Deuteration, Today, Tomorrow

Sarah Youngs

ISIS Deuteration Facility

Science & Technology Facilities Council

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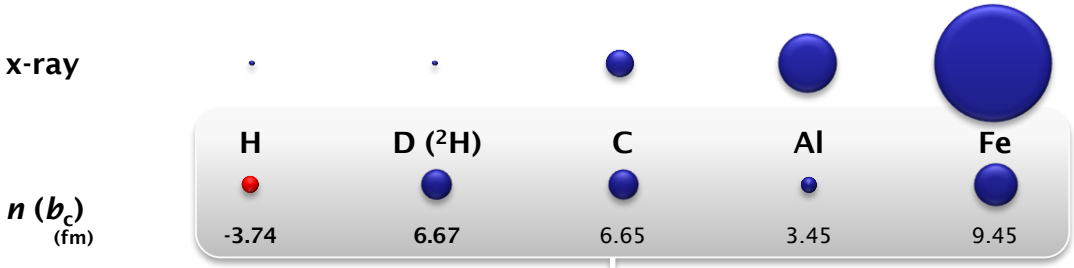
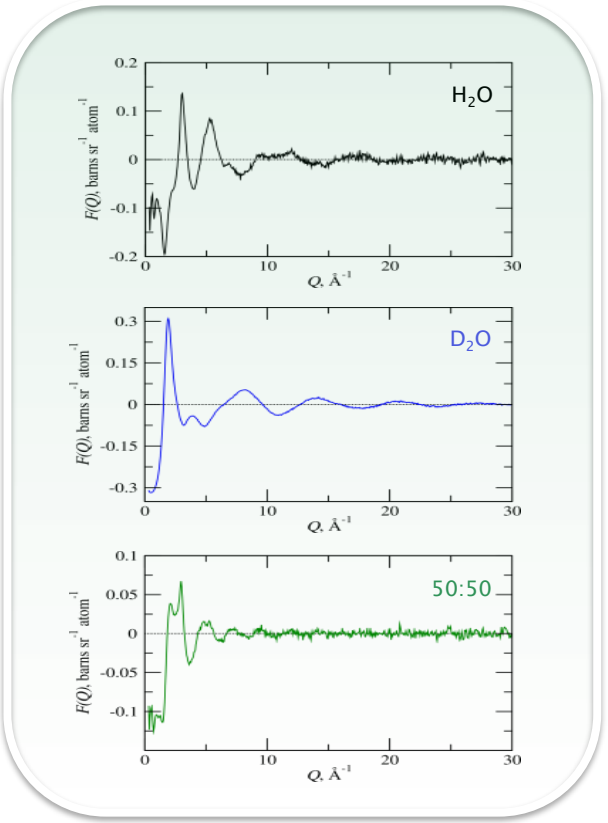
Why Deuteration?



Scattering Lengths

$$F(Q) = \sum_{i,j} (2 - \delta_{ij}) c_i c_j \boldsymbol{b_i b_j} S_{ij}(Q)$$

Composition Structure



Perform multiple measurements on the same system, with different substitutions

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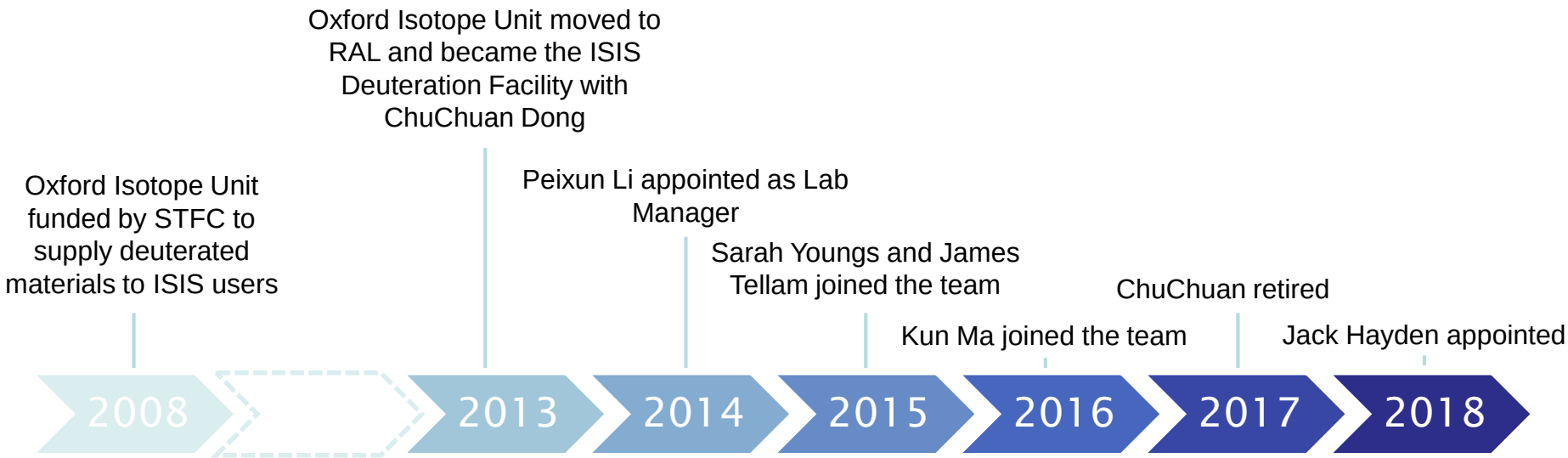
History of the Facility



