

Contents

Reactivity of Aziridinium Salts in Different Solvents Unraveled by a Combined Theoretical and Experimental Approach	1
Hannelore Goossens, Dietmar Hertsen, Karen Mollet, Saron Catak, Matthias D'hooghe, Frank De Proft, Paul Geerlings, Norbert De Kimpe, Michel Waroquier, and Veronique Van Speybroeck	
Characterization of the Chemical Reactivity and Selectivity of DNA Bases Through the Use of DFT-Based Descriptors	35
Vanessa Labet, Christophe Morell, Vincent Tognetti, Olga A. Syzgantseva, Laurent Joubert, Nelly Jorge, André Grand, and Jean Cadet	
Characterising Heterocyclic Rings Through Quantum Chemical Topology	71
Mark Z. Griffiths and Paul L.A. Popelier	
Valence Bond Theory in Heterocyclic Chemistry	103
Zahid Rashid, Ria Broer, Joop H. van Lenthe, and Remco W.A. Havenith	
Aromaticity of Organic and Inorganic Heterocycles	129
Ferran Feixas, Jordi Poater, Eduard Matito, and Miquel Solà	
Chemical Bonding and Aromaticity in Poly-heterocyclic Compounds	161
Truong Ba Tai, Vu Thi Thu Huong, and Minh Tho Nguyen	
Index	189