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Group Theory for Chemists: Fundamental Theory and Applications

Kieran C Molloy

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This undergraduate text deals with basics of group theory and its application to the analysis of vibrational spectra, molecular orbital description of bonding, ligand field theory and other themes within inorganic chemistry. Concise and student- friendly, the book adopts a diagrammatic rather than a rigorous mathematic approach, providing support for lecture courses in chemical group theory offering students opportunities to test their understanding. Problem solving is stressed with numerous self-assessment questions and problem exercises, along with tutorial hints and solutions to selected problems. Part 1 covers the essentials of symmetry and group theory, including symmetry elements and operations, point groups and representations. Part 2 focuses on the application of group theory to vibrational spectroscop building step-wise to show how group theory guides the analysis of vibrational spectra. A brief overview of infrared and Raman spectroscopy techniques is followed by a complete worked example to reiterate key points from earlier sections. Part 3 describes the application of group theory to a molecular orbital approach to chemical bonding. After laying a foundation of the basic rules for forming molecular orbitals using H, and H as examples, the book addresses more complex problems by comparing angular and linear structures for water and planar and pyramidal structures for ammonia. A description of the application of group theory to the bonding in octahedral main group and transitional metal complexes then follows, including an analysis of the influencing crystal field splitting energies. The book concludes with a description of the bonding in ferrocene, bringing together all the ideas presented in earlier sections.

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