	2013	2014	2015	2016	2017
Proposal numbers	53	64	79	86	42*
Staff members	2	4	5	4	5*
Student numbers	0	0	3	2	3
Visiting Researchers	0	0	0	2	2

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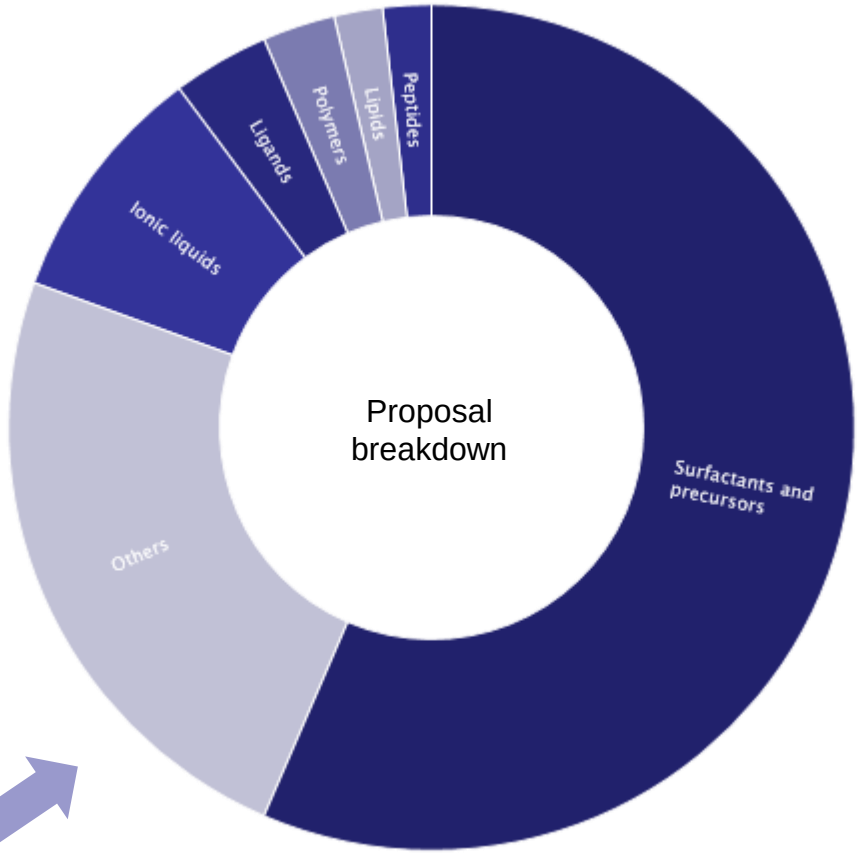
Deuteration Requests

Deuteration FAP members:

