

tive barrier, while an antisymmetrized product (Slater determinant) of the same functions yields a satisfactory barrier value (see Table I). Since the only difference

Table I. Comparison of Energy Contributions to the Ethane Barrier

	"Fixed" geometry, kcal	"Optimized" geometries, kcal
Bare nucleus	+4.7	-74.0
Hartree product	-0.5	-2.2
Antisymmetrized product	2.6	3.1

between the Hartree product and Slater determinant calculation is the antisymmetrization of the wave function in the latter, the present result serves to confirm the conclusion based on the fixed geometry calculation; namely, the repulsive overlap of the closed-shell bond functions manifested as a result of the Pauli exclusion principle is the essential element in the internal rotation barrier of ethane; the additional delocalization introduced in an SCF function for the molecule is less important.

Since a detailed analysis of the new calculation would essentially duplicate the one given previously, we do not reproduce it here. However, it is of interest to

note that the use of optimized geometries leads to a very large negative barrier from the bare nuclei, which contrasts with the fixed geometry result (see Table I). Thus, in the optimized geometry calculation, the "classical" shielding of the nuclei by the localized electrons, as described by the Hartree product function, plays a significant role in cancelling the effect of the geometry change on the barrier; *i.e.*, the difference in the nuclear-electron attraction integrals approximately balances the proton contribution. Such shielding occurs also in the fixed geometry calculation (see Table I), although the terms are much smaller in magnitude and of opposite sign.⁷

In conclusion, it should be cautioned that the present calculation, which confirms the previous analysis of the internal rotation barrier in ethane, does not in any way require that the same essential elements be responsible for the barriers in all molecules; *e.g.*, for systems with lower symmetries, such as H₂O₂, other contributions may be important as well.

(7) The large electron-nuclear interaction contribution suggests that the barrier may be more sensitive to bond polarity in the optimized, than in the fixed, geometry model.⁶

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Book Reviews*

Atlas of Electronic Spectra of 5-Nitrofurans Compounds. By J. EIDUS, A. YA. EKMANE, K. K. VENTERS, and S. A. HILLER. Ann Arbor Science Publishers, Inc., distributed by International Scholarly Book Services, Inc., Portland Ore. 1970. xiii + 153 pp. \$12.00.

This is a translation of a book published in Latvia in 1958. The motivation for dealing with such a narrow group of substances is their importance in medical and veterinary practice. After a 44-page section dealing with general electronic absorption characteristics of furans, there follow in graphic form, supplemented by numerical values for the maxima and their intensities, the uv-visible spectra of 50 5-nitrofurans derivatives. Each spectrum is shown twice, once plotted with a linear and once with a logarithmic intensity scale. The references cited include many from difficultly accessible Russian sources.

Dictionnaire Chimique Anglais-Français. By R. CORNUBERT (Faculté des Sciences, Nancy). Dunod, Paris. 1970. xii + 217 pp. 48 F.

The usual chemical dictionaries available to the English-speaking chemist are those leading from French to English, and do not satisfy the occasionally felt need for the reverse. This paper-bound volume fills such a need.

Discovering Natural Laws: The Experimental Basis of Physics. By MILTON A. ROTHMAN (Trenton State College). Doubleday and Co., Inc., Garden City, N. Y. 1972. xii + 227 pp. \$1.45 (paper); \$5.95 (hardbound).

This is a book that falls outside the conventional curriculum, but it has something to give to the undergraduate and graduate student, the high school student, the layman, and the teacher. It takes up the universally accepted laws, such as the conservation laws, and presents the specific experimental foundations on which they are based. The author, who is both a teacher of physics and a writer of science fiction, writes easily and well, and his work can be enjoyed

by chemists and physicists of widely varying extents of scientific sophistication.

Environment and Society in Transition. Edited by P. ALBERTSON and M. BARNETT. New York Academy of Science, New York, N. Y. 1971. 699 pp. \$30.00.

