Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Crystallisation of Sodium Dodecyl Sulfate-Water Micellar Solutions with Structurally Similar Additives: Counterion Variation

Ruhina M. Miller[a], João T. Cabral[b], Eric S. J. Robles[c], Nicholas J. Brooks[a], Oscar Ces[*a]

[a]Department of Chemistry and Institute of Chemical Biology-CDT and [b]Department of Chemical Engineering, Imperial College London, London SW7 2AZ, United Kingdom

[c]The Procter & Gamble Company, Newcastle Innovation Centre, Newcastle-Upon-Tyne NE12 9TS, United Kingdom

*o.ces@imperial.ac.uk

Materials

*M*Cl	Supplier	Purity (%)
KCl	VWR	≥ 99.0
RbCl	Acros Organics (Fischer Scientific)	≥ 99.8
CsCl	Sigma-Aldrich	≥ 99.999
$MgCl_2$	Sigma-Aldrich	≥ 98.0
$CaCl_2$	VWR	≥ 99.9
$SrCl_2$	Acros Organics (Fischer Scientific)	≥ 99.0

Table S1. The metal chlorides ("*M*Cl") used to synthesize the dodecyl sulfate salts, the suppliers and purity levels.

Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES)

Experimental

Details of the wavelengths (λ) and viewing configurations used for ICP-OES data collection are listed in Table S2. Other relevant settings include: RF power (1300 watts), solution uptake rate (1.5 ml min^{-1}) and gas flow rates – plasma (15 L min^{-1}), auxilllary (argon/Ar, 0.5 L min^{-1}) and nebulizer (Ar, 0.8 L min^{-1}). For Cs only the following adjustments were made: RF power (800 watts), solution uptake rate (3.0 ml min^{-1}) and auxillary (Ar, 0.2 L min^{-1}); the reduced power and higher solution uptake rate lowers the energy available for the formation of ionic species in the plasma.

M	λ (nm)	Configuration
Ca	317.933	Axial
Cs	894.400	Axial
K	766.490	Axial
Li	670.784	Radial
Mg	285.213	Axial
Na	589.592	Radial
Rb	780.023	Axial
Sr	407.771	Radial

Table S2. λ (nm) and viewing configurations chosen for ICP-OES data collection of the listed metals.

Calculations

ICP-OES was used to determine the percentage of Na and counterion in different samples. To run these the samples had to be diluted significantly. The calculations below detail how the percentage of Na or counterion (K has been used as an example) was determined for an undiluted then diluted sample. Afterwards, these were normalised based on the percentage in the original composition for ease of intepretation, specifically 20% for Na and 1% for the counterions.

Na (M_w) = 22.99 (1.1)

SDS (M_w) = 288.37 (1.2)

Na (%) in SDS = 7.97 (1.3)

Na (%) in 20% SDS = 1.59 (1.4)

Na (%) in 10μL of 20% SDS diluted with 10 ml (10,000 μL) of H_2O = 0.0016 (2.1)

Na (ppm) = 15.94 (2.2)

Na (relative to 20%) = X/15.94*20 (2.3)

K (M_w) = 39.10 (3.1)

KDS (M_w) = 304.48 (3.2)

K (%) in KDS = 12.84 (3.3)

K (%) in 1% KDS = 0.13 (3.4)

K (%) in 10μL of 1% KDS diluted with 10 ml (10,000 μL) of H_2O = 0.00013 (4.1)

K (ppm) = 1.28 (4.2)

K (relative to 1%) = X/1.28*1 (4.3)

Dynamic Light Scattering (DLS)

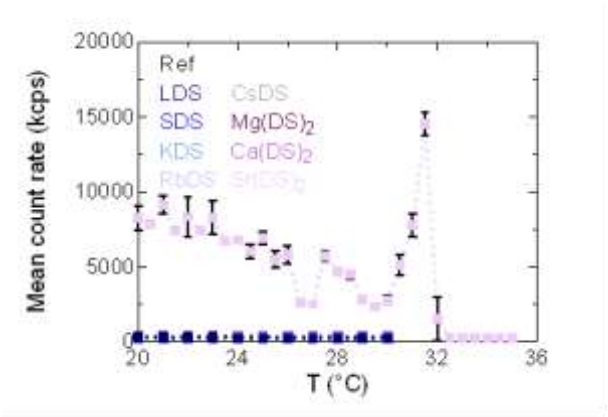

Figure S1. DLS was used as a turbidimeter. Mean count rate (kcps) against temperature for all 20% SDS-H_2O solutions with 1% additive, heated at 1.0 (0.5) °C stepwise intervals to 30 (37) °C for all additives (except $Sr(DS)_2$). The spike for $Sr(DS)_2$ is where the particles are within the spectral window for DLS. The temperature at which the curve flattens off is where the precipitate has fully dissolved: 33 ± 0.5 °C.

Optical Microscopy

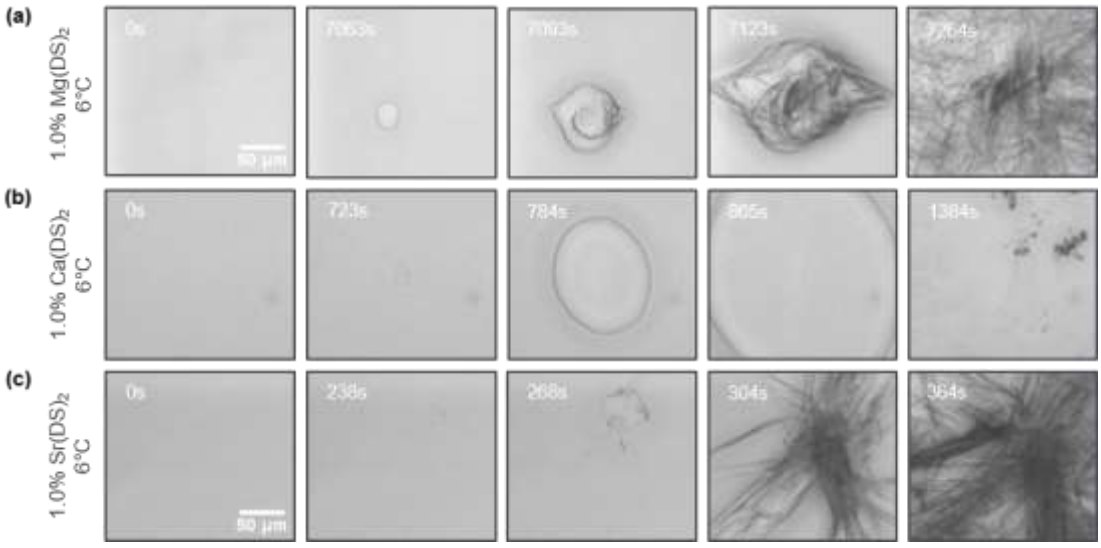

Figure S2. Optical microscopy images showing the crystallization of 20% SDS-H_2O solutions spiked with 1% additive based on group 2 counterions. Samples were quenched to T = 6 °C and held isothermally until crystallisation was complete. (a) $Mg(DS)_2$. (b) $Ca(DS)_2$. (c) $Sr(DS)_2$.