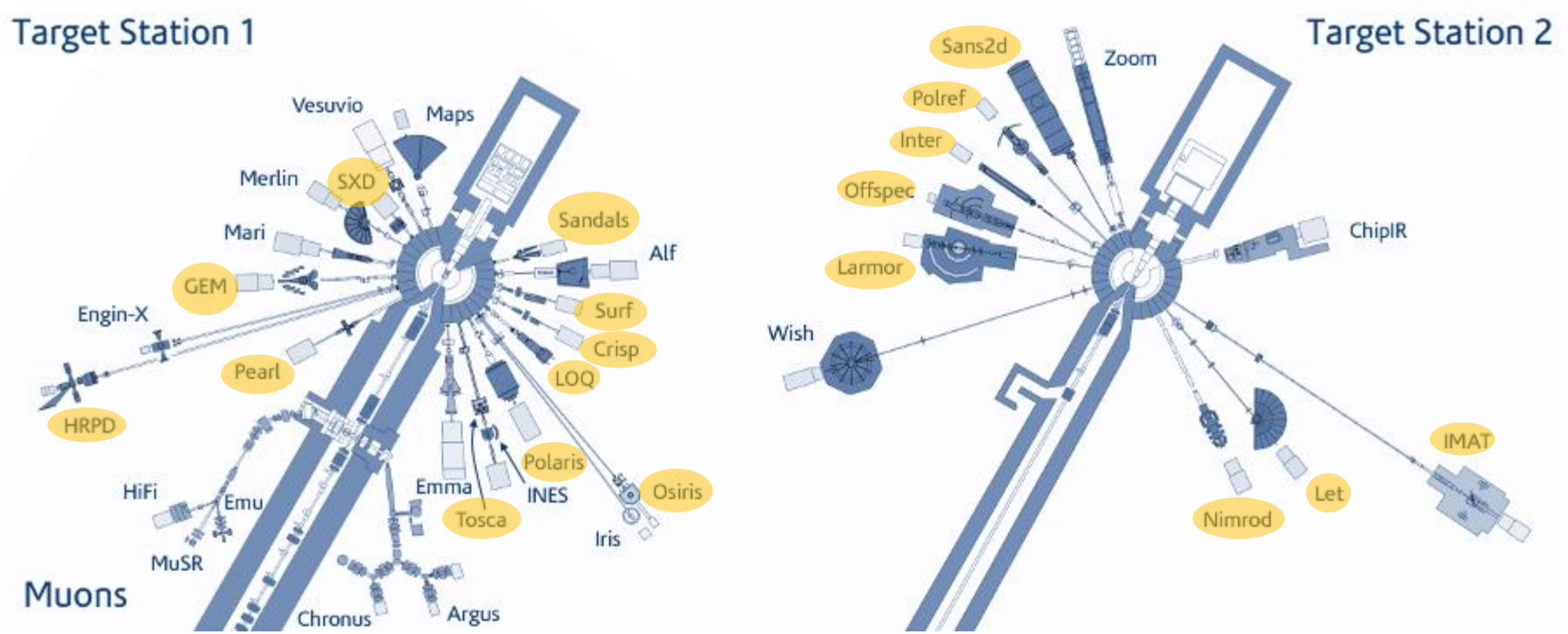
Bob Thomas
Jian Lu
John Webster
Daniel Bowron
Peixun Li
Marek Jura
Sarah Youngs



ISIS Science Areas covered:

- FAP 1: Diffraction
- FAP 2: Liquids
- FAP 3: Large Scale Structures
- FAP 4: Excitations
- FAP 5: Molecular Spectroscopy

