

Table III. Examples of the Examination by the Matching

	The Input Information							
	0-0	2-1	3-2	-	-	2-1	2-1	1-0
CH ₃ CH ₂ (?)	0-0	2-1	3-2	-	-	2-1	2-1	1-0
(?)CH ₂ CH ₂ (?)	-	-	-	1-0	3-2	1-1	1-0	0-0
Candidate								
C-C-OH	0	x	x	0	x	x	x	0
C-C-C-OH	x	0	x	0	x	x	0	0
C-C-C-OH	0	x	x	0	x	x	x	0
C-C-C-OH	x	0	x	0	x	x	0	0
C-C-C-OH	0	x	x	0	x	x	x	0
C-C-C-OH	x	0	x	0	x	x	0	0
C-C-C-OH	x	0	0	0	x	x	0	x
C-C-C-OH	x	0	x	0	x	x	0	0
C-C-C-OH	x	0	x	0	0	0	0	x

^a 0: registered as an informational homologue. x: rejected.

number of the possibilities is

$$\prod_{i=1}^M (\text{MAX}_i - \text{MIN}_i + 1)$$

If the candidate satisfies any of the possibilities, it is registered as an informational homologue; otherwise it is rejected. In the algorithm, homologues of a partial structure on segments and the connectivities between them, considering afferent

segments, are extracted from a candidate structure according to a number between MAX and MIN. This operation continues until any set of the inequalities on numbers of partial structures becomes true. If there is no way to make it true, the candidate is rejected. Aspects of the matching procedure are not always simple. For example, *n*-butane (CH₃CH₂-CH₂CH₃) can survive, though all structures which contain any ethyl group are denied, if an ethylene group (CH₂CH₂) is permitted. In other words, extracting an ethylene group hides the existence of ethyl. Table III shows several examples of the matching process.

CONCLUSIONS

SIEDS enumerates all structures of the informational homologues and displays them in the form of structural diagrams. By means of the system, chemists may easily and quickly recognize an extent at which they arrive in the elucidation of organic structures, and, in cases that identification or determination of structures is not accomplished, they can consider how to obtain further structural information.

REFERENCES AND NOTES

- (1) Y. Kudo and S. Sasaki, *J. Chem. Doc.*, **14**, 200 (1974).
- (2) (a) S. Sasaki, Y. Kudo, S. Ochiai, and H. Abe, *Mikrochim. Acta*, 726 (1971); (b) S. Sasaki, Y. Kudo, S. Ochiai, and I. Fujioka, *Jpn. Anal.*, **22**, 25 (1973); (c) CHEMICS (Combined Handling of Elucidation Methods for Interpretable Chemical Structures) system; e.g., CHEMICS-F will be reported in the near future.
- (3) Y. Kudo, *Kagaku no Ryoiki Zokan*, **98**, 115 (1972).
- (4) Y. Kudo and S. Sasaki, *J. Chem. Inf. Comput. Sci.*, preceding paper in this issue.
- (5) M. F. Lynch, J. M. Harrison, W. G. Town, and J. E. Ash, "Computer Handling of Chemical Structure Information", Macdonald, London, and American Elsevier, New York, 1971, p 36.
- (6) S. Sasaki, H. Abe, Y. Kudo, S. Ochiai, and Y. Ishida, *Kagaku no Ryoiki*, **26**, 981 (1972).
- (7) This is a improved instrument of JAL-30X, which is a system controlled by a console typewriter with a joystick: Y. Kudo, and S. Ochiai, *Anal. Instrum.*, (*Bunseki-Kiki*), **11**, 654 (1973).
- (8) L. M. Masinter, N. S. Sridharan, J. Lederberg, and D. H. Smith, *J. Am. Chem. Soc.*, **96**, 7702 (1974).

LETTERS TO THE EDITOR

Dear Sir:

I read with interest the paper, "Automatic Abstracting Research at CAS", by Pollack and Zamora in the *Journal of Chemical Information and Computer Sciences*, Vol. 15, No. 4, 1975.

On page 229, Table V is entitled, "Abbreviations and Symbols used in ACS Publications". In this table a period is used after all abbreviations and upper-case letters for the symbol for nuclear magnetic resonance. This is, of course, contrary to the information published by the American Chemical Society in "Handbook for Authors of Papers in the Journals of the American Chemical Society", 1st ed, pp 44 and 45.

It appears to me the authors became a little bit too enthusiastic in the title of Table V, especially since CAS deviates from the "Handbook...". It would seem to me that CAS should either conform to the recommendations in the "Handbook..." or the title of Table V should have been "Abbreviations and Symbols used in CAS Publications".

The authors are also inconsistent in the use of the hyphen, viz., p 228: in the title of Table IV the word, "Non-Substantive", is used, which is obviously incorrect; however, in the text in line 3 under "Final Editing" and also in the

heading of the next paragraph the correct form, "nonsubstantive", is used.

The Division of Chemical Information is primarily concerned with communication of correct information, yet we continually allow inconsistent, nonconforming, and inaccurate statements to be published. This is very confusing, and, in this case, it makes the job of editing manuscripts in-house for subsequent publication in ACS journals very difficult and at times impossible when two ACS publications print two entirely different versions of a table.

