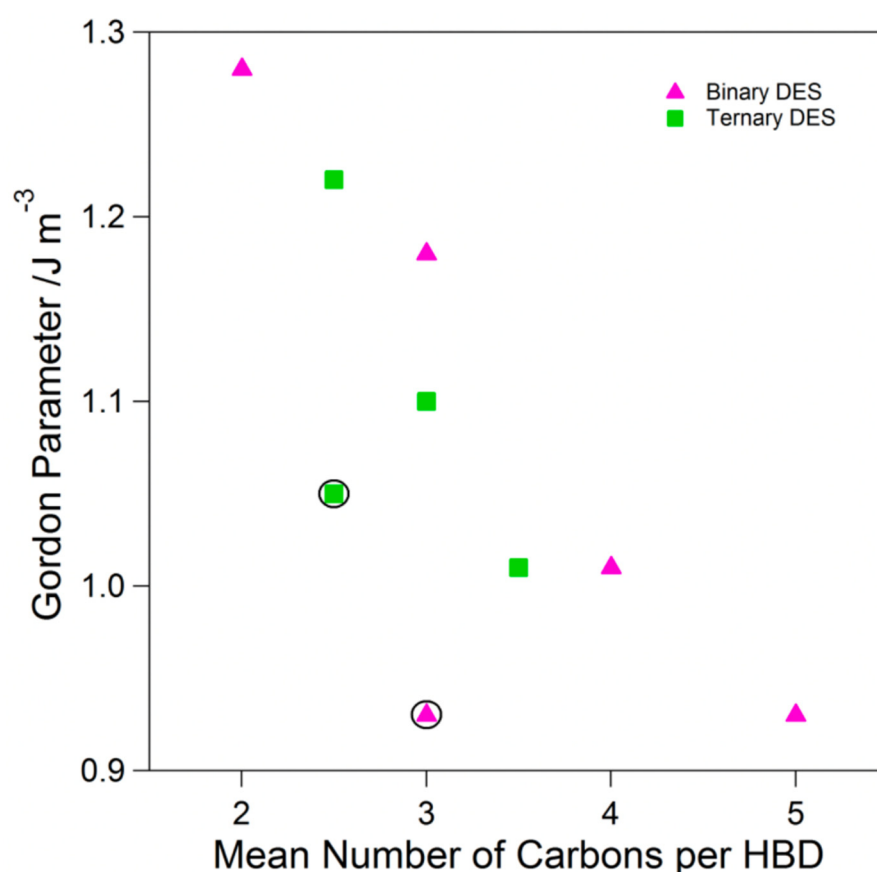


Figure S2. Calculated Gordon Parameter of the prepared DES as a function of mean number of HBD alkyl carbon atoms. As in Figure S1, datapoints are encircled to distinguish 1,2-propanediol.

Table S1. Calculated neutron scattering length densities (SLDs) for the various protonated and deuterated DES components. SLDs were calculated following the procedure reported by Sanchez-Fernandez *et al.* using their reported individual neutron scattering lengths and molecular volumes.[1] For ethylene glycol, scattering lengths, densities, and molecular volumes were derived from the work of Sears,[2] and Azizian and Bashavard.[3].

component	Neutron SLD (10^{-7} \AA^{-2})
H-ethaline	2.75
D-ethaline	59.8
H-C ₁₂ TAB	-3.9
<i>d</i> ₃₄ -C ₁₂ TAB	70.3

Table S2. Calculated X-ray scattering length densities. X-ray SLDs were calculated using the atomic number of the constituent atoms, and the densities of the liquids. Here, the surfactant was just modelled as the alkyl tail, due to the lack of contrast for the headgroup alone.

component	X-ray SLD (10^{-5} \AA^{-2})
ethaline	1.07
2-propethaline	1.06
3-propethaline	1.06
C ₁₂ H ₂₅	1.35

