

## Contents

**Preface** *xvii*

<b>1</b>	<b>History and Development of Ionic Liquids</b>	<b>1</b>
	<i>Sumana Brahma and Ramesh L. Gardas</i>	
1.1	Introduction	1
1.2	Constituents of ILs	2
1.3	The Brief History	3
1.4	Ionic Liquid-Like Systems	6
1.5	The Generation of ILs	6
1.5.1	First-Generation ILs	7
1.5.2	Second-Generation ILs	7
1.5.3	Third-Generation ILs	8
1.6	Structural Development of ILs	9
1.6.1	Task-Specific ILs (TSILs)	9
1.6.2	Chiral ILs	10
1.6.3	Switchable Polarity Solvent ILs	11
1.6.4	Bio-ILs	11
1.6.5	Poly-ILs	12
1.6.6	Energetic ILs	13
1.6.7	Metallic ILs	14
1.6.8	PIILs	15
1.6.9	Acidic ILs	15
1.6.10	Basic ILs	15
1.6.11	Neutral ILs	16
1.6.12	Supported ILs	16
1.6.13	Magnetic ILs	16
1.7	Scope of ILs	17
1.8	Commercialization of ILs	18
1.9	Conclusions	20
	Acknowledgments	21
	References	21

<b>2</b>	<b>Growth of Ionic Liquids and their Applications</b>	<b>29</b>
	<i>Sudakhina Saikia, Himadri Borah, Pangkita Deka, and Rekha R. Dutta</i>	
2.1	Introduction	29
2.1.1	Cations	30
2.1.2	Anions	30
2.2	Growth of Ionic Liquids	30
2.2.1	Quaternization	30
2.2.2	Anion Exchange	32
2.2.3	Acid–Base Neutralization	32
2.2.4	Direct Combination	33
2.2.5	Microwave-Assisted Synthesis	33
2.2.6	Ultrasound-Assisted Synthesis	33
2.3	Applications of Ionic Liquids	33
2.3.1	Electrochemistry	33
2.3.1.1	Electrodeposition	34
2.3.1.2	Electrosynthesis	34
2.3.1.3	Electrocatalysis	34
2.3.2	Solvents and Catalysis	35
2.3.2.1	Ionic Liquids as Solvents for Organic Synthesis	35
2.3.2.2	Ionic Liquids as Solvents for Inorganic Synthesis	37
2.3.2.3	Ionic Liquids as Catalysts for Organic Reactions	38
2.3.3	Separation	41
2.3.4	Heat Transport and Storage	41
2.3.5	Analytics	42
2.3.6	Engineering	42
2.3.7	Performance Additives	43
2.3.8	Biotechnology	43
2.4	Conclusion and Future Prospects	44
	References	44
<b>3</b>	<b>Study of Physicochemical Properties of Ionic Liquids</b>	<b>51</b>
	<i>Tridib Mondal and Palas Samanta</i>	
3.1	Introduction	51
3.2	Physicochemical Properties of Ionic Liquids	52
3.2.1	Density	52
3.2.2	Melting Point	53
3.2.3	Thermal Stability and Decomposition	56
3.2.4	Conductivity	56
3.2.5	Solubility	58
3.2.6	Surface Tension	58
3.2.7	Viscosity	59
3.2.8	Polarity	60
3.2.9	Diffusion	60
3.2.10	Vapor Pressure	61
3.2.11	Miscibility	61