Instruments Covered



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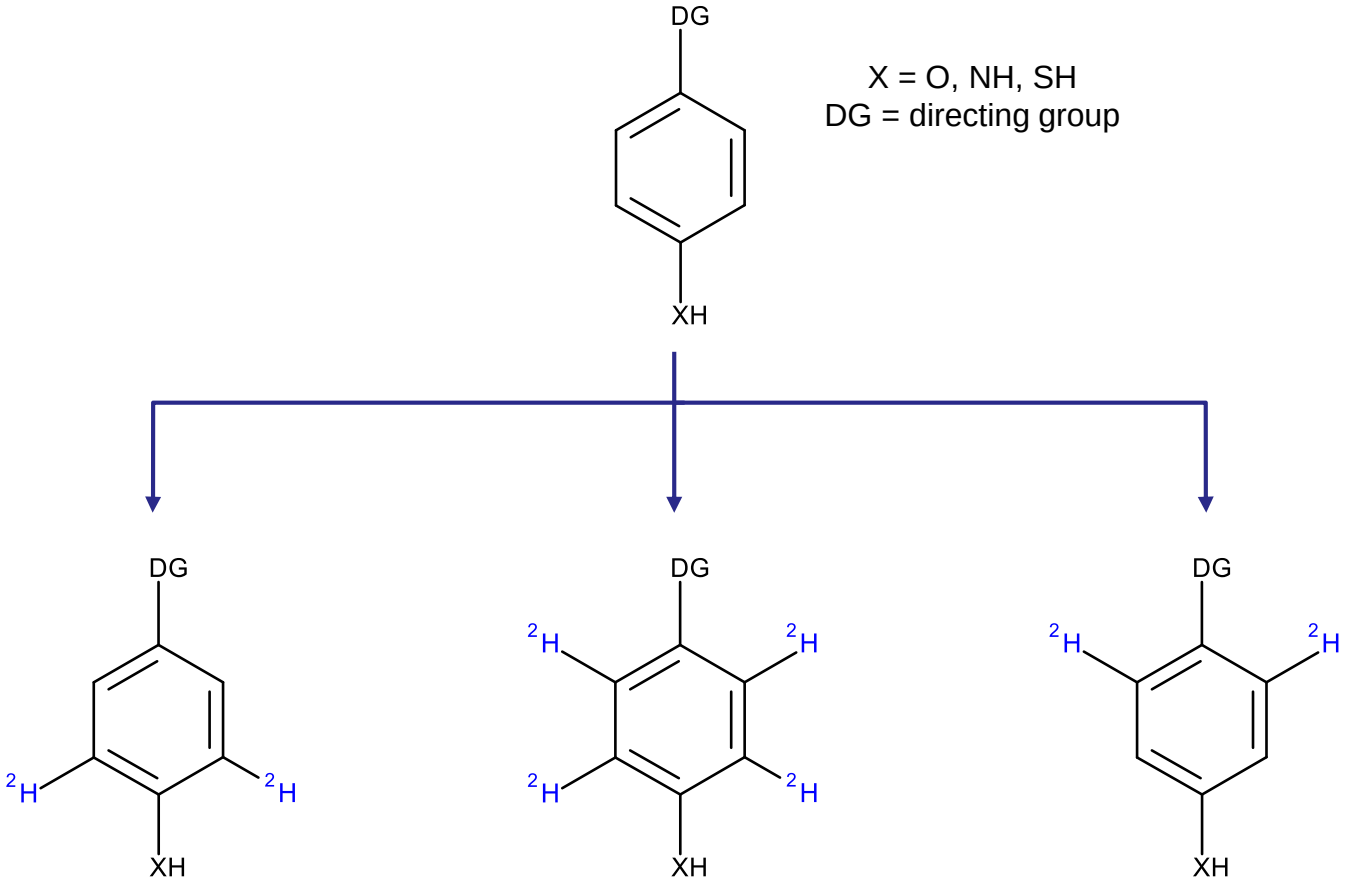
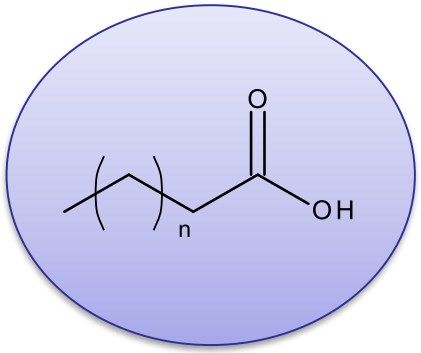
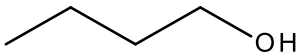
Methods for Deuteration

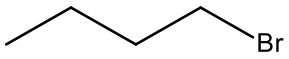


Traditional Compound Requests

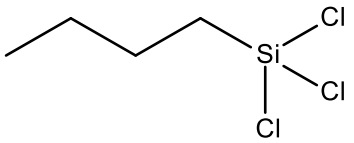


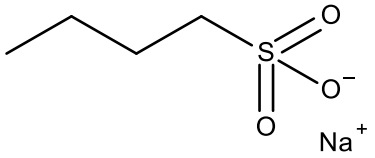
Fatty Acids

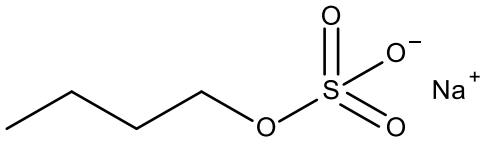


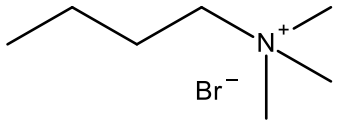


Alcohols/bromides









Surfactants and derivatives

Increasing complexity

Current Facility

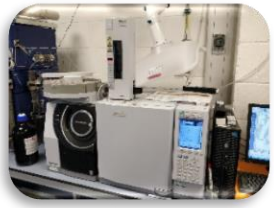
Microwave Reactor

H Cube

Peptide Synthesiser

High Pressure Reactors

Flash and prep-HPLC Columns



GCMS

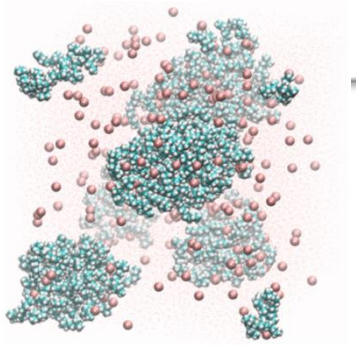
Surfactants

LANGMUIR
Article
pubs.acs.org/Langmuir

Decyltrimethylammonium Bromide Micelles in Acidic Solutions: Counterion Binding, Water Structuring, and Micelle Shape

