ACKNOWLEDGMENT

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Diverse Uses and Future Prospects for Wiswesser Line-Formula Notation

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The many and varied uses found for Wiswesser Line Notation (WLN) in the 1970s are reviewed. The advantages of WLN-based systems for storage and retrieval of chemical structures have been proved over several years of increasingly wide usage. Future prospects for the notation are briefly considered in the light of these advantages and certain shortcomings.

Wiswesser Line Notation (WLN)[1] is a compact way of uniquely and unambiguously representing the complete topology of a chemical molecule by a linear sequence of characters. It is used by around 150 organizations worldwide in industrial, governmental, and educational fields. In addition, between 30 and 40 educational institutions teach WLN even though they do not maintain files of notations. The Chemical Notation Association (CNA) mails information to Canada, U.S., United Kingdom, France, Italy, Sweden, Japan, Denmark, Netherlands, Israel, Switzerland, India, Australia, West Germany, Romania, Austria, Belgium, Norway, and Yugoslavia. The rules of WLN are available in English, French, German, and Japanese translations.[2]

Numerous programs have been written to handle WLN, some part of in-house systems and some, such as the CROSSBOW[3] programs, commercially available. The CROSSBOW suite comprises programs for registration with WLN/molecular formula check, fragment generation, bit and string search, connection table generation, atom-by-atom search, structure display, and KWIC listing. Sixteen different organizations, to date, are using the CROSSBOW system.

Most organizations handling WLN need a checker program which generally validates notation syntax and then generates a molecular formula from the notation for comparison with an input molecular formula. ICI and other companies have used such programs for years. The CROSSBOW one is commercially available.[3] Other well-known checker programs are the ones used by the Institute for Scientific Information in connection with Index Chemicus Registry System (ICRS)[4] and the program WISCT (commercially available[5]) written at Pomona College to verify WLNs and generate connection tables. WISCT is also used to generate connection tables for the MACCS system.[6]

There are two WLN-string-search programs on the market, RADIICAL[7] from ISI (*R*etrieval and *A*utomatic *D*issemination of *I*nformation from the *I*ndex *C*hemicus and *L*ine Notation) and CROSSBOW. Reckitt and Colman in England have purchased certain CROSSBOW programs but use the IBM package INQUIRE to search notations, molecular formulas, and CROSSBOW fragments.

Many American companies, and Pfizer in England, have in-house software for checking and searching WLNs and for generating connection tables (from WLN) to be used in atom-by-atom search and structure display. On the connection table front, CROSSBOW,[3] WISCT,[5] and MACCS[6] are for sale. Two software houses, CIMI[8] and Fraser-Williams (Scientific Systems) Ltd.,[3] specialize in writing WLN systems for customers. Granito of CIMI has written a program to generate ring codes from WLN[9,10] (i.e., the code of the Pharma Documentation Ring).

Finally, this brief survey exemplifying (but not comprehensively covering) WLN software would not be complete without mentioning the PATHFINDER program originally written by the Dow Chemical Company but now available from Chemical Abstracts Service[11] (or in England via the United Kingdom Chemical Information Service—UKCIS). The program is used to check locant paths in ring systems with bridges and/or crossed bonds. It could, of course, be used for any ring system but it is of most use for "tricky" notations where the encoder is not sure whether he has picked the optimum path for lettering ring atoms.

From software we move to examples of the various data bases that have been created by using WLN. The biggest is ICRS.[4] ISI supply very up-to-date tapes, on a monthly basis, of novel compounds appearing in the literature, together with bibliographic data and various flags and subject terms. they

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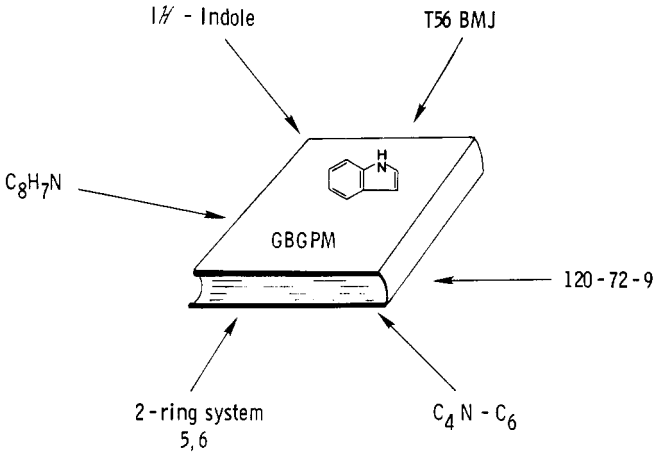

Figure 1.

have thus created a data base, since the early 1960s, of about two and a half million compounds. Cumulated indexes on microfiche and KWIC listings of WLNs on microfilm are also available from ISI.[4]

Another major collection of notations is "The Parent Compound Handbook",[12] available from Chemical Abstracts Service (or UKCIS in England). The handbook gives structural formulas for the parents of all published ring systems. Each parent is given a five-letter accession code. There are six indexes so that the structures can be accessed by parent name, WLN, molecular formula, Chemical Abstracts Registry Number, ring analysis, or ring substructure (see Figure 1). Some specialized data bases are available in machine-readable form from CIMI—for example, CIMI-DRUGFILE and the WLNs for compounds in the Merck Index.[13] The present edition of this reference book contains no notations, but it does carry an explanatory chapter on WLN.

