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.

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

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

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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-

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port.[4] That report then seemed like the answer to a young organic student's prayers, in its promises of systematic descriptions for organic structures. In 1939, at the 102nd National Meeting of the American Chemical Society in Baltimore, I was thrilled to be introduced to Dr. Patterson through his protégé, Mildred Grafflin, then working with me at the Hercules Experiment Station and sharing mutual interests in the sticky challenges of terpene nomenclature. Patterson urged me to continue exploring my idea of describing ring systems exactly like open-chain structures, in terms of a continuous path of connections. No other chemist then was pursuing that simplifying approach. The concept now is dignified by the graph-theoretical name of "Hamiltonian line" or a "Hamiltonian circuit" when the path finishes where it started.[5] Patterson's laborious 25-year collection of all the then-known ring systems into a single ACS monograph focused attention on the heart of the notation-designing problem—that of ring analysis.[6] For experimental material on this personal research, I started a card file on all possible tricycloalkanes up to C20.

In 1945 I concluded 3 years as a chemical engineering instructor at Cooper Union in New York City with three inspirational stimulants for the WLN: (1) a systematic notation for the sets of dimensions in fluid flow and physical chemistry—lower case letters for m, l, t dimensions (in boldface if vectors) and upper case for the more complex electric, magnetic, and thermal dimensions; (2) simple Schoenflies-type symbols for molecular symmetry types, avoiding his superscripts and subscripts; (3) publication of a color-coded explanation of the Periodic System and atomic structure (which appeared just as the Atomic Age began).[7] These pictures of atom-bound electrons showed that there are no such things as double or triple bonds. Pauling himself acknowledged their fictional but still useful nature in his 1960 revision.[8] The only physicochemical reality is the electronic cloud, sharply defined as spherical standing-wave patterns in atoms, elliptical patterns in diatomic molecules, and more complicated patterns in polyatomic molecules.[9]

Molecular modeling was a lifetime fascination with me, and the strongest inspiration for the WLN was my 1946 invention of a very low-cost atomic model that has strong "overlapping orbital" snap fasteners.[10] The 1:100 000 000-scale models were stamped from optically flawed sheets of cellulose acetate plastic in experimental lots of 10 000 at a time.

These glittering 3-D (three-dimensional) inspirations to the 1-D (one-dimensional) WLN delineations never have been displayed at a national or international chemistry meeting, but in a world-famous "Glitter City", this exposure seems appropriate and opportune. Your will see nothing like them in other molecular models shown in the exhibition area by vendors or in the Poster Show of the Chemical Education Division.

Close examination shows that these heartily surviving models can make (1) brightly colored playthings for children, (2) chemically instructive necklaces with hand-painted zig-zag bonding lines, (3) carefully linked long chains that illustrate fine details of tough isotactic polyethylene polymers, and (4) hand-painted single-atom explanations of the onefold to fourfold Schrödinger wave patterns.

While my 1946 atomic models had these several attractions, the tetrahedral forms had the classical limitation to sharply distinct single, double, or triple bonds. My awareness of this theoretical objection soon led to the 1949 notation that had a desired freedom from chemical bondage in its additive acyclic symbol set.

HOW THE WLN BEGAN

The WLN first appeared as a serendipic assembly in December 1949: these functional-group (upper-case letter) and alkyl-chain (Arabic numeral) symbols had been the last and least important details of an earlier Dewey-decimal type of formula-ring-branch classifying notation. It started with the total number of nonhydrogen atoms and used longest connected paths (then continuing through the longest chain) in *all* ring descriptions. The old ring notations like "(66)" for naphthalene were kept, but the other features were abandoned in favor of the long-familiar Loschmidt delineations.[11] In my color-coded 1949 diagrams, I emphasized functional groups rather than carbon chains, and I made this orientation a WLN rule early in 1950. The quintessence of my aim in 1950 was to use *just one mark* for each frequently met atomic group—and only for these deserving few. A smart Vegas "word gambler" would know that such a symbol set would be a winner on simplicity and conciseness—greatest expressive power per mark—because the frequency data have century-old stability.

Here then was the intended freedom from chemical bondage that emerged in the first three features of the WLN: (1) use single letter symbols for frequently met atomic groups, (2) use Arabic numerals for alkyl chains and Patterson's ring numbers, and (3) use LOwer CAse letTErs to LOCATE ring positions, through a self-determined longest path—which later became the heart of the Dow and Chemical Abstracts "WLN PATHFINDER" programs.[12-14]

TRIBUTES TO BUILDERS OF THE PRESENT WLN

In 1953 Frederic R. Benson, then at Remington-Rand's Research Center in South Norwalk, CT, showed how the WLN was useful for substructure searching, even with the primitive card-actuated tabulating equipment that was demonstrated in the special exhibition area of the ACS meeting in Chicago.[15] Fred was smarter than we were in 1953: he never used the methyl contractions that the Chemical Notation Association finally abandoned in 1965, to further simplify the WLN records for the ever more sophisticated computer programs.

