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Annual Report of the ACS Committee on Nomenclature for 1976

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Nomenclature committees, both national and international, were very active in 1976, resulting in substantial progress in many different fields. The ten more important meetings and accomplishments are summarized.

1. 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. In addition, some decisions regarding the spelling of names of parent hydrides and their radicals were taken. Also, ways of working more closely with ACS Divisions, journal editors and authors, editors of handbooks, as well as general means of promoting good nomenclature were explored. Interest in reviving work on pronunciation of chemical words was expressed. "Notes on Nomenclature", a nomenclature column by Fernelius, Loening, and Adams, started at the instigation of this committee, continues to appear in the *Journal of Chemical Education* (four publications this year; see Appendix II) and to be very well received.

2. K. L. Loening was appointed in the summer as the new chairman of the IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS). The reorganized Committee held its first meeting in Oxford, England, in September. An inventory of all IUPAC activities dealing with nomenclature and/or symbols was compiled, and progress of specific projects was reported. A classification scheme for all nomenclature and symbols documents, indicating the various stages of development, was recommended. Specific documents dealing with quantities in clinical chemistry, definitions, terminology and symbols for rheological properties of colloidal systems and surfaces, and initialed abbreviations in the chemical literature were reviewed. General problems dealing with administrative matters and dissemination of IUPAC recommendations were examined at length.

3. The IUPAC Inorganic Nomenclature Commission met in September in Paris, France. Topics under discussion included names for elements beyond 105, ions and radicals, boron compounds, inorganic hydrides, cluster compounds, ligand locants, sulfur compounds, chains and rings, inorganic polymers, and stereochemical designations for coordination compounds. Two documents, "How to Name an Inorganic Compound" and "Names for Ions and Radicals" (Expanded Table II of the Red Book), have been submitted for publication.

4. The IUPAC Organic Nomenclature Commission met in September in Deauville, France. It concentrated its efforts on two main topics: (1) Section G, a structure-based systematic substitutive nomenclature (formerly revision of Sections A, B, C, and D; this is the project in which Joy Merritt of the CAS Nomenclature Division is carrying out the detailed work under the supervision of Drs. Grünewald, Cross, Powell, and Loening); and (2) Section H, nomenclature for isotopically modified compounds. Work on Section G is on schedule, to be completed in 1977. Work on Section H has been completed and the document should be in print in 1977. Some progress has also been made on nodal nomenclature, a general new nomenclature system.

5. The IUPAC Macromolecular Nomenclature Commission met in June in Dorking, England. Work on the updated version of "Nomenclature of Regular Single-Strand Organic Polymers" has been completed and the document has been submitted for publication in *Pure and Applied Chemistry*. The Commission is continuing its work on (1) stereochemical definitions and notations for macromolecules, (b) nomenclature and symbolism of copolymers, (c) subsidiary definitions of terms relating to polymers, (d) definitions for physical properties of polymers, (e) definition and nomenclature of ladder polymers, (f) nomenclature of inorganic polymers, (g) classification and family names of polymers, and (h) interpenetrating polymer networks. Of these items, (a) and (b) are at the most advanced stage with tentative recommendations expected to be issued in 1977.

6. The IUPAC-IUB Commission on Biochemical Nomenclature (CBN) met in New York in the spring. As usual, the Commission has issued a number of nomenclature recommendations in 1976 (see Appendix I). Work is progressing in the area of enzymes, tetrapyrroles, carbohydrates, biochemical phosphorus compounds, lipids, prostaglandins, and other special fields.

7. A joint IUNS-CBN meeting on vitamin nomenclature was held in May in Rochester, N.Y., under the chairmanship of K. L. Loening. Differences in nomenclature practices regarding vitamins, especially tocopherols, of chemists, biochemists, and nutritionists were largely resolved.

8. The IUPAC Interdivisional Committee on Machine Documentation in the Chemical Field held its annual meeting in Lenzerheide, Switzerland, and voted to dissolve itself.

9. All ACS Divisional nomenclature committees were active in 1976 to varying degrees. These are the ones of the Division

of Analytical Chemistry, Division of Carbohydrate Chemistry, Division of Fluorine Chemistry, Division of Inorganic Chemistry, Division of Organic Chemistry, Division of Physical Chemistry, and Division of Polymer Chemistry.

10. The Office of Biochemical Nomenclature of NRC functioned effectively in 1976. Close liaison between it and the Nomenclature Division of CAS is being maintained.

