

# Contents

<b>1</b>	<b>Topological Approaches of the Bonding in Conceptual Chemistry . . . . .</b>	<b>1</b>
	Bernard Silvi, M. Esmail Alikhani, Christine Lepetit and Remi Chauvin	
<b>Part I Topological Methods: Definition, State of the Art and Prospects</b>		
<b>2</b>	<b>On Quantum Chemical Topology . . . . .</b>	<b>23</b>
	Paul L.A. Popelier	
<b>3</b>	<b>Localization-Delocalization Matrices and Electron Density-Weighted Adjacency/Connectivity Matrices: A Bridge Between the Quantum Theory of Atoms in Molecules and Chemical Graph Theory . . . . .</b>	<b>53</b>
	Chérif F. Matta, Ismat Sumar, Ronald Cook and Paul W. Ayers	
<b>4</b>	<b>Extending the Topological Analysis and Seeking the Real-Space Subsystems in Non-Coulombic Systems with Homogeneous Potential Energy Functions. . . . .</b>	<b>89</b>
	Shant Shahbazian	
<b>5</b>	<b>Exploring Chemistry Through the Source Function for the Electron and the Electron Spin Densities . . . . .</b>	<b>101</b>
	Carlo Gatti, Ahmed M. Orlando, Emanuele Monza and Leonardo Lo Presti	
<b>6</b>	<b>Emergent Scalar and Vector Fields in Quantum Chemical Topology . . . . .</b>	<b>131</b>
	A. Martín Pendás, E. Francisco, A. Gallo Bueno, J.M. Guevara Vela and A. Costales	

<b>7</b>	<b>Topology of Quantum Mechanical Current Density Vector Fields Induced in a Molecule by Static Magnetic Perturbations . . .</b>	<b>151</b>
	P. Lazzeretti	
<b>8</b>	<b>Topological Analysis of the Fukui Function . . . . .</b>	<b>227</b>
	P. Fuentealba, C. Cardenas, R. Pino-Rios and W. Tiznado	
<b>9</b>	<b>Topological Tools for the Study of Families of Reaction Mechanisms: The Fundamental Groups of Potential Surfaces in the Universal Molecule Context . . . . .</b>	<b>243</b>
	Paul G. Mezey	
<b>10</b>	<b>Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity . . . . .</b>	<b>257</b>
	Juan Andrés, Lourdes Gracia, Patricio González-Navarrete and Vicent S. Safont	
 <b>Part II Topological Methods for the Characterization of <math>\pi</math>-Electron Delocalization and Aromaticity</b>		
<b>11</b>	<b>Paradise Lost—<math>\pi</math>-Electron Conjugation in Homologs and Derivatives of Perylene . . . . .</b>	<b>297</b>
	Ivan Gutman and Slavko Radenković	
<b>12</b>	<b>Rules of Aromaticity . . . . .</b>	<b>321</b>
	Ferran Feixas, Eduard Matito, Jordi Poater and Miquel Solà	
<b>13</b>	<b>Localized Structures at the Hückel Level, a Hückel-Derived Valence Bond Method . . . . .</b>	<b>337</b>
	Yannick Carissan, Nicolas Goudard, Denis Hagebaum-Reignier and Stéphane Humbel	
<b>14</b>	<b>Magnetic Properties of Conjugated Hydrocarbons from Topological Hamiltonians . . . . .</b>	<b>361</b>
	Jean-Paul Malrieu, Nicolas Ferré and Nathalie Guihéry	
 <b>Part III Topological Methods for the Characterization of Weak Bonding Interactions</b>		
<b>15</b>	<b>What Can Be Learnt from a Location of Bond Paths and from Electron Density Distribution. . . . .</b>	<b>399</b>
	Sławomir J. Grabowski	
<b>16</b>	<b>Following Halogen Bonds Formation with Bader's Atoms-in-Molecules Theory . . . . .</b>	<b>435</b>
	Vincent Tognetti and Laurent Joubert	

<b>17</b>	<b>Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds. A New Perspective. . . . .</b>	<b>461</b>
	Kateryna Mykolayivna Lemishko, Giovanni Bistoni, Leonardo Belpassi, Francesco Tarantelli, M. Merced Montero-Campillo and Manuel Yáñez	
<b>18</b>	<b>A Complete NCI Perspective: From New Bonds to Reactivity . . . .</b>	<b>491</b>
	Christophe Narth, Zeina Maroun, Roberto A. Boto, Robin Chaudret, Marie-Laure Bonnet, Jean-Philip Piquemal and Julia Contreras-García	
<b>19</b>	<b>Diversity of the Nature of the Nitrogen-Oxygen Bond in Inorganic and Organic Nitrites in the Light of Topological Analysis of Electron Localisation Function (ELF) . . . . .</b>	<b>529</b>
	Slawomir Berski and Agnieszka J. Gordon	
<b>20</b>	<b>Quantum Chemical Topology in the Field of Quasirelativistic Quantum Calculations . . . . .</b>	<b>553</b>
	Mohamed Amaouch, Eric Renault, Gilles Montavon, Nicolas Galland and Julien Pilmé	
	<b>Index . . . . .</b>	<b>583</b>

Applications of Topological Methods in Molecular  
Chemistry

Chauvin, R.; Lepetit, C.; Silvi, B.; Alikhani, E. (Eds.)

2016, IX, 586 p. 248 illus., 81 illus. in color., Hardcover

ISBN: 978-3-319-29020-1