Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Insights into Water Extraction and Aggregation Mechanisms of Malonamide-Alkane Mixtures

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Fitting of SAXS patterns

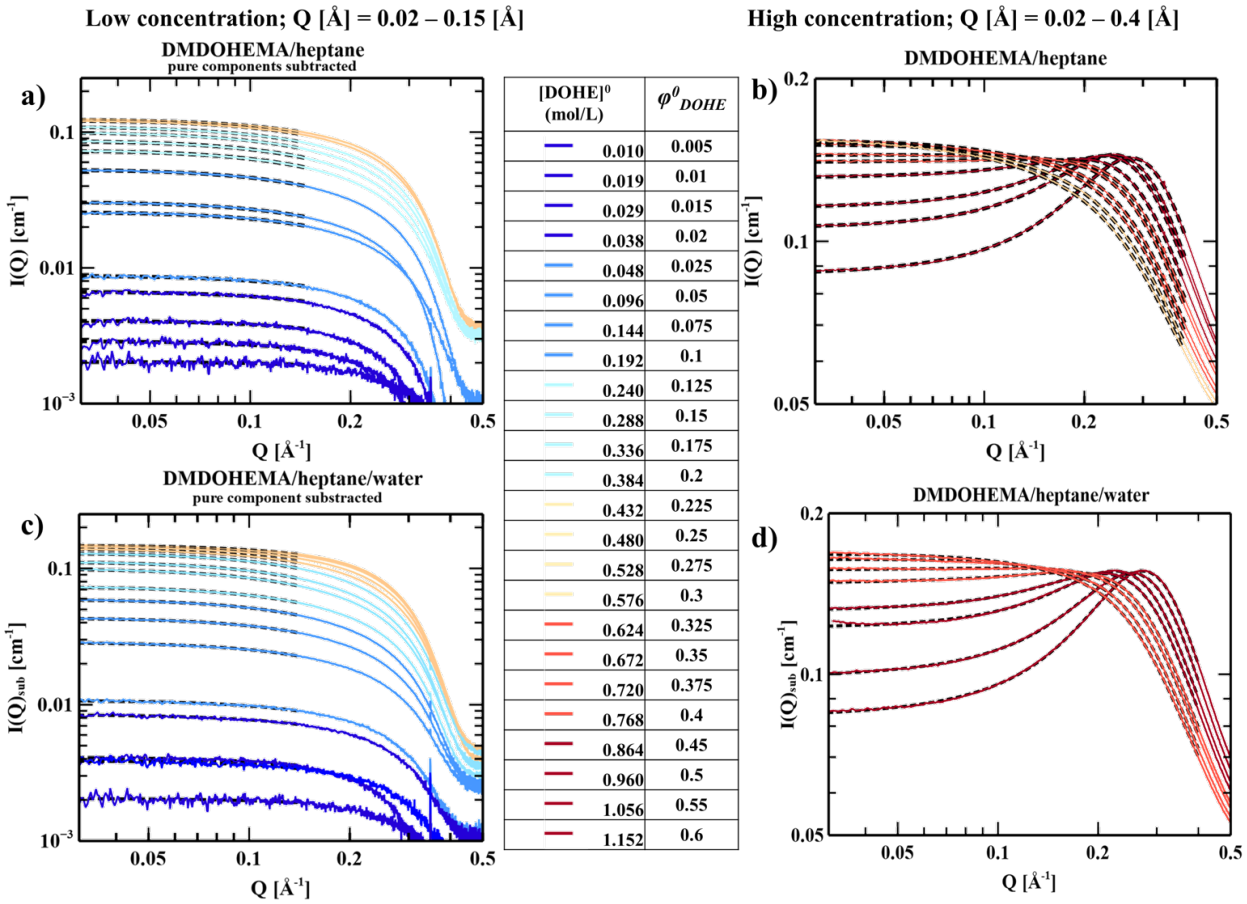

Figure S.1: SAXS fitting of DOHE in C7 without water contact a) at low concentration of DOHE with background subtracted b) at high concentration of DOHE without background subtracted; with water contact c) at low concentration of DOHE with background subtracted d) at high concentration of DOHE without background subtracted.