This soft-bound book is Volume 184 of the Annals of the Academy and contains the proceedings of the International Joint Conference of the American Geographical Society and the American Division of the World Academy of Art and Science, held in 1970. It consists of a large number of papers by a distinguished and international group of specialists drawn from the general areas of space and earth science, biological and medical sciences, physical sciences and engineering, anthropology, sociology and psychology, and economics, political science and law. Chemistry is represented by "Recent Advances in Chemical Sciences" by Ernst Bergmann, and "The Chemical Sciences" by Minoru Tsutsui. The discussions and reports of various working groups, some general addresses, and a summary and conclusion to the conference complete the work, which has no index.

Isonitrile Chemistry. Edited by IVAR UGI (University of Southern California). Academic Press, New York, N. Y. 1971. xii + 278 pp. \$14.50.

Isoocyanides have had a long but thin history and were not generally regarded as important until the 1960's, when a new and more practical synthesis was developed by Ugi and his coworkers. It is now timely that a book on the subject should appear, and it is most appropriate that Dr. Ugi should be the editor.

The treatment in this book is quite comprehensive and includes not only the usual organic chemistry but also chapters on the structure of isocyanides, the isocyanide-nitrile rearrangement, and metal complexes having isocyanide ligands. The ten chapters are written by fifteen contributors, who are from Germany, Japan, and the United States. There are many long tables, and the coverage of the subjects is similar to that in "Organic Reactions" chapters in

* Unsigned book reviews are by the Book Review Editor.

most instances. The chapter on synthesis of isocyanides appropriately dwells heavily on the dehydration of formamides, but it is unfortunate that comparison with other methods is not adequate. A 12-page table lists all known isocyanides with yields and references, but unfortunately, the method of synthesis is not specified. For ethyl isocyanide, for example, seventeen references are given, which in fact report several different preparative routes, but the reader is not told to which method or reference the tabulated yield of 65% belongs.

The chapters are written from the literature published through 1968. A 22-page addendum presents developments in 1969 and a part of 1970, in abstract form. There are both author and subject indexes.

Science in Liberal Arts Colleges. By W. R. SNELLING and R. F. BORUCH. Columbia University Press, New York, N. Y. 1972. xvi + 285 pp. \$8.50.

This book reports the results of a study sponsored by the Research Corporation about the influences that affect a student's decision to major in the sciences. It speaks primarily to educators and counselors and is particularly timely in this period when the needs of society for chemists and physicists are being critically reexamined.

Problems in Structural Inorganic Chemistry. By WILLIAM E. HATFIELD (University of North Carolina) and RICHARD A. PALMER (Duke University). W. A. Benjamin, New York, N. Y. 1971. xi + 328 pp. \$15.00 (cloth); \$4.95 (paper).

This book is intended as supplemental material for beginning graduate courses as well as for a self-study guide. The areas covered, which are representative of modern inorganic chemistry, are Nomenclature, Elementary Structure and Stereochemistry, Atomic Structure, Molecular Symmetry and Group Theory, Chemical Bonding, Vibrational Spectroscopy, Electronic Spectroscopy, Magnetic Susceptibility, Magnetic Resonance, and Basic Crystallography. In addition to Physical Constants, the following extensive appendices are included: Character Tables, Rules for Evaluation of Direct Products in Symmetry Groups, Correlation Tables for Selected Point Groups, and Tanabe-Sugano Diagrams for d^2-d^8 .

The 262 problems are mainly quantitative in nature and range in difficulty from review type to rather complicated computational ones. Clear detailed solutions are presented for one-third of the problems; brief solutions or final answers are given for a second third; solutions are omitted for the remainder. Instead of extensive introductory material, texts, reference books, or research publications are cited as appropriate sources for review or self-study.

The authors are to be commended for putting together this book in so painstaking and careful a manner. The problems are generally excellent. They are stimulating and, in the best sense of the word, mind expanding. The authors' stated aims have been admirably achieved; I recommend it highly.

L. J. Boucher, *Carnegie-Mellon University*

Heat-Resistant Polymers (a translation of *Termoistoikie Polimery*). By V. V. KORSHAK (Institute of Hetero-Organic Compounds, Academy of Sciences of the USSR). Translated by J. SCHMORAK (Israel Program for Scientific Translations). International Scholarly Book Services, Inc., Portland, Ore. 1971. v + 435 pp. \$28.00.

