Supplementary Information for "Relationship between Liquid Nanostructure in Solvents and the Strength of the Hofmeister Effect in Extraction Experiments" Mark N. Kobrak, Dmytro Nykypanchuk, and Camiel H. C. Janssen

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### I. Notes on SAXS Methodology and Analysis

# Methodology for Sample Preparation for SAXS Study

Trihexylamine (96%), trioctylamine (98%), octanoic acid (98%), decanoic acid (>99.5%), oleic acid (99%), copper (II) nitrate (*puriss.*), copper (II) chloride dihydrate (≥99%) and copper (II) sulfate pentahydrate (98%) were purchased from Sigma Aldrich and used as received. HPLC-grade water (Sigma) was used to prepare the metal solutions. Amine and acid mixtures were prepared by addition in the appropriate mole ratio, followed by vortex mixing (Fisher Vortex Genie II) for 2 minutes and subsequent mixing for 1 hour on a New Brunswick Scientific C25 Incubator Shaker at room temperature. Mixtures were left resting overnight. Copper salt solutions were prepared in 100 mM concentrations. Extraction experiments were performed by weight as described in the Methodology section. Samples were mixed for 2 minutes on a vortex mixer (Vortex Genie II) followed by 1 hour of shaking on a New Brunswick Scientific C25 Incubator Shaker. Samples were centrifuged using a Sorvall Evolution Centrifuge at 3500 RPM, and separated by syringe.

# Notes on the Interpretation of SAXS Experiments

It would be desirable to use the strength of the scattering signal to gain insight on the extent of nanostructure in the system, but this is problematic. The scattering contrast depends on elemental composition of nanostructure. The experiments incorporate different inorganic anions, each with different x-ray scattering cross-sections, and there is no way to be certain what fraction of the extracted copper ion or inorganic anion might be associated with the liquid nanostructure, as opposed to being distributed randomly through the solution (and therefore invisible to the SAXS experiment).

#### **II. Experimental SAXS Data**



**Figure S1**: SAXS results for trihexylamine/octanoic acid mixtures after extraction from 100 mM stock solution. Top: 3 Amine:1 Acid; Center: 1 Amine:1 Acid; Bottom: 1 Amine:3 Acid. Signals are normalized against the peak near q=1.5 Å<sup>-1</sup> to facilitate comparison.



**Figure S2**: SAXS results for trioctylamine/decanoic acid mixtures after extraction from 100 mM stock solution. Top: 3 Amine:1 Acid; Bottom: 1 Amine:1 Acid. Signals are normalized against the peak near q=1.5 Å<sup>-1</sup> to facilitate comparison.



**Figure S3**: SAXS results for trioctylamine/oleic acid mixtures after extraction from 100 mM stock solution. Top: 3 Amine:1 Acid; Center: 1 Amine:1 Acid; Bottom: 1 Amine:3 Acid.

#### III. Experimental Data and Fitting Information for A-Series SAXS Results

Prior to fitting, all scattering data was normalized such that the peak near  $q=1.4 \text{ Å}^{-1}$  had a value of 1, facilitating comparison between different samples. SAXS signals were fitted using a function consisting of four Lorentzian curves and a baseline with a linear slope:

$$S(q) = a + bq + \sum_{i=1}^{4} \frac{A_i}{(q - q_{0i})^2 + w_i^2}$$

a is the baseline intercept, b is the slope,  $A_i$ ,  $q_{0i}$ , and  $w_i$  are the amplitude, center, and width of the ith peak.

Units for parameters presented in tables:

- a arbitrary
- b  $(1/Å^{-1})$
- A<sub>i</sub> arbitrary
- *q*<sub>0i</sub> Å<sup>-1</sup>
- w<sub>i</sub> arbitrary

Parameters of the resulting fits are given below, along with the range for the 95% confidence interval, though constraints necessary for fitting make the confidence interval questionable. Peak numbers as presented in the table are arbitrary, and included merely for indexing.

The general pattern for the resulting fit is a Lorentzian centered at low q corresponding to a shoulder near q=0, a single Lorentzian describing the feature near q=0.4 Å<sup>-1</sup>, and two Lorentzian curves necessary to describe the feature near q=1.5 Å<sup>-1</sup>.