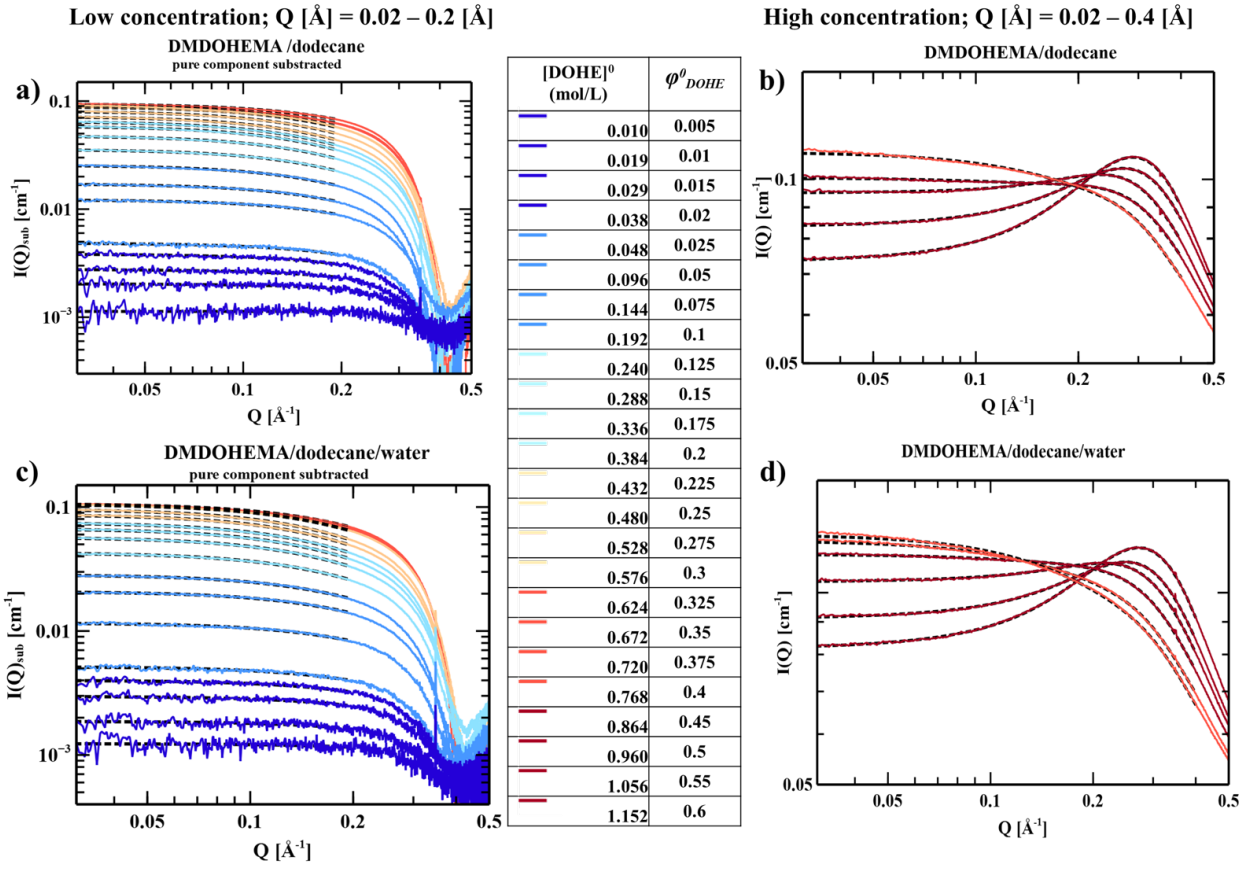

Figure S.2: SAXS fitting of DOHE in C12 without water contact a) at low concentration of DOHE with background subtracted b) at high concentration of DOHE without background subtracted; with water contact c) at low concentration of DOHE with background subtracted d) at high concentration of DOHE without background subtracted.

Composition of Maximum in Scattering

The maxima in I_{OZ} are fit to polynomials with the form

$$I_{\mathrm{OZ}} = \sum_i a_i(\varphi_E - b_i)^{2i} \tag{S.1}$$

using $i = 1, 2$.

