

Book Reviews

International Review of Science. Second Series. The Butterworth Group, Borough Green, Kent, England. 1975.

My review is based on an examination of the seven volumes listed below. I was very favorably impressed by the series, and it would be difficult to conceive of a physical chemist or chemical physicist who would not profit from it. The individual articles provide generally a basic introduction for the beginner, new developments for the expert and a comprehensive list of references for both. I give below a brief synopsis of the articles in Volumes 1, 2, and 4 in which I attempt to reveal both contents and flavor. For the remaining four volumes, only the titles are listed.

Volume 1. Theoretical Chemistry. Edited by A. D. BUCKINGHAM. (The volume is properly dedicated to the late Charles Coulson and contains a complete list of his publications.) xiii + 396 pp. £13.45.

Blinder (Green's functions) gives a classical comprehensive treatment in which he works out the harmonic oscillator and coulomb Green's functions in detail with emphasis on the dynamic form. Necessary conditions and a spectral variation principle are proposed for approximate Green's functions.

Balent-Kurti (rotationally inelastic collisions) organizes the material by means of a flow diagram for the several approximations. It consists of two main branches; the first contains approximations to the fully quantal formulation, the other utilizes classical mechanics. On each branch are two subbranches; in one the S matrix (or time-development operator) maintains unitarity and in the other it does not. This is an extremely helpful organization of the complex material.

Richards and Walker (electronic structure) give a critical survey of closed- and open-shell Hartree-Fock calculations relating to molecular geometries, conformational barriers, ionization potentials, spin-orbit coupling constants, etc.

Epstein (momentum distributions) discusses the experimental determination of momentum distribution and their Fourier transformation to electron densities. "Like octopi" momentum distributions look alike to most people but, in fact, they do vary strongly with bond type.

M. Schwarz (ESCA) takes us on a tour through early semiempirical models, various levels of ab initio quantum mechanical calculations, and finally through intermediate models which are readily applicable and reasonably accurate.

Jortner and Mukamel (radiationless transitions) presents a sophisticated review of most of what one needs to know about this important subject. Their discussions of doorway states, effective Hamiltonians, and statistical limits are particularly useful.

Handy (method of moments) demonstrates for small molecules the superiority of expansions in correlated wave functions over conventional CI. Unfortunately, four (or maybe ten) electrons is the practical upper limit. The "method of moments" (transcorrelated wave functions) is fully described and is proposed as a practical method for extending the beneficial effect of correlation.

Bader (charge distribution) compares molecular charge densities obtained by Hartree-Fock, by configuration interaction, from atoms and from experiment. Schemes for partitioning charge distributions and their application to calculations of potential fields are also discussed.

Messmer (solid-state bonding) presents in physical chemistry languages a brief review of solid-state theory from the point of view of dielectric, band, and localized bond theories. These are applied to one-dimensional, amorphous, and defect solids.

Weinberger and K. Schwarz ($X\alpha$ method) give a clear and detailed description of the scattering of free electrons off of muffin tins, the exchange approximation, the self-consistent field, and the transition state concept. They then list some recent developments and close with a balanced assessment of the method.

Volume 2. Molecular Structure and Properties. Edited by A. D. BUCKINGHAM. xiii + 404 pp. £13.45.

Lide (high-resolution spectroscopy) develops briefly the theory of the vibrating rotor and then compares geometries as determined by spectroscopy and electron diffraction.

Muenter and Dyke (molecular beam spectroscopy) discuss electric dipole, electric polarizability, nuclear hyperfine, quadrupole coupling, spin-rotation, spin-spin, and Zeeman interactions in a variety of strong and weakly bonded species.

Howard (van der Waals molecules) describes the uses of infrared, Raman, and ultraviolet spectroscopy, mass spectrometry, molecular beam spectroscopy, and electron diffraction in the study of these weakly bounded species.

McLauchlan (NMR spectroscopy) describes the use of experimental relaxation times for the determination of molecular geometries of both diamagnetic and paramagnetic molecules. He also discusses briefly molecular orientation, the nuclear Overhauser effect, and the lanthanide shift.

Bogaard and Orr (electric dipole polarizabilities) present both theory and experimental data of static and dynamic polarizabilities. The experimental data come from a variety of sources: refractive index, dielectric constant, normal and hyper-Rayleigh and Raman scattering, quadratic Stark effect, Kerr effect, intermolecular forces, etc.

Clark (hyperfine interaction) develops the spin-Hamiltonian for magnetic dipole, nuclear quadrupole, and contact and electron current interaction and applies it to a wide variety of problems in molecular structure. His discussion includes the Sternheimer and nuclear volume effects as well as isomer and isotope shifts.

Egelstaff, Gray, and Gubbins (equilibrium properties of molecular fluids) provide an excellent summary of di- and polyatomic fluid theory from the standpoint of equilibrium statistical mechanics, integral equations, scaled particle theory, perturbation theory, and computer simulation. The article concludes with a summary of experimental virial coefficients, equations of state, and structure factors.

