lations and shrinking book orders on increasingly effective library resource sharing via photocopying and interlibrary loan rather than on the real problem of proliferation of materials and inflation. Yet publishers persist with the idea that if they can discourage interlibrary loan and photocopying, libraries will be forced to spend more money to buy books and journals. This is nonsensical since libraries cannot spend money which they do not have. The fact is that with or without effective sharing mechanisms, with rising prices and declining support, libraries simply do not have the funds to maintain their previous acquisition levels. If libraries cannot afford to buy the materials users need and if the law prohibits libraries from photocopying what they do not own, then users will simply have to do without.[12] These hard facts could have severe consequences for the academic scientific research community.

The academic research scientist should lobby to throw out the CONTU rule of five which is really nothing more than a ban on copying. The photocopying of copyrighted scientific material by academic researchers is not unfair; it is necessary, and it should be legal. Scientists should not be denied access to information, and libraries should be permitted to perform the vital role in the information transfer process.

Private sector vs. public sector, profit vs. nonprofit, publishers vs. librarians, publishers vs. users—these animosities are inhibiting and counterproductive to the goals of education and research. However, many of those in the information business are planning systems in isolation from the user. The new mechanized systems should be designed to serve human needs rather than subject users to the tyranny of the system. The consequences may be Orwellian for the researcher as the systems become more powerful and more expensive than is justified by the procurers and users of scientific information. The very basis of traditional librarianship, which is basically ownership of information sources and maintenance of direct service to users, is at stake.

The processes for the transfer of scientific information are changing dramatically, and they will change even more in the next decade. The Copyright Act of 1976 and CONTU guidelines for copyrighted materials are merely a stopgap before newer methods of handling information are fully developed. Copyrighted materials are necessary to the development of science. Librarians need the help of the scientists, as creators, evaluators, and users of scientific information, to see that libraries can continue to provide current, timely, and inexpensive information.

REFERENCES AND NOTES

(1) First International Conference of Scientific Editors, Jerusalem, 1977; "Scientific Information Transfer"; Balaban, Miriam, Ed.; D. Reidel: Dordrecht, Holland, 1978; preface.
(2) Broad, William J. "The Publishing Game: Getting More for Less". *Science (Washington, D.C.)* **1981**, *211*, 1137–1139.
(3) Chemical Information Review Committee. "Information Transfer and Use in Chemistry"; British Library: London, 1978; Research and Development Reports No. 5385; 0308-2385, p 1.
(4) Garvey, William D. "Communication: The Essence of Science"; Pergamon: Oxford, 1979; Chapter 1.
(5) Kent, A. K. "Scientific and Technical Publishing in the 1980's". *Chem. Br.* **1980**, *16*, 152–153.
(6) Ploman, Edward W.; Hamilton, L. Clark "Copyright"; Routledge & Kegan Paul: London, 1980; Chapter 1.
(7) Tseng, Henry P. "The Ethical Aspects of Photocopying as They Pertain to the Library, The User and the Owner of Copyright". *L. Libr. J.* **1979**, *72*, 86–90.
(8) Timberg, Sigmund "A Modernized Fair Use Code for the Electronic as Well as the Gutenberg Age". *Northwestern Univ. L. Rev.* **1980**, *75*, 192–244.
(9) "Copyright Report"; University of Oklahoma Libraries, Internal Report, 1980.
(10) Berger, Patricia W., Library Division, National Bureau of Standards. Statement, hearing before Library of Congress Copyright Office, June 11, 1980; unpublished paper.
(11) Stedman, John C., University of Wisconsin, Professor of Law. Statement, Copyright Office Hearings on Section 108, Jan 19, 1980; unpublished paper.
(12) DeGennero, Richard. "Copyright, Resource Sharing, and Hard Times: A View From the Field". *Am. Libr.* **1977**, 430–435.

Introduction to the Symposium on the Uses and Applications of the Wiswesser Line Notation Today†

MURRAY D. ROSENBERG

Technical Information Section, Research and Development Department, Philip Morris Research Center, Richmond, Virginia 23261

Received February 11, 1982

This introduction sets forth key considerations on the uses and applications of the Wiswesser line notation today. The contributions of the international gathering of speakers in the symposium are introduced in this context.

INTRODUCTION

The historical development and past uses/applications of the Wiswesser line-formula chemical notation or, more simply, Wiswesser line notation (WLN) have been published profusely in the past.[1] The most recent years have been relatively quiet on current uses of the WLN. However, it is the most widely used system of structure symbolism in the world today. The rules for the WLN are provided in a large, easy-to-use workbook.[2]

I believe this symposium and others involving computer graphics linked with chemistry clearly shows the maturing of thought and philosophy concerning systems involving chemical structure description beyond traditional chemical nomenclature.

OVERVIEW

It is only appropriate that a symposium on the Wiswesser line notation should start with its creator, Dr. William J.

† Presented on Aug 27, 1980, as part of the symposium on Uses and Applications of the Wiswesser Line Notation Today during the 180th National Meeting of the American Chemical Society (Second Chemical Congress of the North American Continent), Las Vegas, NV.

0095-2338/82/1622-0087$01.25/0

Wiswesser, presenting an historical overview of the WLN from its conception to present. Wiswesser also will close the symposium with his future views for the WLN.[3]

The papers by Warr,[4] Johns,[5] Bond,[8] and Fritts[9] represent the use of the WLN by large chemical and pharmaceutical firms. The papers cover advantages and disadvantages from the user/firm viewpoint.

