

INDEX

- Abbreviations, xv–xxiv
- Ab Manan, Norfaizah, xiii, 117
- Absorption, of vapour, 294
- Absorption isotherms, 172–173
of ammonia, 173
- Absorption/stripping process, 91
- Acid chloroaluminates, 17
- Acidic catalysts, ionic liquids as, 14–19
- Acidic ionic liquids, applications of, 15–18
- Acidic solvents, ionic liquids as, 14–19
- Acidising techniques, 13
- Acid removal, from organic mixtures, 8–9
- Acids. *See also* Amino acid entries; Lewis acid-entries
conjugated, 231
neutralization with protic, 232
- Acylation, 25
- Additive solvents, ionic liquids as, 12
- Additives with specific properties, ionic liquids as, 12–14
- Adhesion problem, 102, 103
- Adsorption, cation, 168
- Advanced biasing procedures, 153
- Advanced materials, radiolytic preparation of, 261
- Aggregates
of ionic liquids, 207
of ions, 218
- Aggregation behaviour, 170
- Air–ionic liquid interface, 295
- Alcohol carbonylation, 21
- Aldehydes, alkyl aromatic, 17–18
- Aldol condensation, 25
- Alkoxyamine preparation, 25–26
- 1-Alkyl-3-methylimidazolium cations, conformers of, 60–62
- 1-Alkyl-3-methylimidazolium ionic liquids
phase behaviour of, 59–85
thermal behaviours of, 59, 80
- Alkyl aromatic aldehydes, 17–18
- Alkylation, of aromatic rings, 17
- Alkylation reactions, 19
of paraffins, 16–17
- Alkyl chain lengths, 280, 281, 284, 292, 295
- Alkyl chains
fluorinated, 293
ion-phobic, 102
- Alkyl groups, melting points and, 280–282
- 1-Alkylimidazolium cation, molecular structure of, 277
- Alkylpyridinium dicyanamide, 4
- Alkyl sulfate ionic liquids, 2–4
long chain, 2–3
- Alkyl sulfates, 246
high purity, 3
onium, 3–4
phosphonium, 4
- Alpha radiolysis, 266
- Amines, isomeric, 106
- Amine treatments, 10
- Amino acid cations, molecular structure of, 277
- Amino acid extraction, 205
- Ammonia, absorption isotherms of, 173
- Ammonium cation, molecular structure of, 278
- Ammonium halides, 14

- Analytical techniques, 297
- Angell strength parameter, 294
- Anion abbreviations, xvii–xviii
- Anion–anion interactions, 171
- Anion behaviour, 168
- Anion–cation interactions, 171
- Anion constituents, of polymerised ionic liquids, 94
- Anion donor ability, 229–230
- Anion effect, 282–283
- Anion head groups, 290–291, 292
- Anionic structures, perfluorinated, 232
- Anionic surfactants, 13–14
- Anions
- CO₂ solubility and, 42
 - dipolar, 246
 - fluorinated, 221, 222
 - ionic liquids with cyanoborate, 4–5
 - ionic liquids with phosphorus-containing, 4
 - kosmotropic and chaotropic, 199
 - oxidisable, 263
- Anti-solvents, CO₂ as, 49
- Antistatic agents, in polymers, 12–13
- Aprotic ionic liquids, 235, 250, 251, 252
- Aqueous solutions, molecular dynamics simulations of, 170
- Aromatic aldehydes, alkyl, 17–18
- Aromatic cations, 266
- Aromatic extraction, 123
- Aromatic hydrocarbons, carbonylation of, 17–18
- Aromaticity, influence of, 265–266
- Aromatic organic liquids, 265
- Aromatic ring alkylation, 17
- Aspartame synthesis, 194
- Asym** (asymmetric form) conformers, 61, 64, 78, 79, 80
- Asymmetric framework method, 124, 134
- Atomic configurations, 153
- Atomistic simulations
- of cations, 156–157
 - classical, 150
- Barrier materials
- ionic liquid membranes as, 104–105
 - ionic liquids as, 87
- Baseline stability, of calorimetry trace, 67
- BASF™ company, 8
- BASIL™ technology, 8
- Behaviour. *See also* Environmental behaviour; Materials behaviour; Phase behaviour entries; Phase transition behaviours; Properties; Swelling behaviour; Thermal behaviours
- aggregation, 170
 - anion, 168
 - dielectric, 237
 - freezing–melting, 279
 - of matter, 150
 - premelting, 64–65
- Bernard, Didier, xiii, 1
- β parameter, 160
- Biasing procedures, advanced, 153
- Binary gas solubilities, 173
- Binary interaction parameters, 45
- Binary ionic liquid + supercritical CO₂ systems, 52
- Binary ionic liquid + supercritical CO₂ phase behaviour predictions for, 45
- Binary ionic liquid + supercritical CHF₃ systems, 42–43, 52
- Binary (ionic liquid + supercritical fluid) systems
- classification of, 43–44
 - liquid–vapour phase behaviour of, 43–44
 - modelling of, 44–46
 - phase behaviour of, 41–46
- Binary solid–liquid equilibrium (SLE) systems, 123
- Binary systems, phase behaviour of, 40
- Biocatalysis
- single-phase and multiphase systems for, 197–198
 - two-phase (biphasic) systems for, 195
 - in whole cell systems, 203–206
- Biocatalysts, history of, 193–194
- Biocatalytic reactions
- future aspects of, 208–210
 - in industrial processes, 193, 194
 - influence on environment, 207
 - in ionic liquids, 193–216

- Biocatalytic syntheses, reported in ionic liquids, 196
- Biodegradability, 206, 207
- Biofuel production, from lignocellulosic biomass, 29
- Biomass valorisation, patent applications concerning, 28–29
- “Biomimetic” ionic liquids, 158
- Biopolymers, 198
 additional, 28
 ionic liquids and, 26–28
- Bioreactive systems, ionic liquid membranes for, 109
- Biorefineries, 26
- Biphasic processes, for alkoxyamine preparation, 25–26
- Biphasic systems, 203–204
 for biocatalysis, 195
 reaction rates in, 50
- Bondi method, 125, 127
- Bonnet, Philippe, xiii, 1
- Born–Fajans–Haber cycle, 283
- Bromides, DSC measurements of, 62–65
- [C₂mim]⁺-based ionic liquids
 physicochemical properties of, 221–226, 229–232, 232–233
 transference number and ionicity of, 226–229
- [C₄mim][PF₆], phase behaviour of, 67–73
- Calibration curves, 230, 232–233
- Calorimetric curves, 68
- Calorimetry trace, baseline stability of, 67
- Carbon dioxide. *See* CO₂ entries;
 Supercritical CO₂
- Carbon nanotubes (CNTs), 13, 168, 169
- Carbon nanotube solvation, 169
- Carbonylation
 of alcohol, 21
 of aromatic hydrocarbons and paraffins, 17–18
 continuous, 21
 of saturated hydrocarbons, 18
- Catalyst inhibition, 204
- Catalyst reuse, 107–108
- Catalytic systems, ionic liquids as solvents for, 19–26
- Cation abbreviations, xv–xvii
- Cation adsorption, 168
- Cation–anion interactions, 171
- Cation changes, phase transitions linked with, 59–65
- Cation constituents, of polymerised ionic liquids, 94
- Cation families, force fields for, 157
- Cation head groups, 289, 290–291
- Cationic transference numbers, 226–227
- Cation reorientation, 244, 245
- Cations
 aromatic, 266
 atomistic simulations of, 156–157
 conformers of 1-alkyl-3-methylimidazolium, 60–62
 imidazolium-based, 163
 ionic liquid, 98, 111
 ionic liquids with lactam, 5
- Cation structures
 in crystalline phases, 69–73
 found in ionic liquids, 277–278
- CEES (2-chloroethyl ethyl sulfide)
 vapour transport, 104–105
- Cell systems biocatalysis in, 203–206
- Cell toxicity prediction, 207–208
- Cellulase, hyperthermophilic, 209–210
- Cellulose
 dissolution and processing of, 26–27
 sulfation/sulfonation of, 27
- Chaotropic anions, 199
- Charge–charge interactions, 168
- Chemical potential, 132
 excess, 171
- Chemical processing, in ionic liquid + supercritical fluid systems, 48–51
- Chemical production, from lignocellulosic biomass, 29
- Chemical transformations, microwave-assisted, 24
- CHF₃ systems, binary ionic liquid + supercritical, 42–43, 52
- Chiral ionic liquids
 applications of, 110
 with membranes, 110
- Chloroaluminate(III) ionic liquids, 16, 17
 preparation of, 15
 regeneration of, 19
- Chloroaluminates, acid, 17
- Chlorolactams, 11–12

