the three properties in some of the other cases.

Notice that we have avoided constructing a "configurational isomerism" relation in this paper. This strategy avoids confusion that can arise from application of the reflexive property. It is not clear whether it makes sense to say that a molecule is "configurationally isomeric" to itself.

Groups and Subgroups. A group is a set with binary operation (here symbolized by juxtaposition) and identity element I that has the following four properties:

(1) AB is in the set for any A and B in the set (closure).

(2) $(AB)C = A(BC)$ for any A, B, and C in the set (associative law).

(3) $AI = IA = A$ for any A in the set (identity rule).

(4) There is, for any A in the set, an element A^{-1} in the such that $A^{-1}A = AA^{-1} = I$ (inverse rule).

A subgroup of a group is a subset of the group which is still a group under the bigger group's binary operation.

Most of the computational trickery in this paper involves operations with inverses and the identity. The rearrangement and skeletal symmetry groups for a CCCM are subgroups of the group of all permutation matrices (of the size of the CCCM), and they therefore contain the identity matrix **I**. This matrix, with ones down the main diagonal and zeros elsewhere, shows up in various places. The matrix **I** can be inserted freely into a congruence or equation. Notice that by definition $\mathbf{I} = \mathbf{I}^{-1}$. A proof often depends on the judicious insertion of the identity matrix **I** in the form $(\mathbf{A}^{-1}\mathbf{A})$ or $(\mathbf{U}^{-1}\mathbf{U})$, for instance.

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ACS Committee on Nomenclature: Annual Report for 1985

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Nomenclature committees, both national and international, were very active in 1985, resulting in substantial progress in many different fields. A summary of the more important meetings and accomplishments follows.

The *ACS Committee on Nomenclature* held its annual meeting at CAS in November.† Progress of the work of the divisional committees and international commissions was reviewed. The format for the periodic table recommended by the Committee in 1983 and proposed by the IUPAC Commission on Nomenclature of Inorganic Chemistry with very minor modifications is finding acceptance throughout the world, although some objections are still being voiced. Improved communication with high school chemistry teachers is being developed with A. Saturnelli of the Bureau of Science Education of the New York State Education Department. Editors of ACS journals continue as ex officio members of the Committee. To establish closer contact with interested individual ACS members, the Committee held two successful open meetings in Miami Beach and Chicago and plans to continue to hold open meetings regularly on Mondays from 2 to 4 p.m. at the national meetings. Closer liaison with other ACS bodies such as the Committees on Education and Science as well as various Divisions continues to be of concern. Cooperation with nomenclature groups in disciplines related to chemistry continues to be pursued. Contact has been established with the ASTM Committee on Medical Terminology. Efforts to contact appropriate groups in physics and pharmacology are in progress. The promotion of and input into International Union of Pure and Applied Chemistry (IUPAC) recommendations is, as always, a primary objective of the Committee. In the view of the Committee, the nomenclature of biotechnology requires urgent attention. Since this is an interdisciplinary subject, a subcommittee was formed to study the topic and to explore the best way to proceed. The Subcommittee on Chemical Pronunciation continues to be active.

The *IUPAC Interdivisional Committee on Nomenclature and Symbols* (IDCNS) continued to function effectively this year. It held its annual meeting in Lyon, France, in August. In addition to the IUPAC publications listed in the Appendix, specific documents in process and thus not yet recorded in this

† Abbreviations used, not identified in the text, are ACS, American Chemical Society; CAS, Chemical Abstracts Service; JCBN, Joint Commission on Biochemical Nomenclature; and NC-IUB, Nomenclature Committee of International Union of Biochemistry.

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Appendix deal with the following topics: description of carbon as a solid, data on adsorption from solution at the solid/solution interface, interphases in systems of conducting phases, infrared reference spectra of molecules in the vapor phase, etc. Several chapters of the revised Red Book from the Commission on Nomenclature of Inorganic Chemistry are also undergoing the review procedure. The IUPAC document on copolymer nomenclature is the first to have gone through the revised IUPAC publication procedure and has now appeared in *Pure and Applied Chemistry* (see Appendix). Other documents are being processed. Work on the Compendium of IUPAC Terminology is continuing, although slowed by the untimely death of V. Gold.

The *IUPAC Commission on the Nomenclature of Inorganic Chemistry* met in August in Lyon, France. Four chapters for the revised Red Book, Aims, Functions and Methods of Nomenclature; Elements, Atoms and Group of Atoms; Formulae; Ions, Radicals and Salts, and a document on polyanions have been completed and are going through the IUPAC publication review procedure. Six chapters have been approved by the Commission: Grammar, Names Based on Stoichiometry, Solids, Neutral Molecular Compounds, Oxo Acids, and Coordination Compounds. Work on the nomenclature for boron compounds is still in progress. The Commission reaffirmed its position on the periodic table and on the systematic names of the elements of atomic numbers greater than 100. Other topics under study are rings and chains, organometallic compounds, advanced stereochemical topics, metal clusters, and abbreviations.