A31W				A31S				
"baseline intercept"	0.022	+/-	0.036	"baseline intercept"	-0.003	+/-	0.030	
"baseline slope"	0.038	+/-	0.013	"baseline slope"	0.049	+/-	0.011	
"peak 4 center"	0.543	+/-	0.007	"peak 4 center"	0.512	+/-	0.010	
"peak 4 width"	0.270	+/-	0.027	"peak 4 width"	0.287	+/-	0.024	
"peak 4 amplitude"	0.013	+/-	0.004	"peak 4 amplitude"	0.019	+/-	0.005	
"peak 3 center"	1.366	+/-	0.006	"peak 3 center"	1.368	+/-	0.004	
"peak 3 width"	0.217	+/-	0.006	"peak 3 width"	0.222	+/-	0.005	
"peak 3 amplitude"	0.037	+/-	0.005	"peak 3 amplitude"	0.042	+/-	0.003	
"peak 2 center"	1.541	+/-	0.051	"peak 2 center"	1.580	+/-	0.034	
"peak 2 width"	0.272	+/-	0.031	"peak 2 width"	0.223	+/-	0.032	
"peak 2 amplitude"	0.012	+/-	0.007	"peak 2 amplitude"	0.005	+/-	0.002	
"peak 1 center"	0.087	+/-	0.070	"peak 1 center"	0.069	+/-	0.069	
"peak 1 width"	0.143	+/-	0.075	"peak 1 width"	0.202	+/-	0.087	
"peak 1 amplitude"	0.001	+/-	0.001	"peak 1 amplitude"	0.005	+/-	0.005	
A31C				A31N				
"baseline intercept"	0.004	+/-	0.031	"baseline intercept"	0.005	+/-	0.022	
"baseline slope"	0.050	+/-	0.012	"baseline slope"	0.049	+/-	0.008	
"peak 4 center"	0.472	+/-	0.009	"peak 4 center"	0.451	+/-	0.006	
"peak 4 width"	0.272	+/-	0.021	"peak 4 width"	0.246	+/-	0.013	
"peak 4 amplitude"	0.020	+/-	0.005	"peak 4 amplitude"	0.019	+/-	0.003	
"peak 3 center"	1.366	+/-	0.007	"peak 2 center"	1.374	+/-	0.007	
"peak 3 width"	0.217	+/-	0.008	"peak 2 width"	0.217	+/-	0.009	
"peak 3 amplitude"	0.036	+/-	0.007	"peak 2 amplitude"	0.035	+/-	0.008	
"peak 2 center"	1.526	+/-	0.061	"peak 3 center"	1.536	+/-	0.058	
"peak 2 width"	0.271	+/-	0.030	"peak 3 width"	0.289	+/-	0.025	
"peak 2 amplitude"	0.013	+/-	0.009	"peak 3 amplitude"	0.017	+/-	0.011	
"peak 1 center"	0.012	+/-	0.127	"peak 1 center"	0.005	+/-	0.096	
"peak 1 width"	0.139	+/-	0.030	"peak 1 width"	0.123	+/-	0.013	
"peak 1 amplitude"	0.005	+/-	0.005	"peak 1 amplitude"	0.005	+/-	0.005	



A11W				A11S			
baseline intercept	0.009	+/-	0.022	baseline intercept	0.015	+/-	0.019
baseline slope	0.050	+/-	0.008	baseline slope	0.050	+/-	0.007
peak 4 center	0.455	+/-	0.006	peak 4 center	0.423	+/-	0.007
peak 4 width	0.245	+/-	0.015	peak 4 width	0.218	+/-	0.013
peak 4 amplitude	0.016	+/-	0.003	peak 4 amplitude	0.018	+/-	0.004
peak 2 center	1.374	+/-	0.007	peak 2 center	1.378	+/-	0.007
peak 2 width	0.210	+/-	0.008	peak 2 width	0.212	+/-	0.008
peak 2 amplitude	0.033	+/-	0.007	peak 2 amplitude	0.034	+/-	0.007
peak 3 center	1.535	+/-	0.051	peak 3 center	1.549	+/-	0.054
peak 3 width	0.280	+/-	0.022	peak 3 width	0.270	+/-	0.026
peak 3 amplitude	0.017	+/-	0.009	peak 3 amplitude	0.014	+/-	0.008
peak 1 center	0.104	+/-	0.038	peak 1 center	0.036	+/-	0.198
peak 1 width	0.126	+/-	0.059	peak 1 width	0.184	+/-	0.166
peak 1 amplitude	0.001	+/-	0.001	peak 1 amplitude	0.004	+/-	0.011
A 1 1 C				A 4 4 A 1			
AIIC				AIIN			
baseline intercept	0.029	+/-	0.016	baseline intercept	0.021	+/-	0.015
baseline intercept	0.029 0.048	+/- +/-	0.016 0.005	A11N baseline intercept baseline slope	0.021 0.048	+/- +/-	0.015 0.005
baseline intercept baseline slope peak 1 center	0.029 0.048 0.416	+/- +/- +/-	0.016 0.005 0.001	A11N baseline intercept baseline slope peak 1 center	0.021 0.048 0.417	+/- +/- +/-	0.015 0.005 0.001
baseline intercept baseline slope peak 1 center peak 1 width	0.029 0.048 0.416 0.165	+/- +/- +/- +/-	0.016 0.005 0.001 0.004	A11N baseline intercept baseline slope peak 1 center peak 1 width	0.021 0.048 0.417 0.178	+/- +/- +/- +/-	0.015 0.005 0.001 0.004
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude	0.029 0.048 0.416 0.165 0.014	+/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude	0.021 0.048 0.417 0.178 0.016	+/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center	0.029 0.048 0.416 0.165 0.014 1.520	+/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center	0.021 0.048 0.417 0.178 0.016 1.386	+/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width	0.029 0.048 0.416 0.165 0.014 1.520 0.291	+/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width	0.021 0.048 0.417 0.178 0.016 1.386 0.206	+/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021	+/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029	+/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021 1.382	+/- +/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017 0.010	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029 1.528	+/- +/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010 0.069
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 width	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021 1.382 0.204	+/- +/- +/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017 0.010 0.016	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 width	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029 1.528 0.299	+/- +/- +/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010 0.069 0.018
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 amplitude	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021 1.382 0.204 0.028	+/- +/- +/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017 0.010 0.016 0.012	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 amplitude	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029 1.528 0.299 0.023	+/- +/- +/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010 0.069 0.018 0.016
baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 width peak 3 amplitude peak 4 center	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021 1.382 0.204 0.028 0.104	+/- +/- +/- +/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017 0.010 0.016 0.012 0.048	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 amplitude peak 4 center	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029 1.528 0.299 0.023 0.119	+/- +/- +/- +/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010 0.069 0.018 0.016 0.012
AIIC baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 width peak 4 center peak 4 width	0.029 0.048 0.416 0.165 0.014 1.520 0.291 0.021 1.382 0.204 0.028 0.104 0.043	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	0.016 0.005 0.001 0.004 0.001 0.080 0.019 0.017 0.010 0.016 0.012 0.048 0.055	A11N baseline intercept baseline slope peak 1 center peak 1 width peak 1 amplitude peak 2 center peak 2 width peak 2 amplitude peak 3 center peak 3 width peak 4 center peak 4 width	0.021 0.048 0.417 0.178 0.016 1.386 0.206 0.029 1.528 0.299 0.023 0.119 0.057	+/- +/+ +/- +/- +/- +/- +/- +/- +/- +/-	0.015 0.005 0.001 0.004 0.001 0.008 0.014 0.010 0.069 0.018 0.016 0.012 0.021



