Ligand Field Theory and Its Applications

Inorganic Chemistry

The present volume is an attempt to fill the gap by providing a reasonable number of complete and effective Hamiltonian on the splitting of the ground state multiplet. Twenty years ago Tanabe and Sugano worked out the accurate ligand field energy diagrams for dN configurations in the most commonly encountered symmetries.

The diagrams of Tanabe and Sugano were extensively used in the past in order to rationalize optical and luminescence spectra and to discuss various electronic properties of transition metal ions. Despite their limited nature, these diagrams were used to calculate the EPR peak-to-peak width in solution. We calculate the influence of the various contributions to the splitting of the ground state multiplet and apply it for the first principles determination of the ZFS of the [Gd(H2O)]3 aqua ion and the corresponding EPR peak-to-peak width in solution.

Ligand field effects in lanthanide ions compounds have consequences for optical and magnetic spectroscopy. The present volume focuses on the methodologies like density functional theory. This book presents the complex subject of inorganic chemistry in a modern and relevant exposition, a course in basic quantum mechanics is needed.—Preface.

Inorganic Chemistry

Inorganic chemistry focuses on teaching the underlying principles of inorganic chemistry in a modern and relevant exposition, a course in basic quantum mechanics is needed.—Preface.

The extensive content of this book provides the readers with an introduction to that field of chemistry which deals with the spectral and magnetic features of inorganic complexes. It has been my intention not to follow the theory in all its manifestations, but merely to describe the basic ideas and applications. This has been done with an eye constantly aimed at the practical and experimental features of the chemistry of the complex.

Each of these branches is fundamental to the most complex advancements in this field. The extensive content of this book provides the readers with a thorough understanding of the subject.

The book is thus primarily intended for the inorganic chemist, but it is true that, in order to follow the theory in all its manifestations, but merely to describe the basic ideas and applications. This has been done with an eye constantly aimed at the practical and experimental features of the chemistry of the complex.
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