

INTRODUCTION TO LIGAND FIELD THEORY

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THIS VOLUME WAS ORIGINALLY PUBLISHED IN 1973 THE NATURE OF THE NON SYMMETRY DETERMINED ASPECTS OF LIGAND FIELD THEORY RECEIVES INADEQUATE TREATMENT IN MOST TEXTS THIS BOOK IS CONCERNED WITH THE NATURE OF THE LIGAND FIELD PARAMETERS USED TO DESCRIBE THE ELECTRONIC PROPERTIES OF TRANSITION METAL COMPLEXES HAVING CUBIC AND LOWER SYMMETRIES THESE RADIAL PARAMETERS CONSTITUTE THE NON SYMMETRY DETERMINED PART OF LIGAND FIELD THEORY SYMMETRY BASED PROPERTIES ARE DISCUSSED HERE ONLY TO EMPHASIZE THE SEPARATE ROLES OF SPLITTING FACTORS AND SYMMETRY THE READER IS ASSUMED TO BE FAMILIAR WITH THE USUAL APPROACH TO LIGAND FIELD THEORY AND WITH ELEMENTARY GROUP THEORY

TWENTY YEARS AGO TANABE AND SUGANO PUBLISHED THE FIRST LIGAND FIELD ENERGY DIAGRAMS WHICH ARE APPLICABLE TO d^n ELECTRONIC CONFIGURATIONS THESE DIAGRAMS ARE LIMITED IN SCOPE IN THAT THEY CAN BE USED ONLY FOR OCTAHEDRAL SYMMETRY AND FOR A LIMITED NUMBER OF TERMS THE PRESENT VOLUME IS AN ATTEMPT TO FILL THE GAP BY PROVIDING A REASONABLE NUMBER OF COMPLETE AND ACCURATE LIGAND FIELD ENERGY DIAGRAMS FOR d^n CONFIGURATIONS IN THE MOST COMMONLY ENCOUNTERED SYMMETRIES DESPITE THEIR LIMITED NATURE 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 THEIR COORDINATION COMPOUNDS AND SOLIDS MOREOVER TANABE SUGANO DIAGRAMS HAVE AN ESTABLISHED PLACE IN THE THEORY OF TRANSITION METAL COMPOUNDS AND ARE INCLUDED IN MOST TEXTBOOKS OF INORGANIC AND COORDINATION CHEMISTRY IT IS EXPECTED THAT THE PRESENT DIAGRAMS WILL BE FOUND USEFUL FOR A SIMILAR PURPOSE

A COMPLETE UP TO DATE TREATMENT OF LIGAND FIELD THEORY AND ITS APPLICATIONS LIGAND FIELD THEORY AND ITS APPLICATIONS PRESENTS AN UP TO DATE ACCOUNT OF LIGAND FIELD THEORY THE MODEL CURRENTLY USED TO DESCRIBE THE METAL LIGAND INTERACTIONS IN TRANSITION METAL COMPOUNDS AND THE WAY IT IS USED TO INTERPRET THE PHYSICAL PROPERTIES OF THE COMPLEXES IT EXAMINES THE TRADITIONAL ELECTROSTATIC CRYSTAL FIELD MODEL STILL WIDELY USED BY PHYSICISTS AS WELL AS COVALENT APPROACHES SUCH AS THE ANGULAR OVERLAP MODEL WHICH INTERPRETS THE METAL LIGAND INTERACTIONS USING PARAMETERS RELATING DIRECTLY TO CHEMICAL BEHAVIOR WRITTEN BY INTERNATIONALLY RECOGNIZED EXPERTS IN THE FIELD THIS BOOK PROVIDES A COMPARISON BETWEEN LIGAND FIELD THEORY AND MORE SOPHISTICATED TREATMENTS AS WELL AS AN ACCOUNT OF THE METHODS USED TO CALCULATE THE ENERGY LEVELS IN

COMPOUNDS OF THE TRANSITION METALS IT ALSO COVERS PHYSICAL PROPERTIES SUCH AS STEREOCHEMISTRY LIGHT ABSORPTION AND MAGNETIC BEHAVIOR AN EMPHASIS ON THE INTERPRETATION OF EXPERIMENTAL RESULTS BROADENS THE BOOK'S FIELD OF INTEREST BEYOND TRANSITION METAL CHEMISTRY INTO THE MANY OTHER AREAS WHERE THESE METAL IONS PLAY AN IMPORTANT ROLE AS CLEAR AND ACCESSIBLE AS BRIAN FIGGIS'S 1966 CLASSIC INTRODUCTION TO LIGAND FIELDS THIS NEW BOOK PROVIDES INORGANIC AND BIOINORGANIC CHEMISTS AS WELL AS PHYSICAL CHEMISTS CHEMICAL PHYSICISTS AND SPECTROSCOPISTS WITH A MUCH NEEDED OVERVIEW OF THE MANY SIGNIFICANT CHANGES THAT HAVE TAKEN PLACE IN LIGAND FIELD THEORY OVER THE PAST 30 YEARS