In 1960 Elbert G. ("Al") Smith published a pioneering report on "Machine Searching for Chemical Structures".[16] The greatest thing that ever happened to the WLN was that my invited WLN report caught Al's intellectual fancy.[17] He soon had the world's largest one-man file of IBM cards with chemical notations and physical property data; his WLN-proofing deck grew to some 80 000 as he went through the Hodgman-CRC, Lange, and Heilbron organic collections. His 1960 report on the beginnings of this file became the WLN user alert for the 1960s. He provided the parliamentary foundations for the Chemical Notation Association (CNA) in 1965 (earning a 3-term presidency) and, with that CNA users' guidance, wrote the greatly improved computer-oriented second edition of the WLN manual.[44] This WLN revision began in Aug 1960, when he and Howard Bonnett typed 14 single-spaced pages of "Proposals for Changes in the Wiswesser Notation". His revision of the WLN manual was a labor of love, with all royalties given to the CNA treasury. He had spent two sabbaticals on WLN pursuits, the second on the Ring Index proving ground. He then provided the card file for the WLN-Ring Index report.[35]

As though all that thankless work were not enough, he coauthored the 3rd edition of the WLN manual with Peter A. Baker.[45] Year after year he promoted the WLN through tutorials in San Francisco, New York, and Chicago, plus WLN seminars and lectures in three trips to Japan and one to Europe, mainly at his own expense. Smith too is indebted to Patterson's revised 1960–1965 Ring Index: "Without that compendium of reported ring structures, I never could have discovered the pseudobridged ring business as I did, or finally have seen the necessity for citing internal spiro atoms in the notation".[18] This additional Smith refinement depended en-

tirely on the Landee–Bowman equation developed at Dow, which was central to computer checking of notations containing complicated ring systems.[19]

In the 1960s, Alan Gelberg also enthusiastically promoted early interest in the WLN, first establishing the huge WLN file at Edgewood Arsenal with Peter Sorter and Charlie Granito. There they generated the clever concept of "permuted" WLN indexes.[20] While there, Alan organized and cochaired a 2-day conference on WLN User Reports and then went on to establish Diamond Alkali's (now Diamond Shamrock's) WLN file with Charlie Granito.[21] Alan showed Penn State's pesticide pioneer, Don Frear, a WLN Index for all of the structures in Frear's Pesticide Index and long afterward helped Joe High, Freeland Romans, and me put the WLN into its 5th edition and into recent editions of the Herbicide Handbook.[22,23] Every year since 1969 Alan has been providing updated notation eduction in an evening class on Chemical Information at the American University in Washington, DC.[24] His numerous publications on WLN applications started in 1962 and continued through the 1970s.[25,26]

In the mid-1950s, Howard T. Bonnett established the foundations of the WLN investments at G. D. Searle that Trisha Johns described at Las Vegas.[46] There he implemented some of the earliest uses of WLN in computer systems that graduated from punched cards to magnetic tapes.[27] Later, Peter F. Sorter transplanted the WLN roots from Edgewood Arsenal to Hoffmann-La Roche.[28] He made a WLN file of the 1960 Merck Index, just to show its value to his supervisors. At Edgewood, I think he won a small bet that he could encode the next 200 compounds coming into the Industry Liaison office in 1 h!

In 1964 Franc Landee, founder of Dow's Computation Research Laboratory, showed the first WLN-generated structure displays to an international computer meeting in Moscow and to this Division's meeting in Philadelphia.[29] Dow's subsequent WLN innovations and extensions also are noted in this symposium.[47]

HISTORIC STRUCTURE DISPLAY FROM WLN

In 1967 Ernie Hyde and Lucille Thomson, at the 153rd National American Chemical Society Meeting in Miami Beach, described their COBOL-programmed conversions of WLN to fragment-code lists, connectivity matrices, and structure displays.[30] These became the foundations for CROSSBOW (Computer Retrieval of Organic SubStructures by means of Wiswesser), a suite of programs now made available with other WLN-indexed services through Fraser Williams, Ltd.[48,49]

In 1968 Alan Gelberg and Charles E. Granito chaired this Division's first symposium on notation systems, in San Francisco.[31] Al Smith gave his first WLN tutorial at that ACS meeting, and I still remember having to help bring in more tables for the unexpected standing attendance.

In that same year Gene Garfield's Institute for Scientific Information (ISI) committed the world's largest investment in the WLN with the Index Chemicus Registry System (ICRS) and its subsequent chemical information services.[32] Murray D. Rosenberg, chairman of this symposium, also developed his interest in WLN with Granito at ISI.[33] Charlie Granito provided some of those challenging developments before he left ISI to concentrate on WLN systems services around the world; once or twice every year Charlie teaches a week-long workshop on WLN in Philadelphia. He also has given tutorials in Europe.