Notations for psychotropic drugs may be looked up in a U.S. National Institute of Mental Health publication.[14] This will be mentioned again later. The Pesticide Manual published by the British Crop Protection Council[15] has an alphanumeric listing of WLNs, and the Pesticide Index published by the Entomological Society of America[16] also contains notations.

The Commercially Available Organic Chemicals Index (CAOCI) was originally produced by a consortium of chemical companies in the U.K., but it is now updated and marketed by Fraser-Williams (Scientific Systems) Ltd.[3] The original CAOCI indexed WLN, molecular formula, chemical name, and supplier data from more than 50 catalogs, and the file had about 120 000 entries with about 52 000 unique WLNs. Fraser-Williams have rationalized and reduced the number of catalogs, but they index more compounds from each catalog, since they now include inorganics, biochemicals, etc. The structural data are available in machine-readable form, and there are various indexes on microfiche. Incidentally the Aldrich Chemical Company was using WLN before the advent of CAOCI.

An incomplete list of WLNs of toxic chemicals used to be available on tape with the Registry of Toxic Effects of Chemical Substances (RTECS).[17] The notations were later withdrawn, but in 1979 it was announced that WLNs would be added for all structures in the near future. About 27 000 "prime names" are on file. Notations for all RTECS compounds *have* been coded for the Environmental Chemicals Data and Information Network (ECDIN)[18] of the European Economic Community. Compounds in the "List of Organic Chemicals and their Customs Classification", the so-called Brussels classification, have also been coded for ECDIN.

There are also files of physical chemical data with associated Wiswesser Line Notations. The Thermodynamics Research Center in Texas and Pedley's work at the University of Sussex, England, are notable in the thermodynamic field. Pedley has used his system to publish tables of thermochemical data, but the WLNs are not yet available in machine-readable form.[19]

Pollack has worked on a substructure index for correlating spectral data,[20] and the CRC Press has published on "Atlas of Spectral Data" wherein spectral characteristics and physical constants of organic compounds can be accessed by WLN[21] (Pollack having provided the WLN expertise).

In Australia, Needleman is using WLN as a tool in a computer-aided learning program,[22] and Vaughan has published on the handling of WLNs and related physical data.[23] Hansch and Leo of Pomona College, Claremont, CA, have published extensively in the field of structure–property relationships.[5,24-26] Their data base of physical constants, such as log *P* values, plus WLNs is commercially available.[5] Adamson and Bawden have also published on structure–property correlation[27-29] and so has Saggers.[30-32]

Several teams have independently used WLN in reaction indexing research. Osinga,[33-35] Lynch,[36-38] Eakin and Warr,[39] and Gelernter[40,41] are cited here. In connection with his SYNCHEM and SYNCHEM2 programs Gelernter has worked on the computer generation of WLNs.[40,41] Teams at NIH[42,43] and the Dow Chemical Company[44] have also worked in this field. In fact the NIH team was able to generate canonical WLNs for 81% of the compounds in one of their data bases, and their program was used to produce WLNs for the psychotropic drugs publication mentioned earlier.[14]

Having exemplified work done using WLN in the past, we shall now briefly consider the use of WLN in ICI Pharmaceuticals Division at present. A recent publication described the online integrated chemical and biological data base at ICI and placed particular emphasis on the sophisticated biological control functions of the system.[45] Chemical and biological searches (independent or integrated) as well as registration and WLN checking are carried out online. Atom-by-atom searching and structure display are done overnight on hit files which have been suitably merged online.

The CROSSBOW system is also used for batchwise searching of CAOCI, ICRS, and Hansch data bases. It is hoped that in 1982 CAOCI data will be incorporated into the online data base.

Various other enhancements are planned for 1982, the most obvious to the outsider being online structure display. Terminals linked to the online data base are now available for use by research chemists, and it will be a great improvement when chemists inputting molecular formulas or reference numbers can receive structural formulas in response to their single enquiries for chemical data, sample data, and biological test results. Chemists cannot at present run substructure or biological searches. Longer term plans are to provide extra, more user-friendly facilities. The future system could still involve WLN since it is not intended to take chemical registration out of the hands of information scientists. The system will revolve around a canonical connection table, and WLN, while not essential for registration, would still be an input option.

The heavy investment put into WLN by ICI and many organizations makes it unlikely that WLN usage will cease for many years to come. Nevertheless the exponents of WLN are going to have to work seriously on some of its disadvantages if WLN is to have a future. Tautomerism, Markush structures, and stereochemistry are three fields requiring research.

The WLN rules are such that any precisely defined structure can be encoded, and tautomers, e.g., 2-hydroxypyridine and 2-pyridone, have different WLNs. This "old-fashioned bond fixation" has both its advantages and its disadvantages in the field of tautomeric and certain mesomeric structures (e.g., chelates).

