present study, which focuses on the current literature.
(4) Zass, E.; Mueller, S. *Chimia* **1986**, *40*, 38-50.
(5) REACCS gives access to two other reaction data bases, derived from Theilheimer's *Synthetic Methods of Organic Chemistry* and *Organic Synthesis*, respectively, not included in the present study, which focuses on the current literature.
(6) Larson, E. R.; Danishefsky, S. *J. Am. Chem. Soc.* **1983**, *105*, 6715.
(7) Tal, D. M.; Frisch, G. D.; Elliott, W. H. *Tetrahedron* **1984**, *40*, 851.

ACS Committee on Nomenclature: Annual Report for 1987

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Nomenclature committees, both national and international, were very active in 1987, resulting in substantial progress in many different fields. A summary of the more important meetings and accomplishments follows.

The ACS Committee on Nomenclature continues to be active. Editors of ACS journals are ex officio members of the Committee. The Committee held its annual meeting at Chemical Abstracts Service (CAS) in November. The Committee continues its efforts to communicate with the ACS membership as well as all other groups who have an interest in chemical nomenclature. As part of this effort, open meetings were held again at the ACS National Meetings in Denver and New Orleans, and the Committee continues to look into simultaneous divisional nomenclature programming at a future national meeting. Good communication with high school chemistry teachers is being maintained through A. Saturnelli and the Bureau of Science Education of the New York State Education Department. Cooperation with the American Society for Testing Materials (ASTM) Committee on Medical Terminology has been established on an ongoing basis. Close liaison with other ACS bodies such as the Committees on Education and Science as well as various Divisions is being pursued. The promotion of and input into International Union of Pure and Applied Chemistry (IUPAC) recommendations is, as always, a primary objective of the Committee. A subcommittee is investigating problems relating to the nomenclature of biotechnology by focusing on the nomenclature of altered proteins. The subcommittee on Chemical Pronunciation continues to be active. The Chairman made an oral report on the activities of the Committee to the ACS Board of Directors at its December meeting.

The IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS) continued to function effectively this year. It held its annual meeting in Boston in August. In addition to the IUPAC publications listed in the Appendix, specific documents in process and thus not yet recorded in this Appendix deal with the following topics: steroids; mass spectroscopy; X-ray spectroscopy; representation and symbolism of reaction mechanisms; and organic chemical transformations. The final chapters of the revised Red Book from the Commission on Nomenclature of Inorganic Chemistry have undergone the review procedure. The *Compendium of IUPAC Terminology* has been published, and work on an expanded second edition has been initiated. Publication is expected in 1988. The final manuscript of the revised manual "Quantities, Units, and Symbols in Physical Chemistry" has been completed, and its publication is imminent. Kurt Loening's chairmanship of IDCNS terminated in 1987 at the Boston meeting. The new chairman is Professor N. Sheppard of the U.K.

The IUPAC Commission on the Nomenclature of Inorganic Chemistry met in August in Boston. All 11 chapters of the revised Red Book have been completed and approved and are receiving final editing. A document on rings and chains has been sent to referees, and recommendations on polyanions have been published (see Appendix). The Commission again 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 organometallic compounds, advanced stereochemical topics, metal clusters, and abbreviations.

