

Contents

Editor's Preface ix

Contributors to Volume 42 xi

Cycloaromatization reactions: the testing ground for theory and experiment 1

IGOR ALABUGIN, BORIS BREINER and MARIAPPAN MANOHARAN

- 1 Introduction: bonds lost and bonds formed, or chemical bookkeeping 1
 - 2 Cycloaromatization reactions: breaking π -bonds and breaking the rules 2
 - 3 The diversity of cycloaromatization reactions 3
 - 4 The relative role of σ - versus π -effects at the early reaction stage 6
 - 5 σ -Effects on reactant stability 10
 - 6 π -Effects on reactant stability 22
 - 7 Transition state effects: communication of orthogonal orbitals in the transition state of radical-anionic cyclizations 23
 - 8 Effects on product stability 27
 - 9 Conclusion 31
- References 31

***N*-Acyloxy-*N*-alkoxyamides – structure, properties, reactivity and biological activity** 35

STEPHEN A. GLOVER

- 1 Introduction 35
 - 2 Synthesis 39
 - 3 Structure 43
 - 4 Chemical reactivity 59
 - 5 Biological activity of *N*-acyloxy-*N*-alkoxyamides 97
 - 6 Conclusions 115
- Acknowledgements 116
References 117

The Interplay between experiment and theory: computational NMR spectroscopy of carbocations 125

HANS-ULLRICH SIEHL

- 1 Introduction 125
- 2 Alkyl and cycloalkylmethyl cations 126

- 3 Vinyl cations 133
- 4 Cycloalkyl cations 142
- 5 μ -Hydrido-bridged carbocations 144
- 6 Bicyclic and polycyclic carbocations 145
- 7 π -Stabilized carbocations 150
- 8 Heteroatom stabilized carbocations 156
- 9 Final remarks 158
- 10 Conclusions 160
- Acknowledgments 160
- References 160

Dynamics of guest binding to supramolecular systems: techniques and selected examples

167

TAMARA C.S. PACE and CORNELIA BOHNE

- 1 Introduction 167
- 2 Techniques 169
- 3 Examples of supramolecular dynamics studies 185
- 4 Conclusions 216
- Acknowledgements 217
- References 217

Mechanisms of oxygenations in zeolites

225

EDWARD L. CLENNAN

- 1 Introduction 225
- 2 Zeolites 226
- 3 Experimental considerations 230
- 4 Intrazeolite photooxygenations 232
- Acknowledgement 261
- References 262

Metal-catalyzed alcoholysis reactions of carboxylate and organophosphorus esters

271

R. STAN BROWN and ALEXEI A. NEVEROV

- 1 Introduction 271
- 2 Background theory 274
- 3 Titrations in alcohol 276
- 4 Metal ion alcoholysis and titration in alcohol 278
- 5 Transition metal ion and Ln^{3+} catalysts of transesterifications of neutral carboxylate and organophosphate esters 284

CONTENTS

vii

6	Transition metal ion and La^{3+} -catalysis of the alcoholysis of phosphate diesters	308
7	Conclusions	324
	Acknowledgements	325
	References	325

Author Index	333
---------------------	------------

Cumulative Index of Authors	351
------------------------------------	------------

Cumulative Index of Titles	353
-----------------------------------	------------

Subject Index	363
----------------------	------------