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Nota di contenuto	Molecular Symmetry; Contents; Preface; 1 Symmetry Elements and Operations; 1.1 Introduction; 1.2 Symmetry Elements and Operations; 1.2.1 Proper Rotations: Cn; 1.2.2 The Plane of Symmetry: ; 1.2.3 The Inversion Centre: i; 1.3 Examples of the Impact of Geometric Symmetry on Chemistry; 1.3.1 Oxygen Transfer via Metal Porphyrins; 1.3.2 Nuclear Magnetic Resonance: Chemical Equivalence; 1.4 Summary; 1.5 Self-Test Questions; Further Reading; 2 More Symmetry Operations and Products of Operations; 2.1 Introduction; 2.2 Background to Point Groups; 2.3 Closed Groups and New Operations 2.3.1 Products of Operations2.3.2 Fixed Symmetry Elements; 2.3.3 The Final Missing Operation, Improper Rotations: Sn; 2.3.4 Equivalences for

Improper Rotation Operations; 2.4 Properties of Symmetry Operations; 2.4.1 Equivalent Operations and Equivalent Atoms; 2.4.2 The Inverse of an Operation; 2.4.3 The Order of the Product; Operations that Commute; 2.5 Chirality and Symmetry; 2.6 Summary; 2.7 Completed Multiplication Tables; 2.8 Self-Test Questions; 3 The Point Groups Used with Molecules; 3.1 Introduction; 3.2 Molecular Classification Using Symmetry Operations
3.3 Constructing Reference Models with Idealized Symmetry3.4 The Nonaxial Groups: Cs,Ci,C1; 3.4.1 Examples of Molecules for the Nonaxial Groups: Cs,Ci,C1; 3.5 The Cyclic Groups: Cn, Sn; 3.5.1 Examples of Molecules for the Cyclic Groups: Cn, Sn; 3.6 Axial Groups Containing Mirror Planes: Cnh and Cnv; 3.6.1 Examples of Molecules for Axial Groups Containing Mirror Planes: Cnh and Cnv; 3.7 Axial Groups with Multiple Rotation Axes: Dn, Dnd and Dnh; 3.7.1 Examples of Axial Groups with Multiple Rotation Axes: Dn,Dnd and Dnh; 3.8 Special Groups for Linear Molecules:C v and Dh
3.9 The Cubic Groups: Td and Oh3.10 Assigning Point Groups to Molecules; 3.11 Example Point Group Assignments; 3.11.1 Example 1: Conformations of Cyclohexane; 3.11.2 Example 2: Six-Coordinate Metal Complexes; 3.12 Self-Test Questions; 4 Point Group Representations, Matrices and Basis Sets; 4.1 Introduction; 4.2 Symmetry Representations and Characters; 4.2.1 Water, H2O, C2v; 4.2.2 Direct Products; 4.3 Multiplication Tables for Character Representations; 4.4 Matrices and Symmetry Operations; 4.5 Diagonal and Off-Diagonal Matrix Elements; 4.5.1 Ammonia, NH3, C3v
5.4 Properties of Point Groups and Irreducible Representations

Sommario/riassunto

Symmetry and group theory provide us with a formal method for the description of the geometry of objects by describing the patterns in their structure. In chemistry it is a powerful method that underlies many apparently disparate phenomena. Symmetry allows us to accurately describe the types of bonding that can occur between atoms or groups of atoms in molecules. It also governs the transitions that may occur between energy levels in molecular systems, which in turn allows us to predict the absorption properties of molecules and hence their spectra. Molecular Symmetry lays out the fo