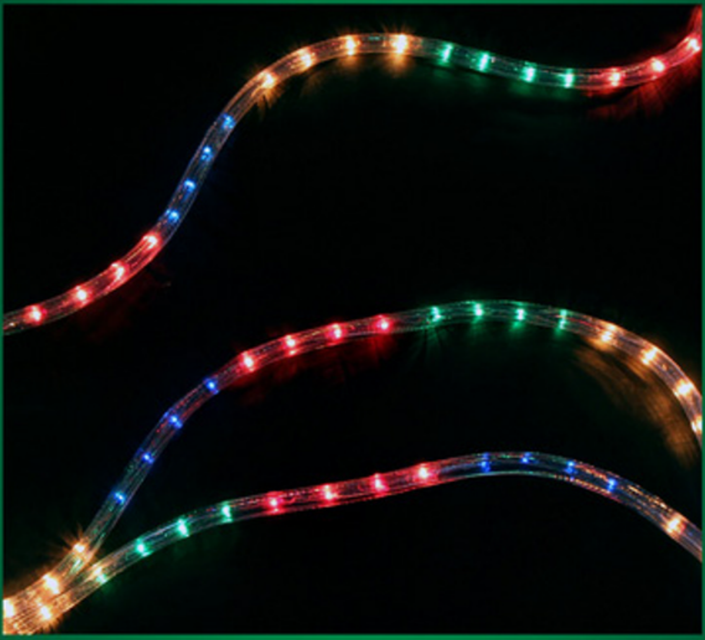
Ionic Liquids Completely UnCOILed

Critical Expert Overviews



Edited by

NATALIA V. PLECHKOVA
KENNETH R. SEDDON

WILEY

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CONTENTS OF "IONIC LIQUIDS UNCOILED"

CONTENTS OF "IONIC LIQUIDS FURTHER UnCOILed"

COIL CONFERENCES

COIL-1	Salzburg	Austria	2005
COIL-2	Yokohama	Japan	2007
COIL-3	Cairns	Australia	2009
COIL-4	Washington	USA	2011
COIL-5	Algarve	Portugal	2013
COIL-6	Jeju Island	South Korea	2015
COIL-7	Ottawa	Canada	2017
COIL-8	Belfast[a]	UK	2019

[a] Precise location still to be confirmed.

PREFACE

This is the third and final book of three volumes of critical overviews of the key areas of ionic liquid chemistry. The first volume was entitled *Ionic Liquids UnCOILed*; the second was *Ionic Liquids Further UnCOILed*. The history and rationale behind this trilogy were explained in the preface to Volume 1 and so will not be repeated here. But we did instruct the authors as follows: 'It is important to emphasise that these are meant to be critical reviews. We are not looking for comprehensive coverage, but insight, appreciation and prospect. We want the type of review which can be read to give a sense of importance and scope of the area, highlighting this by the best published work and looking for the direction in which the field is moving. We would also like the problems with the area highlighting, *e.g.* poor experimental technique, poor selection of liquids, and variability of data'. Looking back over all three books, we are amazed at the quality of reviews produced and their 'timeless' nature – they are fresh and inciteful.

This final book includes eleven critical expert overviews of differing aspects of ionic liquids – the final chapter could almost be a stand-alone book. It is our continuing view that, in the second decade of the twenty-first century, reviews that merely regurgitate a list of all papers on a topic, giving a few lines or a paragraph (often the abstract!) to each one, have had their day – 5 min with an online search engine will provide that information. But we are sure that the growth of open-access journals and books from predatory online publishers will guarantee their prolonged existence. Such reviews belong with cassette tapes, typewriters and the printed journal – valuable in their day, but of little value now. The value of a review lies in the expertise and insight of the reviewer and their willingness to share it with the reader. It takes moral courage to say 'the work of […] is irreproducible, or of poor quality, or that the conclusions are not valid' – but in a field expanding at the prestigious rate of ionic liquids, it is essential to have this honest feedback. Otherwise, errors are propagated. Papers still, in 2015, appear using hexafluorophosphate or tetrafluoroborate ionic liquids for synthetic or catalytic chemistry, and calculations on 'ion pairs' are still being used to rationalise liquid state properties! We trust this volume, containing eleven excellently perceptive reviews, will help guide and secure the future of ionic liquids. We believe the reviews in our volumes should be compulsory reading for all research workers in the field.