This is a very useful monograph reviewing both the syntheses and properties of heat-resistant polymers. Originally published in Russian in 1969, the emphasis is on the relationship between the properties of a polymer and its structure. There is a brief introductory chapter on heat resistance and thermal resistance of polymers (differentiated by changes in mechanical strength and chemical changes in structure, respectively) and methods for their determination. This is followed by chapters surveying the main classes of polymers which are of interest as thermoresistant materials: carbon-chain polymers, heterochain polymers, heterocyclic polymers (the longest chapter), and element-organic (containing boron, silicon, phosphorus, and metals) and purely inorganic polymers. The presentation and depth are very much in the style of *Russian Chemical Reviews*. The subject index is comprehensive and there are separate author indexes for Russian and non-Russian authors.

As to be expected in a translated work, the literature gap problem is intensified. The non-Russian work is reviewed into about 1966 and the Russian work into 1968. Also, the indexes give page references to the original Russian text which, in the translation, appear as marginal text notations. These often are out of sequence, but specific material is relatively easy to find because of the extensive use of structures, graphs, and tabular summaries.

This monograph can be recommended as a comprehensive introduction and review of the subject matter (despite the absence of literature coverage for the past five years) and as a convenient summary of work which has appeared in the less accessible Russian patent and journal literature.

Daniel T. Longone, *The University of Michigan*

Disposal of Sewage and Other Waterborne Wastes. By KARL IMHOFF, W. J. MULLER, and D. K. B. THISTLETHWAYTE. Ann Arbor Science Publishers, Inc., Ann Arbor, Mich. 1971. x + 405 pp. \$16.80.

This is the second edition of a textbook in English inspired by Dr. Karl Imhoff's "Taschenbuch der Stadtentwaesserung," which has appeared in 22 editions since he first published it in 1906. Its especial significance is that it takes cognizance of the need for a well-rounded practical reference book for men having a wide variety of backgrounds and varied degrees of responsibility for the disposal of waste water. The authors have recognized also that there is a difference in the techniques applicable to different situations in different countries or regions. To make the book complete in its coverage, the first section is devoted to a summary of the amounts, variations, and composition of domestic sewage and industrial wastes. What the analyst measures in waste water and the importance of each constituent measured are explained in clear language. The major portion of the book, however, is devoted to the subject of waste-water disposal in natural or engineered systems. In a series of well-balanced chapters, arranged essentially in the same sequence as are the processes applied to a waste water, the reader is acquainted with how each process functions and what it accomplishes. In every case, specific numerical values are reported for loading rates, percentage removals, and other factors important in design or in evaluating the efficiency of a treatment process. These values are then applied in specific examples which illustrate design or evaluating techniques. The material is presented by the authors in simple understandable language which summarizes clearly the state of the art of waste-water disposal. It should, as the authors intended, serve the needs of a great variety of technical and engineering personnel for a book which is at the same time both a textbook and a practical reference work.

P. H. McGauhey, *Sanitary Engineering Research Laboratory, University of California*

Handbook of Naturally Occurring Compounds. Volume II. Terpenes. T. K. DEVON (Pfizer Medical Research Laboratories, Groton, Conn.) and A. I. SCOTT (Sterling Chemistry Laboratory, Yale University, New Haven, Conn.). Academic Press, Inc., New York, N. Y. xi + 576 pp. 28.5 × 22 cm. \$21.00.

Natural products chemists keeping up with the literature, or beginning research in an area new to them, face a formidable challenge in the 1970's. So many new compounds are being studied, and the work is published in so many journals round the world, that there is an urgent need for up-to-date, reliable compendia giving useful entries into the literature. This book fills this need admirably for terpenoids. It lists most of the naturally occurring terpenoids to which structures have been assigned. The name, molecular formula, structural formula, molecular weight, optical rotation, melting point, and literature entry reference (some from 1971) are provided for each compound. A compound may be found from a name index, a formula index, and classification numbers based upon skeletal types. The biogenetic relationships between skeletal types are indicated by charts. The book is easy to use, and in addition is a pleasure to browse through, like a good dictionary.

This book will be outstandingly useful to all chemists working with terpenes. Its modest price and the prospect of regular updating enhance its appeal.

P. W. Le Quesne, *University of Michigan*