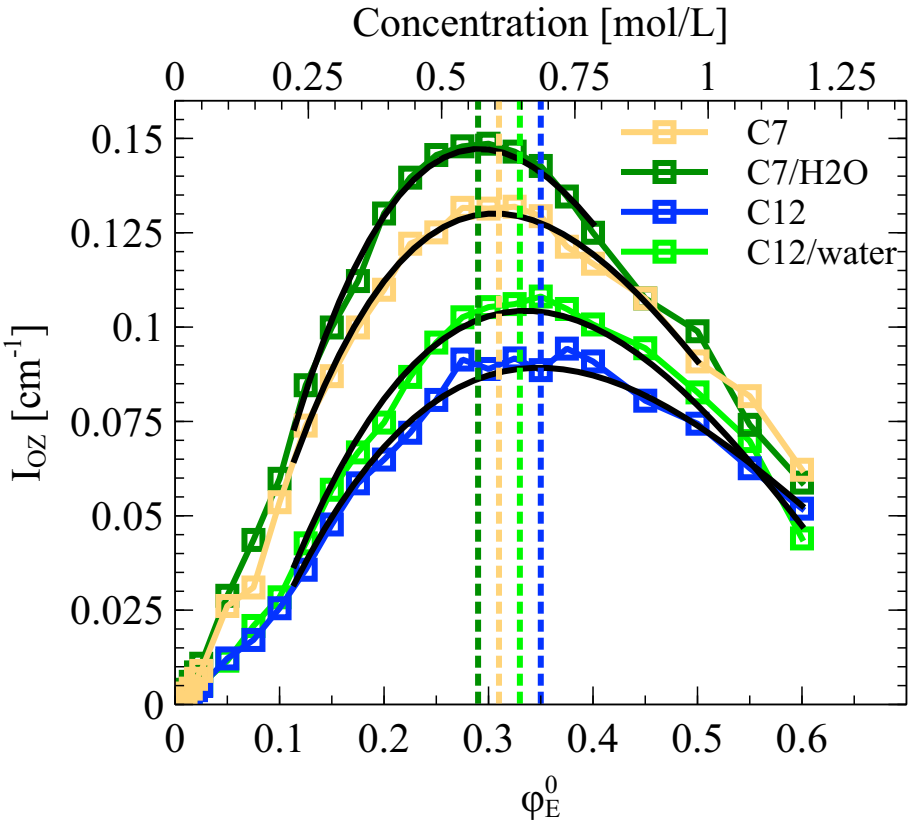

Figure S.3: Polynomial fits to estimate the composition of the maximum in scattering intensity, I_{OZ}, for each system: DMDOHEMA/C12 (blue), DMDOHEMA/C12/water (green), DMDOHEMA/C7 (black), and DMDOHEMA/C7/water (red). Fits are shown with orange lines, and vertical lines denote the maximum value for each particular system of the corresponding color. Composition values are given in Table 3.

KF measurements of DMDOHEMA in 3 M $LiNO_3$

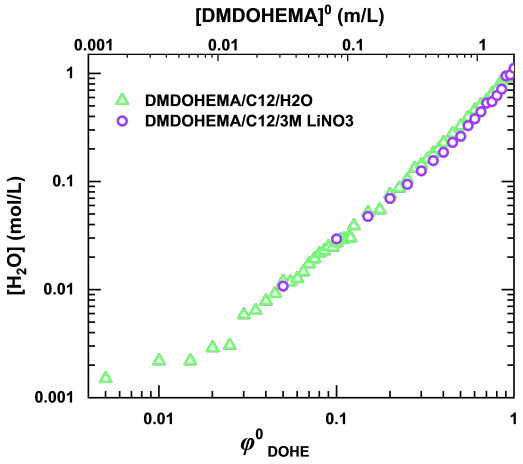

Figure S.4: Organic phase water concentration, $[H_2O]$, upon extraction into DMDOHEMA/dodecane mixtures as a function of initial DMDOHEMA concentration, $[DOHE]^0$ for pure water and 3 M $LiNO_3$ aqueous phases.

Molecular Dynamics

Table S.1: MD simulation compositions and periodic cubic box sizes. Concentrations are given in mol/L.

DOHE			Water		n-Dodecane	Simulation box
φ^0_{ext}	conc.	num.	conc.	num.	num.	length (Å)
0.26	0.5	301	0.11	66	1961	99.07
0.51	1.0	590	0.33	199	1298	99.56