Daniel T. Bowron[†] and Karen J. Edler[*,‡]

[†]ISIS Pulsed Neutron and Muon Source, Science and Technolog
Oxford, Didcot OX11 0QX, U.K.
[‡]Department of Chemistry, University of Bath, Claverton Down,

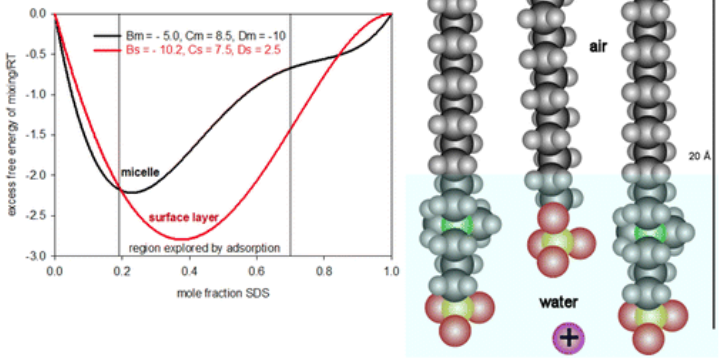


THE JOURNAL OF PHYSICAL CHEMISTRY B
Article
pubs.acs.org/JPCB

Analysis of the Asymmetric Synergy in the Adsorption of Zwitterionic–Ionic Surfactant Mixtures at the Air–Water Interface below and above the Critical Micelle Concentration

Peixun Li,[†] Kun Ma,[†] Robert K. Thomas,[*,†] and Jeffrey Penfold[†,‡]

[†]Physical and Theoretical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford, OX1 3QZ, U.K.
[‡]Rutherford-Appleton Laboratory, Science & Technology Facilities Council, Chilton, Didcot, OX11 0QX, U.K.

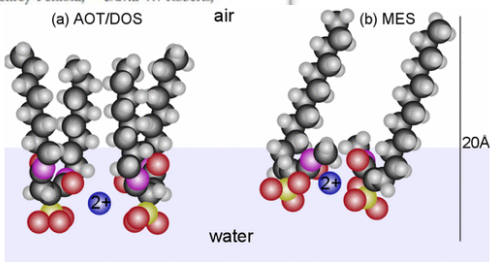


LANGMUIR
Article
pubs.acs.org/Langmuir

Adsorption of Methyl Ester Sulfonate at the Air–Water Interface: Can Limitations in the Application of the Gibbs Equation be Overcome by Computer Purification?

Hui Xu,[†] Peixun Li,[‡] Kun Ma,[‡] Rebecca J. L. Welbourn,[‡] Jeffrey Penfold,[‡,§] David W. Roberts,[∥] Robert K. Thomas,[*,§] and Jordan T. Petkov[†,⊥]

[†]KLK Oleo, SDN BHD, Menara KLK, Muliara Damansara, 47810 Petaling
[‡]Rutherford-Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, Unit
[§]Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxfor
[∥]Liverpool John Moores University, Liverpool, U.K.



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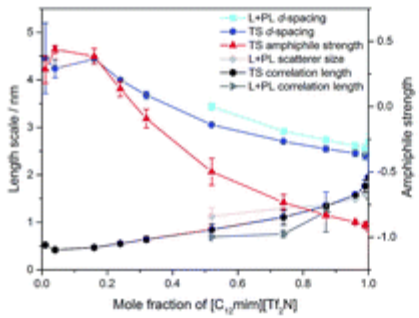
Ionic Liquids

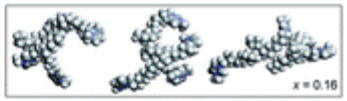
Faraday Discussions
Cite this: *Faraday Discuss.*, 2018, **206**, 265

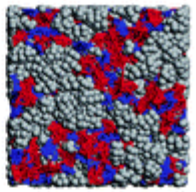
PAPER View Article Online

Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering†

Christopher P. Cabry,[a] Lucia D'Andrea,[a] Karina Shimizu,[b] Isabelle Grillo,[c] Peixun Li,[d] Sarah Rogers,[d] Duncan W. Bruce,[*a] José N. Canongia Lopes[*be] and John M. Slattery[*a]