3.3	Conclusion and Perspectives	62
	Acknowledgments	62
	References	62
<b>4</b>	<b>Ionic Liquids as Green Solvents: Are Ionic Liquids Nontoxic and Biodegradable?</b>	<b>69</b>
	<i>Helen Treasa Mathew, Kumar Abhisek, Shashikant Shivaji Vhatkar, Arvind Kumar, and Ramesh Oraon</i>	
4.1	Introduction	69
4.2	Toxicity and Biodegradability of Ionic Liquids	71
4.2.1	Toxicological Effects and Toxicity Mechanisms of ILs	71
4.2.2	Scope of Biodegradable and Nontoxic ILs	76
4.3	Applications of Ionic Liquids as Green Solvents	78
4.3.1	Ionic Liquids as Green Solvents in Biomass Utilization and Extraction	78
4.3.2	Ionic Liquids as Green Solvents in Energy Applications	80
4.3.3	Ionic Liquids as Green Solvents in Biomedical Applications	81
4.4	IoNanofluids	82
4.4.1	Properties of INFs	82
4.4.2	Applications of INFs	85
4.4.3	Are IoNanofluids Nontoxic and Biodegradable?	86
4.5	Conclusion	88
	References	88
<b>5</b>	<b>Promising Uses of Ionic Liquids on Carbon–Carbon and Carbon–Nitrogen Bond Formations</b>	<b>97</b>
	<i>Sudeshna Kalita and Anup Singhania</i>	
5.1	Introduction	97
5.2	Carbon–Carbon Bond Formation Reactions	98
5.2.1	C–C Cross-Coupling Reactions	98
5.2.1.1	Heck Coupling	98
5.2.1.2	Suzuki Coupling	103
5.2.1.3	Sonogashira Coupling	106
5.2.1.4	Stille Coupling	109
5.2.1.5	Hiyama Coupling	109
5.2.2	Aldol Condensation	111
5.2.3	Claisen–Schmidt Condensation Reaction	113
5.2.4	Friedel–Crafts Alkylation	114
5.2.5	Diel–Alder Reaction	114
5.2.6	Henry Reactions	115
5.2.7	Other C–C Bond Formation Reaction	116
5.3	Carbon–Nitrogen Bond Formation Reaction	117
5.3.1	Biginelli Reaction	117
5.3.2	N-Allylation Reactions	120
5.3.3	Mannich Reaction	121

5.3.4	Other C—N Bond Formation Reactions	123
5.4	Conclusion	131
	References	131
<b>6</b>	<b>Ionic Liquids in Separation Techniques</b>	<b>141</b>
	<i>Hailu Demissie, Fidelis O. Ajibade, Eden Mulu, Jean J.R. Kinhou, Temitope F. Ajibade, Kayode H. Lasisi, Nathaniel A. Nwogwu, and Daniel A. Ayejoto</i>	
6.1	Introduction	141
6.2	General Characteristics of ILs	143
6.3	The Use of ILs in Separation Technology	145
6.3.1	IL-Based Solid–Liquid Extractions	145
6.3.2	Simple SLEs	146
6.3.3	Microwave-Assisted Extractions	147
6.3.4	Ultrasound-Assisted Extractions	147
6.3.5	Liquid–Liquid Extraction	148
6.3.6	ILs as Mobile Phase Additives in Liquid Chromatography	149
6.3.7	ILs Used as Surface-Bonded Stationary Phases	151
6.4	Conclusions and Future Perspectives	153
	References	153
<b>7</b>	<b>Polymers and Ionic Liquids</b>	<b>161</b>
	<i>Hailu Demissie, Fidelis O. Ajibade, Jean J. R. Kinhou, Eden Mulu, Temitope F. Ajibade, Ehiaghe A. Elimian, Bashir Adelodun, Pankaj Kumar, and Oluwaseyi A. Ajala</i>	
7.1	Introduction	161
7.2	Properties of ILs	163
7.3	Synthesis of PILs	166
7.4	Types and Application of Common PILs	167
7.5	Conclusion	167
	References	172
<b>8</b>	<b>Effect of Ionic Liquids on Electrochemical Biosensors and Other Bioelectrochemical Devices</b>	<b>179</b>
	<i>Himadri Borah, Upakul Dutta, and Rekha R. Dutta</i>	
8.1	Introduction	179
8.2	The Importance of Ionic Liquids in Electrochemistry	181
8.2.1	Larger Electrochemical Window	181
8.2.2	Ionic Conductivity	182
8.2.3	Hydrophobicity	183
8.2.4	Viscosity	183
8.2.5	Catalytic Performance	184
8.3	Fabrication of IL-Based Sensing Layers	184
8.3.1	Direct Mixing	184
8.3.2	Physical Adsorption	185
8.3.3	Casting and Rubbing	185

- 8.3.4 Electrodeposition 185
- 8.3.5 Sol–Gel Encapsulation 185
- 8.3.6 Layer-by-Layer (LbL) Method 186
- 8.3.7 Sandwich-Type Immunoassay 186
- 8.4 IL-Based Electrochemical Biosensors 186
- 8.4.1 Application of RTILs in Construction of Electrochemical Biosensors 187
- 8.4.1.1 CNMs-ILs-Based Electrochemical Biosensor as Cancer Biomarker 189
- 8.4.1.2 CNMs-ILs-Based Electrochemical Biosensor for Cardiac Diseases 190
- 8.4.1.3 CNMs-ILs-Based Electrochemical Biosensor for Immunoglobulins 190
- 8.4.1.4 CNMs-ILs-Based Electrochemical Biosensor for Neurotransmitters 190
- 8.4.1.5 CNMs-ILs-Based Electrochemical Glucose Biosensors 191
- 8.5 Application of Ionic Liquids in Bioelectrochemical Devices 191
- 8.6 Conclusions and Future Prospects 191
- References 192