- Classical atomistic simulations, 150
 Classical potential functions, 150
 Close-boiling mixtures treatment, 8
 CO₂ (carbon dioxide). *See also*
 Supercritical CO₂
 as anti-solvent, 49
 as co-solvent, 49, 51
 CO₂ absorption isotherms, 172–173
 CO₂ capture
 in fossil fuel burning power plants,
 101
 ionic liquids for, 30
 CO₂ gas permeabilities, 104
 CO₂ mixtures, molecular dynamics
 simulation studies of, 170–171
 CO₂/N₂ separations, 102
 CO₂ removal, 10–11
 from process streams, 48
 CO₂ separation, 99–104
 gelled membranes in, 103–104
 industrial applications of, 100–101
 MMMs in, 102–103
 poly(RTILs) in, 101–102
 CO₂ solubility, 41–42, 46, 130
 CO₂ systems
 binary ionic liquid + supercritical,
 41–42
 ternary ionic liquid + supercritical,
 46–48
 Cofactor regeneration, 203
 Cohesive energy density, 158–159
 COIL conferences, viii
 Cole–Cole (CC) model, 242, 243, 249, 250
 Cole–Davidson (CD) model, 242, 243,
 250
 Collective properties, of ionic liquids,
 154
 Common ionic liquids, incremental
 changes to, 180
 Composite liquid–polymer structures,
 95–97
 Composite membranes, with three
 components, 95, 96
 Compounds
 diblock, 130
 enantiomeric separation of, 110
 extraction of, 204–206
 Computational equipment/methods,
 advanced, 260
 Computations, engineering, 134–135
 Computed viscosities, 162
 Computer-aided design modelling
 (CADM), 121
 “Conceptual” tools, 118
 Conductance dispersion, 239, 247, 248
 Conductivity. *See also* Direct current
 (DC) electrical conductivity;
 Electrical conductivity (σ);
 Electrically conducting systems;
 Molar conductivity entries
 frequency-dependent, 238
 ionic, 163–164, 218
 thermal, 164
 Conductivity maximum per ion, 170
 Conductivity measurements, 220, 228.
 See also Molar conductivity
 measurements
 Conductivity values, 222–224
 COnductor-likeScreeningMOdel for
 Real Solvents (COSMO-RS), 88,
 132–133, 134, 283
 Conformational cation changes, phase
 transitions linked with, 59–65
 Conformational structures, 60
 Conformers
 of 1-alkyl-3-methylimidazolium
 cations, 60–62
 multiple, 60, 81
 Conjugated acids, 231
 Conjoint polymers, 19
 Contactors. *See* Membrane contactors
 Continuous biphasic processes, with
 ionic liquids and supercritical CO₂,
 49–50
 Continuous carbonylation, 21
 Continuous fractional component (CFC)
 method, 172–173
 Continuous processes. *See also*
 Continuous biphasic processes
 design of, 118
 with ionic liquids, supercritical CO₂,
 and miscibility switch phenomenon,
 50–51
 Controlled density reduction, 50
 Copolymers, hydrogenated, 12
 Correlation functions, in molecular
 simulations, 152
 Co-solvents, CO₂ as, 49, 51
 Coulombic forces, 217
 melting points and, 280–281

- Coulombic interactions, 81, 124, 230, 232
- Crespo, João G., xiii, 87
- Critical expert overviews, ix–x
- Critical points, 174
- Cross-linkable/linked gemini RTILs (GRTILs), 94, 105. *See also* Room temperature ionic liquids (RTILs)
- Crystal** α phase, 68, 69–71
- Crystal** β phase, 68, 69
- Crystal–crystal phase transitions, 67, 68–69, 81
- Crystal** γ phase, 68, 69–71
- Crystalline domains, 73–74, 76, 80
- Crystalline grains, 79
- Crystalline structure, 87–88
- Crystallisation
- intermittent, 77–80, 81
 - of ionic liquids, 62–65
 - model for, 73–74
 - rhythmic, 74–77, 80, 81
 - smooth, 78
- Crystallisation/melting, timescale of, 76
- Crystallisation peak, 65
- Crystallisation timescale, 76, 78
- Crystals, simulations of, 178–179
- Crystal structures, 72–73
- predicting, 178
- Cubic equations of state, 44–45
- Cumulative radiation exposure, 261
- Cyanoborate anions, ionic liquids with, 4–5
- Cyclic experiments, 77
- Databases, 119, 156
- force field, 179–180
 - of ionic liquids, 276
- Data production, 276
- Debye–Falkenhagen (DF) theory, 247, 248
- Debye process, 240, 242
- Degradation, of ionic liquids, 208
- Demixing
- instantaneous, 51
 - spinodal, 51
- Denaturation, 199
- Dense membranes, modified, 97
- Density, 283–288. *See also* Energy density
- computing, 157–158
 - at different temperatures, 288
- Density functional theory (DFT), 60
- Density measurements, 220
- Density oscillations, 167
- Depolymerisation, of starch, 28
- Derivative quantity calculations, 158
- Designer functionalities, for ionic liquids, 118. *See also* Process design
- Desulfurisation, of oil, 29
- Desulfurisation technology, 10
- 1,3-Dialkylimidazolium cation, molecular structure of, 277
- 1,3-Dialkylimidazolium ionic liquids, 41, 42, 52
- vapourisation enthalpy of, 158–159
- Dialkyl sulfates, 4
- Diblock compounds, 130
- Dielectric behaviour, 237
- Dielectric constants, 251–252
- static, 235, 236, 237, 238, 240, 241, 248–253
- Dielectric continuum approach, 253
- Dielectric continuum theory, 248, 253
- Dielectric dispersion, 238, 241
- Dielectric dispersion curves, frequency-dependent, 235
- Dielectric loss, 238, 241, 244
- Dielectric modes, 236
- Dielectric permittivity, frequency-dependent relative, 238
- Dielectric properties, of ionic liquids, 235–258
- Dielectric relaxation, 236, 240. *See also* Ion cloud relaxation; Non-exponential relaxation
- Dielectric relaxation spectroscopy (DRS), 236, 237, 248–249. *See also* DRS studies
- developments of, 254
- Dielectric response, 235–236, 240, 241
- molecular processes affecting, 243–248
- Dielectric spectra, 236, 237, 253, 254
- of ionic liquids, 240–243
 - phenomenological description of, 240–243
- Dielectric theory, 237–238
- of electrically conducting systems, 237–240, 241
- Differential scanning calorimetry (DSC), 60, 220. *See also* DSC entries

- Diffusivity, 99, 104, 227
 ionic, 224
- Diffusivity measurements, 226
- Dipolar anions, 246
- “Dipolar” processes, 236
 affecting dielectric response, 243–246
- Dipolar VOCs, 252. *See also* Volatile organic compounds (VOCs)
- Dipole moments, 252
 electric, 253
 molecular, 253
- Direct current (DC) electrical conductivity, 236
- Dispersion
 conductance, 239, 247, 248
 dielectric, 238, 241
- Dissociativity, 228
- Dissolved cellulose, 26–27
 textile applications for, 27
- Domains. *See also* Crystalline domains; Premelting domains
 hydrophobic and hydrophilic, 245
 polar and non-polar, 155
 rhythmic transition of, 76
- Double imidazolium cation, molecular structure of, 277
- Double layer, ionic liquid, 168
- Double-layer stacking formation, 168
- Downstream processes/processing, 197, 203
- DRS studies, 240. *See also* Dielectric relaxation spectroscopy (DRS)
- DSC instruments, nano-Watt-stabilised, 66. *See also* Differential scanning calorimetry (DSC)
- DSC measurements, of bromides, 62–65
- DSC/Raman spectroscopy
 measurements, 66–67
- DSC traces, 75, 76, 77, 79
- Dynamical relaxation processes, in
 molecular simulations, 151
- Dynamic heterogeneity, 162
- Dynamic hydrogen bonding, 167–168
- Dynamic performance tests, 98
- Dynamic water clusters, 105
- Eco-efficiency analysis, 208
- Effective ionic concentration, 233
- Efficiency system design, 118
- Electrical conductivity (σ), frequency-dependent, 238. *See also* Direct current (DC) electrical conductivity
- Electrically conducting systems,
 dielectric theory of, 237–240, 241
- Electric dipole moment, 253
- Electrochemical applications, ionic liquid membranes for, 108–109
- Electrochemical molar conductivity, 227–228
- Electrode polarisations, 236, 241, 249–250
- Electrolyte NRTL (e-NRTL) model, 124
- Electron decay, 267–268
- Electron reactivity, presolvated, 263
- Electrons, solvated, 267, 269
- Electron spin resonance studies, 263
- Enantiomeric separation, of compounds, 110
- Energy density, cohesive, 158–159
- Energy recycle design, 118
- Engineering computations, 134–135
 for ionic liquids, 120
 for process design, 121–122
- Engineering simulations, 117–148
- Enhanced selectivity, ionic liquid systems with, 110
- Enthalpy
 molar crystallisation, 78
 vapourisation, 155, 158–159, 174
- Environmental behaviour, of ionic liquids, 210
- Environmental impact, of ionic liquids, 206–208
- Environmentally benign solvents, 39
- Environmentally friendly ionic liquids, 207
- Enzymatic catalysis, 106
- Enzymatic fuel cells, development of, 109
- Enzymatic membrane reactors, ionic liquid membranes for, 109
- Enzyme-catalysed reactions, water content/activity in, 200–201
- Enzyme classes (ECs), 194, 195
- Enzymes
 as biocatalysts, 193
 in biocatalytic syntheses, 196
 hydrolysing, 27