The *IUPAC Organic Nomenclature Commission* met in Lyon, France, in August. The Commission continued its study of the reorganization and revision of the present edition of the IUPAC organic rules, its evaluation of expanded documentation in specific subject areas, and development of new techniques for longer range consideration. In connection with the latter, projects dealing with nomenclature for delocalized ions and radicals, oxo acids, and nodal numbering are continuing to develop. Recommendations for generating numerical prefixes beyond 200, published as provisional rules in 1983, were fully approved. A convention of describing rings and ring systems with cumulative double bonds was approved for circulation as provisional recommendations for public comment. Comprehensive documentation on classical ions and radicals, natural products, and fusion nomenclature is well advanced. A glossary of class names and terms has been compiled. In addition, projects on revision of Section E (Stereochemistry), indicated hydrogen, and numbering priorities are under study.

The *IUPAC Macromolecular Nomenclature Commission* met in Lyon, France, in August. The Commission completed its work on the nomenclature of crystalline polymers and on polymerizations involving chiral monomers or resulting in optically active polymers. The Commission is continuing its work on (a) polymers in dilute solutions, (b) polymers in the bulk, (c) subsidiary definitions of terms relating to polymers, and (d) interpenetrating polymer networks. The latter topic is also being actively worked on by the ACS Nomenclature Committee. The Commission is working on the compilation of all of its recommendations into book form. Recommendations on nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers and on source-based nomenclature for copolymers have been published (see Appendix).

In *biochemical nomenclature* both JCBN and NC-IUB met jointly in Utrecht, The Netherlands, in May. A new edition of the book *Enzyme Nomenclature* was published (see Appendix). Recommendations for naming incompletely specified bases in nucleic acid sequences were published in 1985 (see Appendix). Documents dealing with the nomenclature of glycoproteins, folic acid, and prenols have been completed. A new 4th edition of the compendium *Biochemical Nomenclature and Related Documents* is being assembled. A substantial revision of the 1971 edition of the steroid rules is expected to be ready for approval in 1986. Work continues on preparation of recommendations for the nomenclature of tetrapyrroles, prostaglandins, carbohydrates, neurotransmitters, leukotrienes, and other biochemical specialties. Revisions of the lipid and terpene rules are planned.

At the *ACS Divisional level*, ten divisions are represented on the ACS Nomenclature Committee. These are the Division of Analytical Chemistry, Division of Carbohydrate Chemistry, Division of Chemical Information, Division of Fluorine Chemistry, Division of Inorganic Chemistry, Division of Medicinal Chemistry, Division of Nuclear Chemistry and Technology, Division of Organic Chemistry, Division of Physical Chemistry, and Division of Polymer Chemistry. Nomenclature activities within these divisions varied widely.

The Chairman of the Committee is the CAS Director of Nomenclature and, through these combined offices, maintains close liaison between ACS nomenclature committees, CAS, and other organizations. During 1985, cooperation with outside organizations continued to be substantial. In the area of drug names, we again have made a considerable contribution to the USAN (U.S. Adopted Names) program of the American Medical Association and the INN (International Nonproprietary Names) program of the World Health Organization. In addition, we advise on drug nomenclature relating to the U.S. Pharmacopeia. Similar contributions in the area of pesticide names are being made to the programs of the American National Standards Institute and the International Standards Organization. We now cooperate or provide services in the nomenclature field to the following organizations:

American Chemical Society
American Institute of Nutrition
American Medical Association
American National Standards Institute
American Pharmaceutical Association
American Society of Hospital Pharmacists
British Crop Protection Council
British Pharmacopeia
British Veterinary Codex Committee
Canada Department of Agriculture
Canadian Standards Association
Drug Enforcement Association
Food and Agricultural Organization
Food and Drug Administration
International Agency for Research on Cancer
International Standards Organization
International Union of Biochemistry
International Union of Crystallography
International Union of Nutritional Sciences
International Union of Pure and Applied Chemistry
National Cancer Institute
National Institutes of Health
National Library of Medicine
National Research Council
U.S. Department of Agriculture
U.S. Department of the Army
U.S. Fish and Wildlife Service
U.S. Pharmacopeia
World Health Organization

In addition, correspondence with individual authors and editors was processed regularly. CAS continues to be the headquarters for the distribution of nomenclature pamphlets and other nomenclature information.

APPENDIX: OFFICIAL NOMENCLATURE PUBLICATIONS, 1985

IUPAC

Analytical Chemistry Division: Commission Analytical Nomenclature and International Confederation for Thermal Analysis, Nomenclature Committee. "Nomenclature for Thermal Analysis, IV", Recommendations 1985. *Pure Appl. Chem.* **1985**, *57*(11), 1737–1740.

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Analytical Chemistry Division: Commission on Spectrochemical and Other Optical Procedures for Analysis. "Nomenclature, Symbols, Units and Their Usage in Spectrochemical Analysis. V. Radiation Sources", Recommendations 1985. *Pure Appl. Chem.* **1985**, *57*(10), 1453–1490.

