

safety. It would have also been desirable to see more papers interrelating engineering safeguards (design) and site evaluations.

The International Atomic Energy Agency should be commended for having organized in a very methodical manner these Proceedings. They contain a great deal of information bearing on the field of reactor safety and have been clearly presented. It is rather apparent that the Proceedings will serve as a very useful reference to all members of the reactor community and particularly to those of us involved in performing safety evaluations.

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#### **Advances in Chemical Physics, Volume V.**

I. Prigogine, Editor,  
Interscience Publishers (1963).

More articles of interest to physical-inorganic chemists are contained in this volume than in previous volumes of this series. The intention of the authors, as stated in the Introduction, is to present their point of view on their subject so that it is comprehensible to research workers who are not expert in their particular field. The bibliographies alone are worth the price of the book.

#### *New Developments in the One-Electron Theory of $\pi$ -Electron Systems*, H. Hartmann (17 references)

An extension of Hückel's theory for  $\pi$ -electron systems is given. For readers unfamiliar with this theory, a readable account is given in "Quantum Chemistry" by Daudel, Lefebvre, and Moser.

The paper explains the observation of Scheibe that, in all molecules with  $\pi$ -electron systems, the difference between the ionization energy and the energy of the first excited state, of the same multiplicity as the ground state, is nearly the same. The method for developing the explanation is to add to the 2  $p$  states used by Hückel in forming the

molecular orbitals higher atomic states of the same symmetry. The formal development of the theory is then carried out in such a way that Hückel's assumptions about the Coulomb, resonance, and overlap integrals are retained.

Resonance energies, charge densities and bond orders are also discussed.

#### *Convex Molecules in Gaseous and Crystalline States*, Taro Kihara (24 references)

"A body is called convex if any line segment whose end points are inside lies entirely in that body." The theory developed in this article is therefore applicable to a broad spectrum of molecules which we are used to thinking of as octahedra, tetrahedra, etc.

The geometry of convex bodies is first developed. The pertinent parameters of surface area,  $S$ , volume,  $V$ , and mean curvature integrated over the surface,  $M$ , are given for several commonly occurring molecular bodies. After discussing diffusion coefficients, the second virial coefficient is developed in terms of  $S$ ,  $V$ , and  $M$  using the Lennard-Jones 6-12 potential. The parameters for the Lennard-Jones potential obtained from the second virial coefficient allow a calculation of the cohesive energy per molecule at the minimum nearest-neighbor distance for crystalline states. The effects of multipole interactions in crystals are then discussed.

#### *Spectroscopy of Transition-Group Complexes*, Chr. Klixbüll Jørgensen (270 references)

The most imposing aspect of this review is a thirty-six page table of absorption spectra of transition-group complex ions. The author's discussion gives, however, a most useful skeleton outline of crystal-field theory and molecular-orbital theory as applied to  $d$  and  $f$  transition-metal complexes. The pertinent quantum-mechanical development is first given for atoms and molecules with particular emphasis on the use of group theory. The energy levels of a very large number of individual complexes of  $d$  and  $f$  groups are discussed in a detailed and critical manner.

#### *Theories on the Magnetic Properties of Compounds*, Shoichiro Koide and Takehiko Oguchi (103 references)

This review, which in many respects complements that of Jørgensen, covers the literature on the 3  $d$  group metals very thoroughly. Energy levels are discussed theoretically considering the various electronic/electronic and electronic/nuclear interactions. A most interesting analysis of the effect of molecular vibrations in allowing  $d \rightarrow d$

and  $f \rightarrow f$  transitions is presented. Tinkham has observed hyperfine structure in his paramagnetic spectra of  $\text{Mn}^{2+}$  ions in a  $\text{ZnF}_2$  crystal. A detailed evaluation of this is given in terms of the migration of fluorine electrons to the manganese. Exchange interactions between magnetic ions in crystals are also analyzed.

*Forbidden Transitions in Organic and Inorganic Systems*, Andrew D. Liehr  
(34 references)

Since electric dipole transitions are allowed only between states of different parities, the transition  ${}^2\text{E}_g \rightarrow {}^2\text{T}_2g$  of  $\text{Ti}^{3+}$  ion in an octahedral crystal field is forbidden. Asymmetric vibrations, which destroy the center of symmetry, mix in states of odd parity, however, to allow the transition to take place. This type of problem, which is also discussed by Koide and Oguchi, is developed in more detail by Liehr. The case of benzene is discussed as well as that of  $\text{Ti}(\text{H}_2\text{O})_6^{3+}$ .

*The Formal Statistical Theory of Transport Processes*, James A. McLennan, Jr.  
(27 references)

The hydrodynamical equations of motion are derived from the principles of statistical mechanics. A hydrodynamic process is defined as one for which the local thermodynamic variables and velocity are determined by the history of their boundary values. External forces, which cause the deviation from equilibrium, are introduced. Among the topics considered are macroscopic conservation laws and thermodynamic variables, entropy production, transport relations, and ionized media.

*Quantum Mechanical Interpretation of Nuclear Quadrupole Coupling Data*,  
E. Scrocco (43 references)

The author's main concern is to present some of the mathematical formalisms which are being developed in quantum chemistry. Among more recent work, the author emphasizes the contributions of Parks and Parr and McWeeny.

*Collinson Theory of Chemical Reaction Rates*,  
B. Widom  
(23 references)

Bimolecular reactions, which are caused by random collisions between pairs of molecules, are studied. The time interval between collisions is assumed long compared to the period of vibration of the molecules.

Through the use of kinetic theory, rate constants are derived for steady-state systems in which the products are instantaneously removed from the reactants and for systems in which the reactant states are characterized by the Boltzmann distribution. Arguments are presented to show that in general these constants will be different and that this difference is measurable.

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