Quantum Modeling of Spin-Selective Processes of the Triplet State. Edition No. 1

Description: This book provides insights on spin-selective processes which occur in short-lived triplet (T) excited states. The T state is invariably of lower energy than the excited singlet (S) state, derived from the same single-electron transition. The triplet state has three spin sublevels which are split even in the absence of an external magnetic field. The zero-field splitting (ZFS) is determined mostly by spin-spin characteristic of the orbital nature of the excited state. The difference in the magnetic sublevel radiative rates makes it possible to detect microwave transitions between triplet spin substates via changes in phosphorescence intensity, which is the origin of the ODMR technique in triplet state spectroscopy. The electric dipole activity of the spin sub-levels in the phosphorescent triplet-singlet transitions is estimated in this book by means of the quadratic response technique. The first ab initio attempt is performed in order to understand the origin of spin-selective solvent effects on ODMR signals. The first part of book reviews aspects of the theory of quantum chemistry, the second part presents the different sample applications.


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