- influence of ionic liquids on, 198–200
 in ionic liquids, 194–197
 patent applications concerning, 28–29
 solubilisable, 109
- Enzyme solubility, 198
- Enzyme types, screening for, 209
- EoS methods/models, 123, 128–132, 134.
See also Equations of state (EoS);
 Group contribution EoS (GC-EoS)
 model
- Eötvös equation, 296
- Equations of state (EoS). *See also* EoS
 methods/models
 cubic, 44–45
 group contribution, 45
 statistical-mechanics-based, 45
- Equilibrating vapour phase, 201
- Equilibrium MD (EMD) simulation,
 161
- Equimolar mixtures, MD studies of,
 177–178
- Equipment
 for ionic liquid thermal analysis,
 65–67
 for mass transfer processes, 91
- Estimation tools, 134–135
- Ether glycols, 23–24
- 1-Ethyl-3-methylimidazolium ionic
 liquids, 217, 219, 221, 226–227, 228,
 229, 231–232, 233. *See also*
 [C₂mim]⁺-based ionic liquids
- Excess chemical potential, 171
- Expanded ensemble (EE) approach,
 171–172
- Experimental data, simulations vs.,
 154–155
- Experimental data collection, 122
- Exploratory research, 181
- “Extended Hamiltonian” methods, in
 molecular simulations, 151
- Extracting agents, ionic liquids as, 7–8
- Extraction of compounds, 204–206
- Extractive fermentation, 204
- Extrapolation procedures, 162
- Far infrared (FIR) methods, 236
- Fermentation, extractive, 204
- Fine particles recovery, 13
- Fixed-charge models, 161, 166
- Flowsheeting software packages, 122
- Flowsheet programs, 118
- Fluid catalytically cracked (FCC) off-gas,
 17
- Fluid multiphase systems, ternary, 43–44
- Fluid theory models, statistical
 association, 45–46
- Fluorinated alkyl chains, 293
- Fluorinated anions, 221, 222
- Fluorination, 24–25
 of halogenated compounds, 18
- Fluorination catalysis, liquid phase, 18
- Force field databases, 156, 179–180
- Force field parameters, for ionic liquids,
 157
- Force fields, 178–180
 for cation families, 157
 developing, 179
 for imidazolium-based ionic liquids,
 178
 in molecular simulations, 150–151
 non-polarisable, 166
 polarisable, 157, 161, 166
 refined, 180
 setting, 156–157
 united-atom, 157
 validation of, 178–179
- Fossil fuel burning power plants, CO₂
 capture in, 101
- Free energy methods/schemes, 171, 172
 multistage, 172
- Freezing–melting behaviour, 279
- Frequency analyses, 74
- Frequency-dependent dielectric
 dispersion curve, 235
- Frequency-dependent electrical
 conductivity, 238
- Frequency-dependent relative dielectric
 permittivity, 238
- Frequency distribution curves, 76
- Friedel–Crafts acylation, 25
- Fuel cells
 development of enzymatic, 109
 ionic liquid membranes for, 108–109
- Fugacity coefficients, 129
- Functional group parameters, 126
- Functionalised ionic liquids, 209
- Function analysis, radial distribution,
 168

- Gamma radiation damage, 266
- Gas absorption isotherms, 172–173.
See also Vapour entries
- Gases
non-polar, 172
separation of, 99–104
solubility of, 129–130
- Gas–liquid interfaces, 164–169
ionic, 165–166
- Gas permeabilities, CO₂, 104
- Gas phase behaviour, 131–132
- Gas phase quantum calculations, 159
- Gas separation membrane performance, 100
- Gas solubility, 88–90, 131
- Gas–vapour permeation applications, 97
- Gatterman–Koch reaction, 17–18
- GC non-random lattice–fluid EoS (GCNRLF-EoS) model, 131. See also Equations of state (EoS); Group contribution EoS (GC-EoS) model
- Gelled ionic liquids, 95–97
- Gelled membranes, in CO₂ separation, 103–104
- Gelled RTILs, 95–97. See also Room temperature ionic liquids (RTILs)
- Gemini RTILs (GRTILs), 94. See also Room temperature ionic liquids (RTILs)
- Gibbs energies (G^E), 129, 283
- Gibbs excess (G^E) models, 123–128
- Gibbs free energy models, 88
- Glass transition temperatures, 279
- Gold nanoparticles, 269–270
- Granted patents, 28
- Gravimetric balance, 41
- Green-Kubo expression, 163–164
- “Green” solvents, 40, 90
- Group contribution EoS (GC-EoS) model, 45, 131–132. See also Equations of state (EoS)
- GT** (*gauche trans*) conformations, 62, 64, 65, 69–70, 72, 73, 75–76
- GT** (*gauche' trans*) conformations, 62, 69–73
- Guanidinium cation, molecular structure of, 278
- Guanidinium ionic liquids, 5
- Guo, Liangliang, xiii, 275
- G-values, 265–266
- Halides, 14, 15
- Haloalkanes, 16–17
- Halogenated compound fluorination, 18
- Halogen-free ionic liquid synthesis, 2
- Hamiltonian methods, in molecular simulations, 151
- “Hardware” tools, 120
- Head groups
anion, 290–291, 292
cation, 289, 290–291
- Heat capacity, 159. See also Temperature entries; Therm- entries
- Heat transfer cycles, 77
- Helmholtz energy, 129–130, 131
- Henry’s Law constants, 171, 172, 173
- High-frequency processes, 242
- High purity alkyl sulfates, 3
- High-purity ionic liquids, 5–6, 267
- Hofmeister series, 199–200
- Holes, radiolytically induced, 263
- Hollow fibre membrane contactor, 91
- Homogeneous systems, 50
- Homo-metathesis, 22
- Hydrocarbons, carbonylation of saturated, 18
- Hydrocarbon stream drying, 25
- Hydrocarbon streams, sulfur compound removal from, 9–10
- Hydrochloric acid recovery, 8–9
- Hydrodesulfurisation process, 10
- Hydrodynamic approaches, 244, 245
- Hydroformylation, 20–21
- Hydrogenated copolymers, 12
- Hydrogenation, of conjunct polymers, 19
- Hydrogen bonding, 289
dynamic, 167–168
- Hydrolysing enzymes, 27
- Hydrolysis, of polyamides, 18
- Hydrophilic domains, 245
- Hydrophilic ionic liquids, 198–199
- Hydrophilic poly(diols-RTIL)s, 104–105.
See also Room temperature ionic liquids (RTILs)
- Hydrophobic domains, 245
- Hydrophobic ionic liquids, 105
- Hydrophobicity, 199–200