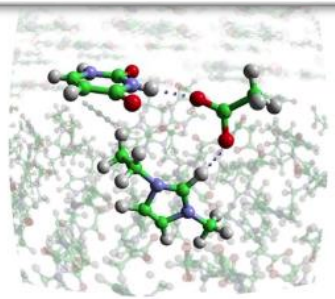




ChemPubSoc Europe DOI: 10.1002/cphc.201600984 CHEMPHYSCHEM Articles

Solvation Structure of Uracil in Ionic Liquids

Sarah E. Norman,[a, b] Adam H. Turner,[b] John D. Holbrey,[b] and Tristan G. A. Youngs*[a]



RSC Advances

PAPER View Article Online

Structure of ionic liquids with amino acid anions *via* neutron diffraction†

Cite this: *RSC Adv.*, 2015, **5**, 67220

S. E. Norman,‡*[a] A. H. Turner[a] and T. G. A. Youngs[b]

The liquid structures of the ionic liquids 1-ethyl-3-methylimidazolium alaninate and 1-ethyl-3-methylimidazolium serinate are fully elucidated through the application of neutron diffraction techn
serin
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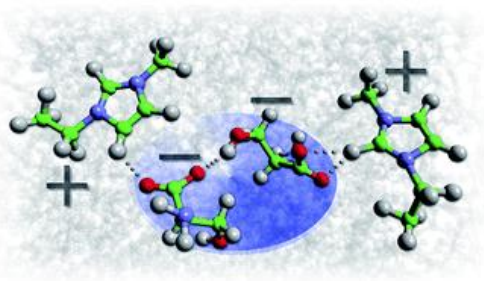
Received 15th April 2015
Accepted 28th July 2015
DOI: 10.1039/c5ra06785e
www.rsc.org/advances



PCCP

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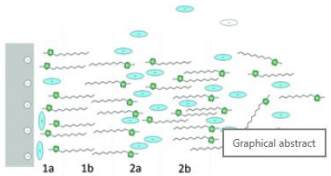
Direct measurements of ionic liquid layering at a single mica–liquid interface and in nano-films between two mica–liquid interfaces†

Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 297

Lucy R. Griffin,[a] Kathryn L. Browning,[a] Stuart M. Clarke,*[a] Alexander M. Smith,[b] Susan Perkin,[b] M. W. A. Skoda[c] and Sarah E. Norman[c]



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Deep Eutectic Salts

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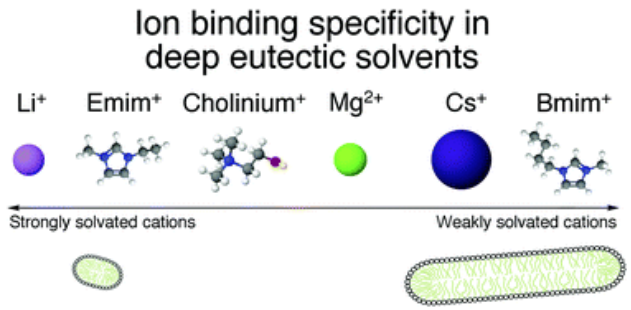
Cite this: Phys. Chem. Chem. Phys., 2018, 20, 13952

Counterion binding alters surfactant self-assembly in deep eutectic solvents†

A. Sanchez-Fernandez, O. S. Hammond, K. J. Edler, T. Arnold, J. Doutch, R. M. Dalgliesh, P. Li, K. Ma and A. J. Jackson



The Journal of Physical Chemistry Letters

Letter

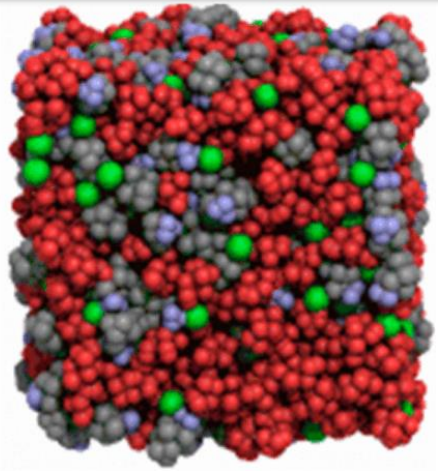
Cite This: J. Phys. Chem. Lett. 2018, 9, 3922−3927