## 9 Nanopharmaceuticals With Ionic Liquids: A Novel

### Approach 195

*Bharadwaj Ittishree, Lipeeka Rout, Vinod Kashyap, and Rahul Sharma*

- 9.1 Introduction 195
- 9.2 Applications of Ionic Liquids in Various Fields 196
- 9.3 Nanotechnology and Ionic Liquids 197
- 9.4 Use of Ionic Liquids in Nanocarrier Development (Reported Work) 198
- 9.5 Ionic Liquid-Assisted Metal Nanoparticles 198
- 9.6 Conclusion 201
- References 201

## 10 Anticancer Activity of Ionic Liquids 203

*Atreyee Banaspati and Nirupamjit Sarmah*

- 10.1 Introduction 203
- 10.2 Classification of Ionic Liquids 205
- 10.3 Toxicity of Ionic Liquids 207
- 10.4 Anticancer Potential of Ionic Liquids 209
- 10.5 Conclusions and Future Scope 213
- References 214

## 11 Importance of Ionic Liquids in Plant Defense: A Novel

### Approach 221

*Mamun Mandal and Abhijit Sarkar*

- 11.1 Introduction 221
- 11.2 Generation of ILs and Their Application 222
- 11.3 Role of ILs in Plant Defense Mechanisms 224
- 11.3.1 ILs as Antibacterial Agents 224
- 11.3.2 ILs as Antifungal Agents 225
- 11.3.3 ILs as an Herbicide and Plant Growth Promoters 226

11.3.4	Effects of ILs as Deterrents	227
11.3.5	Application of ILs as Bioactive Formulations	228
11.3.6	Role of ILs in SAR Induction Mechanism	228
11.4	IL Products in Future Management of Agri Industries: An Innovative Approach	229
11.5	Conclusions	230
	References	230
<b>12</b>	<b>Theoretical Description of Ionic Liquids</b>	<b>235</b>
	<i>Daniel A. Ayetoro, Nathaniel A. Nwogwu, Kelechi E. Igwe, Ehiaghe A. Elimian, Hailu Demissie, Temitope F. Ajibade, Abdulhamid Yusuf, Kayode H. Lasisi, Pankaj Kumar, Bashir Adelodun, and Fidelis O. Ajibade</i>	
12.1	Introduction	235
12.2	Ionic Liquid Dynamics	237
12.2.1	Self-Diffusion	237
12.2.2	Viscosity	238
12.3	Theoretical Advances in Force Fields and Electronic Structures	239
12.4	Mixtures in Ionic Liquids	241
12.4.1	Ionic Liquids and Interfaces	241
12.4.2	Ionic Liquids and Water	243
12.5	Applications of Ionic Liquids in Chemical Processes	245
12.5.1	Preamble	245
12.5.2	Separation and Purification	245
12.5.3	Reaction Media in Chemical and Biochemical Catalysis	245
12.6	Future Developments	247
12.7	Conclusion	248
	References	248
<b>13</b>	<b>Theoretical Understanding of Ionic Liquid Advancements in the Field of Medicine</b>	<b>255</b>
	<i>Mrinal K. Si</i>	
13.1	Introduction	255
13.2	A Brief History of Ionic Liquids and Deep Eutectic Solvents	257
13.3	Biomedical Applications	257
13.3.1	Solubilization of Drugs	257
13.3.2	Protein Stabilization	258
13.4	Summary and Future Aspects	260
13.4.1	Developing a Microscopic Understanding to Enable Task-Specific Design	260
	References	260
<b>14</b>	<b>Recent Developments in Ionic Liquid Research from Environmental Perspectives</b>	<b>265</b>
	<i>Prarthana Bora and Swapnali Hazarika</i>	
14.1	Introduction	265
14.2	Applications of Ionic Liquids	267

