

# Preface

Symmetry is a general principle, which plays an important role in various areas of knowledge and perception, ranging from arts and aesthetics to natural sciences and mathematics. According to Barut,<sup>1</sup> the symmetry of a physical system may be looked at in a number of different ways. We can think of symmetry as representing

- the impossibility of knowing or measuring some quantities, e.g., the impossibility of measuring absolute positions, absolute directions or absolute left or right;
- the impossibility of distinguishing between two situations;
- the independence of physical laws or equations from certain coordinate systems, i.e., the independence of absolute coordinates;
- the invariance of physical laws or equations under certain transformations;
- the existence of constants of motions and quantum numbers;
- the equivalence of different descriptions of the same system.

Chemists are more used to the operational definition of symmetry, which crystallographers have been using long before the advent of quantum chemistry. Their ball-and-stick models of molecules naturally exhibit the symmetry properties of macroscopic objects: they pass into congruent forms upon application of bodily rotations about proper and improper axes of symmetry. Needless to say, the practitioner of quantum chemistry and molecular modeling is not concerned with balls and sticks, but with subatomic particles, nuclei, and electrons. It is hard to see how bodily rotations, which leave all interparticle distances unaltered, could affect in any way the study of molecular phenomena that only depend on these internal distances. Hence, the purpose of the book will be to come to terms with the subtle metaphors that relate our macroscopic intuitive ideas about symmetry to the molecular world. In the end the reader should have acquired the skills to make use of the mathematical tools of group theory for whatever chemical problems he/she will be confronted with in the course of his or her own research.

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<sup>1</sup>A.O. Barut, *Dynamical Groups and Generalized Symmetries in Quantum Theory*, Bascands, Christchurch (New Zealand) (1972)

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