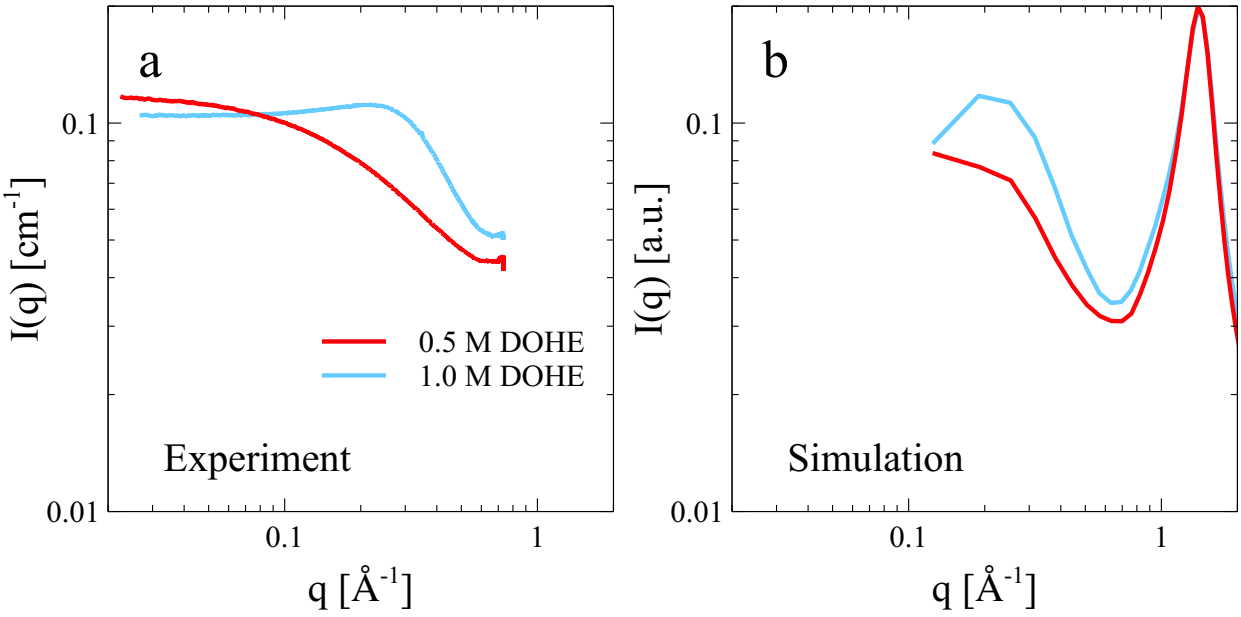

Figure S.5: Experimental SAXS patterns for water-contacted 0.49 and 0.98 M DMDOHEMA in dodecane (left) are compared to the simulation-calculated SAXS patterns for 0.5 and 1.0 M DMDOHEMA in dodecane with extracted water (right).

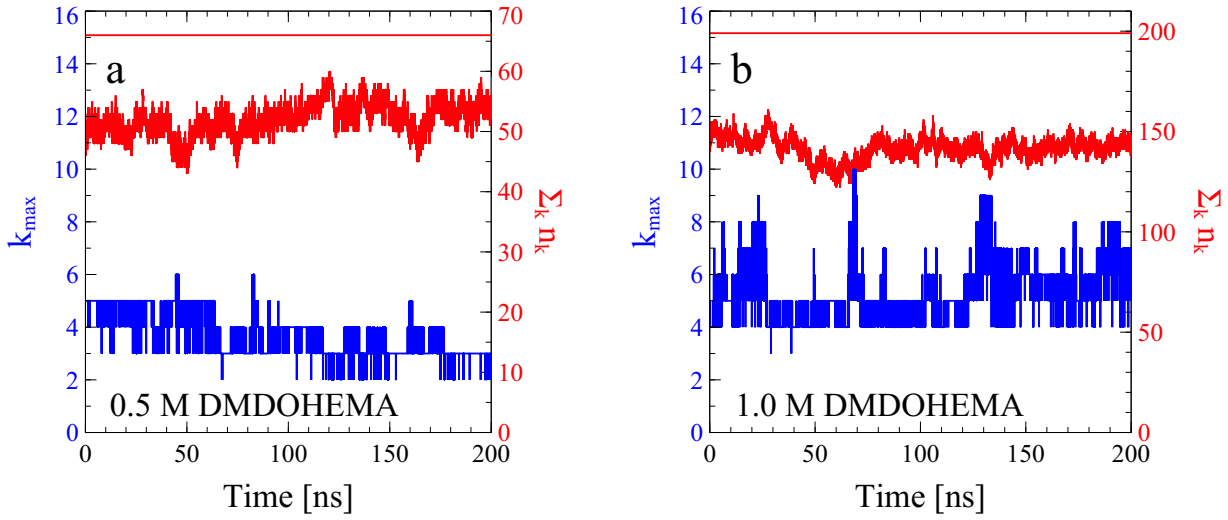

Figure S.6: The size of the single largest water cluster (k_{max}) is shown on the blue left axis and the total number of clusters of all sizes ($\sum_k n_k$) is shown on the red right axis as a function of simulation time. For reference, the total number of water molecules is shown on the red axis at a solid red line. Data for 0.5 M DMDOHEMA in dodecane is shown in panel A, and data for 1.0 M DMDOHEMA is shown in panel B.