Natalia V. Plechkova
Kenneth R. Seddon

ACKNOWLEDGEMENTS

This volume is a collaborative effort. We, the editors, have our names emblazoned on the cover, but the book would not exist in its present form without the support from many people. Firstly, we thank our authors for producing such splendid, critical chapters and for their open responses to the reviewers' comments and to editorial suggestions. We are also indebted to our team of expert reviewers, whose comments on the individual chapters were challenging and thought provoking, and to Martyn J. Earle for his photographic assistance. The backing from the team at Wiley, led by Dr. Arza Seidel, has been fully appreciated – it is always a pleasure to work with such a professional group of people. Finally, this book would never have been published without the unfailing, enthusiastic support from Deborah Poland and Sinead McCullough, whose patience and endurance continue to make the impossible happen. So we thank again everyone involved in the project – we are proud to have been associated with them.

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ABBREVIATIONS

Ionic Liquids

GNCS	guanidinium thiocyanate
GRTIL	gemini room-temperature ionic liquid
[HI-AA]	hydrophobic derivatised amino acid
IL	ionic liquid
poly(GRTIL)	polymerised gemini room-temperature ionic liquid
poly(RTIL)	polymerised room-temperature ionic liquid
RTIL	room-temperature ionic liquid
$[PSpy]_3[PW]$	$[1\text{-}(3\text{-sulfonic acid})\text{propylpyridinium}]_3[PW_{12}O_{40}]\cdot 2H_2O$

Cations

$[bm(2\text{-}Me)im]^+$	1-butyl-2,3-dimethylimidazolium
$[(bz)C_1C_5im]^+$	1-benzyl-2-methyl-3-pentylimidazolium
$[C_{10}btz]^+$	3-decylbenzothiazolium
$[C_{11}btz]^+$	3-undecylbenzothiazolium
$[C_{12}btz]^+$	3-dodecylbenzothiazolium
$[1\text{-}C_m\text{-}3\text{-}C_nim]^+$	1,3-dialkylimidazolium
$[C_nmim]^+$	1-alkyl-3-methylimidazolium
$[C_nC_mim]^+$	1-alkyl-3-alkylimidazolium
$[Hmim]^+$	1-methylimidazolium
$[C_1mim]^+$	1,3-dimethylimidazolium
$[C_1C_1im]^+$	1,3-dimethylimidazolium
$[C_1C_1C_1im]^+$	1,2,3-trimethylimidazolium
$[C_1C_1mim]^+$	1,2,3-trimethylimidazolium
$[C_2im]^+$	1-ethylimidazolium
$[C_2C_1im]^+$	1-ethyl-3-methylimidazolium
$[C_2C_1C_1im]^+$	1-ethyl-2,3-dimethylimidazolium
$[C_2C_1C_1im]^+$	1-ethyl-2,3-dimethylimidazolium
$[C_2mim]^+$	1-ethyl-3-methylimidazolium
$[C_1C_1(2\text{-}NO_2)im]^+$	1,3-dimethyl-2-nitroimidazolium
$[C_1C_1(2\text{-}Me\text{-}4\text{-}NO_2)im]^+$	1,3-dimethyl-2-methyl-4-nitroimidazolium