A13W				A13S			
"baseline intercept"	0.025	+/-	0.009	"baseline intercept"	0.024	+/-	0.011
"baseline slope"	0.050	+/-	0.003	"baseline slope"	0.050	+/-	0.004
"peak 1 center"	0.509	+/-	0.032	"peak 1 center"	0.502	+/-	0.037
"peak 1 width"	0.140	+/-	0.022	"peak 1 width"	0.155	+/-	0.023
"peak 1 amplitude"	0.003	+/-	0.002	"peak 1 amplitude"	0.004	+/-	0.002
"peak 2 center"	1.400	+/-	0.007	"peak 2 center"	1.399	+/-	0.008
"peak 2 width"	0.199	+/-	0.015	"peak 2 width"	0.197	+/-	0.016
"peak 2 amplitude"	0.027	+/-	0.009	"peak 2 amplitude"	0.025	+/-	0.010
"peak 3 center"	1.547	+/-	0.062	"peak 3 center"	1.523	+/-	0.050
"peak 3 width"	0.314	+/-	0.015	"peak 3 width"	0.311	+/-	0.015
"peak 3 amplitude"	0.025	+/-	0.013	"peak 3 amplitude"	0.029	+/-	0.012
"peak 4 center"	0.400	+/-	0.003	"peak 4 center"	0.396	+/-	0.002
"peak 4 width"	0.086	+/-	0.005	"peak 4 width"	0.087	+/-	0.005
"peak 4 amplitude"	0.004	+/-	0.001	"peak 4 amplitude"	0.005	+/-	0.001
A13C				A13N			
"baseline intercept"	0.027	+/-	0.009	"baseline intercept"	0.024	+/-	0.010
"baseline slope"	0.050	+/-	0.004	"baseline slope"	0.050	+/-	0.004
"peak 1 center"	0.515	+/-	0.037	"peak 1 center"	0.502	+/-	0.038
"peak 1 width"	0.154	+/-	0.026	"peak 1 width"	0.152	+/-	0.023
"peak 1 amplitude"	0.003	+/-	0.002	"peak 1 amplitude"	0.003	+/-	0.002
"peak 2 center"	1.555	+/-	0.060	"peak 2 center"	1.403	+/-	0.006
"peak 2 width"	0.321	+/-	0.015	"peak 2 width"	0.202	+/-	0.013
"peak 2 amplitude"	0.026	+/-	0.013	"peak 2 amplitude"	0.027	+/-	0.008
"peak 3 center"	1.402	+/-	0.007	"peak 3 center"	1.547	+/-	0.047
"peak 3 width"	0.203	+/-	0.014	"peak 3 width"	0.335	+/-	0.015
"peak 3 amplitude"	0.028	+/-	0.009	"peak 3 amplitude"	0.031	+/-	0.011
"peak 4 center  "	0.401	+/-	0.002	"peak 4 center"	0.397	+/-	0.003
"peak 4 width"	0.089	+/-	0.004	"peak 4 width"	0.088	+/-	0.005
"peak 4 amplitude"	0.005	+/-	0.001	"peak 4 amplitude"	0.005	+/-	0.001



#### IV. Experimental Data and Fitting Information for B-Series SAXS Results

Prior to fitting, all scattering data was normalized such that the peak near  $q=1.4 \text{ Å}^{-1}$  had a value of 1, facilitating comparison between different samples. SAXS signals were fitted using a function consisting of four Lorentzian curves and a baseline with a linear slope:

$$S(q) = a + bq + \sum_{i=1}^{4} \frac{A_i}{(q - q_{0i})^2 + w_i^2}$$

a is the baseline intercept, b is the slope,  $A_{i}$ ,  $q_{0i}$ , and  $w_{i}$  are the amplitude, center, and width of the ith peak.

Units for parameters presented in tables:

- a arbitrary
- b  $(1/Å^{-1})$
- A<sub>i</sub> arbitrary
- **q**<sub>0i</sub> Å<sup>-1</sup>
- w<sub>i</sub> arbitrary

Parameters of the resulting fits are given below, along with the range for the 95% confidence interval, though constraints necessary for fitting make the confidence interval questionable. Peak numbers as presented in the table are arbitrary, and included merely for indexing.