Eakin[10] and Coulson[11] cover the applications from the view of the commercial information firm.

Walker[6] and Rosenberg[7] provide a historical look at the development of an information product based on WLN, its use in a real setting, and suggested improvements in the service.

CONCLUSIONS

In the introduction of this symposium, it was stated that with the hundreds of industrial and government users of the WLN over the world, the volume of publications about its application has been decreasing. This may be an effect of the intense use of the Chemical Abstracts Services' (CAS) registry numbers and the newly seen advances in direct input and output of chemical structure information via computer graphics terminals.

While it is evident the end user of any chemical information, be it chemist or information scientist, would prefer a chemical structure diagram, the use of WLN as an *intelligent* registration of chemical uniqueness for a sophisticated computer system should not be underrated. Some of the desirable characteristics include its ability to become transparent to all but the involved chemical information scientist, its low cost per computer entry, its portability, and its transferability.

While the feverish activity involved in the past over WLN has abated, there remain these key activities for its continued usage: (1) In existing large files of structures encoded in WLN; (2) as an entry point for a sophisticated system, directly or indirectly, prior to its conversion to a connectivity table (CT); (3) as a screen for searches prior to expensive CT searching which will provide valid answers; (4) to generate storable structure-related information for small files of chemicals.

REFERENCES AND NOTES

(1) A complete bibliography of all publications involving the Wiswesser line notation is available from the creator of the notation: Dr. William J. Wiswesser, USDA-SEA-Weed Science Research, P.O. Box 1209, Frederick, MD 21701.
(2) Smith, E. G.; Baker, P. A. "The Wiswesser Line-Formula Chemical Notation", 3rd ed.; Chemical Information Management, Inc.: Cherry Hill, NJ, 1976.
(3) Wiswesser, W. J. "How the WLN Began in 1949 and How It Might Be in 1999". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(4) Warr, W. A., "Diverse Uses and Future Prospects for Wiswesser Line-Formula Notation". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(5) Johns, T. M.; Clare, M. "Getting the Most Out of the WLN. WLN as a Structural Summary Medium". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(6) Walker, S. B. "Development of CAOCI and Its Use in the ICI Plant Protection Division". Presented at the 2nd Chemical Congress of the North American Continent, San Francisco, CA, Aug 1980; Abstract CINF 23.
(7) Rosenberg, M. D.; DeBardeleben, M. Z.; DeBardeleben, J. F. "Chemical Supply Catalog Indexing: Now and the Future–an Ideal Place for Use of the Wiswesser Line Notation (WLN)". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(8) Bond, V. B.; Bowman, C. M.; Davison, L. C.;f Roush, P. F.; Young, L. F. "Applications of the Wiswesser Line Notation at the Dow Chemical Company". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(9) Fritts, L. E.; Schwind, M. M. "Using the Wiswesser Line Notation (WLN) for Online, Interactive Searching of Chemical Structures". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(10) Eakin, D. R. "Graphics Challenge WLN–Can WLN Hold Fast". *J. Chem. Inf. Comput. Sci.*, paper included in this issue.
(11) Coulson, H. J.; Sher, I. H. Luiso, K.; Lawlor, H.; Sarkisian, J. E. "WLN at ISI–Applications in Commercial Information Services"; unpublished.

How the WLN Began in 1949 and How It Might Be in 1999[†]

WILLIAM J. WISWESSER
U.S. Department of Agriculture, Frederick, Maryland 21701

Received August 24, 1981

In December 1949 the first WLN (Wiswesser Line-Formula Notation) symbols were developed as a new "least effort" method for standardizing the old line-formula delineations that Loschmidt had introduced in 1861. The set of letter symbols was comprehensively simplified in June 1950, but these 30-year-old first WLN's employed the full symbol set of the standard typewriter keyboard; thus they probably will resemble structural delineations of the 21st century closer than the present WLN descriptions. Basic features of an advanced WLN (AWLN), with a greatly expanded character set, are summarized.

INTRODUCTION

This is a doubly great honor, the experience of a lifetime for me, first to have an international symposium on this notation which I started in 1949 and then, at the next ACS meeting, to be the recipient for the Herman Skolnik Award of the Division of Chemical Information. For these honors I thank all of you who have made the WLN what it is today. My obligation now is to describe and document its historic, mathematical, and theoretical foundations or "roots".

The taproot of the WLN might be pinpointed to a hisotry-making discovery 50 years ago when H. Mark and R. Wierl determined the first 41 structures of gaseous molecules by wave-mechanical analysis of a diffracted precision electron beam.[1] Here at last were verified dimensions of free-moving molecules! Two related personal interests appeared in 1931, as I was graduating from high school: Linus Pauling started his reports on the nature of electronic bonds,[2] and Henze and Blair summarized a 19th century mathematical problem of counting alkyl and alkane isomers.[3a] In 1955 I discovered the first direct solution to Arthur Cayley's 1857 problem of counting alkane isomers—by partitioning CH_2 groups around and between the *X*, *Y* branches, thus proving the "Mathematical Foundations for a Chemical Notation" based on the WLN symbol set.[3b]

Austin M. Patterson, father of American chemical nomenclature, became by "guidefather" through the maze of organic chemistry in 1933, when he published the Liege re-

[†] Presented at the "Sympsoium on Uses and Applications of the Wiswesser Line Notation (WLN) Today", Las Vegas, NV, Aug 27, 1980. Also presented in part as the acceptance address for the Herman Skolnik Award of the Division of Chemical Information, American Chemical Society, Houston, TX, April, 1981.