

Chemical Group Theory: Introduction and Fundamentals (Mathematical Chemistry)

Danail Bonchev, Dennis H. Rouvray

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In chapter 1, after an outline of some historical aspects of the use of symmetry in chemistry is given, the scene is set by introducing a number of group theoretical techniques that have been employed by chemists. Chapter 2 considers in detail the nature and the differing types of groups that have been employed by chemists and others in their description of chemical systems. In chapter 3 a comparatively new mathematical formalism is presented that is now being increasingly used for the interpretation of stereochemical phenomena. The symmetry of molecules is analyzed from a group-theoretical perspective in chapter 4, while in chapter 5 the symmetry of the chemical graphs that are commonly used to represent both organic and inorganic molecules is addressed. Chapters 4 and 5 together encompass applications such as the enumeration of many different chemical isomers and analysis of the symmetry characteristics of a variety of recently synthesized molecules such as the fullerenes. The concluding chapter 6



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