Krishnamurthi feels that Algorithmic Wiswesser Notation[46-48] could be of use in a Markush structure project, and Lynch's team at Sheffield have been considering this in ongoing work on Markush structure representation. As regards stereochemistry, a special subcommittee of the Chemical Notation Association made great progress in stereochemical suffixes for WLNs up until 1979, but no work is being carried out at present. CNA (UK) had high hopes of organizing a research project in WLN, stereochemistry suffixes, structure display, and graphics, but no suitable student could be found for the academic year 1980–1981.

The principle disadvantage of WLN is that it is not user friendly. This can only be overcome by programs which will derive a canonical WLN from something else (but no one has yet produced a cost-effective program to do this for over 90% of compounds), by writing programs to generate canonical connection tables from noncanonical WLNs, or by accepting the intervention of a skilled "middle man".

However, one must recognize that WLN has some great advantages. Compared with most chemical names and connection tables, it is a very compact way of completely representing the topology of a molecule. It has a proven, past performance with large files and is in worldwide usage. Obviously one has to balance the cost of hardware plus software against the costs of extra WLN-skilled personnel, but in many organizations WLN is a cost-effective tool for registration and search. WLNs are readable, listable, and permutable. They are easily printed and transmitted on tape. Chemically meaningful entities are easily detectable in them and in fragment codes generated from them. Systems such as CROSSBOW require little prior processing of files (e.g., tree structuring or inversion) before searches can be run. Relatively cheap hardware and software are used. Moreover, there is only the one line notation with worldwide usage, whereas connection tables being used are many and varied. WLN is therefore useful for interchange of data the world over. For these reasons WLN must have a future in the 1980's.

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Graphics Challenge WLN. Can WLN Hold Fast?†

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Chemist-oriented graphics systems are now available, allowing the research chemist to manipulate structures by using computer techniques. The presentation looks at the role these graphics systems play in research and compares it with the role which standard WLN-based systems play. It discusses the techniques necessary to support chemical information retrieval and the development required for WLN to meet the challenge of chemist-oriented graphics. A graphics-oriented enhancement of CROSSBOW is discussed. A machine aligned connection table (MACT) is proposed, as is an interface between WLN and Chemical Abstracts Connectivity Tables.

INTRODUCTION

The chemist in research has seen many changes in the last decade; one such change has been the use of computerized technique to support his main synthetic effort. These include the following:

On-line reference retrieval systems now supplement his conventional library publications.
Substructure and structure retrieval systems available on company data banks replace previous manual card indexes.
Drug design techniques are now in use with computerized structure–activity correlation.
Structure elucidation usually involves some form of computerized interpretation following spectroscopic analysis.
Many chemists see molecular modeling as a vital aid to interpreting their research results.
Other chemists now use computerized methods to aid synthetic pathway design.

Computers are thus very vital to chemical research, and the chemist's involvement with computers is changing. The advent of interactive graphics systems means the chemist can have meaningful dialogues with computer systems in the chemist's own language—the structure diagram. This is particularly important for applications such as molecular modeling and synthetic pathway design, where interaction with the system is essential.

But some chemists are now putting on pressure to ensure that they can have direct access to computer files for other purposes—such as substructure retrieval. Will any problems be solved by giving chemists direct access to company files? Where does this leave the existing WLN-based systems? Can they move forward and meet the challenge? Or is it time to move away from WLN? Will graphics just be an expensive toy? These are questions being asked by many people in many organizations in America, Europe, and Japan, and it is important that the people making these decisions evaluate carefully the options before them.

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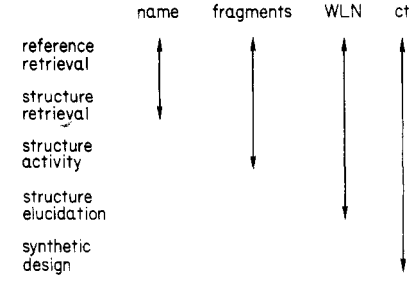
STRUCTURE REPRESENTATION

Firstly, however, perspective is important. WLN is not an alternative to graphics—WLN is merely a method of structure representation. Computerized chemical handling systems principally use one or more of the following ways of describing the chemical to the computer:

Chemical Nomenclature. This covers everything from simple common and trade names to complex systematic nomenclature such as that used by Chemical Abstracts.
Fragment Codes. This covers from the simple manual fragment code typified by the Derwent Ring Code to the complex algorithmically generated systems used by the BASIC or IDC groups.
Notations. Almost exclusively WLN, but some companies and organizations have developed other notational systems.
Connection Tables. These vary from simple atom-bond connectivity matrices to the more complex, involving stereochemistry, etc. Graphics-based systems rely almost solely on connection tables.

The use of a particular structural representation in a given application obviously varies from organization to organization. In general terms the following diagramatic representation is seen to apply:



Connection tables are used extensively where detailed structure manipulation is required. But the picture is much

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