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Physical Chemistry Division: Commission on Molecular Structure and Spectroscopy. Clinical Chemistry Division: Commission on Quantities and Units. "Names, Symbols, Definitions and Units of Quantities in Optical Spectroscopy", Recommendations 1984. *Pure Appl. Chem.* **1985**, *57*(1), 105–120.

IUPAC–IUB

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IUB

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Jeannin, Yves; Holden, Norman E. "The Nomenclature of the Heavy Elements". *Nature (London)* **1985**, *313*, 744.

BOOK REVIEWS

A Handbook of Computational Chemistry. By Tim Clark (Universität Erlangen-Nürnberg). Wiley, New York, 1985. x + 332 pp. $35.00.

This book is subtitled *A Practical Guide to Chemical Structure and Energy Calculations*, and this is an accurate statement of what Dr. Clark has achieved in this excellently organized and clearly written work. Any chemist wishing to carry out and interpret calculations using standard programs of the molecular mechanics, semiempirical MO, or ab initio varieties will find this to be an extremely practical guide indeed. Although aimed at chemists who have no special theoretical background (beyond some familiarity with point-group symmetry notation), many of the experienced community will also find this book to be an asset.

A brief introductory chapter orients the reader with respect to the advantages, capabilities, and costs of computational chemistry as well as to some of the computer-specific questions of program language, compatibility with computer type, and program availability. Included is a table listing the currently available program packages of the types described in later chapters, sources of supply, computers they run on, and comments about some of their special features.

Chapter 2 (80 pp), "Molecular Mechanics", begins with an introduction to the physical model underlying the MM1 and MM2 programs of Allinger and the EAS program of Engler, Andose, and Schleyer. The techniques of geometry optimization and calculation of strain energy are included. A brief but effective discussion of the parametrization of such programs is followed by detailed instructions on setting up the input data for the MMP2 program, with cycloheptane as an example. A thorough and very reader-friendly job is done with this. (Clark intends the reader to read this book in sequence, and he does a careful job as he introduces each new idea.) Once the input is explained and displayed, we are shown a complete listing of the output and "walked through" it in detail. Next, we are shown how to modify the input to put a methyl group onto cyclohexane, again with display of input and output. Following this comes an example of a conjugated system, 1,3-cycloheptadiene, enabling Clark to explain how a quantum chemical calculation is interfaced with the force field model in MMP2. Treatments of norcaradiene, 1,3,5-cycloheptatriene, and *tert*-butyl cation finish up this chapter.

Chapter 3 (46 pp), "Molecular Orbital Theory", is an attempt to set out the terminology and ideas that are unavoidable in subsequent discussions of LCAO–MO–SCF calculations. This is done well. Clark has picked his points and examples wisely from this enormous subject, taking just enough to provide a basis for later chapters. A reader who has had 3 years of university chemistry could cope with this chapter. (The potential reader should note that the discussion of MO coefficient *values* on pp 93–95 is correct only if overlap is assumed to be zero.) This chapter establishes the connection between an MO's pictorial nature and the numbers that will come out of a computer. It also treats the problems of self-consistent field calculations, unpaired electrons, spin contamination, group orbitals, and the perturbational viewpoint of qualitative molecular orbital theory. Embedded in this chapter is a long section dealing with computational niceties: How are such programs organized? What is a Z-matrix, and how do we program it in? How do we utilize symmetry when ordering a program to optimize a molecule's geometry? How do we find special points on a potential surface? This is all illustrated carefully with examples.

Chapter 4 (92 pp), "Semiempirical Methods", concerns itself with MINDO/3 and MNDO programs and illustrates input and output with the MOPAC package purveyed by QCPE. Care is taken to alert the reader to the subtleties of choosing the right method for a given problem. This is done both by explicit discussion and by reference to the literature. Several examples of input and output are given detailed treatment: CH_2 singlet and triplet (UHF and half-electron), MNDO; ethylene and diborane with localization of MOs, MNDO. There is a commendable discussion of some of the ways such calculations can go wrong, and ways of recognizing and correcting such problems. The chapter ends with a 44-page bibliography of MINDO/3 or MNDO calculations reported in the literature through Volume 98 of *Chemical Abstracts*.

The fifth and final chapter (84 pp), "*Ab Initio* Methods", is essentially a primer in the use and interpretation of GAUSSIAN 82. It starts with a description of primitive Gaussians, split shells and polarization functions—the paraphernalia peculiar to such high-level calculations. Clark does not lose his touch here. He picks out the essentials and describes them from a physical and pictorial vantage that will appeal to the uninitiated reader. Examples continue to be used to good effect. We see CH_2 singlet and triplet states contrasted again, with the singlet done both as an open-shell and as a closed-shell system. We also see a "correlated" triplet methylene example, done at the Moeller-Plesset second-order (MP2) level. The treatment of this ab initio method is impressive and quite current.

This book meets a real need in a uniformly competent and efficient manner. It will be seen on many desktops (as opposed to bookshelves) in the next decade.

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