Experimental report

06/01/2021

Proposal: 9-12-579 **Council:** 4/2019

Title: The Self-assembly and Structural Evolution of glycerol monooleate in oil with Water Doping

Research area: Engineering

This proposal is a new proposal

Main proposer: Thomas MCCOY

Experimental team: Thomas MCCOY
Alexander ARMSTRONG
Alexander ROUTH
Belinda FONSEKA

Local contacts: Sylvain PREVOST

Samples: D2O
dodecane-d26
Glycerol monooleate
dodecane-h26

Instrument	Requested days	Allocated days	From	To
D11	2	2	24/09/2019	26/09/2019

Abstract:

The precise mechanism by which organic friction modifiers adsorb to a metal surface and reduce friction and wear remains unclear. Conflicting results exist between the currently accepted theory for lubrication and molecular dynamics simulations.In order to utilise these compounds optimally, this mechanism must be precisely understood, informing the next generation of friction modifiers that drastically improve the lifetimes of engines and significantly reduce fuel emissions.

Supplementary Material - Temperature and hydration effects of friction modifying surfactant in dodecane

Thomas M. McCoy,[1] Alexander J. Armstrong,[1] Belinda R. Fonseka,[2]
Sylvain Prevost,[3] Beatrice Cattoz,[4] Peter J. Dowding,[4]
Alexander F. Routh[1,*]

[1]BP Institute and Department of Chemical Engineering and Biotechnology,
University of Cambridge, CB3 0EZ, United Kingdom
[2]BP Institute and Department of Chemistry,
University of Cambridge, CB3 0EZ, United Kingdom
[3]Institut Laue Langevin, Grenoble, 38000, France
[4]Infineum UK Ltd, Abingdon, OX13 6BB, United Kingdom

*To whom correspondence should be addressed; E-mail: afr10@cam.ac.uk

Details of fitting parameters used in the modelling of small-angle neutron scattering (SANS) data are presented within, as well as additional graphs showing all datasets. For all SANS modelling, the ellipsoid model in SasView was used without including a polydispersity contribution.[1] A summary of the physicochemical properties for the sample components are shown in Table S1.

Table S1: Physicochemical properties of compounds used in this study.

Additive	Molecular weight g/mol	Density g/mL	Dipole moment D	SLD $\times 10^{-6}$ Å^{-2}
Gylcerol monooleate	356.55	0.94		0.21
Oleic acid	282.47	0.90	2.47	0.08
Toluene	92.14	0.87	0.36	1.09
Phenol	94.11	1.07	1.22	1.45
H_2O	18.02	1.00	1.85	−0.56
D_2O	20.03	1.11	1.86	6.36
D-dodecane	196.50	0.86	0.07	6.71

References

[1] Feigin, L., Svergun, D. I., Taylor, G. W. General principles of small-angle diffraction. In *Structure analysis by small-angle X-ray and neutron scattering*. Springer, **1987**, pages 25–55.