The IUPAC Organic Nomenclature Commission met in Boston in August. The Commission continued its study of the reorganization and revision of the present edition of the IUPAC organic rules and the development of new techniques for longer range consideration. In connection with the latter, projects dealing with nomenclature for cyclophanes, oxo acids, and nodal numbering are continuing to develop. Recommendations for generating numerical prefixes beyond 200 have been published (see Appendix). A convention for describing rings and ring systems with cumulative double bonds was approved for publication. 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 Commission on Macromolecular Nomenclature met in Boston in August. The Commission completed its work on a report offering about 75 definitions of terms dealing with crystalline polymers, agreed on a revision of the report on stereochemistry, and appointed a working party to coordinate the publication of the *Compendium on Macromolecular Nomenclature*. The Commission discussed and made progress on documents dealing with (a) the classification of polymerization reactions (mechanism and stoichiometry), (b) the nomenclature of cross-linked and nonlinear (branched, star, etc.) polymers and of polymer networks, (c) the structure-based nomenclature of irregular polymers, (d) the conventions for structural formulas of polymers, (e) the terminology for static and dynamic mechanical properties of polymers in bulk state, and (f) the nomenclautre of ladder polymers. Work was initiated on the document dealing with the terminology of liquid crystals. In 1987, recommendations on the use of abbreviations were published (see Appendix), and two reports on classification of polymers and on solutions were completed and submitted for publication.

In biochemical nomenclature both the Joint Commission on Biochemical Nomenclature (JCBN) and the Nomenclature Committee of the International Union of Biochemistry (NC-IUB) met jointly in Szeged, Hungary, in May. Recommendations dealing with the nomenclature of folic acid, prenols, and tetrapyrroles have been published (see Appendix).

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A new fourth edition of the compendium *Biochemical Nomenclature and Related Documents* should be published in the very near future. Work on a substantial revision of the 1971 edition of the steroid rules has been completed, and the recommendations are going through the review procedure. Work continues on preparation of recommendations for the nomenclature of prostaglandins, carbohydrates, neurotransmitters, leukotrienes, and other biochemical specialties. Revisions of the lipid and terpene rules are planned.

At the ACS Division level, 10 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 1987 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 Committee on Polycyclic Aromatic Compounds
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
United Nations Division of Narcotic Drugs
U.S. Department of Agriculture
U.S. Department of the Army
U.S. Fish and Wildlife Service
U.S. Pharmacopeia
World Health Organization

Public awareness and understanding of the importance and the role of chemical nomenclature in science communications was actively promoted by various members of the Committee by means of individual presentations, publications, refereeing, and advisory activities. 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: NOMENCLATURE PUBLICATIONS, 1987

IUPAC

Compendium of Chemical Terminology, IUPAC Recommendations. Victor Gold, Kurt L. Loening, Alan D. McNaught, Pamil Sehmi, Compilers; Blackwell: Oxford, U.K., 1987; 456 pp.

Applied Chemistry Division: Commission on Water Quality; International Association on Water Pollutions Research & Control (IAWPRC), Working Group. "Notations for Use in the Description of Wastewater Treatment Processes". *Water Res.* **1987**, *21*(2), 135–139.

Clinical Chemistry Division: Commission on Quantities and Units; International Federation of Clinical Chemistry, Scientific Committee, Analytical Section, Expert Panel on Quantities and Units. "Quantities and Units in Clinical Chemistry: Nebulizer and Flame Properties in Flame Emission and Absorption Spectrometry", Recommendations 1986. *Pure Appl. Chem.* **1986**, *58*, 1737–1742.

Inorganic Chemistry Division: Commission on Atomic Weights and Isotopic Abundances. "Atomic Weights of the Elements 1985". *Pure Appl. Chem.* **1986**, *58*, 1677–1692.

Inorganic Chemistry Division: Commission on Nomenclature of Inorganic Chemistry. "Nomenclature of Polyanions". *Pure Appl. Chem.* **1987**, *59*, 1529–1548.

Macromolecular Division: Commission on Macromolecular Nomenclature. "Use of Abbreviations for Names of Polymeric Substances", Recommendations 1986. *Pure Appl. Chem.* **1987**, *59*, 691–693.

Organic Chemistry Division: Commission on Nomenclature of Organic Chemistry. "Extension of Rules A-1.1 and A-2.5 Concerning Numerical Terms Used in Organic Chemical Nomenclature", Recommendations 1986. *Pure Appl. Chem.* **1986**, *58*, 1693–1696.