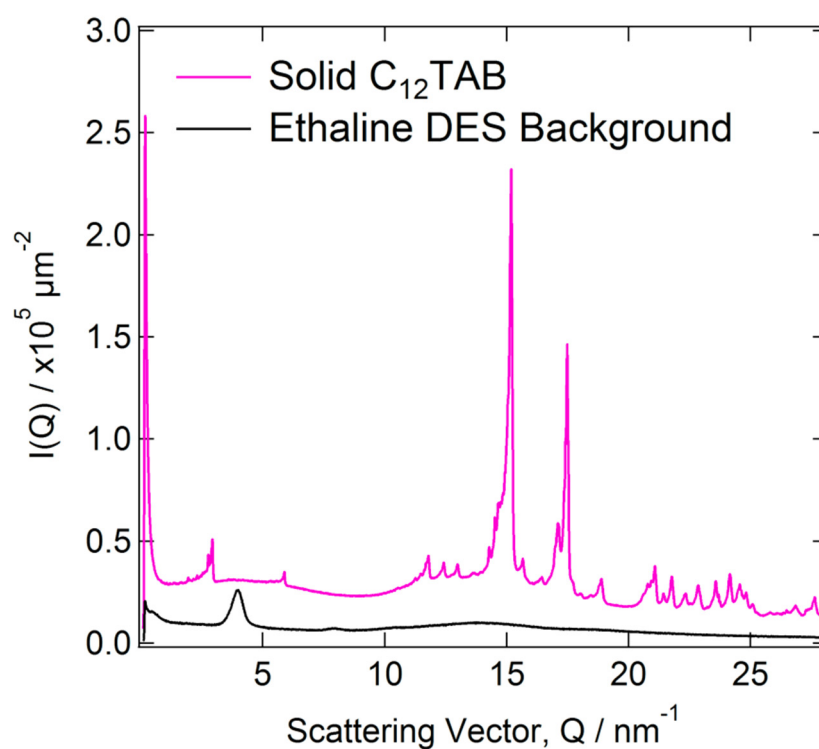


Figure S3. SWAXS data collected for reference samples of pure, solid C_{12}TAB powder at 30°C (pink trace), and pure ethaline DES in a Kapton cell, fully melted at 60°C (black trace). Note that these SWAXS data are displayed on a linear, not log-log scale.

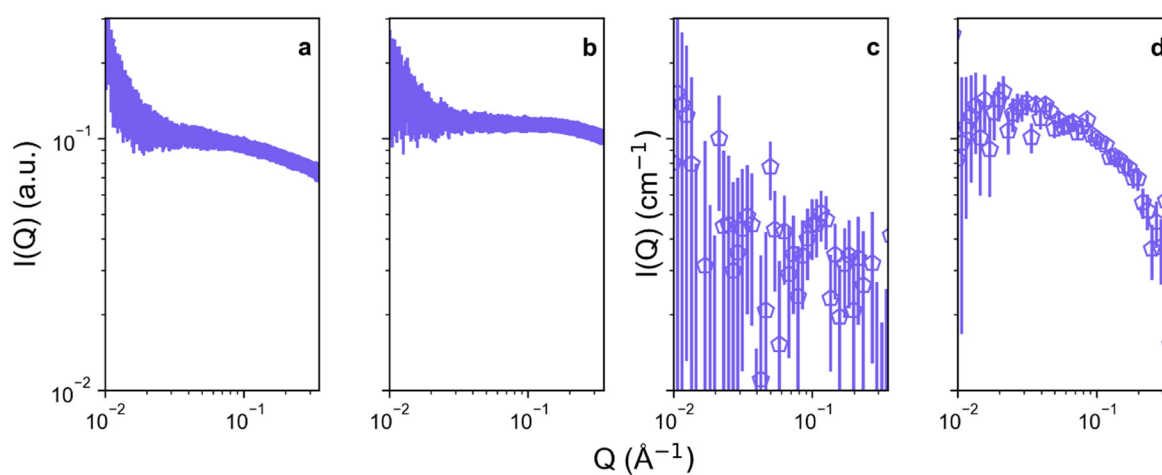


Figure S4. SAXS data of 2 wt.% C_{12}TAB in ChCl:EG (a); SAXS data of 2 wt.% C_{12}TAB in 2-prope-thaline (b); SANS data of 2 wt.% $\text{D-C}_{12}\text{TAB}$ in H-ethaline (c); SANS data of 2 wt.% H- C_{12}TAB in D-ethaline (d). All data are shown with matching x- and y-axis scaling.

References

1. Sanchez-Fernandez, A.; Arnold, T.; Jackson, A.J.; Fussell, S.L.; Heenan, R.K.; Campbell, R.A.; Edler, K.J. Micellization of Alkyltrimethylammonium Bromide Surfactants in Choline Chloride:Glycerol Deep Eutectic Solvent. *Phys Chem Chem Phys* **2016**, *18*, 33240–33249, doi:10.1039/C6CP06053F.
2. Sears, V.F. Neutron Scattering Lengths and Cross Sections. *Neutron News* **1992**, *3*, 26–37, doi:10.1080/10448639208218770.
3. Azizian, S.; Bashavard, N. Surface Properties of Diluted Solutions of Cyclohexanol and Cyclopentanol in Ethylene Glycol. *J. Colloid Interface Sci.* **2005**, *282*, 428–433, doi:10.1016/j.jcis.2004.08.135.