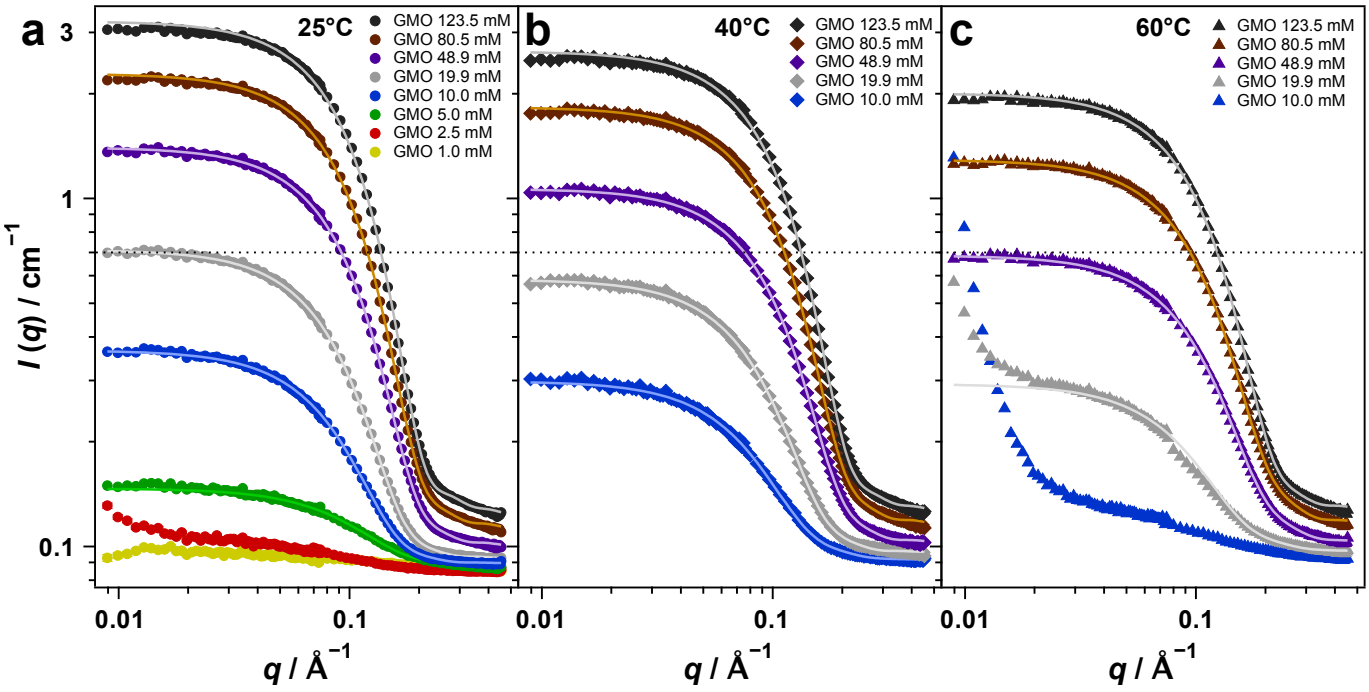

Figure S1: (a)

Table S2: Ellipsoid model fitting parameters of glycerol monooleate (GMO) in D-dodecane at different concentrations and temperatures.

	25°C			40°C			60°C		
[GMO] mM	Scale factor	$R_{Eq.}$ nm	$R_{Ax.}$ nm	Scale factor	$R_{Eq.}$ nm	$R_{Ax.}$ nm	Scale factor	$R_{Eq.}$ nm	$R_{Ax.}$ nm
5.0	7.12×10^{-4}	2.30	0.91	-	-	-	-	-	-
10.0	1.75×10^{-3}	2.69	1.27	1.24×10^{-3}	2.96	1.10	-	-	-
19.9	3.87×10^{-3}	2.61	1.37	3.10×10^{-3}	2.69	1.27	1.90×10^{-3}	2.58	0.90
48.9	9.99×10^{-3}	2.40	1.32	8.54×10^{-3}	2.35	1.19	6.66×10^{-3}	2.29	0.97
80.5	1.66×10^{-2}	2.37	1.35	1.48×10^{-2}	2.32	1.25	1.23×10^{-2}	2.28	1.07
123.5	2.45×10^{-2}	2.30	1.40	2.20×10^{-2}	2.26	1.31	1.87×10^{-2}	2.22	1.19

Table S3: Ellipsoid plus fractal model fitting parameters of 20 mM glycerol monooleate (GMO) in D-dodecane at 60°C.

[GMO] mM	Ellipsoid scale factor	$R_{Eq.}$ nm	$R_{Ax.}$ nm	Fractal scale factor	$R_{Frac.}$ nm	Fractal dimension	Cutoff length nm
19.9	1.95×10^{-3}	2.58	0.90	1.00×10^{-3}	27.50	1.40	60.00

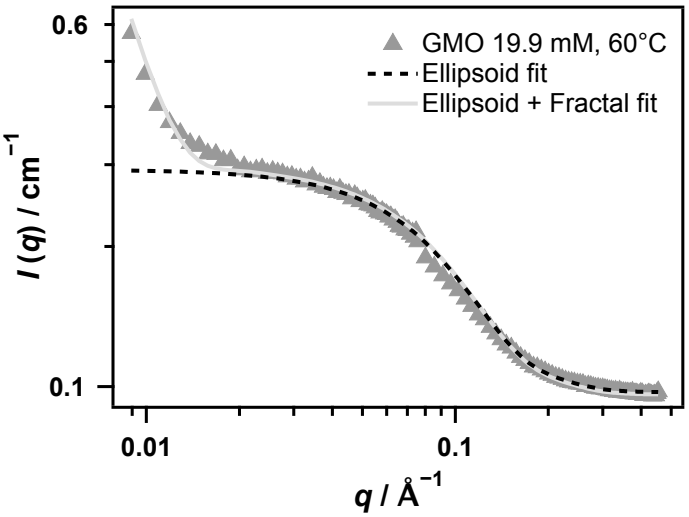

Figure S2: (a)