$[C_1C_1(4\text{-}NO_2)im]^+$	1,3-dimethyl-4-nitroimidazolium
$[C_2C_1(4\text{-}NO_2)im]^+$	1-ethyl-3-methyl-4-nitroimidazolium
$[C_3mim]^+$	1-propyl-3-methylimidazolium
$[C_3C_3im]^+$	1,3-dipropylimidazolium
$[^iC_3mim]^+$	1-*iso*-propyl-3-methylimidazolium
$[^iC_3\ ^iC_3im]^+$	1,3-di-*iso*-propylimidazolium
$[(^iC_3)_2im]^+$	1,3-di-*iso*-propylimidazolium
$[C_4C_1im]^+$	1-butyl-3-methylimidazolium
$[C_4mim]^+$	1-butyl-3-methylimidazolium
$[^iC_4mim]^+$	1-*iso*-butyl-3-methylimidazolium
$[^sC_4mim]^+$	1-*sec*-butyl-3-methylimidazolium
$[^tC_4mim]^+$	1-*tert*-butyl-3-methylimidazolium
$[(^tC_4)_2im]^+$	1,3-di-*iso*-butylimidazolium
$[C_4C_4im]^+$	1,3-dibutylimidazolium
$[^tC_4{}^tC_4im]$	1,3-di-*tert*-butylimidazolium
$[C_4C_1(4,5\text{-}Br_2)im]^+$	1-butyl-3-methyl-4,5-bromoimidazolium
$[C_5mim]^+$	1-pentyl-3-methylimidazolium
$[C_6mim]^+$	1-hexyl-3-methylimidazolium
$[C_6C_1im]^+$	1-hexyl-3-methylimidazolium
$[C_6C_6im]^+$	1,3-dihexylimidazolium
$[C_7mim]^+$	1-heptyl-3-methylimidazolium
$[C_8mim]^+$	1-octyl-3-methylimidazolium
$[C_9mim]^+$	1-nonyl-3-methylimidazolium
$[C_{10}mim]^+$	1-decyl-3-methylimidazolium
$[(C_{10})_2im]^+$	1,3-didecylimidazolium
$[C_{11}mim]^+$	1-undecyl-3-methylimidazolium
$[C_{12}mim]^+$	1-dodecyl-3-methylimidazolium
$[(C_{12})_2im]^+$	1,3-didodecylimidazolium
$[C_{13}mim]^+$	1-tridecyl-3-methylimidazolium
$[C_{14}mim]^+$	1-tetradecyl-3-methylimidazolium
$[C_{15}mim]^+$	1-pentadecyl-3-methylimidazolium
$[C_{16}mim]^+$	1-hexadecyl-3-methylimidazolium
$[C_{17}mim]^+$	1-heptadecyl-3-methylimidazolium
$[C_{18}mim]^+$	1-octadecyl-3-methylimidazolium
$[C_2C_1mim]^+$	1-ethyl-2,3-dimethylimidazolium
$[C_3C_1mim]^+$	1-propyl-2,3-dimethylimidazolium
$[C_8C_3im]^+$	1-octyl-3-propylimidazolium
$[C_{12}C_{12}im]^+$	1,3-bis(dodecyl)imidazolium
$[C_1OC_2mim]^+$	1-(2-methoxyethyl)-3-methylimidazolium
$[C_4dmim]^+$	1-butyl-2,3-dimethylimidazolium
$[C_4C_1C_1im]^+$	1-butyl-2,3-dimethylimidazolium
$[C_4C_1mim]^+$	1-butyl-2,3-dimethylimidazolium
$[C_6C_{7O1}im]^+$	1-hexyl-3-(heptyloxymethyl)imidazolium
$[C_2F_3mim]^+$	1-trifluoroethyl-3-methylimidazolium
$[C_4vim]^+$	3-butyl-1-vinylimidazolium