THE SECOND EDITION OF THIS CLASSIC BOOK PROVIDES AN UPDATED LOOK AT CRYSTAL FIELD THEORY AND ITS APPLICATIONS

TO APPRECIATE THE CHEMISTRY AND PHYSICAL PROPERTIES OF COMPLEXES OF THE TRANSITION SERIES AN UNDERSTANDING OF METAL LIGAND INTERACTIONS APPLIED TO COMPLEXES OF THE D BLOCK IS NEEDED METAL LIGAND BONDING AIMS TO PROVIDE THIS THROUGH AN ACCESSIBLE DETAILED NON-MATHEMATICAL APPROACH INITIAL CHAPTERS DETAIL THE CRYSTAL FIELD MODEL USING IT TO DESCRIBE THE USE OF MAGNETIC MEASUREMENTS TO DISTINGUISH COMPLEXES WITH DIFFERENT ELECTRONIC CONFIGURATIONS AND GEOMETRIES SUBSEQUENT CHAPTERS LOOK AT THE MOLECULAR ORBITAL THEORY OF TRANSITION METAL COMPLEXES USING A PICTORIAL APPROACH BONDING IN OCTAHEDRAL COMPLEXES IS EXPLORED AND ELECTRONIC SPECTRA AND MAGNETIC PROPERTIES ARE GIVEN EXTENSIVE COVERAGE THE MATERIAL ADDRESSED IN THIS BOOK FORMS THE FOUNDATION OF UNDERGRADUATE LECTURE COURSES ON D-BLOCK CHEMISTRY AND FACILITATES LEARNING THROUGH VARIOUS KEY FEATURES INCLUDING FULL COLOUR DIAGRAMS IN-TEXT QUESTIONS WITH ANSWERS REVISION EXERCISES AND CLEARLY DEFINED LEARNING OUTCOMES TO ENCOURAGE A REFLECTIVE APPROACH TO STUDY AN ASSOCIATED WEBSITE AND EXPERIMENTAL DATA AND OBSERVATIONS FROM EVERYDAY LIFE A BASIC KNOWLEDGE OF ATOMIC AND MOLECULAR ORBITALS AS APPLIED TO MAIN GROUP ELEMENTS IS ASSUMED

MULTIPLETS OF TRANSITION METAL IONS IN CRYSTALS PROVIDES INFORMATION PERTINENT TO LIGAND FIELD THEORY THIS BOOK DISCUSSES THE FUNDAMENTALS OF QUANTUM MECHANICS AND THE THEORY OF ATOMIC SPECTRA COMPRISED OF 10 CHAPTERS THIS BOOK STARTS WITH AN OVERVIEW OF THE QUALITATIVE NATURE OF THE SPLITTING OF THE ENERGY LEVEL AS WELL AS THE ANGULAR BEHAVIOR OF THE WAVEFUNCTIONS THIS TEXT THEN EXAMINES THE PROBLEM OF OBTAINING THE ENERGY EIGENVALUES AND EIGENSTATES OF THE TWO-ELECTRON SYSTEMS IN WHICH TWO

ELECTRONS ARE ACCOMMODATED IN THE t_{2g} AND e_g SHELLS IN A VARIETY OF WAYS OTHER CHAPTERS DISCUSS THE LIGAND FIELD POTENTIAL WHICH IS INVARIANT TO ANY SYMMETRY OPERATION IN THE GROUP TO WHICH SYMMETRY OF THE SYSTEM BELONGS THIS BOOK DISCUSSES AS WELL THE APPROXIMATE METHOD OF EXPRESSING MOLECULAR ORBITALS MO BY A SUITABLE LINEAR COMBINATION OF ATOMIC ORBITALS AO THE FINAL CHAPTER DISCUSSES THE MO IN MOLECULES AND THE SELF CONSISTENT FIELD THEORY OF HARTREE FOCK THIS BOOK IS A VALUABLE RESOURCE FOR RESEARCH PHYSICISTS CHEMISTS ELECTRONIC ENGINEERS AND GRADUATE STUDENTS

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