the reviewers for their helpful comments which led to improvement of the paper.

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ACS Committee on Nomenclature: Annual Report for 1980

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Nomenclature committees, both national and international, were very active in 1980, 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. In addition, ways of working more closely with ACS Divisions, journal editors and authors as well as general means of promoting good nomenclature were explored. The chairman of the committee addressed the editors of ACS journals on the subject of chemical nomenclature at their conference in Columbus; this should lead to closer cooperation between the two groups. The feasibility study on compiling an authoritative chemical dictionary was extended, while the project on visual aids for chemical nomenclature was dropped. Contact was established between the committee and its recently established British equivalent. The subcommittee on chemical pronunciation continues to be active.

The *IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS)* functioned effectively this year. It held its annual meeting in Cambridge in September. 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: straightforward transformations, transport phenomena, biochemical equilibrium data, chemical kinetics, physicochemical quantities and units in clinical chemistry, calorimetric measurements on cellular systems, and various classes of carbohydrates.

The *IUPAC Inorganic Nomenclature Commission* met in September in Cambridge. Topics under discussion included neutral molecules and compounds, ions and radicals, rings and chains, polyhedral clusters, isopoly- and heteropolyanions, oxo acids, inorganic polymers, and stereochemical nomenclature. These topics were discussed in the context of providing a revision of the 1970 edition of the Red Book. Revised recommendations on the nomenclature of nitrogen hydrides and isotopically modified compounds are expected to be issued next year.

The *IUPAC Organic Nomenclature Commission* met in September in Cambridge. The commission continued its study of the reorganization and revision of the present rules according to a more logical arrangement (Section R) and of a more drastic long-range approach (Section G). In connection with Section G, several specific projects are under way: nodal nomenclature, radial nomenclature, "inorganic" ring nomenclature, nomenclature for delocalized ions and radicals, nomenclature of oxo acids, and general priority rules for numbering. The following topics are so well advanced that publications should be forthcoming within a year or two: lambda convention, classical ions and radicals, cyclophanes, and a revision of the Section E rules on stereochemistry. The 1979 provisional recommendations for the revision of the Hantzsch-Widman nomenclature system for naming heteromonocycles have generated so many diverse opinions and comments that the commission requires additional time and study before issuing definitive recommendations.

The *IUPAC Macromolecular Nomenclature Commission* met in September in Naples. The commission is continuing its work on (a) nomenclature and symbolism of copolymers, (b) subsidiary definitions of terms relating to polymers, (c) definitions for physical properties of polymers, (d) substitutive nomenclature for reacted polymers, (e) nomenclature of inorganic polymers, (f) classification and family names of polymers, and (g) interpenetrating polymer networks. Of these items (a), (e), and (f) are at the most advanced stage with recommendations expected to be issued in 1981 or 1982. A definitive version of the recommendations dealing with stereochemical definitions and notations relating to polymers will be issued in 1981.

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

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In *biochemical nomenclature* both JCBN and NC-IUB met jointly in Bellagio in June. Documents published in 1980 include the first supplement to "Enzyme Nomenclature (1978)", conformational nomenclature for five- and six-membered-ring forms of monosaccharides, and an amended version of "Nomenclature of Tetrapyrroles" (see Appendix). Work is progressing on recommendations for the nomenclature of prostaglandins (Joy Merritt is doing the spadework), carbohydrates, vitamins, enzyme kinetics, catecholamines, amino acids, diterpenes, glycoproteins, multienzyme proteins, and other specialized topics. Two documents, "Nomenclature of unsaturated monosaccharides" and "Nomenclature of branched-chain monosaccharides", have been approved as provisional recommendations and are expected to be published in 1981.

All *ACS divisional nomenclature committees* were active in 1980 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.

The *Office of Biochemical Nomenclature* continues to operate. 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 1980 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 Pharmacopoeia
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. 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, 1980

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Computer-Assisted Mechanistic Evaluation of Organic Reactions. 2. Perception of Rings, Aromaticity, and Tautomers

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New algorithms for the perception of rings, aromaticity, and tautomers were developed in conjunction with the CAMEO program for computer-assisted mechanistic evaluation of organic reactions. Briefly, the algorithms contain the following steps: prune the molecule of side chains, find ring(s), subdivide each ring into structural units, sum the units' contributions for the π-electron count, and determine whether tautomerization is possible. A noteworthy aspect of the ring alogrithm is that only rings belonging to the smallest set of smallest rings (SSSR) are found. Results for representative molecules are presented, and rules for determining the aromaticity/tautomer status of rings, especially heterocycles, are discussed.

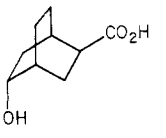
INTRODUCTION

An interactive computer program (CAMEO) is being developed in our laboratory to predict products of organic reactions given starting materials and conditions.[2a] A particularly novel aspect of the program is that mechanistic reasoning is used to predict products rather than relying on data tables for numerous, known, often mechanistically similar transformations.[2b-d] The program has three principal segments: (1) graphics which control the input and output of structures and communication between the user and computer, (2) perception of structural features and reactive sites in the reactants and products, and (3) mechanistic evaluation of potential reaction paths. An overview of CAMEO has been presented previously.[2a] Since substantial innovation has been made in several areas, details on specific procedures will also be presented in a series of papers. The present work focuses on the algorithms that have been developed for the perception of rings, aromaticity, and tautomers. The procedures are general and can be applied to other problems in which the perception of such structural features is required. Listings of the perception routines in CAMEO are available from the authors upon request.

RING PERCEPTION

Background. Enabling a computer to perceive rings is an essential part of any organic synthesis program. The presence of rings restricts conformational freedom, decreasing the feasibility of some intramolecular reactions but enhancing the likelihood of others. Reactivity toward common reagents may be substantially altered; contrast the behavior of cyclopropanone and acetone.

Although one could perceive all possible rings, i.e., all unique closed paths, this is excessive. Only the number which will suffice to define intramolecular relationships must be found. Frērejacque's number,[3] calculated by applying the following equation to a molecule, number of rings = number of bonds - number of atoms + 1, yields the number of rings in the smallest set of smallest rings (SSSR). From the SSSR, one can determine the total ring strain energy, aromaticity, stereochemistry, topology, and the set of synthetically important rings. A recent paper by Gasteiger and Jochim explores the advantages of finding and using the SSSR in detail.[4] It should be noted that envelope rings (rings which can be constructed by the intersections of, and which circumscribe, two SSSR rings, i.e., the six-membered ring in bicyclo[2.2.0]hexane) are not necessary for determining ring strain energy. Difficulties arise when applying this equation to highly symmetrical molecules, for instance the bicyclo[2.2.2]octanes. Following Frērejacque, only two of the three equivalent (if unsubstituted) rings would be perceived. Furthermore, the two rings perceived would vary depending on the order of atom numbers. As unsymmetrical substitution, shown in **1**, can occur, either (1)



1

subsequent processing must be independent of which pair of rings is found, or (2) the ring perception algorithm must find all three rings. The second option was chosen, necessitating the redefinition of the SSSR to include (ignoring substitution) symmetrically equivalent rings.

Previously published programs have constructed the SSSR by several methods. Wipke and Dyott used Welch's first algorithm to find the basis set of rings; then ring assemblies were constructed.[6] Finally all rings were found by means of Gibbs' algorithm. A minimal basis set and a set of "chemically interesting" rings (the basis set plus any ring of ≤ 8 bonds) were then found.[6] Despite the circuitous path, this approach

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