Alan R. McGarvey, Manager
Technical Information Services
Armstrong Cork Company
Lancaster, Pennsylvania

Received December 18, 1975

Dear Sir:

Dr. Pollock and Mr. Zamora have asked me to respond to Mr. McGarvey's letter of 15 December 1975 concerning their article, "Automatic Abstracting Research at CAS", published

in the *Journal of Chemical Information and Computer Sciences*, Vol. 15, No. 4, 1975. Table V, entitled "Abbreviations and Symbols Used in ACS Publications", which was included in the article, is the most current official list of accepted abbreviations agreed to by all ACS editors of primary and secondary journals. The ACS "Handbook for Authors of Papers in the Journals of the American Chemical Society", 1st ed, to which you referred, was published in 1967, and the list of abbreviations which it contains is outdated. I understand that ACS staff are revising the "Handbook", but the revision is not yet ready for publication.

I apologize to the authors and to your readers for allowing

the erroneously hyphenated "Non-Substantive" to get through unedited in the manuscript.

As an in-house editor myself, I can sympathize with efforts to prepare correct manuscripts in the face of seemingly conflicting standards. In our group, we attempt to use the most up-to-date standards, hoping thereby to keep confusion to a minimum.

Newell E. Gilmour, Jr., Technical Writing Manager
Chemical Abstracts Service
The Ohio State University
Columbus, Ohio

Received December 23, 1975

NEWS AND NOTES

NEWS ITEMS

Garfield Receives ASIS Award

Eugene Garfield, President and founder of the Institute for Scientific Information®, received the American Society for Information Science (ASIS) 1975 Award of Merit. Presentation was made in Boston on October 26, at the banquet concluding that national organization's annual convention. The ASIS Award of Merit is given annually for outstanding contributions or service to information science. Dr. Garfield is the eleventh recipient.

ISI Lecturer

The Institute for Scientific Information® (ISI®) has created a new position, Lecturer-Professional Education, designed to help academic institutions enhance their instructional programs on the use of scientific and technical information.

ISI offers without charge a professional reference librarian/educator to serve as a guest lecturer, seminar leader, or panelist who will provide instruction on the role the company's services play in information retrieval for the sciences and the social sciences. Participation by the ISI lecturer will be by invitation from the schools, and presentations will be tailored to meet the needs of graduate or undergraduate students.

The first person to fill the new position is Diane J. Hoffman, a Syracuse University graduate with seven years' experience as a reference librarian.

CAS/NLM Contract

The National Library of Medicine (NLM) has entered into a one-year, \$156,200 contract with the American Chemical Society's Chemical Abstracts Service Division for information and services in support of NLM's Toxicology Information Program. The contract extends cooperative efforts between NLM and CAS in which the CAS Chemical Registry System and other portions of the CAS data base have been used to supply information for NLM's TOXLINE and CHEMLINE computer-based information-retrieval services.

Under the new contract, CAS will assist NLM in resolving substance identification problems, develop and install a maintenance system for updating and creating new generations of NLM's CHEMLINE file, which provides access to substance-related information in the TOXLINE data base and other NLM on-line services, and develop search aids and

indexes to assist users in conducting structure and substructure searches of CAS systematic nomenclature in the CHEMLINE file. CAS also will cooperate with NLM in developing a search profile for extracting from the CAS data base citations, abstracts, and index entries for documents in toxicology and related fields for use in the TOXLINE data base, enrich NLM's *Toxicity Bibliography* file by adding to it the *Chemical Abstracts* chemical substance and general subject index entries for those citations in the file that are also covered by CAS, and evaluate, in cooperation with NLM, the usefulness of tagging toxicology-related data and concepts in CAS's *Chemical-Biological Activities* (CBAC) computer-readable file, which comprises part of the TOXLINE data base.

Chemical Society (London)/CAS Cooperative Program

The Chemical Society (London) and the American Chemical Society are expanding their cooperation in chemical information processing.

Under terms of a new cooperative agreement signed in London November 13, The Chemical Society will pay a share of the operating costs of ACS's Chemical Abstracts Service and provide computer-readable abstracts and index entries for British chemical papers and patents for input to the service's computer data base. The Chemical Society in turn will have the unrestricted right to use the data base and the exclusive right to market Chemical Abstracts Service publications, microform services, computer-readable files, and services derived from them in the British Isles. The British organization also will be represented on the CAS advisory and editorial advisory boards and will consult with the ACS Board of Directors Committee on Chemical Abstracts Service on decisions affecting CAS operations and services.

The Chemical Society's share of Chemical Abstracts Service's expenses will be based in part on the percentage of the total documents abstracted in *Chemical Abstracts* in a given year that originate in the British Isles and in part on the use made of CAS publications and services in the British Isles. The value of The Chemical Society's input will be credited as part of its share of the costs.

ACS concluded a similar cooperative agreement with West Germany's Internationale Dokumentationsgesellschaft fuer Chemie late last year and has been discussing possible cooperative arrangements with representatives of the Japanese chemical community.