Allen and Watts (high polymers) present a general discussion of chain statistics and dynamics of single chains and then specialize to rubber, glasses, and crystalline polymers.

Gerloch (magnetochemical models) computes magnetic susceptibilities of transition metal complexes by means of an effective spin-Hamiltonian which includes exchange, superexchange, and crystal field effects.

Volume 4. Magnetic Resonance. Edited by C. A. McDOWELL. xiii + 239 pp. £13.45.

Atkins (electron spin relaxation in liquids) begins with the separation of low- and high-frequency regimes by a projection operator approach. He then treats molecular rotation, spin-exchange, and spin-rotation by means of equations of motion expressed in terms of the appropriate Liouville operators.

Allendoerfer (ENDOR and free radicals in solution) gives a brief introduction to the theory and methods of electron-nuclear double resonance and summarizes experimental results for neutral and anionic radicals.

Fujiwara (ESR of hot inorganic ions) gives an extensive review of the experimental data on "s" (e.g., Zn, Cd) and "d" (e.g., V, Cr) ions produced by the radiation of a variety of compounds.

Hirota (EPR of radical anions) compares theoretical and experimental ESR hyperfine splittings of the radical anions as a function of their interaction with solvent, counterions, and each other. He then treats intramolecular, intermolecular, rotational, and spin-lattice relaxation processes.

Reeves (ionic processes in membranes) first describes the biological membrane and membrane models suitable for NMR spectroscopy. From this he abstracts chemical shifts, dipole-dipole coupling, quadrupole coupling, and spin relaxation parameters.

Andrew (NMR in solids) describes the reduction of tensor dipolar broadening by powder suspension and by rotation. The resultant improvement in resolution reveals spin multiplets, chemical shifts, Knight shifts anisotropy, etc. The reduction of the broadening by multiple pulse, high magnetic field, and double resonance rare-spin methods is also discussed.

Srinivasan (tunnelling processes) discusses the effect of tunnelling

on line-shapes, spin-lattice relaxation, and hyperfine interaction with particular emphasis on the methyl radical and on defects.

Volume 5. Mass Spectrometry. Edited by A. MACCOLL. xiii + 365 pp. £13.45.

P. J. Derrick: Ion lifetimes. G. D. Flesch and H. J. Svec: Physical inorganic aspects of mass spectrometry. J. H. Bowie and B. D. Williams: Negative-ion mass spectrometry of organic, organometallic, and coordination compounds. V. J. Shiner, Jr., and W. E. Buddenbaum: The role of mass spectrometry in the study of heavy-atom kinetic isotope effects. J. H. Beynon and R. G. Cooks: Ion kinetic energy spectrometry. J. L. Holmes: Isotopic labeling as a tool for determining fragmentation mechanisms. J. F. J. Todd and G. Larson: Quadrupole mass spectrometry.

Volume 7. Surface Chemistry and Colloids. Edited by M. KERKER. xiii + 269 pp. £13.45.

G. A. Somorjai: The structure of solid surfaces. J. A. Mann, Jr., and K. C. Porzio: Capillarity: the physical nature of fluid-fluid interfaces including the problem of biomembrane structure. D. H. Napper and R. J. Hunter: Hydrosols. P. Ekwall and P. Stenius: Aggregation in surfactant systems. P. Becher: Emulsions.

Volume 8. Macromolecular Science. Edited by C. E. H. BAWN. xiii + 303 pp. £13.45.

A. M. North: Relaxation in polymers. W. B. Black: High-modulus organic fibres. M. L. Huggins: Thermodynamics of polymer solutions. T. Saegusa and S. Kobayashi: Polymerization of cyclic imino ethers. Ph. Teyssie, T. Ouhadi, and J. P. Bioul: New prospects in homogeneous ring-opening polymerization of heterocyclic monomers. G. Allen and C. J. Wright: Neutron scattering studies of polymers. A. Ledwith: Photoinitiation, photopolymerization, and photochemical processes in polymers.

Volume 10. Thermochemistry and Thermodynamics. Edited by H. A. SKINNER. xiii + 337 pp. £13.45.

J. L. McNaughton and C. T. Mortimer: Differential scanning calorimetry. G. Pilcher: Thermochemistry of organometallic compounds containing metal-carbon linkages. A. Snelson: Matrix isolation spectroscopy of high-temperature species. Y. S. Touloukian: Reference data on thermophysics. G. Rialdi and R. L. Biltonen: Thermodynamics and thermochemistry of biologically important systems. D. R. Douslin: The PVT properties of fluids. A. Cezairliyan and C. W. Beckett: Measurement of thermal properties at high pressures by transient techniques. R. A. J. Shelton: Alloy thermochemistry. D. I. Marchidan: Thermodynamics of molten salts.