The general pattern for the resulting fit is a single Lorentzian describing the feature near  $q=0.4 \text{ Å}^{-1}$ , and either one or two Lorentzian curves necessary to describe the feature near  $q=1.5 \text{ Å}^{-1}$ ; other Lorentzians are either centered in the range  $q=2-3 \text{ Å}^{-1}$  to represent highly localized interactions or moved "off-plot" during the fit, meaning that they are irrelevant to the fit.

B31W				B31S			
"baseline intercept"	0.067	+/-	11633.800	"baseline intercept"	0.070	+/-	423.390
"baseline slope"	0.000	+/-	190.292	"baseline slope"	0.000	+/-	3.354
"peak 1 center"	0.434	+/-	0.005	"peak 1 center"	0.451	+/-	0.006
"peak 1 width"	0.169	+/-	0.024	"peak 1 width"	0.173	+/-	0.017
"peak 1 amplitude"	0.003	+/-	0.001	"peak 1 amplitude"	0.003	+/-	0.001
"peak 2 center"	1.386	+/-	0.001	"peak 2 center"	1.385	+/-	0.001
"peak 2 width"	0.237	+/-	0.004	"peak 2 width"	0.240	+/-	0.003
"peak 2 amplitude"	0.051	+/-	0.003	"peak 2 amplitude"	0.053	+/-	0.002
"peak 3 center"	2.517	+/-	1.671	"peak 3 center"	2.719	+/-	1.360
"peak 3 width"	0.390	+/-	1.939	"peak 3 width"	0.476	+/-	1.187
"peak 3 amplitude"	0.006	+/-	0.167	"peak 3 amplitude"	0.012	+/-	0.112
"peak 4 center"	62.546	+/-	703646000.000	"peak 4 center"	333.071	+/-	32014900.000
"peak 4 width"	0.400	+/-	15318200.000	"peak 4 width"	0.400	+/-	64203.400
"peak 4 amplitude"	1.977	+/-	90005400.000	"peak 4 amplitude"	155.095	+/-	17155200.000
B31C				B31S			
"baseline intercept"	0.043	+/-	0.495	"baseline intercept"	0.073	+/-	0.011
"baseline slope"	0.012	+/-	0.426	"baseline slope"	0.000	+/-	0.015
"peak 2 center"	0.389	+/-	0.015	"peak 1 center"	0.372	+/-	0.001
"peak 2 width"	0.177	+/-	0.033	"peak 1 width"	0.145	+/-	0.003
"peak 2 amplitude"	0.006	+/-	0.005	"peak 1 amplitude"	0.008	+/-	0.000
"peak 1 center"	1.393	+/-	0.001	"peak 2 center"	2.000	+/-	0.386
"peak 1 width"	0.237	+/-	0.004	"peak 2 width"	0.531	+/-	0.779
"peak 1 amplitude"	0.051	+/-	0.002	"peak 2 amplitude"	0.012	+/-	0.057
"peak 3 center"	4.071	+/-	151.566	"peak 3 center"	1.410	+/-	0.001
"peak 3 width"	0.358	+/-	224.753	"peak 3 width"	0.240	+/-	0.004
"peak 3 amplitude"	0.119	+/-	18.533	"peak 3 amplitude"	0.051	+/-	0.002
"peak 4 center"	0.000	+/-	1.141	"peak 4 center"	2.523	+/-	1.579
"peak 4 width"	0.254	+/-	1.086	"peak 4 width"	0.183	+/-	0.545
"peak 4 amplitude"	0.006	+/-	0.076	"peak 4 amplitude"	0.002	+/-	0.026



B11W				B11S		
"baseline intercept"	0.065	+/-	0.013	"baseline intercept"	0.048 +/-	3403.160
"baseline slope"	0.000	+/-	0.017	"baseline slope"	0.030 +/-	27.690
"peak 1 center"	0.405	+/-	0.006	"peak 1 center"	0.356 +/-	0.001
"peak 1 width"	0.186	+/-	0.016	"peak 1 width"	0.125 +/-	0.003
"peak 1 amplitude"	0.005	+/-	0.001	"peak 1 amplitude"	0.008 +/-	0.000
"peak 2 center"	1.389	+/-	0.001	"peak 2 center"	1.410 +/-	0.001
"peak 2 width"	0.235	+/-	0.003	"peak 2 width"	0.230 +/-	0.002
"peak 2 amplitude"	0.050	+/-	0.002	"peak 2 amplitude"	0.047 +/-	0.001
"peak 3 center"	1.948	+/-	0.057	"peak 3 center"	129.847 +/-	68340000.000
"peak 3 width"	0.228	+/-	0.179	"peak 3 width"	0.400 +/-	1161000.000
"peak 3 amplitude"	0.002	+/-	0.005	"peak 3 amplitude"	56.956 +/-	49114000.000
"peak 4 center  "	2.387	+/-	0.109	"peak 4 center"	149.742 +/-	29010000.000
"peak 4 width"	0.473	+/-	0.494	"peak 4 width"	0.400 +/-	359005.000
"peak 4 amplitude"	0.017	+/-	0.046	"peak 4 amplitude"	94.674 +/-	54045600.000
B11C				B11N		
"baseline intercept"	-0.044	+/-	0.042	"baseline intercept"	0.070 +/-	0.012
"baseline slope"	0.050	+/-	0.034	"baseline slope"	0.000 +/-	0.015
"peak 1 center"	0.616	+/-	0.085	"peak 1 center"	0.357 +/-	0.001
"peak 1 width"	0.442	+/-	0.175	"peak 1 width"	0.150 +/-	0.004
"peak 1 amplitude"	0.015	+/-	0.018	"peak 1 amplitude"	0.009 +/-	0.001
"peak 2 center"	1.416	+/-	0.001	"peak 2 center"	2.000 +/-	0.267
"peak 2 width"	0.225	+/-	0.005	"peak 2 width"	0.342 +/-	0.441
"peak 2 amplitude"	0.046	+/-	0.003	"peak 2 amplitude"	0.003 +/-	0.016
"peak 3 center"	0.357	+/-	0.001	"peak 3 center  "	1.406 +/-	0.001
"peak 3 width"	0.087	+/-	0.002	"peak 3 width"	0.234 +/-	0.002
"peak 3 amplitude"	0.006	+/-	0.000	"peak 3 amplitude"	0.050 +/-	0.001
"peak 4 center"	2.020	+/-	0.162	"peak 4 center"	2.575 +/-	2.463
"peak 4 width"	0.795	+/-	1.053	"peak 4 width"	0.278 +/-	1.095
"peak 4 amplitude"	0.038	+/-	0.162	"peak 4 amplitude"	0.005 +/-	0.080



