ABSTRACT OF THE THESIS

This thesis is concerned with theoretical investigations on interaction of electromagnetic radiations with molecules. In particular, we have studied, for the first time, the spin-resolved Auger electron spectroscopy and double ionization of free gaseous molecules, and photoelectron spectroscopy of those molecular targets which are rotationally state selected and oriented in space in their gas phase using electrostatic hexapole field techniques. All the three of these processes are assumed to take place following the absorption of a single photon in electric dipole approximation. In these studies, whereas light has been treated classically, a molecule is described by quantum mechanical methods. Therefore, the essential theoretical techniques used in our semi-classical studies of photon-molecule interactions are, among others,non-relativistic quantum mechanics, group theory, and Racah algebra.

The theoretical expressions developed in this thesis are exact and in their most general form. These are applicable to all molecular systems whose symmetry properties can be described by one of the 32 point groups. But, the specific examples considered herein for Auger electron spectroscopy and for double ionization are the molecules which belong to one of the $C_{\infty v}$, $D_{\infty h}$, or T_d point groups; for photoelectron spectroscopy are the molecular targets of C_{3v} or T_d symmetries.

It is our hope that the results of this thesis would be of considerable utility in understanding the structure and dynamics of molecules, as well as in unraveling the hitherto unknown aspects of molecular mechanics.

Keywords : Group theory, Electric dipole approximation, Racah algebra, Auger electron spectroscopy, Spin-polarization, Correlations, Circular dichroism, Electrostatic hexapole field, State selection, Orientation, Photoelectron spectroscopy.