Volume 11. Chemical Crystallography. Edited by J. M. ROBERTSON. xii + 228 pp. £13.45.

J. C. Speakman: Aspects of hydrogen bonding. P. Coppens: Measurement of electron densities in solids by x-ray diffraction. J. M. Robertson: Chemistry and crystallography of caryophyllene. J. D. Dunitz and H. B. Burgi: Nonbonded interactions in organic molecules. R. Mason and D. P. M. Mingos: Structural organotransition metal chemistry. A. McL. Mathieson: Structures of natural products: alkaloids.

F. A. Matsen, *The University of Texas at Austin*

Gmelin Handbuch der Anorganischen Chemie. Achte Auflage. Mangan. Teil C3. Verbindungen mit Sauerstoff und Metallen der 3 bis 6. Gruppen des Periodensystems. Mangan-Stickstoff-Verbindungen. Teil C6. Verbindungen mit Schwefel, Selen und Tellur. System No. 56. Hauptredakteure: C3, EDITH SCHLEITZER-STEINKOPF; C6, HARTMUT KATSCHER. Springer-Verlag, New York, N.Y. C3 1975, C6 1976. C3, xii + 307 pp. C6, xxxii + 360 pp. 18.5 × 25.5 cm. Prices: C3, \$260.50; C6, \$336.60.

Inasmuch as these two volumes both relate to manganese compounds, they are conveniently reviewed together.

Teil C3 completes the chemistry of manganese-oxygen compounds, begun with Teil C1 (manganese oxides, 1973) and Teil C2 (oxo-manganese ions and respective compounds with group 1 and 2 metals,

1975), and includes manganese-nitrogen compounds. Within the major chapters of the first portion of Teil C3 (230 pp), oxo-manganese-metal systems are described by periodic group. For periodic groups 6-8, the absence of main-group metals restricts discussions to subgroup metals. Within the various chapters on these systems, the differing arrangements used in presenting the numerous compounds and solid solutions are described in introductory reviews in both English and German. The discussions are replete with numerical constants, crystal-structure representations, and phase diagrams. Particular emphasis has been given to the magnetic and electrical properties of the various compounds and phases, e.g., those of the lanthanides. The second portion of Teil C3 (77 pp) deals with manganese nitrides; double nitrides with other metals; azides and azido complexes; imido complexes; manganese(II) amide and amido complexes; manganese(II) nitrite and nitrito complexes; manganese(II) nitrate, its aqueous solutions, nitratomanganates(II), and double nitrates; and manganese(III) nitrate, oxonitrate, and nitratomanganates(III). Physical properties, including phase diagrams, are covered in detail, as are also methods of synthesis. Literature coverage is through 1974, with many more recent citations.

Teil 6 is divided into separate sections dealing respectively with compounds of sulfur (268 pp), selenium (42 pp), and tellurium (50 pp). Each major section is again introduced by reviews in both English and German. Treatments of manganese(II) sulfide and sulfate, and of the hydrates of the latter, are particularly extensive. A very extensive section on ternary compounds of manganese, other metals, and sulfur gives much data on phase relationships and crystal structures. Treatment of the sulfate, its double salts, and their hydrates is very detailed. Other oxosulfur compounds include sulfites, thiosulfates, and thionates. Limited discussion of manganese-sulfur-halogen compounds is included. Treatment of selenium derivatives parallels and closely resembles that of the sulfur compounds. Tellurium compounds include tellurides, oxotellurates, and halotellurates. The only polonium compound described is MnPo. Very extensive treatments of magnetic properties are included for most compounds. Literature coverage is complete through 1975, with some more recent data added.

Like all volumes in the Gmelin series, these are meticulous in their presentation, logically and clearly organized, and attractively produced.

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Quantum Theory of Open Systems. By E. B. DAVIES (St. John's College, Oxford). Academic Press, New York, N.Y. 1976. x + 171 pp. \$16.50.

Professor Davies has produced a very timely synthesis of two important fields of current theoretical research. The theory of open systems as a key to the physics and chemistry of biological structures (and other self-organizing systems) has recently made headlines from the 1977 Nobel prize recognition given to I. Prigogine's foundational work in that area. Paralleling the growth in understanding of open systems, but in the field of the pure mathematics of physics, there has been the development of von Neumann's operator approach to quantum theory as a rigorous but practical alternative to what have been the more standard approaches in the past. Davies' marriage of these two lines of work seems quite successful if one is not expecting an introductory level text in either area.

The mathematical background required of the reader is adequately described in the preface: "... a knowledge of functional analysis at the graduate level together with a general familiarity with the formalism of quantum theory." Overall, the emphasis is clearly on the development of the mathematical language, and, while examples of applications are described, they are not developed. The practical-minded reader should certainly look for an introduction to the physics and chemistry of open systems in something like Haken's "Synergetics"¹ before attempting Davies' book.

(1) H. Haken, "Synergetics", Springer-Verlag, New York, N.Y., 1977.

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