The Chairman of the Committee is CAS Director of Nomenclature and, through these combined offices, maintains close liaison between ACS nomenclature committees, CAS, and other organizations. During 1976 cooperation with outside organizations continued to be substantial. In the area of drug and pesticide names considerable contributions were made 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, 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 Veterinary Codex Committee
Canada Department of Agriculture
Canadian Standards Association
Drug Enforcement Association
Food and Agricultural Organization
Food and Drug Administration
International Standards Organization
International Union of Biochemistry
International Union of Nutritional Sciences
International Union of Pure and Applied Chemistry
National Cancer Institute
National Library of Medicine
National Research Council
U.S. Department of Agriculture
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 I. OFFICIAL NOMENCLATURE PUBLICATIONS 1976

IUPAC

1. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Rules for the nomenclature of organic chemistry. Section E: stereochemistry" (Recommendations 1974).
   Pure Appl. Chem. **1976**, 45(1), 11–30.
2. Organic Chemistry Division. Commission on Nomenclature of Organic Chemistry, "Nomenclature of organic chemistry: Section F—natural products and related compounds".
   IUPAC Inf. Bull., Append. Provis. Nomencl., No. 53, Dec 1976, 22 pp.
3. Physical Chemistry Division. Commission on Electrochemistry, "Manual of symbols and terminology for physicochemical quantities and units. Appendix III. Electrochemical nomenclature" (Recommendations approved 1973).
   Elektrokhimiya **1975**, 11(12), 1780–93.
4. Physical Chemistry Division. Commission on Colloid and Surface Chemistry, "Manual of symbols and terminology for physicochemical quantities and units. Appendix II. Definitions, terminology and symbols in colloid and surface chemistry. Part II. Heterogeneous catalysis" (Rules approved 1975).
   Pure Appl. Chem. **1976**, 46(1), 71–90.
5. Physical Chemistry Division. Commission on Colloid and Surface Chemistry, "Selected definitions, terminology, and symbols for rheological properties".
   IUPAC Inf. Bull., Append. Provis. Nomencl., No. 57, Dec 1976, 8 pp.
6. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Definition and symbolism of molecular force constants".
   IUPAC Inf. Bull., Append. Provis. Nomencl., No. 56, Dec 1976, 12 pp.
7. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Nomenclature and use of symbols in mass spectrometry" (Recommendations 1976).
   Analusis **1976**, 4(8), 378–82.
8. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Nomenclature and conventions for reporting Mössbauer spectroscopic data" (Recommendations 1975).
   Pure Appl. Chem. **1976**, 45(3–4), 211–16.
9. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Presentation of NMR data for publication in chemical journals. B. Conventions relating to spectra from nuclei other than protons" (Recommendations 1975).
   Pure Appl. Chem. **1976**, 45(3–4), 217–19.
10. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Nomenclature and spectral presentation in electron spectroscopy resulting from excitation by photons" (Recommendations 1975).
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11. Physical Chemistry Division. Commission I.1 on Physicochemical Symbols, Terminology and Units, "Expression of results in quantum chemistry".
    IUPAC Inf. Bull., Append. Provis. Nomencl., No. 49, Sept 1976, 5 pp.
12. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Recommendations for the presentation of infrared absorption spectra in data collections".
    IUPAC Inf. Bull., Append. Provis. Nomencl., No. 50, Sept 1976, 8 pp.
13. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy, "Symbolism and nomenclature for mass spectroscopy".
    IUPAC Inf. Bull., Append. Provis. Nomencl., No. 51, Sept 1976, 10 pp.
14. Physical Chemistry Division. Commission I.6 on Colloid and Surface Chemistry, "Reporting experimental data dealing with critical micellization concentrations (cmc's)".
    IUPAC Inf. Bull., Append. Provis. Nomencl., No. 52, Sept 1976, 8 pp.
15. Inorganic Chemistry Division. Commission on Atomic Weights in Consultation with Committee on Teaching of Chemistry. "Table of atomic weights to four significant figures".
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    J. Chin. Chem. Soc. (Taipei) **1976**, 23(1), Al.
    Kem. Tidskr. **1976**, 88(7–8), 52 (Swed.).
16. Inorganic Chemistry Division. Commission on Atomic Weights, "Atomic Weights of the elements 1975".
    Pure Appl. Chem. **1976**, 47(1), 75–95.
17. Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry and the Commission on Nomenclature of Organic Chemistry, "Nomenclature of organic chemistry: Section D. D-1. Nomenclature systems".
    Chem. Listy **1976**, 70(6), 591–602 (Czech.).
18. Inorganic Chemistry Division. Commission on Nomenclature of Inorganic Chemistry and the Commission on Nomenclature of Organic Chemistry, "Nomenclature of organic chemistry: Section D. D-5. Organic compounds containing phosphorus, arsenic, antimony or bismuth".
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elements of atomic numbers greater than 105".
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20. Analytical Chemistry Division. Commission on Electroanalytical Chemistry, "Classification and nomenclature of electroanalytical techniques" (Rules approved 1975).
Pure Appl. Chem. **1976**, 45(2), 81–97.
21. Analytical Chemistry Division. Commission on Spectrochemical and Other Optical Procedures for Analysis, "Nomenclature, symbols, units and their usage in spectrochemical analysis II. Data interpretation" (Rules approved 1975).
Pure Appl. Chem. **1976**, 45(2), 99–103.
22. Analytical Chemistry Division. Commission on Spectrochemical and Other Optical Procedures for Analysis, "Nomenclature, symbols, units and their usage in spectrochemical anaysis III. Analytical flame spectroscopy and associated non-flame procedures" (Rules approved 1975).
Pure Appl. Chem. **1976**, 45(2), 105–23.
23. Analytical Chemistry Division. Commission on Electroanalytical Chemistry, "Recommendations for sign conventions and plotting of electrochemical data" (Rules approved 1975).
Pure Appl. Chem. **1976**, 45(2), 131–4.
24. Analytical Chemistry Division. Commission on Electroanalytical Chemistry, "Status of the Faraday Constant as an analytical standard".
Pure Appl. Chem. **1976**, 45(2), 123–30.
25. Analytical Chemistry Division. Commission on Spectrochemical and Other Optical Procedures for Analysis, "Nomenclature, symbols, units and their usage in spectrochemical analysis IV. X-ray emission spectroscopy".
IUPAC Inf. Bull., Append. Provis. Nomencl., No. 54, Dec 1976, 26 pp.