- Hydrosilation, 22–23
 Hydroxyl groups, 296
 Hyperthermophilic cellulase, 209–210
 Hypothetical critical points, 174
- Ideal heat capacity, 159
 Imidazolium-based cations, 163
 Imidazolium-based ionic liquids, 128, 129, 130, 280. *See also* Imidazolium ionic liquids
 force field for, 178
 “refined” force fields for, 157
 Imidazolium-based RTILs, 101, 104. *See also* Room temperature ionic liquids (RTILs)
 Imidazolium halides, 15
 Imidazolium ionic liquids, 3, 276. *See also* Imidazolium-based ionic liquids
 Imidazolium ring, 165, 166, 167
 Imidazolium ring plane, 169
 Imidazolium salts, 22–23
 Immobilisation procedures, quality of, 97
 Immobilised ionic liquids, 6
 Immobilised ions, 102
 Impedance measurements, 226
 Impurities
 in ionic liquids, 201–202
 toxicity effect of, 206–207
 Incident radiation, 262
 Industrial applications
 of CO₂ gas separation, 100–101
 of ionic liquid membranes, 90
 Industrial processes, biocatalytic reactions in, 193, 194
 Infinite-dilution activity coefficients, 132
 “Infinite-dilution” solubility, 172
 Instantaneous demixing, 51
 Integrated absorption/stripping process, 91
 Integrated membrane–ionic liquid systems, 90
 Interfacial simulations, 165–166
 Intermittent crystallisation, 77–80, 81
 Intermolecular interactions, 287–288
 Intermolecular vibrations, 247
 Inter-wall distance, 169
 Ion aggregates, 218
 Ion cloud relaxation, 247–248
 Ionic compounds, polar, 7
 Ionic concentration, effective, 233
 Ionic conductivity, 163–164, 218
 Ionic diffusivity, 224
 Ionicity, 226, 228–229, 232
 correlation with ionic structures and physicochemical properties, 229–232
 in ionic liquids, 217–234
 Ionicity values, 230
 Ionic liquid + supercritical fluid systems
 chemical processing in, 48–51
 phase behaviour of, 41–46, 46–48
 reactions and separations in, 49–51
 separations in, 48–49
 Ionic liquid abbreviations, xv
 Ionic liquid additives, for oil drilling/oil wells, 13
 Ionic liquid aggregates, 207
 Ionic liquid–air interface, 295
 Ionic liquid antistatic agents, in polymers, 12–13
 Ionic liquid-based polymer membranes, 108
 Ionic liquid cations, 98
 “Ionic liquid chemistry,” 98
 Ionic liquid complications, 134
 Ionic liquid confinement, 168–169
 Ionic liquid databases, 276
 Ionic liquid degradation, 208
 Ionic liquid deposition, 206
 Ionic liquid design/designability, 218, 276
 Ionic liquid diffusion, 208
 Ionic liquid diversity, 260–261, 276
 Ionic liquid double layer, 168
 Ionic liquid–gas interface, 165–166
 Ionic liquid interfaces, with non-polar solvents, 166
 Ionic liquid–liquid interface, 166
 Ionic liquid lubricants, 12
 Ionic liquid membrane technology, 87–116
 future directions for, 109–111
 Ionic liquid membranes
 applications of, 99–109
 as barrier materials, 104–105
 characterisation of, 97–99
 industrial applications of, 90
 structure and morphology of, 90–97
 Ionic liquid mixtures, 170

- Ionic liquid preparations, for radiation chemistry studies, 266–268
- Ionic liquid properties
 origin of, 217–234
 temperature dependencies of, 222–224
 tuneability of, 111
- Ionic liquid radiation chemistry, 259–274
 future prospects for, 270
 nanoparticle synthesis and, 268–270
- Ionic liquid radiolysis products, 261–262
- Ionic liquid recycling, 10
- Ionic liquids. *See also* Room temperature ionic liquids (RTILs)
 as acidic catalysts and solvents, 14–19
 additional applications for, 11–12
 as additive solvents, 12
 as additives with specific properties, 12–14
 advantages of, 209
 alkyl sulfate, 2–4
 applications of, 28, 88
 applications of acidic, 15–18
 aprotic, 235, 250, 251, 252
 biocatalytic reactions in, 193–216
 biocatalytic syntheses reported in, 196
 “biomimetic,” 158
 biopolymers and, 26–28
 cation–anion constituents of
 polymerised, 94
 cations in, 111
 cation structures found in, 277–278
 chloroaluminate, 16, 17
 for CO₂ capture, 30
 continuous biphasic processes with supercritical CO₂ and, 49–50
 continuous processes with, 50–51
 crystallisation of, 62–65
 with cyanoborate anions, 4–5
 definitions and properties of, 87–90
 densities of conventional, 285–286
 1,3-dialkylimidazolium, 41, 42
 dielectric properties of, 235–258
 dielectric spectra of, 240–243
 engineering computations for, 120
 environmental behaviour of, 210
 environmental impact of, 206–208
 environmentally friendly, 207
 enzymes in, 194–197
 as extracting agents, 7–8
 force field parameters for, 157
 functionalised, 209
 gelled, 95–97
 generalities concerning, 264
 “green” character of, 90
 guanidinium, 5
 high-purity, 5–6, 267
 hydrophilic, 198–199
 hydrophobic, 105
 imidazolium, 3, 276
 imidazolium-based, 128, 129, 130, 280
 immobilised, 6
 improved use of, 2–6
 impurities in, 201–202
 incremental changes to common, 180
 influence on enzymes and substrate, 198–200
 interest in, 1–2
 ionicity in, 217–234
 with lactam cations, 5
 Lewis acidic, 15
 as ligands, 21
 LLE simulations of, 176
 low-temperature, 15
 low-viscosity, 240, 253
 as lubricants, 29–30
 with magnetic properties, 110–111
 as membranes, 87
 microwave-assisted chemical transformations with, 24
 molecular dynamics simulations of, 167
 molecular simulation of, 149–192
 molecular simulations of pure, 170
 in multi-component systems, 170–171
 neutral, 25
 onium, 24
 organic compound recovery from, 48–49
 partial crystallisation of, 6
 performance of, 297
 in petrochemistry, 1–37
 phase behaviour of 1-alkyl-3-methylimidazolium, 59–85
 phase transition behaviours of, 73–80
 with phosphorus-containing anions, 4
 physicochemical properties of, 275–307

- polymer membranes and, 93
 pre-selection of, 132
 preparation of chloraluminat(III), 15
 preparing, 267
 production under ultrasonication, 6
 products and processes related to, 117, 118
 properties and data points for, 279
 properties of, 40, 153–155
 protic, 250–251, 295–296
 pyridinium, 3, 270
 as reaction media, 50
 “refined” force fields for imidazolium-based, 157
 regeneration of chloraluminat(III), 19
 room temperature, 59
 self-diffusiveness/self-diffusivities of, 152, 154, 159–161, 161–162, 170
 separation processes using, 6–12
 solubility in, 171–173
 as solvents for catalytic systems, 19–26
 as solvents in SLMs, 106
 with specific functionalities, 118
 starch and, 27–28
 static dielectric constant of, 248–253
 sulfate, 2
 supercritical fluids in, 39–57
 task-specific, 92–93, 94
 terahertz spectra of, 243
 thermal analyses of, 60
 thermal measurements of, 66
 thermodynamic models for, 122–133
 thermodynamic properties of, 134
 unique properties of, 59–60
 volatile organic compounds *vs.*, 253
 water-immiscible, 197, 198
- Ionic liquid science, radiation chemistry and, 261–262
- Ionic liquid–solid interface, 166–169
- Ionic liquid stability, nuclear fuel recycling and, 264–266
- Ionic liquid structural features, 283
- Ionic liquid/supercritical fluid systems, phase behaviour of, 40–48
- Ionic liquid/supporting membrane systems, 106–107
- Ionic liquid synthesis, 219
 halogen-free, 2
- Ionic liquid systems
 with enhanced selectivity, 110
 stimuli-responsive, 110–111
- Ionic liquid thermal analysis
- Ionic liquid–vacuum interface, 165
- “Ionic” processes, 236
 affecting dielectric response, 246–247
- Ionic structures, ionicity correlation with, 229–232
- Ionising radiation, 259, 262
- Ion pairing, 246
- Ion-pair modes, 246
- Ion-phobic alkyl chains, 102
- Irradiation, microwave, 24, 28. *See also* Radiation entries
- Isomeric amines, 106
- Isomerisation, 18
- Isomers, rotational, 60–61, 62
- Isopropyl groups, melting points and, 281–282
- Isoquinolinium cation, molecular structure of, 277
- Isothermic–isobaric Gibbs ensemble MC (GEMC) method, 172, 175. *See also* Monte Carlo (MC) simulations
- Isotherms, absorption, 172–173
- Kamlet–Taft parameter, 253
- Karl Fischer titration, 201, 289
- Kilohertz regime, 247, 250
- Kirkwood formula, 252
- Kohlrausch–Williams–Watts (KWW) function, 242
- Kosmotropic anions, 199
- Kragl, Udo, xiii, 193
- Kroon, Maaik C., xiii, 39
- Lactam cations, ionic liquids with, 5
- Lactams, 11–12
- Lactobacillus* species, 204, 207
- Lattice-fluid (LF-EoS) model, 131. *See also* Equations of state (EoS)
- Lennard–Jones fluids, 166
- Lewis acidic ionic liquids, 15
- Lewis acids, 14
- Lewis bases, 20–21
- Lewis basicity, 217, 218–219, 222, 230
- Librational processes, 244
- Life cycle analysis, 208

