

Contents

Preface — V

List of contributing authors — XI

Bapan Saha and Pradip Kumar Bhattacharyya

1 Role of heteroatoms and substituents on the structure, reactivity, aromaticity, and absorption spectra of pyrene: a density functional theory study — 1

- 1.1 Introduction — 1
- 1.2 Theoretical and computational details — 2
- 1.3 Results and discussions — 3
 - 1.3.1 Geometry of the chosen systems — 4
 - 1.3.2 HOMO shapes and HOMO perspectives — 6
 - 1.3.3 Variations in global hardness and philicity, and dipole moment — 10
 - 1.3.4 Variations in aromatic character — 13
 - 1.3.5 Variations in UV visible spectra — 14
- 1.4 Conclusions — 16
- References — 17

Samuel Tetteh and Albert Ofori

2 Effect of delocalization of nonbonding electron density on the stability of the M–C_{carbene} bond in main group metal-imidazol-2-ylidene complexes: a computational and structural database study — 21

- 2.1 Introduction — 21
- 2.2 Methods — 23
 - 2.2.1 CSD Analyses — 23
 - 2.2.2 Computational Details — 24
- 2.3 Results and discussion — 24
 - 2.3.1 Binding energy — 28
 - 2.3.2 Natural bond orbital (NBO) analyses — 29
 - 2.3.3 Thermodynamic stability — 30
- 2.4 Conclusions — 31
- References — 32

Liliana Mammino

3 Educational components in the supervision of chemistry postgraduate students: experiences and reflections — 35

- 3.1 Introduction — 36
 - 3.1.1 Background information — 36
 - 3.1.2 Continuity aspects and novel components in postgraduate mentoring — 37

3.1.3	General and specific features of learning how to do research in computational chemistry —	37
3.2	Approaches selected for educational research focusing on the postgraduate level —	38
3.3	Mentoring and learning in postgraduate studies —	40
3.3.1	The main operations in postgraduate work —	40
3.3.2	The literature review operation —	41
3.3.3	Designing a project —	42
3.3.4	Performing the planned activities —	42
3.3.5	Preparation of presentations —	43
3.3.6	Writing: the most challenging operation —	44
3.3.7	Planning a thesis and organising its material —	54
3.3.8	Fostering independence —	56
3.4	Discussion and conclusions —	57
	References —	58

Miroslava Nedyalkova, Ralitsa Robeva, Atanaska Elenkova and Vasil Simeonov

4	Chemometric exploratory data analysis for patients with diabetes type 2 and diabetic complications —	61
4.1	Introduction —	61
4.2	Methods and results —	62
4.2.1	Input data —	62
4.3	Results and discussion —	64
4.3.1	Clustering of the parameters (HCA) —	66
4.4	Conclusions —	76
	References —	76

Moses M. Edim, Hitler Louis, Emmanuel A. Bisong, Apebende G. Chioma, Obieze C. Enudi, Tomsmith O. Unimuke, Asuquo B. Bassey, David Prince, Queen O. Sam, Emmanuel I. Ubana and Tiya H. Mujong

5	Electronic structure theory study of the reactivity and structural molecular properties of halo-substituted (F, Cl, Br) and heteroatom (N, O, S) doped cyclobutane —	79
5.1	Introduction —	80
5.2	Computational details —	80
5.3	Results and discussion —	85
5.3.1	Vibrational analysis —	85
5.3.2	Bond Polarity Index (BPI) —	87
5.3.3	Intrinsic Bond Strength Index (IBSI) —	88
5.3.4	CDFT results using Fukui function on cyclobutane and its associated halogenated and doped-ringed structures —	90

5.3.5	Quantum chemical descriptors —	92
5.3.6	Natural bond orbital analysis (NBO) —	95
5.3.7	Atomic charge analysis —	96
5.3.8	Molecular electrostatic potential (MEP) —	97
5.4	Conclusions —	99
	References —	100