Physical Chemistry Division: Commission on Molecular Structure and Spectroscopy. "A Descriptive Classification of the Electron Spectroscopies", Recommendations 1987. *Pure Appl. Chem.* **1987**, *59*, 1343–1406.

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. *Spectrochim. Acta, Part A* **1987**, *43A*, 1–9.

Physical Chemistry Division: Commission on Molecular Structure and Spectroscopy; Clinical Chemistry Division. Commission on Quantities and Units; International Federation of Clinical Chemistry (IFCC). Scientific Committee, Analytical Section, Expert Panel on Quantities and Units. "Names, Symbols, Definitions and Units of Quantities in Optical Spectroscopy", Approved Recommendation 1985. *J. Clin. Chem. Clin. Biochem.* **1987**, *25*, 327–336.

Physical Chemistry Division: Commission on Molecular Structure and Spectroscopy; Coblentz Society Spectral Evaluation Committee, Vapor Phase Subcommittee. "Specifications for Infrared Reference Spectra of Molecules in the Vapor Phase", Recommendations 1987. *Pure Appl. Chem.* **1987**, *59*, 673–681.

Physical Chemistry Division: Commission on Physicochemical Symbols, Terminology and Units. "Abbreviated List of Quantities, Units and Symbols in Physical Chemistry"; Blackwell: Oxford, U.K., 1987; A4 four sides, thick laminated card.

IUPAC–IUB

Joint Commission on Biochemical Nomenclature. "Nomenclature and Symbols for Folic Acid and Related Compounds", Recommendations 1986. *Eur. J. Biochem.* **1987**, *168*, 251–253. *Pure Appl. Chem.* **1987**, *59*, 833–836.

Joint Commission on Biochemical Nomenclature. "Nomenclature of Glycoproteins, Glycopeptides and Peptidoglycans", Recommendations 1985. *J. Biol. Chem.* **1987**, *262*, 13–18.

Joint Commission on Biochemical Nomenclature. "Nomenclature of Prenols", Recommendations 1986. *Eur. J. Biochem.* **1987**, *167*, 181–184. *Pure Appl. Chem.* **1987**, *59*, 683–689.

Joint Commission on Biochemical Nomenclature. "Nomenclature of Tetrapyrroles", Recommendations 1986. *Pure Appl. Chem.* **1987**, *59*, 779–832.

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REACCS in the Chemical Development Environment. 1

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A number of database management systems suitable for the storage of chemical reaction information are currently available. Criteria used at McNeil Pharmaceutical for the selection of a graphics-based database management system for the storage of proprietary information are presented. Applications for the software are discussed.

INTRODUCTION

Information retrieval is a major problem facing the chemical industry. During the time from when a reaction is first attempted to when it is scaled-up for production, many chemists in various departments may have worked on the project. To prevent duplication of expensive experimental work, an efficient method for the storage and retrieval of data is critical.

For example, at McNeil Pharmaceutical, process work on Tolectin (tolmetin sodium) over the past 20 years has produced many volumes of information in the form of Chemical Research Reports, monthly reports, and notebook experimentals. It became obvious during work on this and other projects that data storage and retrieval for formal written reports was satisfactory. However, these reports normally contained only positive results. They frequently excluded experiments that did not give the desired product, or they only briefly summarized such experiments. In addition, these reports did not typically include all reaction variations representing changes in solvents, catalysts, reaction times, and/or reaction temperatures. Consequently, much of the information contained in research notebooks was not readily accessible. In fact, one could access most of this information only with great difficulty. Rather than spending the time necessary to retrieve the original data, chemists repeated experiments. Obviously, some method was necessary to allow for the storage and rapid retrieval of all chemical reaction data generated by Chemical Development and Chemical Research.

Representatives from the Chemical Development and Medicinal Chemistry departments met on several occasions to clearly define the needs for chemical database software at McNeil and to determine how those needs could be met.[1] The various storage systems that they considered were System

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