- Ligand liquids, 21
- Light gas transport properties, of
three-component composite
membranes, 102, 103
- Lignocellulosic biomass, biofuel and
chemical production from, 29
- Lipases, 194–195
- Liquid clathrates, 14
- Liquid crystalline solutions, 26
- Liquid–gas interfaces, 164–169
ionic, 165–166
- Liquid–liquid equilibrium (LLE)
systems, 123, 124, 125, 127, 131, 132,
149, 175–176
- Liquid–liquid interfaces, 164–169
- Liquid–liquid phase separation, 8
- Liquid membranes, supported, 103–104
- Liquid phase fluorination catalysis, 18
- Liquid phase separations, 105–108
- Liquid–polymer structures, composite,
95–97
- Liquids, supercooled, 79, 279. *See also*
Ionic liquid entries
- Liquid–solid interfaces, 164–169
- Liquid structure, 155
- Liquid–vapour phase behaviour, of
binary systems, 43–44
- LLE calculations, 176. *See also* Liquid–
liquid equilibrium (LLE) systems
- LLE prediction, 133
- Local composition models, 88
- Local melting domains, 78
- Log P value, 207–208
- Long chain alkyl sulfate ionic liquids,
2–3
- Lower critical endpoint (LCEP), 44
- Low-temperature ionic liquids, 15
- Low-viscosity ionic liquids, 240, 253
- Low-viscosity VOCs, 236. *See also*
Volatile organic compounds (VOCs)
- Lu, Xingmei, xiii, 275
- Lubricants, ionic liquid, 12, 29–30
- Macroscopic electric dipole moment
($\mathbf{M}[\mathbf{t}]$), 237
- Macroscopic viscosity, 225
- Maginn, Edward J., xiii, 149
- Magnetic properties, ionic liquids with,
110–111
- Market needs, matching, 119
- Mass transfer limitations, 50, 197–198
- Mass transfer processes, equipment for,
91
- Materials behaviour, process design and,
119
- Mathias–Klotz–Prausnitz (MKP) mixing
rule, 128
- Matrix acidising technique, 13
- Matter, behaviour of, 150
- Maxwell equation predictions, 103
- Maxwell's equations, 237–238
- MC codes, in molecular simulations, 153.
See also Monte Carlo (MC)
simulations
- MD codes, in molecular simulations, 151.
See also Molecular dynamics (MD)
simulations
- Mean square displacement (MSD), 160,
169
in molecular simulations, 152
- Melting
model for, 73–74
rhythmic, 74–77, 80, 81
- Melting/crystallisation, timescale of, 76
- Melting domains, local, 78
- Melting points, 279–283
computing with MD simulations,
176–177
predicting, 176
thermodynamic, 176–177
- Melting process, 63–65
- Melting trace, 74
- Membrane contactors, 90–93
major drawback of, 92
- Membrane disruption, 208
- Membrane–ionic liquid systems, 90
- Membrane performance, 100
- Membrane reactors, enzymatic, 109
- Membranes. *See also* Ionic liquid
membranes; Polymer–electrolyte
membrane (PEM); Polymer
membranes; Three-component
composite membranes (MMMs)
chiral ionic liquids with, 110
gelled, 103–104
ionic liquids as, 87
Nafion[®], 108
proton exchange, 108

- separation selectivity of, 99
- structural integrity of, 103
- supported liquid, 103–104
- swelling behaviour of, 98–99
- two-component, 102
- Membrane systems, 90
- Membrane technology, related to ionic liquids, 87–116
- Metal halides, 14
- Metal nanoparticle synthesis, radiation chemistry in, 269
- Metal salts, 7, 8
- Metathesis, 22
- Methane-to-methanol conversion, 24
- Methanol, methane conversion to, 24
- Methyl groups, melting points and, 281
- Microwave-assisted chemical transformations, with ionic liquids, 24
- Microwave experiments, 242
- Microwave irradiation, 24, 28
- Microwave regime, 240, 247, 250, 253
- Microwave spectra, of ionic liquids, 240–243
- Miscibility switch phenomenon, continuous processes with, 50–51
- Mixture properties, 179
- Mixtures
 - of ionic liquids, 170
 - molecular dynamics simulation studies of CO₂, 170–171
 - ternary, 198
- Mixture thermodynamic properties, predicting, 154
- Modelling. *See also* Cole–Cole (CC) model; Cole–Davidson (CD) model; Computer-aided design modelling (CADM); Electrolyte NRTL (e-NRTL) model; EoS methods/models; Fixed-charge models; Modified UNIFAC (Do) model; Multi-scale modelling approach; Non-random two-liquid (NRTL) activity coefficient model; NRTL segmented activity coefficients (NRTL-SAC) model; Polarisable continuum model (PCM); PR + Stryjek–Vera (PRSV) EoS model;
 - Quadrupolar models;
 - Thermodynamic models;
 - UNIQUAC method/model
- of binary (ionic liquid + supercritical fluid) systems, 44–46
- of phase behaviour, 88
- Modelling groups, 181
- Modified dense membranes, 97
- Modified UNIFAC (Do) model, 127
- Molar conductivity, 225, 226
 - electrochemical, 227–228
- Molar conductivity ratios, 217, 219
- Molar crystallisation enthalpy, 78
- Molecular dipole moments, 252, 253
- Molecular dynamics (MD) simulations, 150–153, 165
 - of aqueous solutions, 170
 - to compute melting points, 176–177
 - drawbacks of, 151–152
 - of ionic liquids, 167
 - standard liquid, 180–181
 - “statistical” properties and, 152
- Molecular dynamics (MD) simulation studies
 - of CO₂ mixtures, 170–171
 - of equimolar mixtures, 177–178
- Molecular mechanics (MM) simulations, 283
- Molecular processes, affecting dielectric response, 243–248
- Molecular simulations
 - advances in, 181
 - defined, 150
 - future perspectives on, 173–181
 - goals of, 153–156
 - of ionic liquids, 149–192
 - of pure ionic liquids, 170
- Molecular volumes, 287, 294
- Molecule configurations, in molecular simulations, 151
- Monte Carlo (MC) simulations, 150–153, 172–173, 175, 176
 - advantages of, 152–153
- Morpholinium cation, molecular structure of, 277
- Morphologies of ionic liquids as membranes, 87
- Motion equations, in molecular simulations, 151