#### V. Experimental Data and Fitting Information for C-Series SAXS Results

Prior to fitting, all scattering data was normalized such that the peak near q=1.4 Å<sup>-1</sup> had a value of 1, facilitating comparison between different samples. SAXS signals were fitted using a function consisting of five Lorentzian curves and a baseline with a linear slope:

$$S(q) = a + bq + \sum_{i=1}^{5} \frac{A_i}{(q - q_{0i})^2 + w_i^2}$$

a is the baseline intercept, b is the slope,  $A_{i}$ ,  $q_{0i}$ , and  $w_{i}$  are the amplitude, center, and width of the ith peak.

Units for parameters presented in tables:

- a arbitrary
- b  $(1/Å^{-1})$
- A<sub>i</sub> arbitrary
- **q**<sub>0i</sub> Å<sup>-1</sup>
- w<sub>i</sub> arbitrary

Parameters of the resulting fits are given below, along with the range for the 95% confidence interval, though constraints necessary for fitting make the confidence interval questionable. Peak numbers as presented in the table are arbitrary, and included merely for indexing.

The general pattern for the resulting fit is two overlapping Lorentzian curves describing the feature near  $q=0.4 \text{ Å}^{-1}$ , and either one or two Lorentzian curves necessary to describe the feature near  $q=1.5 \text{ Å}^{-1}$ ; other Lorentzians are either centered in the range  $q=2-3 \text{ Å}^{-1}$  to represent highly localized interactions or moved "off-plot" during the fit, meaning that they are irrelevant to the fit.

C31W				C31S			
"baseline intercept"	0.000	+/-	0.031	"baseline intercept"	0.000	+/-	0.032
"baseline slope"	0.041	+/-	0.011	"baseline slope"	0.034	+/-	0.123
"peak 2 center"	0.158	+/-	0.069	"peak 2 center"	0.160	+/-	0.042
"peak 2 width"	0.304	+/-	0.300	"peak 2 width"	0.250	+/-	0.117
"peak 2 amplitude"	0.007	+/-	0.018	"peak 2 amplitude"	0.007	+/-	0.009
"peak 1 center"	0.460	+/-	0.022	"peak 1 center"	0.452	+/-	0.019
"peak 1 width"	0.199	+/-	0.046	"peak 1 width"	0.207	+/-	0.037
"peak 1 amplitude"	0.004	+/-	0.004	"peak 1 amplitude"	0.005	+/-	0.003
"peak 4 center"	1.347	+/-	0.028	"peak 4 center"	1.362	+/-	0.029
"peak 4 width"	0.273	+/-	0.026	"peak 4 width"	0.280	+/-	0.041
"peak 4 amplitude"	0.035	+/-	0.016	"peak 4 amplitude"	0.042	+/-	0.022
"peak 5 center"	1.408	+/-	0.013	"peak 5 center"	1.406	+/-	0.014
"peak 5 width"	0.192	+/-	0.026	"peak 5 width"	0.188	+/-	0.042
"peak 5 amplitude"	0.018	+/-	0.016	"peak 5 amplitude"	0.015	+/-	0.021
"peak 3 center"	2.511	+/-	0.140	"peak 3 center"	3.235	+/-	27.658
"peak 3 width"	0.001	+/-	0.232	"peak 3 width"	0.325	+/-	18.123
"peak 3 amplitude"	0.000	+/-	0.000	"peak 3 amplitude"	0.020	+/-	1.076
C31C				C31N			
"baseline intercept"	0.000	+/-	0.103	"baseline intercept"	0.000	+/-	0.120
"baseline slope"	0.028	+/-	0.270	"baseline slope"	0.001	+/-	0.449
"peak 2 center"	0.197	+/-	0.069	"peak 2 center"	0.058	+/-	0.151
"peak 2 width"	0.278	+/-	0.223	"peak 2 width"	0.291	+/-	0.519
"peak 2 amplitude"	0.012	+/-	0.032	"peak 2 amplitude"	0.013	+/-	0.062
"peak 5 center"	0.441	+/-	0.033	"peak 1 center"	0.385	+/-	0.038
"peak 5 width"	0.198	+/-	0.052	"peak 1 width"	0.247	+/-	0.067
"peak 5 amplitude"	0.005	+/-	0.005	"peak 1 amplitude"	0.012	+/-	0.016
"peak 1 center"	1.374	+/-	0.020	"peak 4 center"	1.362	+/-	0.032
"peak 1 width"	0.273	+/-	0.047	"peak 4 width"	0.299	+/-	0.068
"peak 1 amplitude"	0.045	+/-	0.021	"peak 4 amplitude"	0.040	+/-	0.024
"peak 4 center"	1.407	+/-	0.015	"peak 5 center"	1.405	+/-	0.011
"peak 4 width"	0.180	+/-	0.051	"peak 5 width"	0.195	+/-	0.033
"peak 4 amplitude"	0.011	+/-	0.020	"peak 5 amplitude"	0.019	+/-	0.021
"peak 3 center"	2.563	+/-	2.320	"peak 3 center"	2.530	+/-	1.661
"peak 3 width"	0.774	+/-	5.271	"peak 3 width"	0.795	+/-	3.606
		,	0.005	"nonly 2 annulity do"	0.062	./	1 215