pubs.acs.org/JPCL

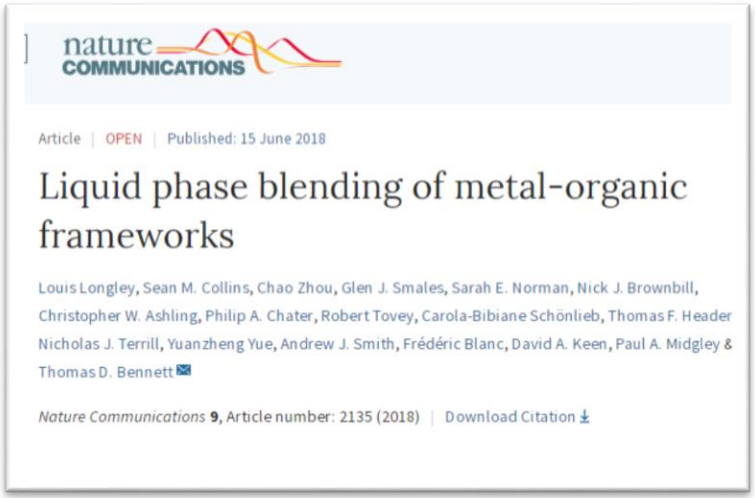
Amphiphilically Nanostructured Deep Eutectic Solvents

Samila McDonald,† Thomas Murphy,† Silvia Imberti,‡ Gregory G. Warr,§ and Rob Atkin*,∥

†Priority Research Centre for Advanced Fluids and Interfaces, Newcastle Institute for Energy and Resources (NIER), The University of Newcastle, Newcastle, New South Wales 2308, Australia
‡STFC, Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom
§School of Chemistry and Sydney Nano Institute, University of Sydney, Sydney, New South Wales 2006, Australia
∥School of Molecular Sciences, The University of Western Australia, Perth, Western Australia 6009, Australia



Metal Organic Framework Ligands



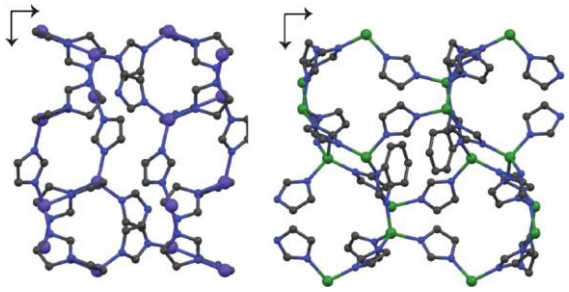
nature COMMUNICATIONS

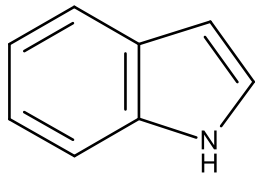
Article | OPEN | Published: 15 June 2018

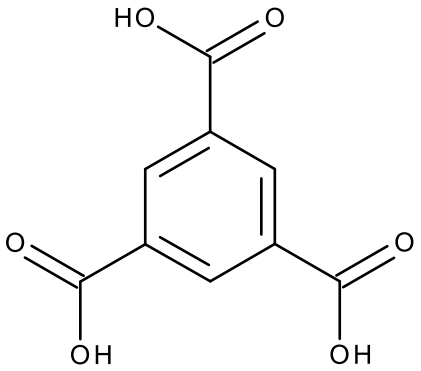
Liquid phase blending of metal-organic frameworks

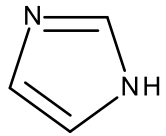
Louis Longley, Sean M. Collins, Chao Zhou, Glen J. Smales, Sarah E. Norman, Nick J. Brownbill, Christopher W. Ashling, Philip A. Chater, Robert Tovey, Carola-Bibiane Schönlieb, Thomas F. Header Nicholas J. Terrill, Yuanzheng Yue, Andrew J. Smith, Frédéric Blanc, David A. Keen, Paul A. Midgley & Thomas D. Bennett

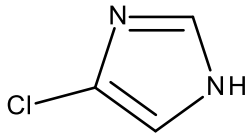
Nature Communications **9**, Article number: 2135 (2018) | Download Citation