- Multi-component systems, ionic liquids
in, 170–171
- Multiphase systems
for biocatalysis, 197–198
ternary fluid, 43–44
- Multiple conformers, 60, 81
- Multi-scale modelling approach,
120–121
- Multi-scale simulations, 117
- Multistage free energy methods, 172
- Multi-walled carbon nanotubes
(MWCNTs), 168, 169
- Nafion® membranes, 108
- Nanofiltration technology, 107
- Nanomaterials, 29
- Nanoparticles, 269
- Nanoparticle synthesis
ionic liquid radiation chemistry and,
268–270
radiation chemistry in, 269
radiolytic, 269, 270
- Nanotubes (NTs), 168, 169
- Nano-Watt-stabilised DSC instruments,
66. *See also* Differential scanning
calorimetry (DSC)
- Natural gas purification, 10–11
- Natural gas sweetening, 101
- “Neoteric” media, 260–261
- Nernst–Einstein (NE) equation, 163,
225
- Network analysers, vectorial, 240
- Neutral functional groups, 126
- Neutral ionic liquids, 25
- Neutralization, with protic acids, 232
- Newtonian viscosity, 162
- Nickel-catalysed olefin oligomerisation,
20
- Nishikawa, Keiko, xiii, 59
- Nitrogen-containing polar compound
separation, 11
- Noble, Richard D., xiii, 87
- Non-equilibrium MD (NEMD)
simulation, 162
- Non-exponential relaxation, 245
- Non-Gaussian parameters, 160
- Non-planar** conformers, 61
- Non-polar domains, 155
- Non-polar gases, 172
- Non-polarisable force fields, 166
- Non-polar solute–ionic liquid systems,
127
- Non-polar solvents, ionic liquid interface
with, 166
- Non-random two-liquid (NRTL) activity
coefficient model, 123–128, 134
UNIQUAC method *vs.*, 126
- Novel products, developing, 119
- NRTL segmented activity coefficients
(NRTL-SAC) model, 125. *See also*
Non-random two-liquid (NRTL)
activity coefficient model
- Nuclear fuel recycling, ionic liquid
stability and, 264–266
- Nuclear magnetic resonance (NMR)
measurements, 228. *See also*
Pulsed-gradient spin-echo (PGSE)–
nuclear magnetic resonance (NMR)
measurements
- Nuclear magnetic resonance (NMR)
spectroscopy, 160, 264, 265
- Ohmic loss, 239
- Oil desulfurisation, 29
- Oil drilling/oil wells, ionic liquid
additives for, 13
- OKE spectra, 244. *See also* Optical Kerr
effect (OKE)
- Olefinic compounds, hydroformylation
reaction of, 20–21
- Olefinic oligomers, 17
- Olefin oligomerisation, 15–16
transition-metal catalysed, 20
- Olefins, separation of, 7–8
- Oligomerisation
of olefins, 15–16, 17
transition-metal catalysed olefin, 20
- Oligomers, olefinic, 17
- Olivier-Bourbigou, H el ene, xiv, 1
- One-phase systems, 203. *See also*
Single-phase systems
- Onium alkyl sulfates, 3–4
- Onium ionic liquids, 24
- Onium salts, 6
- Operation models, 122
- Optical Kerr effect (OKE), 242. *See also*
OKE spectra
- Optimization techniques, 122

- Organic compound recovery, from ionic liquids with supercritical CO₂, 48–49
- Organic liquids, aromatic, 265
- Organic mixtures, acid removal from, 8–9
- Organic molecular compounds, melting points of, 280
- Organic-rich phase, in ternary ionic liquid + supercritical CO₂ systems, 47
- Organic solute extraction, 39
- Organic solvent nanofiltration technology, 107
- Organic solvents, 195
advantages of, 193, 194
- Organic substrates, solubility of, 197
- Organomodified polysiloxanes, 22–23
- Orrick–Erbar method, 293
- Overviews, value of, ix–x
- Oxazolidinium cation, molecular structure of, 277
- Oxidisable anions, 263
- Oxygen-containing polar compound separation, 11
- Paraffin alkylation, 16–17
- Paraffins carbonylation of, 17–18
- Parameters
assigning, 156
non-Gaussian, 160
- Partial crystallisation, of ionic liquids, 6
- Patent applications, 28–29
- Patents, 2, 18, 19
granted, 28
- Peak-top temperature, 78, 79
- Peng–Robinson (PR) EoS, 128–129. *See also* Equations of state (EoS)
- Penicillin G extraction, 205–206
- Pentaalkylimidazolium cation, molecular structure of, 277
- Perfluorinated anionic structures, 232
- Permeability (*P*), defined, 99. *See also* CO₂ gas permeabilities
- Permittivities
frequency-dependent relative dielectric, 238
static, 249
- Permittivity formalism, 239
- Peters, Cor J., xiv, 39
- Petrochemistry, ionic liquids in, 1–37
- Phase behaviour
of 1-alkyl-3-methylimidazolium ionic liquids, 59–85
of binary (ionic liquid + supercritical fluid) systems, 41–46
of binary or ternary systems, 40
of [C₄mim][PF₆], 67–73
of gases, 131–132
of ionic liquid/supercritical fluid systems, 40–48
methods to determine, 40–41
modelling, 88
of ternary (ionic liquid + supercritical fluid) systems, 46–48
- Phase behaviour data, 52
- Phase behaviour predictions, for binary ionic liquid CO₂ systems, 45
- Phase change properties, 179
- Phase toxicity, 207
- Phase transition behaviours, novel, 73–80
- Phase transition peaks, 68
- Phase transitions, 67–69
linked with conformational cation changes, 59–65
slow, 81
- Phosphonium alkyl sulfates, 4
- Phosphonium cation, molecular structure of, 277
- Phosphorus-containing anions, ionic liquids with, 4
- Photolysis, 25
- Physical properties, predicting, 119, 15–164
- Physicochemical properties, 232. *See also* Density entries; Melting points; Surface tension; Viscosities (η)
of [C₂mim]⁺-based ionic liquids, 221–226
ionicity correlation with, 229–232
of ionic liquids, 217, 219, 275–307
methodology for measuring, 219–221
- Pigamo, Anne, xiv, 1
- Piperazinium cation, molecular structure of, 278
- Piperidinium cation, molecular structure of, 278
- Planar** conformers, 61

- Plechkova, Natalia V., x
- Plutonium, processing spent, 264–265
- Polar domains, 155
- Polar ionic compounds, 7
- Polarisable continuum model (PCM), 125
- Polarisable force fields, 157, 161, 166
- Polarisation
 electrode, 249–250
 space charge, 247
- Polarity parameters, 252
- Polarity probes, 251–252
- Polar substances, 194
- Polar VOCs, 252. *See also* Volatile organic compounds (VOCs)
- Polyalphaolefins (PAOs), 15–16
- Polyamide hydrolysis, 18
- Poly(di-ol-RTIL)s, 104–105. *See also* Room temperature ionic liquids (RTILs)
- Polymer–electrolyte membrane (PEM), 108–109
- Polymer gas separation membrane performance, 100
- Polymeric ammonium cation, molecular structure of, 278
- Polymer ionic liquid membranes, 93–95
- Polymerisation inhibitors, 25–26
- Polymerised ionic liquids, cation–anion constituents of, 94
- Polymerised membrane gemini RTILs (poly[GRTILs]), 94. *See also* Room temperature ionic liquids (RTILs)
- Polymerised membrane RTILs (poly[RTILs]), 93–94, 95, 96, 97, 99. *See also* Poly(RTIL) composite membrane materials
 in CO₂ separation, 101–102
- Polymer membranes
 ionic liquid-based, 108
 ionic liquids and, 93
- Polymers
 conjunct, 19
 ionic liquid antistatic agents in, 12–13
- Polymer synthesis, 23–24
- Poly(RTIL) composite membrane materials, 104. *See also* Room temperature ionic liquids (RTILs)
- Polysiloxanes, organomodified, 22–23
- Polytetramethylene ether glycols, 23, 24
- Polytrimethylene ether glycols, 23–24
- Pore loadings, 169
- Porous membrane contactors, 90–93
- Post-predictive simulations, 154
- Potential functions, classical, 150
- Power plants, CO₂ capture in fossil fuel burning, 101
- Predicted solubility, 132
- Predicting cell toxicity, 207–208
- Predicting crystal structures, 178
- Predicting melting points, 176
- Predicting physical properties, 119, 153–164
- Predicting relative trends, 161
- Predictions, qualitative trend, 158
- Predictive models, 88
- Premelting behaviour, 64–65
- Premelting domains, 73–74
- Presolvated electron reactivity, 263
- Pressure differences, in gas–vapour permeation applications, 97
- Pressure sensitive compositions, 14
- Pressure tensor, 161
- Primary ionic liquid radiolysis products, 261–262
- Process design
 engineering computations for, 121–122
 materials behaviour and, 119
- Process simulation tools, 117
- Process simulators, 134
- Process streams, CO₂ removal from, 48
- “Process synthesis” tools, 118
- Process systems engineering (PSE), 120
- Process toxicity, 208
- Product design, 119. *See also* Process design
- Product design applications, 121
- Properties. *See also* Additives with specific properties; Behaviour; Dielectric properties; Ionic liquid properties; Light gas transport properties; Magnetic properties; Mixture properties; *P-V-T* properties; Physical properties; Physicochemical properties; Phase change properties; Self-diffusiveness/self-diffusivities;