C11W				C115		
"baseline intercept"	0.000	+/-	9104.050	"baseline intercept"	0.006 +/-	0.023
"baseline slope"	0.043	, +/-	82.551	"baseline slope"	0.044 +/-	0.008
"peak 1 center"	0.283	, +/-	0.124	"peak 1 center"	0.261 +/-	0.023
"peak 1 width"	0.238	, +/-	0.267	"peak 1 width"	0.207 +/-	0.028
"peak 1 amplitude"	0.007	, +/-	0.029	"peak 1 amplitude"	0.008 +/-	0.004
"peak 2 center"	0.458	+/-	0.070	"peak 2 center"	0.454 +/-	0.029
"peak 2 width"	0.170	+/-	0.115	"peak 2 width"	0.182 +/-	0.036
"peak 2 amplitude"	0.002	+/-	0.008	"peak 2 amplitude"	0.003 +/-	0.003
"peak 3 center"	1.388	+/-	0.009	"peak 3 center"	1.399 +/-	0.003
"peak 3 width"	0.244	+/-	0.033	"peak 3 width"	0.251 +/-	0.030
"peak 3 amplitude"	0.046	+/-	0.011	"peak 3 amplitude"	0.050 +/-	0.007
"peak 4 center"	1.410	+/-	0.021	"peak 4 center"	1.405 +/-	0.008
"peak 4 width"	0.151	+/-	0.100	"peak 4 width"	0.145 +/-	0.099
"peak 4 amplitude"	0.003	+/-	0.013	"peak 4 amplitude"	0.003 +/-	0.010
"peak 5 center"	114.445	+/-	77321400.000	"peak 5 center"	94101.700 +/-	0.000
"peak 5 width"	0.400	+/-	5072780.000	"peak 5 width"	0.400 +/-	0.000
"peak 5 amplitude"	85.063	+/-	234210000.000	"peak 5 amplitude"	99826.500 +/-	0.000
C11C				C11N		
"baseline intercept"	0.000	+/-	0.028	"baseline intercept"	0.000 +/-	0.024
"baseline slope"	0.050	+/-	0.011	"baseline slope"	0.047 +/-	0.008
"peak 2 center"	0.281	+/-	0.004	"peak 1 center"	0.286 +/-	0.006
"peak 2 width"	0.100	+/-	0.013	"peak 1 width"	0.121 +/-	0.013
"peak 2 amplitude"	0.002	+/-	0.001	"peak 1 amplitude"	0.004 +/-	0.002
"peak 5 center"	0.436	+/-	0.063	"peak 2 center"	0.411 +/-	0.040
"peak 5 width"	0.245	+/-	0.068	"peak 2 width"	0.214 +/-	0.028
"peak 5 amplitude"	0.006	+/-	0.006	"peak 2 amplitude"	0.009 +/-	0.005
"peak 4 center"	1.400	+/-	0.003	"peak 3 center"	1795.970 +/-	0.000
"peak 4 width"	0 202	+/-	0.008	"neak 3 width"	0 400 +/-	0.000
"peak 4 amplitude"	0.202	•7	01000	peak o math	0.400 .7	
	0.033	+/-	0.006	"peak 3 amplitude"	1520.700 +/-	0.000
"peak 3 center"	0.033 1.550	+/- +/-	0.006 0.083	"peak 3 amplitude" "peak 4 center"	1520.700 +/- 1.404 +/-	0.000 0.010
"peak 3 center" "peak 3 width"	0.033 1.550 0.354	+/- +/- +/-	0.006 0.083 0.052	"peak 3 amplitude" "peak 4 center" "peak 4 width"	1520.700 +/- 1.404 +/- 0.360 +/-	0.000 0.010 0.147
"peak 3 center" "peak 3 width" "peak 3 amplitude"	0.033 1.550 0.354 0.017	+/- +/- +/- +/-	0.006 0.083 0.052 0.012	"peak 3 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude"	1520.700 +/- 1.404 +/- 0.360 +/- 0.022 +/-	0.000 0.010 0.147 0.010
"peak 3 center" "peak 3 width" "peak 3 amplitude" "peak 1 center"	0.232 0.033 1.550 0.354 0.017 2.409	+/- +/- +/- +/- +/-	0.006 0.083 0.052 0.012 0.108	"peak 3 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 5 center"	1520.700 +/- 1.404 +/- 0.360 +/- 0.022 +/- 1.402 +/-	0.000 0.010 0.147 0.010 0.001
"peak 3 center" "peak 3 width" "peak 3 amplitude" "peak 1 center" "peak 1 width"	0.033 1.550 0.354 0.017 2.409 0.138	+/- +/- +/- +/- +/- +/-	0.006 0.083 0.052 0.012 0.108 0.397	"peak 3 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 5 center" "peak 5 width"	1520.700 +/- 1.404 +/- 0.360 +/- 0.022 +/- 1.402 +/- 0.207 +/-	0.000 0.010 0.147 0.010 0.001 0.001