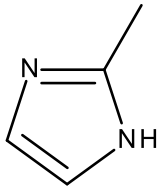












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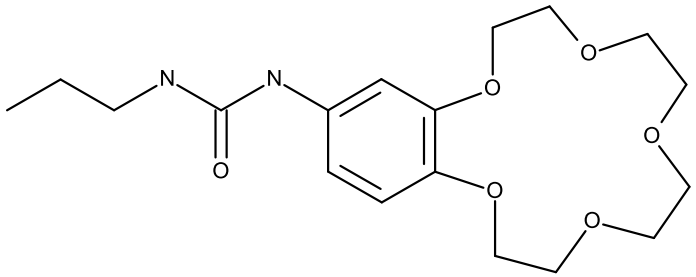
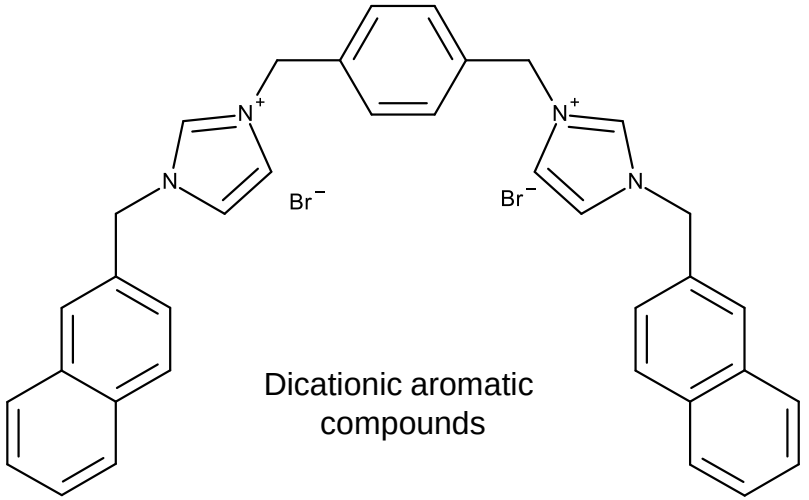
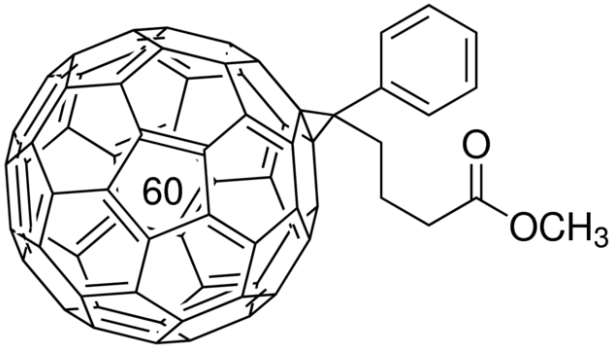
Increasing Complexity



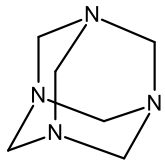
Benzocrown ether



Dicationic aromatic compounds



Functionalised fullerenes



Cage molecule

Moving towards: Batteries, electrolytes, perovskite materials

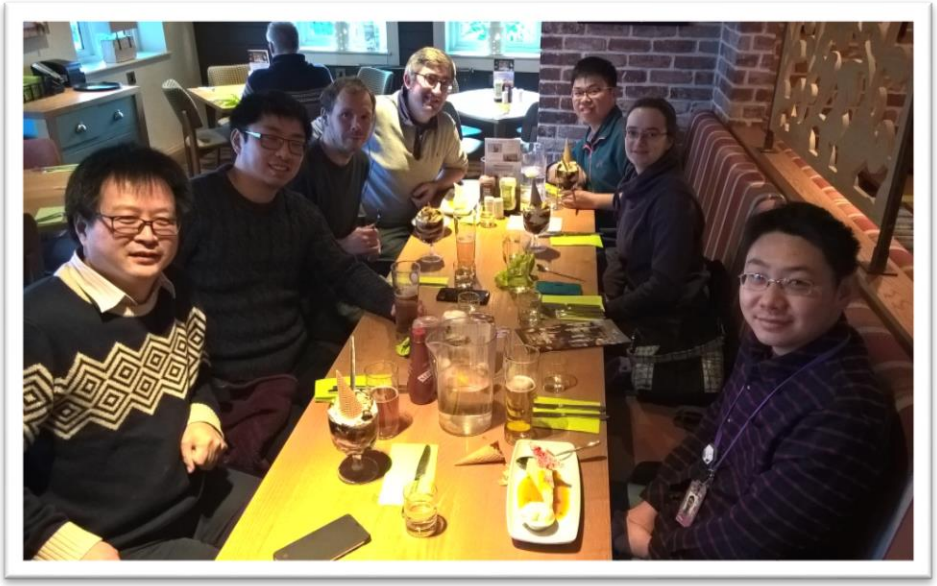
Future of the Deuteration Facility

1. Increasing interaction with user and science groups
2. Help the evolving science programs (more complex materials)
3. Continued development of new deuteration methods

Hosting visitors:

Training the next generation of students and postdocs to carry on with the techniques we develop on site

Acknowledgements



https://www.isis.stfc.ac.uk/Pages/ISIS-Deuteration-Facility-Lab.aspx

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