- “Statistical” properties;
- Thermodynamic properties;
- Transport properties; Viscosities (η)
- collective, 154
- of ionic liquids, 40, 59–60, 87–90, 111, 153–155
- optimising solvent, 235
- origin of ionic liquid, 217–234
- of room temperature ionic liquids, 59
- Property models, 122
- trends in, 155–156
- Property predictions, 119, 153–164
- Protective garment materials, 104–105
- Protein renaturation, 199
- Protic acids, neutralization with, 232
- Protic ionic liquids, 250–251, 295–296
- Proton exchange membranes, 108
- Proton relay molecules, 108
- PR + Stryjek–Vera (PRSV) EoS model, 128. *See also* Equations of state (EoS); Peng–Robinson (PR) EoS
- Pulsed-gradient spin-echo (PGSE)–nuclear magnetic resonance (NMR) measurements, 218, 220, 224. *See also* Nuclear magnetic resonance (NMR) entries
- Pulse radiolysis, 260, 261, 262, 270
- Pure-component parameters, 46
- Pure group parameters, 45
- Pure ionic liquids
 - molecular simulations of, 170
 - VLE of, 174–175
- PUREX process, 264–265
- Purification processes, 11–12
- Purity criteria, 267, 268
- P-V-T* properties, 131
- Pyridazinium cation, molecular structure of, 278
- Pyridinium cation, molecular structure of, 278
- Pyridinium ionic liquids, 3, 270
- Pyridinium salts, 22–23
- Pyrrolidinium cation, molecular structure of, 278
- Pyrrolinium cation, molecular structure of, 278
- Quadrupolar models, 172
- Qualitative trend predictions, 158
- Quantitative structure–property relationships (QSAR), 283
- Quantum calculations, gas phase, 159
- Quantum chemical calculations, 123, 125, 132–133
- Quantum chemistry methods, 150
- Radial distribution function, 155
- Radial distribution function analysis, 168
- Radiation. *See also* Irradiation
 - incident, 262
 - ionising, 259, 262
- Radiation biology/medicine, 260
- Radiation chemistry, 259–261. *See also*
 - Ionic liquid radiation chemistry
 - fundamentals of, 262–264
 - of ionic liquids, 259–274
 - ionic liquid science and, 261–262
 - in metal nanoparticle synthesis, 269
- Radiation chemistry studies, ionic liquid preparations for, 266–268
- Radiation chemistry techniques, 260
- Radiation damage, gamma, 266
- Radiation exposure, cumulative, 261
- Radical polymerisation inhibitors, 25–26
- Radiolysis, pulse, 260, 261, 262, 266
- Radiolysis products, primary ionic liquid, 261–262
- Radiolysis product studies, 263–264
- Radiolysis studies, 267
- Radiolytically induced holes, 263
- Radiolytic damage, 270
- Radiolytic energy deposition, 262
- Radiolytic nanoparticle synthesis, 269, 270
- Radiolytic preparation, of advanced materials, 261
- Radiolytic yield (*G*-value), 265–266
- Raman active bands, 70
- Raman bands, 69
- Raman scattering intensities, 69
- Raman spectra, 71–72
- Raman spectroscopic studies, 60
- Raman spectroscopy, 98
- Raman spectroscopy/DSC measurements, 66–67
- Reaction media, ionic liquids as, 50
- Reaction rates, in biphasic systems, 50

- Reactions and separations, in ionic liquid + supercritical fluid systems, 49–51
- Reaction/separation media, 52
- Reactors, enzymatic membrane, 109
- Redlich–Kwong (RK) EoS model, 129.
See also Equations of state (EoS)
- “Refined” force fields, 180
 for imidazolium-based ionic liquids, 157
- Regeneration, of chloraluminatate(III) ionic liquids, 19
- Registration, Evaluation, Authorization and restriction of Chemical substance (REACH) regulations, 208
- Regular solution theory (RST), 88–89
- Relative dielectric permittivity, frequency-dependent, 238
- Relative trends, predicting, 161
- Renaturation, of proteins, 199
- Reorientational dynamics, 165
- Research, on biocatalytic reactions, 208–210
- Returning temperature, 77
- Reverse-NEMD (RNEMD) simulation, 162
- Reviews, value of, ix–x
- Rhythmic crystallisation/melting, 74–77, 80, 81
- Robeson plots, 100, 101
- Room temperature ionic liquids (RTILs), 88, 93. *See also* Gelled RTILs; Gemini RTILs (GRTILs); Polymerised membrane RTILs (poly[RTILs]); Poly(RTIL) composite membrane materials; RTIL entries
- imidazolium-based, 101, 104
- interest in, 218
- novel phase transition behaviours of, 73–80
- unique properties of, 59
- Rooney, David, xiv, 117
- Root mean square deviation (RMSD), 125, 126, 133
- Rotational isomers, 60–61, 62
- RTIL displacement problem, 103–104.
See also Room temperature ionic liquids (RTILs)
- RTIL membranes, supported, 104
- RTIL “tuning,” 99
- Saccharomyces cerevisiae*, 204, 205
- Saturated hydrocarbons, carbonylation of, 18
- Saturated salt solution equilibration, 201
- Scanning electron microscopy (SEM), 98
- Screening, for enzyme types, 209
- Seddon, Kenneth R., x
- Selectivity, 99
 improving and controlling, 194
 ionic liquid systems with enhanced, 110
- Self-diffusion coefficients, 220, 224, 225, 227
- Self-diffusiveness/self-diffusivities
 in calculating viscosity, 161–162
 of ionic liquids, 152, 154, 159–161, 170
- Self-dissociativity, 218
- Separation media, 52
- Separation membrane performance, 100
- Separation processes, using ionic liquids, 6–12
- Separations
 CO₂/N₂, 102
 in ionic liquid + supercritical fluid systems, 48–49
 in the liquid phase, 105–108
 of nitrogen-containing polar compounds, 11
 of olefins, 7–8
 of oxygen-containing polar compounds, 11
- Separations and reactions, in ionic liquid + supercritical fluid systems, 49–51
- Separation selectivity, of membranes, 99
- Shah, Jindal K., xiv, 149
- Shear rates, 162
- Simulations
 of crystals, 178–179
 engineering, 117–148
 experimental data vs., 154–155
 interfacial, 165–166
 multi-scale, 117
 post-predictive, 154
- Single particle time correlation functions, in molecular simulations, 152
- Single-phase systems, for biocatalysis, 197–198, 203

- SLMs containing ionic liquids (SILMs),
93, 97, 105, 106. *See also* Supported
liquid membranes (SLMs)
in CO₂ separation, 100–101
- Slow phase transitions, 81
- Smooth crystallisation, 78
- “Snap together” chemistry, 94
- Sodium cation, molecular structure of,
277
- Soft SAFT (statistical associating fluid
theory) EoS model, 130. *See also*
Equations of state (EoS); Truncated
perturbed chain polar statistical
associating fluid theory (tPC-
PSAFT) EoS model
- Software packages flowsheeting, 122
- “Software” tools, 120
- Solid–liquid equilibrium (SLE) systems,
123, 149, 176–178
- Solid–liquid interfaces, 164–169
- Solubilisable enzymes, 109
- Solubility
binary gas, 173
of CO₂, 41–42, 46, 130
enzyme, 198
of gases, 129–130, 131
“infinite-dilution,” 172
in ionic liquids, 171–173
measurement of, 99
of organic substrates, 197
predicted, 132
substrate, 194, 198
surfactant, 198
- Solubility parameters, 88–89
- Solute–ionic liquid systems, non-polar,
127
- Solutes, target, 98, 105, 106
- Solute transport, 93
- Solvated electrons, 267, 269
- Solvation dynamics, related to dielectric
response, 248
- Solvation process, 263
- Solvent conformations, 132
- Solvent polarity parameter, 221
- Solvent properties, optimising, 235
- Solvent reuse, 107–108
- Solvents, 91–92
advantages of organic, 193, 194
for cellulose, 26–27
environmentally benign, 39
- “green,” 40, 90
organic, 195
tailored, 88
- Solvents for catalytic systems, ionic
liquids as, 19–26
- Space charge polarisation, 247
- Spectral parameterisation, 242–243
- Spinodal demixing, 51
- Square-well chain-fluid EoS (SWCF-
EoS) model, 130–131. *See also*
Equations of state (EoS)
- Stability, of calorimetry trace, 67
- Stacking formations, double-layer, 168
- Standard liquid MD simulations,
180–181
- Starch
depolymerisation of, 28
ionic liquids and, 27–28
- Static conditions, 249
- Static dielectric constants, 235, 236, 237,
238, 240, 241, 250–251, 252, 253
of ionic liquids, 248–253
- Static permittivities, 249
- Statistical association fluid theory
models, 45–46
- Statistical-mechanics-based equations of
state, 45
- “Statistical” properties, molecular
dynamics simulations and, 152
- Stein, Florian, xiv, 193
- Stejskal–Tanner equation, 220
- Stimuli-responsive ionic liquid systems,
110–111
- Stokes–Einstein–Debye (SED) equation,
245
- Stokes–Einstein relationship, 162
- Structural integrity, of membranes, 103
- Sub-picosecond dynamics, 243
- Substrate accumulation, 203
- Substrates
influence of ionic liquids on, 198–200
organic, 197
- Substrate solubility, 194, 198
- Sulfate ionic liquids, 2
- Sulfation/sulfonation, of cellulose, 27
- Sulfonium cation, molecular structure of,
278
- Sulfur compound removal, from
hydrocarbon streams, 9–10
- Sulfuric acid recovery, 9