C13W				C135		
"baseline intercept"	0.000	+/-	1777.180	"baseline intercept"	0.004 +/-	0.021
"baseline slope"	0.047	+/-	22.238	"baseline slope"	0.050 +/-	0.007
"peak 1 center"	0.299	+/-	0.007	"peak 1 center"	0.287 +/-	0.004
"peak 1 width"	0.106	+/-	0.017	"peak 1 width"	0.094 +/-	0.010
"peak 1 amplitude"	0.002	+/-	0.001	"peak 1 amplitude"	0.002 +/-	0.001
"peak 2 center"	0.425	+/-	0.040	"peak 2 center"	0.431 +/-	0.040
"peak 2 width"	0.189	+/-	0.034	"peak 2 width"	0.207 +/-	0.039
"peak 2 amplitude"	0.005	+/-	0.004	"peak 2 amplitude"	0.006 +/-	0.003
"peak 4 center"	1.401	+/-	0.003	"peak 4 center "	1.401 +/-	0.004
"peak 4 width"	0.207	+/-	0.012	"peak 4 width"	0.203 +/-	0.011
"peak 4 amplitude"	0.034	+/-	0.010	"peak 4 amplitude"	0.032 +/-	0.008
"peak 3 center"	1.457	+/-	0.064	"peak 3 center"	1.498 +/-	0.068
"peak 3 width"	0.381	+/-	0.130	"peak 3 width"	0.340 +/-	0.047
"peak 3 amplitude"	0.020	+/-	0.010	"peak 3 amplitude"	0.018 +/-	0.011
"peak 5 center"	82.593	+/-	73407500.000	"peak 5 center"	2439.530+/-	0.000
"peak 5 width"	0.400	+/-	1269630.000	"peak 5 width"	0.400 +/-	0.000
"peak 5 amplitude"	6.599	+/-	23854000.000	"peak 5 amplitude"	3353,250 +/-	0.000
				pp	0000.200 //	
C13C				C13N		
C13C "baseline intercept"	0.000	+/-	244.973	C13N "baseline intercept"	0.000 +/-	0.022
C13C "baseline intercept" "baseline slope"	0.000 0.050	+/- +/-	244.973 15.379	C13N "baseline intercept" "baseline slope"	0.000 +/- 0.050 +/-	0.022 0.008
C13C "baseline intercept" "baseline slope" "peak 1 center"	0.000 0.050 0.279	+/- +/- +/-	244.973 15.379 0.005	C13N "baseline intercept" "baseline slope" "peak 2 center"	0.000 +/- 0.050 +/- 0.299 +/-	0.022 0.008 0.004
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width"	0.000 0.050 0.279 0.096	+/- +/- +/- +/-	244.973 15.379 0.005 0.018	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/-	0.022 0.008 0.004 0.009
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude"	0.000 0.050 0.279 0.096 0.002	+/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/-	0.022 0.008 0.004 0.009 0.001
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center"	0.000 0.050 0.279 0.096 0.002 0.428	+/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/-	0.022 0.008 0.004 0.009 0.001 0.036
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width"	0.000 0.050 0.279 0.096 0.002 0.428 0.244	+/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 width"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 2 amplitude"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007	+/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 width" "peak 1 amplitude"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 4 center"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392	+/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 4 center" "peak 4 width"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198	+/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 4 center" "peak 4 width" "peak 4 amplitude"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030	+/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015 0.011
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030 1.488	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026 0.212	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/- 1.455 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015 0.011 0.037
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 2 amplitude" "peak 2 width" "peak 4 center" "peak 4 amplitude" "peak 4 amplitude" "peak 3 center" "peak 3 width"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030 1.488 0.292	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026 0.212 0.061	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 amplitude" "peak 4 amplitude" "peak 3 center"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/- 1.455 +/- 0.368 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015 0.011 0.037 0.094
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 2 amplitude" "peak 2 width" "peak 2 amplitude" "peak 4 center" "peak 4 width" "peak 3 center" "peak 3 width" "peak 3 amplitude"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030 1.488 0.292 0.015	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026 0.212 0.061 0.038	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center" "peak 3 width" "peak 3 amplitude"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/- 1.455 +/- 0.368 +/- 0.025 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015 0.011 0.037 0.094 0.010
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 width" "peak 1 amplitude" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 4 center" "peak 4 width" "peak 3 center" "peak 3 width" "peak 3 amplitude" "peak 3 center"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030 1.488 0.292 0.015 12.882	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026 0.212 0.061 0.038 956285.000	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center" "peak 3 width" "peak 3 amplitude" "peak 5 center"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/- 1.455 +/- 0.368 +/- 0.025 +/- 3291.870+/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.004 0.015 0.011 0.037 0.094 0.010 0.000
C13C "baseline intercept" "baseline slope" "peak 1 center" "peak 1 amplitude" "peak 2 amplitude" "peak 2 width" "peak 2 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center" "peak 3 amplitude" "peak 5 center" "peak 5 width"	0.000 0.050 0.279 0.096 0.002 0.428 0.244 0.007 1.392 0.198 0.030 1.488 0.292 0.015 12.882 0.391	+/- +/- +/- +/- +/- +/- +/- +/- +/- +/-	244.973 15.379 0.005 0.018 0.001 0.079 0.101 0.009 0.012 0.029 0.026 0.212 0.061 0.038 956285.000 8329850.000	C13N "baseline intercept" "baseline slope" "peak 2 center" "peak 2 width" "peak 2 amplitude" "peak 1 center" "peak 1 amplitude" "peak 4 center" "peak 4 width" "peak 4 amplitude" "peak 3 center" "peak 3 amplitude" "peak 5 center" "peak 5 width"	0.000 +/- 0.050 +/- 0.299 +/- 0.095 +/- 0.003 +/- 0.430 +/- 0.195 +/- 0.007 +/- 1.407 +/- 0.204 +/- 0.031 +/- 1.455 +/- 0.368 +/- 0.025 +/- 3291.870+/- 0.400 +/-	0.022 0.008 0.004 0.009 0.001 0.036 0.031 0.004 0.004 0.004 0.015 0.011 0.037 0.094 0.010 0.000 0.000 0.000