$[(^iC_3)_2(4,5\text{-}Me_2)im]^+$	1-*iso*-propyl-3,4,5-trimethylimidazolium
$[^iC_3C_1(4,5\text{-}Me_2)im]^+$	1,3-di-*iso*-propyl-4,5-dimethylimidazolium
$[(^tC_4)_2(4\text{-}SiMe_3)im]^+$	1,3-di-*tert*-butyl-4-trimethylsilylimidazolium
$[(allyl)mim]^+$	1-allyl-3-methylimidazolium
$[P_nmim]^+$	polymerisable 1-methylimidazolium
$[C_2mmor]^+$	1-ethyl-1-methylmorpholinium
$[C_2py]^+$	1-ethylpyridinium
$[C_4py]^+$	1-butylpyridinium
$[C_6py]^+$	1-hexylpyridinium
$[C_8py]^+$	1-octylpyridinium
$[C_{14}py]^+$	1-tetradecylpyridinium
$[C_4m_\beta py]^+$	1-butyl-3-methylpyridinium
$[C_4m_\gamma py]^+$	1-butyl-4-methylpyridinium
$[C_6(dma)_\gamma py]^+$	1-hexyl-4-dimethylaminopyridinium
$[C_nC_1pyr]^+$	1-alkyl-1-methylpyrrolidinium
$[C_1C_1pyr]^+$	1,1-dimethylpyrrolidinium
$[C_1C_2pyr]^+$	1-ethyl-1-methylpyrrolidinium
$[C_2C_1pyr]^+$	1-ethyl-1-methylpyrrolidinium
$[C_2mpyr]^+$	1-ethyl-1-methylpyrrolidinium
$[C_3C_1pyr]^+$	1-propyl-1-methylpyrrolidinium
$[C_3mpyr]^+$	1-propyl-1-methylpyrrolidinium
$[C_4mpyr]^+$	1-butyl-1-methylpyrrolidinium
$[C_4C_1pyr]^+$	1-butyl-1-methylpyrrolidinium
$[C_5C_1pyr]^+$	1-pentyl-1-methylpyrrolidinium
$[C_6mpyr]^+$	1-hexyl-1-methylpyrrolidinium
$[C_nC_1pyr]^+$	1-alkyl-1-methylpyrrolidinium
$[C_1C_3pip]^+$	1-methyl-1-propylpiperidinium
$[C_2C_1pip]^+$	1-ethyl-1-methylpiperidinium
$[C_2C_6pip]^+$	1-ethyl-1-hexylpiperidinium
$[C_3C_1pip]^+$	1-methyl-1-propylpiperidinium
$[C_8quin]^+$	1-octylquinolinium
$[dabcoH]^+$	1,4-diazabicyclo[2.2.2]octan-1-ium(1+)
$[dabcoH_2]^{2+}$	1,4-diazabicyclo[2.2.2]octan-1-ium(2+)
$[dmPhim]^+$	1,3-dimethyl-2-phenylimidazolium
$[FcC_1mim]^+$	1-ferrocenyl-3-methylimidazolium
$[H_2NC_2H_4py]^+$	1-(1-aminoethyl)pyridinium
$[H_2NC_3H_6mim]^+$	1-(3-aminopropyl)-3-methylimidazolium
$[HN_{2\,2\,2}]^+$	triethylammonium
$[H_2mor]^+$	morpholinium
$[H_2pip]^+$	piperidinium
$[Hpy]^+$	pyridinium
$[H_2pyr]^+$	pyrrolidinium
$[N_{0\,1\,1\,1}]^+$	trimethylammonium
$[N_{0\,0\,1\,1}]^+$	dimethylammonium
$[N_{0\,0\,0\,1}]^+$	methylammonium

$[N_{1\,1\,1\,1}]^+$	tetramethylammonium
$[N_{1\,1\,1\,2OH}]^+$	cholinium
$[N_{1\,1\,2\,2OH}]^+$	ethyl(2-hydroxyethyl)dimethylammonium
$[N_{1\,1\,1\,4}]^+$	trimethylbutylammonium
$[N_{1\,4\,4\,4}]^+$	methyltributylammonium
$[N_{1\,8\,8\,8}]^+$	methyltrioctylammonium
$[N_{2\,2\,2\,2}]^+$	tetraethylammonium
$[N_{3\,3\,3\,3}]^+$	tetrapropylammonium
$[N_{3\,3\,3\,11}]^+$	tripropylundecylammonium
$[N_{3\,3\,6\,8}]^+$	dipropylhexyloctylammonium
$[N_{4\,4\,4\,4}]^+$	tetrabutylammonium
$[N_{5\,5\,5\,5}]^+$	tetrapentylammonium
$[N_{6\,6\,6\,6}]^+$	tetrahexylammonium
$[N_{6\,6\,6\,14}]^+$	trihexyl(tetradecyl)ammonium
$[N_{10\,10\,10\,10}]^+$	tetradecylimidazolium
$[N_{12\,12\,12\,12}]^+$	tetradodecylammonium
$[NR_3H]^+$	trialkylammonium
$[P_{2\,2\,2(1O1)})]^+$	triethyl(methoxymethyl)phosphonium
$[P_{4\,4\,4\,3a}]^+$	(3-aminopropyl)tributylphosphonium
$[P_{4\,4\,4\,4}]^+$	tetrabutylphosphonium
$[P_{5\,5\,5\,5}]^+$	tetrapentylphosphonium
$[P_{6\,6\,6\,14}]^+$	trihexyl(tetradecyl)phosphonium
$[P_{8\,8\,8\,14}]^+$	tetradecyl(trioctyl)phosphonium
$[P_{10\,10\,10\,10}]^+$	tetradecylphosphonium
$[P_{10\,10\,10}CH_2C(O)NH_2]^+$	amidomethyl-tritetradecylphosphonium
$[P_{10\,10\,10}CH_2CO_2]^+$	carboxymethyl-tritetradecylphosphonium
$[P_{18\,18\,18\,18}]^+$	tetraoctadecylphosphonium
$[PhCH_2eim]^+$	1-benzyl-2-ethylimidazolium
$[pyH]^+$	pyridinium
$[RC_nim]^+$	1,3-dialkylimidazolium
$[Rmim]^+$	1-alkyl-3-methylimidazolium
$[S_{2\,2\,2}]^+$	triethylsulfonium
$[S_{2\,2\,16}]^+$	diethylhexadecylsulfonium
$[(vinyl)mim]^+$	1-vinyl-3-methylimidazolium