IUPAC/IUB

26. Commission on Biochemical Nomenclature, "Nomenclature of cyclitols" (Recommendations 1973).
Biochem. J. **1976**, 153(1), 25–31.
27. Commission on Biochemical Nomenclature, "Enzyme nomenclature" (Recommendations 1972). Supplement 1: corrections and additions (1975).
Biochem. Biophys. Acta **1976**, 429(1), 1–45.
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Probl. Endokrinol. **1976**, 22(1), 112–15 (Russ.).
29. Commission on Biochemical Nomenclature, "Nomenclature of corrinoids" (Recommendations 1973).
Cobalamin: Biochem. Pathophysiol. **1975**, 453–68.
30. Commission on Biochemical Nomenclature, "Definitive rules for nomenclature of steroids".
Kem. Kozl. **1975**, 44(4), 543–88 (Hung.).

APPENDIX II. NOTES ON NOMENCLATURE

1. W. C. Fernelius, Kurt Loening, and Roy M. Adams, "Addition compounds. Historical development of chemical nomenclature. Information sources on nomenclature practices".
J. Chem. Educ. **1976**, 53(6), 354–5.
2. W. C. Fernelius, Kurt Loening, and Roy M. Adams, "Systematic versus index nomenclature. Levels of communication via nomenclature. New edition of the Green Book".
J. Chem. Educ. **1976**, 53(8), 495–6.
3. W. C. Fernelius, Kurt Loening, and Roy M. Adams, "Chemical nomenclature versus that of other sciences. Some U.S. nomenclature practices at variance with those recommended by IUPAC. Isomerism about a double bond: use of *cis* and *trans*".
J. Chem. Educ. **1976**, 53(11), 726–7.
4. W. C. Fernelius, Kurt Loening, and Roy M. Adams, "Differences between "organic" and "inorganic" nomenclature".
J. Chem. Educ. **1976**, 53(12), 773–4.

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Structure-Text and Nomenclature-Text Searching for Chemical Information: an Experiment with the *Chemical Abstracts Integrated Subject File* and Registry System

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The *Chemical Abstracts Integrated Subject File* (the computer-readable file corresponding to the volume subject index of *Chemical Abstracts*) and a subset of the *Chemical Abstracts* Registry System file of connection tables have been used for a comparative test of nomenclature-text and structure-text searching. The structure search used a bit-mask searching technique, with a fragment code derived from the connection tables by the statistical methods of M. F. Lynch's group at the University of Sheffield. The same test questions were used to search corresponding nomenclature-text and structure-text data bases. The conclusions were that the fragment bit-screen search was capable of providing a search service of adequate quality even without an atom-by-atom search, that the fragment search performed on balance with superior cost-effectiveness to the nomenclature search, that the nomenclature search nevertheless gave a quality of performance (recall and precision) that would be regarded as acceptable in a commercial information-retrieval service, and that, within the fragment code, bond-centered fragments gave a superior performance to atom-centered fragments.

INTRODUCTION

The volume subject indexes to *Chemical Abstracts* refer to compounds by means of highly systematic nomenclature, the version used from 1972 to 1976 being Ninth Collective Index (9CI) nomenclature.[1] The computer-readable data base corresponding to these volume subject indexes is known as the *Chemical Abstracts Integrated Subject File* (CAISF).[2] Like the volume subject indexes themselves, CAISF is organized in two parts, the General Subject file and the Chemical Substance file; within each file, the arrangement is alphabetical upon the parent headings. The file therefore differs from most computer-readable information files in that the different pieces of information referring to a document are not found together, but are scattered throughout an alphabetical index.

This file enables information scientists to carry out substructure searches, using the systematic nomenclature as the structure file, and link them to searches of general concepts

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