### VI. Low-q SAXS Results for A31C and A31N

Figure 5 shows the SAXS results for large q, and there is evidence that scattering intensity rises at low q-values. Figure S3 considers the organic phase after Cu(NO<sub>3</sub>)<sub>2</sub> and CuCl<sub>2</sub> extractions.





We have used the Irena<sup>1</sup> package for IgorPro(Wavemetrics)to analyze low-q data for Nitrate and Chloride salts. The data was modelled with an arbitrary distribution of spherical particles, using, for example, the maximum entropy method. The model fit the data well, as indicated by a residual values (see Figure S4).

1. Ilavsky, J. and P. R. Jemian (2009). "Irena: tool suite for modeling and analysis of small-angle scattering." Journal of Applied Crystallography 42: 347-353.



Figure S4: Fitting results for organic phase of A31-Cu(NO<sub>3</sub>)<sub>2</sub> (left) and A31-CuCl<sub>2</sub> (right) extraction experiments, as described in the text.

The fitted mean diameters for the particles are found to be 4.8 and 4.6 nm for Nitrate and Chloride respectively. Considering the polydispersity of the distribution the difference in particle size between the two salts is negligible.

#### VII. Molecular Origin of Nanoscale Peak

It is instructive to compare molecular dimensions in the amine/acid mixture with the characteristic lengthscale for the nanostructures, calculated as  $d = 2 \pi/q$ ; see Figure S5 and Table S1. The lengthscale calculated from the peak position correlates with theoretical spacing calculated based on packing of stretched amine and acid chains in layered structures similar to packing of organic acids in a liquid.<sup>1,2</sup> Overall, the distances found experimentally are always shorter than the maximum expected length for tail-to-tail packing of the stretched chains. The discrepancy could originate from to partial chain coiling, interdigitation, or aliphatic chain tilt with respect to the polar interface defined by the polar head groups, but the specific molecular arrangement in the present systems are unclear.

The set of amine/acid mixtures used in our extraction study is not broad enough to support a final interpretation of molecular arrangement. However, it is worth noting that for the oleic acid containing system (C) we observed two lengthscales at small scattering vectors based on fitting of signal. The long spacing d =22.2 is consistent with observed trend for systems A and B, in that spacing increases commensurately with aliphatic chain length. However, the shorter spacing d = 13.7 is similar to systems A and B. While the origin of the shorter lengthscale is not clear, we theorize that it may correspond to a dimer of the amine with cis-folded oleic acid chain, in which case the overall dimer length for system C would be expected to be similar to that for the trioctylamine/decanoic acid arrangement.

System	E	Calculated length, Å		
	3:1	1:1	1:3	
A	11.6	13.8	15.7	17.6
В	14.5	15.5	18.8*	22.6
C - stretched	-	22.2	21	35.1
C - folded	13.7	13.7	14.8	25.1

Table S1. The characteristic lengthscale of nanostructures in water saturated amine acid mixtures at 1:3, 1:1, 3:1 molar amine to acid ratios as calculated from SAXS data and compared to a maximum length of stretched amine and acid chains arranged tail-to-tail configuration.

\* calculated from Reference 3.





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3. M. N. Kobrak and K. G. Yager, X-Ray scattering and physicochemical studies of trialkylamine/carboxylic acid mixtures: nanoscale structure in pseudoprotic ionic liquids and related solutions, *Phys. Chem. Chem. Phys.*, 2018, **20**, 18639–18646.