Anions

$[Ace]^-$	acetate
$[Ala]^-$	alaninate
$[\beta Ala]^-$	β-alaninate
$[Al(hfip)_4]^-$	tetra(hexafluoro-*iso*-propoxy)aluminate(III)
$[Arg]^-$	arginate
$[Asn]^-$	asparaginate
$[Asp]^-$	asparatinate

$[B_{4444}]^-$	tetrabutylborate
$[BBB]^-$	bis[1,2-benzenediolato(2-)-*O,O′*]borate
$[C_1CO_2]^-$	ethanoate
$[C_1SO_4]^-$, $[O_3SOC_1]^-$	methyl sulfate
$[C_8SO_4]^-$, $[O_3SOC_8]^-$	octyl sulfate
$[C_nSO_4]^-$	alkyl sulfate
$[(C_n)(C_m)SO_4]^-$	asymmetrical dialkyl sulfate
$[(C_n)_2SO_4]^-$	symmetrical dialkyl sulfate
$[CTf_3]^-$	tris{(trifluoromethyl)sulfonyl}methanide
$[Cys]^-$	cysteinate
$[dbsa]^-$	dodecylbenzenesulfonate
$[dca]^-$	dicyanamide
$[FAP]^-$	tris(perfluoroalkyl)trifluorophosphate
$[Gln]^-$	glutaminate
$[Glu]^-$	glutamate
$[Gly]^-$	glycinate anion
$[His]^-$	histidinate
$[Ile]^-$	isoleucinate
$[lac]^-$	lactate
$[Leu]^-$	leucinate
$[Lys]^-$	lysinate
$[Met]^-$	methionate
$[Nle]^-$	norleucinate
$[NDf_2]^-$	bis{bis(pentafluoroethyl)phosphinyl}amide
$[NMes_2]^-$	bis(methanesulfonyl)amide
$[NPf_2]^-$, $[BETI]^-$	bis{(pentafluoroethyl)sulfonyl}amide
$[NTf_2]^-$, $[TFSI]^-$	bis{(trifluoromethyl)sulfonyl}amide
$[O_2CC_1]^-$	ethanoate
$[O_3SOC_2]^-$, $[O_3SOC_2]^-$	ethyl sulfate
$[OMs]^-$	methanesulfonate (mesylate)
$[ONf]^-$	perfluorobutylsulfonate
$[OTf]^-$	trifluoromethanesulfonate
$[OTs]^-$	4-toluenesulfonate, $[4\text{-}CH_3C_6H_4SO_3]^-$ (tosylate)
$[Phe]^-$	phenylalaninate
$[Pro]^-$	prolinate
$[Sacc]^-$	saccharinate
$[Ser]^-$	serinate
$[Suc]^-$	succinate
$[tfpb]^-$	tetrakis(3,5-bis(trifluoromethyl)phenyl)borate
$[Thr]^-$	threoninate
$[Tos]^-$	tosylate
$[Trp]^-$	tryphtophanate
$[Tyr]^-$	tyrosinate
$[Val]^-$	valinate