- Supercooled liquids, 79, 279
- Supercritical CO₂, 39
 continuous biphasic processes with ionic liquids and, 49–50
 continuous processes with, 50–51
 organic compound recovery from ionic liquids with, 48–49
 properties of, 40
- Supercritical fluid + ionic liquid systems, phase behaviour of, 41–46, 46–48
- Supercritical fluids
 commonly used, 40
 in ionic liquids, 39–57
- Supercritical fluid systems, phase behaviour of, 40–48
- Supercritical solvents, 260–261
- Superheating, 178
- Supported ionic liquid-phase (SILP) technology, 21, 29
- Supported liquid membranes (SLMs), 90–93, 103–104. *See also* SLMs containing ionic liquids (SILMs)
 development of, 110
 major drawback of, 92
- Supported RTIL membranes, 104.
See also Room temperature ionic liquids (RTILs)
- Surface charge densities, 168
- Surface diffusion coefficients, 167
- Surface negative charge, 168
- Surface tension, 165, 294–296
- Surfactants, anionic, 13–14
- Surfactant solubility, 198
- Suzuki reactions, 107–108
- Sweetening, of natural gas, 101
- Swelling behaviour, of membranes, 98–99
- Sym** (symmetric form) conformers, 61, 64, 78, 80
- Syntheses. *See also* “Process synthesis” tools
 aspartame, 194
 of ionic liquids, 2, 219
 of polymers, 23–24
 selective improvement of, 209
- Tailored solvents, 88
- Tait equation, 288
- Target solutes, 98, 105, 106
- Task-specific ionic liquids, 92–93, 94
- Techniques, abbreviations for, xviii–xx
- Temperature dependencies, of ionic liquid properties, 222–224, 225
- Temperatures. *See also* Heat entries; Therm- entries
 density at different, 288
 glass transition, 279
 viscosity and, 289
- Terahertz regime, 246
- Terahertz spectra, 253
 of ionic liquids, 243
- Ternary fluid multiphase systems, 43–44
- Ternary (ionic liquid + CO₂ + water) systems, 47–48
- Ternary (ionic liquid + CO₂ + organics) systems, 46–47, 52
- Ternary ionic liquid + supercritical CO₂ systems, 46–48
- Ternary (ionic liquid + supercritical fluid) systems, phase behaviour of, 46–48
- Ternary LLE systems, 127. *See also* Liquid–liquid equilibrium (LLE) systems
- Ternary mixtures, 198
- Ternary systems, 123–124
 phase behaviour of, 40
- Tetraalkylimidazolium cation, molecular structure of, 277
- Tetrazolium cation, molecular structure of, 277
- Textile applications, for dissolved cellulose, 27
- Thermal analyses, 220. *See also* Heat entries; Temperature entries
 equipment for, 65–67
 of ionic liquids, 60
- Thermal behaviours, of 1-alkyl-3-methylimidazolium ionic liquids, 59, 80
- Thermal conductivity, 164
- Thermal energy, 76
- Thermal fluctuations, 80
- Thermal histories, 66, 81
 equipment for, 65–67
- Thermal phenomena, 80–81
- Thermal properties, of [C₂mim]⁺-based ionic liquids, 221–222

- Thermal stability, 209
of [C₂mim]⁺-based ionic liquids, 221, 222
- Thermodynamically rigorous approaches, 177
- Thermodynamic information, in
molecular simulations, 151
- Thermodynamic integration methods, 171, 172
- Thermodynamic melting points, 176–177
- Thermodynamic models, for ionic liquids, 122–133
- Thermodynamic pathways, traversing, 177
- Thermodynamic properties, 157–159
of ionic liquids, 134
predicting, 153–155
- Thermodynamic water activity, 200
- Three-component composite membranes (MMMs), 95, 96
in CO₂ separation, 102–103
light gas transport properties of, 102, 103
- Time-dependent information, in
molecular simulations, 151
- Timescales, in molecular simulations, 151–152
- Tokuda, Hiroyuki, xiv, 217
- Toxicity
phase, 207
process, 208
- Toxicity effects, of impurities, 206–207
- Toxicity evaluation, 206
- Transference numbers, 226–229
cationic, 226–227
- Transition-metal catalysed olefin
oligomerisation, 20
- Transition state theory, 253
- Transport properties, 159–164, 179, 232
predicting, 153–155
- Trialkylimidazolium cation molecular
structure of, 277
- Triazolium cation, molecular structure of, 277
- Trimethylpentene to dimethylhexene (TMP/DMH) molar ratio, 16
- Truncated perturbed chain polar
statistical associating fluid theory
(tPC-PSAFT) EoS model, 129, 130.
See also Equations of state (EoS)
- TT** (*trans trans*) conformations, 62, 64, 65, 69, 71, 72, 73, 75–76
- Tuneability, of ionic liquid properties, 111
- Two-component membranes, 102
- Two-phase systems, 203. *See also*
Biphasic systems
for biocatalysis, 195
“Two-phase”–“three-phase”–“two-
phase”–“one-phase” transition, 47, 49
- Ultrasonication, ionic liquid production
under, 6
- UNIFAC method/model, 123, 126–127, 133
- UNIQUAC method/model, 123, 125–126, 127–128, 133
non-random two-liquid (NRTL)
activity coefficient model *vs.*, 126
- United-atom force field, 157
- Upper critical endpoint (UCEP), 44
- Uranium, processing spent, 264–265
- Uronium cation, molecular structure of, 278
- Vacuum–liquid interfaces, 165
- Valorisation of biomass, patent
applications concerning, 28–29
- van der Waals forces, melting points and, 281
- van der Waals function, 131
- van der Waals interaction parameters, 156
- van der Waals interactions, 167, 168, 218–219, 230, 231, 292, 293
- “Vanilla” MD simulations, 180–181
- Vapour absorption, 294. *See also* Gas
entries
- Vapourisation enthalpy, 155, 158–159, 174
- Vapour–liquid equilibrium (VLE)
systems, 124, 125, 126, 132, 149
of pure ionic liquids, 174–175
- Vapour phase, in ternary ionic liquid +
supercritical CO₂ systems, 47
- Vapour phase studies, 174
- Vapour pressures, 174
- Vapours, separation of, 99–104

- Vapour transport and capture, 93
Vectorial network analysers, 240
Vehicle mechanisms, 218
Vibrations, intermolecular, 247
Viscosities (η), 161–162, 202, 217, 233, 236, 288–294. *See also* Low-viscosity ionic liquids
 computed, 162
 macroscopic, 225
 Newtonian, 162
 temperature and, 289
Viscosity measurements, 220
Viscosity values, 222–224, 294
VLE modelling, 128, 130, 131, 133.
 See also Vapour–liquid equilibrium (VLE) systems
Vogel–Fulcher–Tammann (VFT) equations, 222, 224, 225, 226, 293, 294
Vogel–Tammann–Fulcher (VTF) equations. *See* Vogel–Fulcher–Tammann (VFT) equations
“Void-induced” melting method, 177
Volatile organic compounds (VOCs), 236, 237, 240, 242, 247, 248, 249
 ionic liquids *vs.*, 253
 polar and dipolar, 252
Volume fluctuations, 158
Watanabe, Masayoshi, xiv, 217
Water content/activity, in enzyme-catalysed reactions, 200–201
Water-immiscible ionic liquids, 197, 198
Water transport, 105
Water vapour, 106
Weingärtner, Hermann, xiv, 235
Whole cell systems, 193
 biocatalysis in, 203–206
Widom test particle insertion method, 171, 172
Wilson equation, 126
Wishart, James F., xiv, 259
Wong-Sandler mixing rules, 128
X-ray photoelectron spectroscopy (XPS) techniques, 97
X-ray powder diffraction (XRD), 27
Xylenes, 17
Ye and Shreeve method, 288
Zeolites, 102, 103
Zero-frequency limit, 238
Zero shear rate, 162
Zhang, Suojian, xiv, 275
Zhou, Qing, xiv, 275