Emmanuel A. Bisong, Hitler Louis, Tomsmith O. Unimuke, Victoria M. Bassey,
John A. Agwupuye, Linda I. Peter, Francis O. Ekpen and Aderemi T. Adeleye

6	Theoretical investigation of the stability, reactivity, and the interaction of methyl-substituted peridinium-based ionic liquids —	103
6.1	Introduction —	104
6.2	Computational details —	105
6.3	Results and discussion —	105
6.3.1	Natural bond orbital (NBO) analysis —	105
6.3.2	Analysis of HOMO–LUMO —	110
6.3.3	Atomic dipole moment corrected Hirshfeld (ADCH) atomic charge analysis of pyridinium ion and its interaction with hydrogen nitrate: emphasis on the nitrogen charge —	112
6.3.4	The electrostatic molecular potential (ESP) plot —	112
6.3.5	Binding energy —	113
6.3.6	Atoms-in-molecules (AIM) descriptors and H-atom binding energies —	114
6.4	Conclusions —	115
	References —	115

Tandrima Banerjee and Abhijit Samanta

7	Chemical computational approaches for optimization of effective surfactants in enhanced oil recovery —	119
7.1	Introduction —	119
7.2	Fundamentals of use of surfactant in EOR —	121
7.3	Chemical computational approaches for surfactant —	122
7.3.1	Molecular dynamics (MD) simulation —	122
7.3.2	Dissipative particle dynamics (DPD) simulation —	126
7.4	Application of chemical computational approaches —	130
7.4.1	Application of MD and DFT Simulation in EOR —	130
7.4.2	Application of DPD simulation in EOR —	138
7.5	Conclusions —	141
	References —	142

Olugbenga Morayo Oshakuade and Oluseyi Ezekiel Awe

8 Determination of bulk and surface properties of liquid Bi-Sn alloys using an improved quasi-lattice theory — 149

- 8.1 Introduction — 149
- 8.2 Theoretical framework — 150
 - 8.2.1 Average coordination number ($\bar{z}$) — 150
 - 8.2.2 Quasi-lattice theory for compound forming liquid alloys (QLT) — 152
 - 8.2.3 Surface concentration and surface tension — 158
- 8.3 Results and discussion — 159
 - 8.3.1 Enthalpy and entropy of mixing — 159
 - 8.3.2 Concentration-concentration fluctuations in the long-wavelength limit and Warren-Cowley short-range-order parameter — 160
 - 8.3.3 Surface concentration and surface tension — 161
- 8.4 Conclusions — 162
- References — 163

Kayode E. Adewole, Ahmed A. Ishola and Blessing O. Omolaso

9 Identification of potential histone deacetylase inhibitory biflavonoids from *Garcinia kola* (Guttiferae) using *in silico* protein-ligand interaction — 165

- 9.1 Introduction — 165
- 9.2 Materials and methods — 167
 - 9.2.1 Ligand preparation — 167
 - 9.2.2 Protein preparation — 167
 - 9.2.3 Molecular docking — 167
- 9.3 Results — 167
- 9.4 Discussion and conclusions — 174
 - 9.4.1 Discussion — 174
 - 9.4.2 Conclusions — 176
- References — 176

Medinat O. Osundiya, Segun E. Olaseni, Rasaq A. Olowu, and Olanrewaju Owoyomi

10 Thermodynamics of the micellization of quaternary based cationic surfactants in triethanolamine-water media: a conductometry study — 181

- 10.1 Introduction — 182
- 10.2 Materials and methods — 184
 - 10.2.1 Materials — 184
- 10.3 Results and discussion — 185
 - 10.3.1 Results — 185
 - 10.3.2 Mixed micelle formation. And Solvent Effect — 187
 - 10.3.3 Effect of Temperature on the Mixed micelle formation — 188
 - 10.3.4 Thermodynamics of Mixed-Micelles — 189
- 10.4 Conclusion — 190
- References — 191