Techniques

AA	all-atom parameterisation
AES	Auger electron spectroscopy
AFM	atomic force microscopy
AMBER	Assisted Model Building with Energy Refinement
ANN	associative neural network
APPLE&P	Atomistic Polarisable Potential for Liquids, Electrolytes and Polymers
ARXPS	angle-resolved X-ray photoelectron spectroscopy
ATR-IR	attenuated total reflectance infrared spectroscopy
BPNN	back-propagation neural network
BPP	Bloembergen–Purcell–Pound theory
CADM	computer-aided design modelling
CC	Cole–Cole model
CCC	countercurrent chromatography
CD	Cole–Davidson model
CE	capillary electrophoresis
CEC	capillary electrochromatography
CHARMM	Chemistry at HARvard Molecular Mechanics
COSMO-RS	**Co**nductor-like **S**creening **Mo**del for Real Solvents
COSY	**Co**rrelation Spectroscop**y**
CPCM	conductor-like polarisable continuum model
CPMD	Car–Parrinello molecular dynamics
DFT	density functional theory
DLVO	Derjaguin, Landau, Verwey and Overbeek theory
DRS	dielectric relaxation spectroscopy
DSC	differential scanning calorimetry
ECSEM	electrochemical scanning electron microscopy
EC-XPS	electrochemical X-ray photoelectron spectroscopy
EF-CG	effective force coarse-graining method
EFM	effective fragment potential method
EI	electron ionisation
EIS	electrochemical impedance spectroscopy
EMD	equilibrium molecular dynamics
EOF	electro-osmotic flow
EPSR	empirical potential structure refinement
ES	electrospray mass spectrometry
ESI–MS	electrospray ionisation mass spectrometry
EXAFS	extended X-ray absorption fine structure
FAB	fast atom bombardment
FMO	fragment molecular orbital method
FIR	far-infrared spectroscopy
FTIR	Fourier transform infrared spectroscopy
GAMESS	general atomic and molecular electronic structure system

GC	gas chromatography
GGA	generalised gradient approximations
GLC	gas–liquid chromatography
GSC	gas–solid chromatography
HM	heuristic method
HOESY	heteronuclear Overhauser effect spectroscopy
HPLC	high-performance liquid chromatography
HREELS	high-resolution electron energy loss spectroscopy
IGC	inverse gas chromatography
IPES	inverse photoelectron spectroscopy
IR	infrared spectroscopy
IRAS	infrared reflection–absorption spectroscopy
IR-VIS SFG	infrared visible sum-frequency generation
ISS	ion scattering spectroscopy
LEIS	low-energy ion scattering
L-SIMS	liquid secondary ion mass spectrometry
MAES	metastable atom electron spectroscopy
MALDI	matrix-assisted laser desorption
MBSS	molecular beam surface scattering
MC	Monte Carlo
MD	molecular dynamics
MIES	metastable impact electron spectroscopy
MLP	multilayer perceptron
MLR	multi-linear regression
MM	molecular mechanics
MR	magnetic resonance
MRI	magnetic resonance imaging
MS	mass spectrometry
NEMD	non-equilibrium molecular dynamics
NEXAFS	near-edge absorption fine structure
NIR	near-infrared spectroscopy
NMR	nuclear magnetic resonance
NR	neutron reflectivity
NRTL	non-random two liquid
OPLS	Optimised Potentials for Liquid Simulations
PCM	polarisable continuum model
PDA	photodiode array detection
PES	photoelectron spectroscopy
PFG-NMR	pulsed field-gradient nuclear magnetic resonance
PGSE-NMR	pulsed-gradient spin-echo nuclear magnetic resonance
PPR	projection pursuit regression
QM	quantum mechanics
QSAR	quantitative structure–activity relationship
QSPR	quantitative structure–property relationship
RAIRS	reflection–absorption infrared spectroscopy

RI	refractive index
RMC	reverse Monte Carlo
RNEMD	reverse non-equilibrium molecular dynamics
RNN	recursive neural network
ROESY	rotating-frame Overhauser effect spectroscopy
RP-HPLC	reverse-phase high-performance liquid chromatography
RST	regular solution theory
SANS	small-angle neutron scattering
SCMFT	self-consistent mean field theory
SEM	scanning electron microscopy
SEM-EDX	scanning electron microscopy with energy-dispersive X-ray
SFA	surface forces apparatus
SFC	supercritical fluid chromatography
SFG	sum-frequency generation
SFM	systematic fragmentation method
SIMS	secondary ion mass spectrometry
soft-SAFT	soft statistical associating fluid theory
STM	scanning tunnelling microscopy
SVN	support vector network
TEM	tunnelling electron microscopy
TGA	thermogravimetric analysis
THz-TDS	terahertz time-domain spectroscopy
TLC	thin-layer chromatography
tPC-PSAFT	truncated perturbed chain-polar statistical associating fluid theory
TPD	temperature programmed desorption
UA	united-atom parameterisation
UHV	ultra-high vacuum
UNIFAC	*UNI*QUAC *F*unctional-group *A*ctivity *C*oefficients
UNIQUAC	*UNI*versal *QUA*si*C*hemical
UPLC	ultra-pressure liquid chromatography
UPS	ultraviolet photoelectron spectroscopy
UV	ultraviolet
UV-Vis	ultraviolet-visible
VBT	volume-based thermodynamics
XPS	X-ray photoelectron spectroscopy
XRD	X-ray powder diffraction
XRR	X-ray reflectivity