14.2.1	Ionic Liquids as Solvents and Catalysts	267
14.2.2	Ionic Liquids in Analytical Chemistry	268
14.2.3	Ionic Liquids in Electrochemical Applications	270
14.2.3.1	In Electrodeposition	270
14.2.3.2	Energy Management	270
14.2.3.3	Bioscience	271
14.2.3.4	Biomechanics	271
14.2.4	Ionic Liquids in Industrial Applications	272
14.2.5	Ionic Liquid as Lubricants	273
14.2.6	Ionic Liquids as a Corrosion Resistant Material	274
14.2.7	Ionic Liquids as Additives in Drilling Fluid	275
14.2.8	Ionic Liquids as Absorbents in Gas Capturing	276
14.2.9	Ionic Liquid Crystals	277
14.2.10	Ionic Liquids in Biomedical Applications	278
14.3	Limitations of Ionic Liquids	278
14.4	Conclusion	279
	References	280
<b>15</b>	<b>Ionic Liquids for Sustainable Biomass Conversion in Biorefinery</b>	<b>283</b>
	<i>Rakesh Dutta and Khemnath Patir</i>	
15.1	Introduction	283
15.2	Biomass as a Source of Organic Compounds and Fuels	284
15.3	Biomass Conversion Process	285
15.3.1	Thermochemical Process	285
15.3.2	Lignin Extraction Processes	285
15.3.3	Enzymatic Processes	286
15.4	Value-Added Organic Compounds from Biomass in Ionic Liquids	286
15.5	Production of Biodiesel with Ionic Liquids	291
15.6	Toxicity and Ecotoxicity of ILs for Biorefinery	292
15.6.1	Toxicity of ILs Used in Biorefinery	293
15.6.2	Biodegradation of ILs Used in Biorefinery	293
15.6.3	Conclusion Regarding Toxicity and Biodegradation of ILs	294
15.7	Conclusions	295
	References	295
<b>16</b>	<b>Ionic Liquids for Atmospheric CO<sub>2</sub> Capture: A Techno-Economic Assessment</b>	<b>301</b>
	<i>Kumar Abhisek, Helen T. Mathew, Shashikant S. Vhatkar, Dipti S. Srivastava, Rahul Minz, and Ramesh Oraon</i>	
16.1	Introduction	301
16.2	Different Processes of CO <sub>2</sub> Capture	303
16.2.1	Membrane Separation	304
16.2.2	Cryogenic Separation	305
16.2.3	Absorption	306

- 16.2.3.1 Chemical Absorption 306
- 16.2.3.2 Physical Absorption 311
- 16.2.3.3 Ionic Liquids for Physical Absorption of CO<sub>2</sub> 313
- 16.2.4 Adsorption 314
- 16.2.5 Ionic Liquids as a Catalyst for Chemical Fixation of CO<sub>2</sub> 315
- 16.3 Conclusion 316
- References 317

## **17 Recovery of Biobutanol Using Ionic Liquids 333**

*Kalyani Motghare, Diwakar Shende, Dharam Pal, and Kailas L. Wasewar*

- 17.1 Introduction 333
  - 17.1.1 Biofuel 333
  - 17.1.2 Classification of Biofuels 333
    - 17.1.2.1 First Generation 333
    - 17.1.2.2 Second Generation 334
    - 17.1.2.3 Third Generation 334
    - 17.1.2.4 Fourth Generation 334
  - 17.2 Biobutanol: First-Generation Biofuels 335
  - 17.3 Butanol Production 335
    - 17.3.1 Butanol Production via Biochemical Conversion 335
    - 17.3.2 Butanol Production via Petrochemical Conversion 336
  - 17.4 Butanol Recovery 337
    - 17.4.1 Butanol Recovery Techniques 337
      - 17.4.1.1 Distillation 337
      - 17.4.1.2 Liquid–Liquid Extraction 337
      - 17.4.1.3 Pervaporation 338
      - 17.4.1.4 Gas Stripping 338
      - 17.4.1.5 Perstraction 338
      - 17.4.1.6 Adsorption 339
    - 17.5 Ionic Liquids 339
      - 17.5.1 Ionic Liquids: A Brief History 339
      - 17.5.2 Production of Ionic Liquids 341
      - 17.5.3 Applications of Ionic Liquids 341
    - 17.6 Recovery of Biobutanol Using Ionic Liquids 343
    - 17.7 World Butanol Demand 344
    - 17.8 Conclusion 345
    - Acknowledgments 346
    - References 346

## **18 Bio-Carboxylic Acid Separation by Ionic Liquids 353**

*Anuj Kumar, F.M. Antony, D.Z. Shende, and K.L. Wasewar*

- 18.1 Introduction 353
  - 18.1.1 Applications of Bio-Carboxylic Acids 353



- 18.1.2 Market of Bio-Carboxylic Acids 354
- 18.1.3 Production of Bio-Carboxylic Acids 354
- 18.2 Ionic Liquids 355
- 18.3 Challenges in the Separation of Bio-Carboxylic Acids 357
- 18.4 Methods for Separating Bio-Carboxylic Acids 357
  - 18.4.1 Distillation 357
  - 18.4.2 Evaporation 359
  - 18.4.3 Adsorption 359
  - 18.4.4 Membrane Extraction 359
  - 18.4.5 Solvent Extraction 360
- 18.5 Separation of Bio-Carboxylic Acids by the Reactive Extraction Process 360
- 18.6 Conclusion and Perspectives 364
  - References 364
  