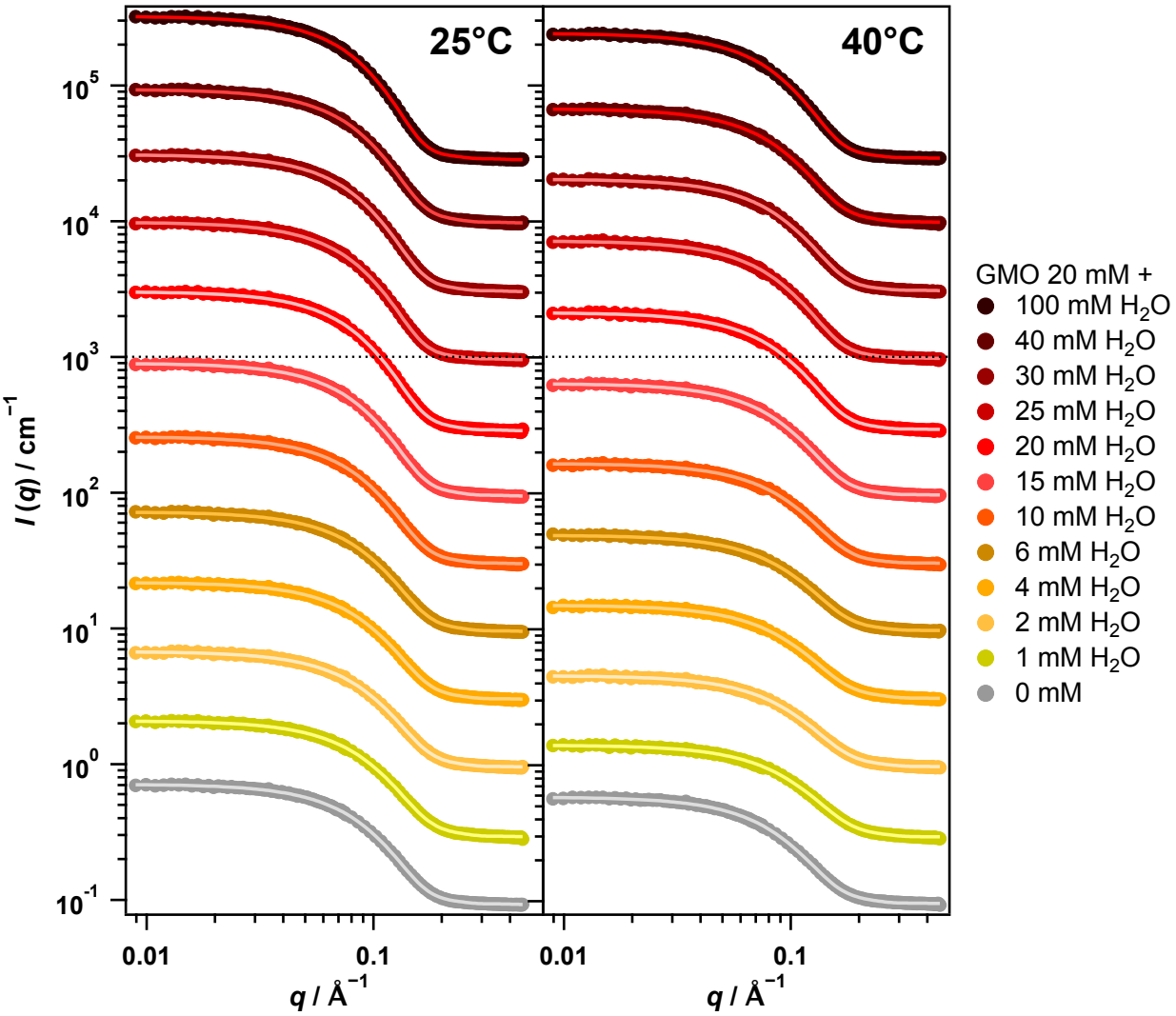

Figure S3: (a)