MISCELLANEOUS

Å	1 ångstrom = 10^{-10} m
ACS	American Chemical Society
ANQ	1-amino-3-nitroguanidine
API	active pharmaceutical ingredient

ATMS	acetyltrimethylsilane
ATPS	aqueous two-phase system
a.u.	atomic units
BASF™	Badische Anilin- und Sodafabrik
BASIL	Biphasic Acid Scavenging Utilising Ionic Liquids
BATIL	Biodegradability and Toxicity of Ionic Liquids
BE	binding energy
BILM	bulk ionic liquid membrane
BNL	Brookhaven National Laboratory
BOD	biochemical oxygen demand
BP	British Petroleum
b.pt.	boiling point
BSA	bovine serum albumin
BT	benzothiophene
BTAH	benzotriazole
BTX	benzene–toluene–xylene mixture
calc.	calculated
CB	Cibacron Blue 3GA
CCDC	Cambridge Crystallographic Data Centre
CE	crown ether
CEES	2-chloroethyl ethyl sulphide
CFC MC	'continuous fractional component' Monte Carlo
cif	crystallographic information file
CL&P	Canongia Lopes and Pádua
CLM	charge lever momentum
CMC	critical micelle concentration
CMPO	octyl(phenyl)-*N*,*N*-diisobutylcarbamoylmethylphosphine oxide
$[C_nMeSO_4]$	alkyl methyl sulfate
CNTs	carbon nanotubes
CNRS	Centre National de la Recherche Scientifique
COIL	Congress on Ionic Liquids
CPU	central processing unit
CSA	chemical shielding anisotropy
CSD	Cambridge Structural Database
CWAs	chemical warfare agents
d	doublet (NMR)
D°_{298}	bond energy at 298 K
1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
DABCO	1,4-diazabicyclo[2.2.2]octane
DBT	dibenzothiophene
DC	direct current
DC18C6	dicyclohexyl-18-crown-6
DF	Debye and Falkenhagen

DH	Debye–Hückel
DIIPA	diisopropylamine
4,6-DMDBT	4,6-dimethyldibenzothiophene
DNA	deoxyribonucleic acid
DMF	dimethylmethanamide (dimethylformamide)
DMH	dimethylhexene
2DOM	two-dimensional ordered macroporous
3DOM	three-dimensional ordered macroporous
DOS	density of states
DPC	diphenyl carbonate
DRA	drag-reducing agent
DSSC	dye-sensitised solar cell
DSTE	double stimulated-echo
E	enrichment
EDC	extractive distillation column
EE	expanded ensemble approach
EoS	equation of state
EOR	enhanced oil recovery
EPA	Environmental Protection Agency
eq.	equivalent
FCC	fluid catalytic cracking
FFT	fast Fourier transform
FIB	focussed ion beam
FMF	Freiburger Materialforschungszentrum
FRIAS	Freiburg Institute for Advanced Studies
FSE	full-scale error
ft	foot
GDDI	generalised distributed data interface
GEMC	Gibbs ensemble Monte Carlo
GSSG	glutathione disulfide
GSH	glutathione
GT	gauche-trans
HDS	hydrodesulfurisation
HEMA	2-(hydroxyethyl) methacrylate
HOMO	highest occupied molecular orbital
HOPG	highly oriented pyrolytic graphite
HV	high vacuum
i.d.	inner diameter
IFP	Institut Français du Pétrole
IgG	immunoglobulin G
IPBE	ion-pair binding energy
IPE	Institute of Process Engineering, Chinese Academy of Sciences, Beijing
ITO	indium tin oxide
IUPAC	International Union of Pure and Applied Chemistry