- 19 Current Trends in QSAR and Machine Learning Models of Ionic Liquids: Efficient Tools for Designing Environmentally Safe Solvents for the Future 369**  
*Supratik Kar and Jerzy Leszczynski*
- 19.1 Ionic Liquids and Their Structural Characteristics 369
- 19.2 Properties of ILs 372
- 19.3 Application of ILs 372
- 19.4 Do ILs Follow Green Chemistry Principles and Are Hazard Free for Environment? 375
- 19.5 Regulatory Proposals for Toxicity Assessment of ILs 376
- 19.6 Why In Silico Modeling Is Needed for ILs 377
- 19.7 Predictive Toxicity Models for ILs 378
- 19.8 Databases of Ionic Liquid 380
- 19.9 Overview and Future Avenues 388
  - Declaration of Competing Interest 389
  - Acknowledgments 389
  - References 389
  
- 20 Advances in Simulation Research on Ionic Liquid Electrolytes 395**  
*Huo Feng and Yue Bowen*
- 20.1 Simulation Method of Ionic Liquid Electrolytes 396
  - 20.1.1 Density Functional Theory 396
  - 20.1.2 Ab Initio Molecular Dynamics Simulation 399
  - 20.1.3 Molecular Dynamics Simulation 402
- 20.2 Advances in Simulation of Ionic Liquid Electrolytes in Batteries 403
  - 20.2.1 Ionic Liquids Are Used as Solvents in Electrolytes 403
  - 20.2.2 Ionic Liquids Are Used as Salts in Electrolytes 407
  - 20.2.3 Ionic Liquids Are Used as Additives in Electrolytes 407

- 20.3 Advances in Simulation of Ionic Liquid Electrolytes in Capacitors 408
  - 20.3.1 Simulation of Ionic Liquid Electrolytes in Flat-Electrode Capacitor 409
  - 20.3.2 Simulation of Ionic Liquid Electrolytes in Porous Electrode Capacitor 410
- 20.4 Conclusion 413
  - References 414
  
- 21 Applications of Ionic Liquids in Heterocyclic Chemistry 419**  
*Suresh Rajamanickam and Binoyargha Dam*
  - 21.1 Introduction 419
  - 21.2 Application of Ionic Liquids in the Syntheses of Various Heterocycles 421
  - 21.3 Conclusion and Future Prospective 440
    - References 440
  
- 22 Application of Ionic Liquids in Drug Development 443**  
*Partha Dutta, Charu Arora, and Sanju Soni*
  - 22.1 Introduction 443
  - 22.2 Classification of Ionic Liquids 444
  - 22.3 General Synthetic Methodologies 444
  - 22.4 An Overview of Applications in Diverse Fields 445
  - 22.5 Specific Applications in the Field of Pharmaceutical Development 447
    - References 451
  
- 23 Application of Ionic Liquids in Biocatalysis and Biotechnology 459**  
*Ehiaghe Agbovhimen Elimian, Fidelis Odedishemi Ajibade, Temitope Fausat Ajibade, Hailu Demissie, Nathaniel Azubuikwe Nwogwu, Kayode Hassan Lasisi, Daniel A. Ayetoro, and Ehizonomhen Solomon Okonofua*
  - 23.1 Introduction 460
  - 23.2 Properties of Ionic Liquids 460
    - 23.2.1 Hydrophobicity 461
    - 23.2.2 Polarity 461
    - 23.2.3 Purity 461
    - 23.2.4 Miscibility of Ionic Liquids 462
    - 23.2.5 Viscosity 462
  - 23.3 Whole-Cell Biotransformations 464
  - 23.4 Ionic Liquids as Solvents for Enzyme Catalysis 467
  - 23.5 Enzyme Selectivity in Ionic Liquids 469
    - 23.5.1 Enantioselectivity 469
    - 23.5.2 Regioselectivity 470
  - 23.6 Ionic Liquid Stability of Enzymes 470

23.7	Application of Ionic Liquids in Bioethanol Production	471
23.8	Ionic Liquids Applied in the Synthesis of Biodiesel	475
23.9	Conclusion	479
	References	479
	<b>Index</b>	489