In 1969 we created the first computer-generated WLN bit screens designed for very high speed and inexpensive substructure searching, with the modest capabilities of the CDC computer then serving the U.S. Army at Fort Detrick. Charlie Granito promptly implemented this idea at ISI and proved that this front end bit screen gave a *30-fold* increase in searching speed. It is the ultimate low-cost solution for searching ISI's ever-increasing multimillion-record files.[34]

In 1969 Chemical Abstracts Service (CAS) published a combination WLN Index and numeric index to the Ring Index structures from Al Smith's card file, converted to tape at Dow.[35] This was followed in 1976 by an order of magnitude improvement in Tommy Ebe's group at CAS—the Parent Compound Handbook, containing over 40 000 WLN descriptions verified by the CAS refinement of Dow's PATHFINDER program. This also is an ever-growing file, with bimonthly updates.[36]

In 1971 Carl Farrell, Dave Chauvenet and Deena Koniver at the NIH's Division of Computer Research and Technology created a major landmark in structure processing with "Computer Generation of WLN" from handwritten diagrams on a Rand writing tablet.[37] It truly was something you had to see to believe, watching the computer terminal chatter out the WLN a few seconds after drawing a two-dimensional structure and then pressing the "finished" key. This program was used to generate most of the WLN descriptions published in Earl Usdin's WYLBUR-composed book, "Psychotropic Drugs and Related Compounds".[38,39] Richard Feldmann and George Miller (then at NIH) provided additional display contributions to the computerized WLN generation from the DCRT group.[40,41]

In 1974 Lehigh University's Science & Engineering Library established a Repository of Reports on WLN, with a bibliography that Gelberg started.[42] We continue to urge all authors of WLN reports to help maintain this publicly available repository with reprints and reports. We will help to provide updated bibliographies like those we give in "CWIK List News" as long as there is a continuing interest and support among members of the Lehigh Valley Section of the American Chemical Society (ACS) and the Chemical Notation Association.

HOW MIGHT THE WLN BE IN 1999?

At Las Vegas we noted that the WLN symbol set had its 30th birthday last summer (June 1), and Aug 20, 1980, Berzelius' 201st birthday anniversary, was the first anniversary of my new experiences with a powerful text-processing system called "WYLBUR", which I have used to advance the WLN with the larger character set available at all online terminals. The advanced WLN (AWLN) starts as the 1949 WLN did—with the enriched full typewriter keyboard: the AWLN is simpler because *one* mark more closely represents *one* meaning, thus avoiding possible misunderstandings with multimeaning symbols like T and Y.

In a WLN paper presented earlier at Las Vegas, I was pleased to hear Trisha Johns" reminder that our WLN is a *linguistic* rather than merely symbolic notation.[46] Being in Caesar's Palace Hotel reminded me that the greatest oversight of those great Greeks and Romans was their failure to use *spaces* to separate their carved or written words: I have a long computer striptease with this message in large upper case (Roman monument) letters: THEGREEKSANDROMANSRANTHEIRLETTERSTOGETHERLIKETHISOVERLOOKINGTHEOBVIOUS ADVANTAGES OF SPACES BETWEEN THE WORDS. This spacing was a Medieval breakthrough! Our WLN was—and perhaps still is—the only linear notation that uses blank spaces to separate the cyclic units of information: spaced lower case letters locate the ring positions and then show what is there. After 25 years of waiting, we finally have lower case distinctions again, with online computer systems that have lower case printing capability. Few chemists appreciate the heritage

B	C	
	I	
	P	S

Figure 1. The "BC" beginning of the AWLN symbol set.

of these cursive characters: they were created about 1000 years ago by the artistic hand of a skilled Vatican Secretary during the reign of Charlemagne and hence were named the Carolingian Miniscule. Some 500 years later, Gutenberg's Latin contemporaries used that superb symbol set to design and "freeze" lower case Roman letters for the world.

CREATIVE COMPUTER CHEMISTRY IN 1999

We can sharpen our forward vision by looking backward just 6 decades: in 1919 Edwin E. Slossen concluded his best selling book on "Creative Chemistry" with a discussion of the indescribably enormous energy of radioactive decay in radium and then ended the book with the general belief that our control of that energy was forever unattainable: "The atom is as much beyond our reach as the moon".[50] Imagine his amazement if he had been told of America's ability to get closeup pictures of Saturn's moons and rings, a chilly billion miles away, or to put a man on the moon, picking up rock samples like a stroller collecting shells at the seashore!

Soon online computer and word-processing terminals will be as commonplace as IBM's Selectric typewriters are today; by 1999 high schools and alert grade schools will have color-coded chemistry in educational entertainment that goes far beyond today's pinball games of skill: computer-weaned grade-school science students might well be able to tap an online "Chemical Picture Book for Children" with advanced WLN descriptions, because they can comprehend printed pictures of molecules as easily as the far more expensive—and unsearchanble—artistic renditions on starters like gaseous FF, HH, II, NN, or OO diad molecules and OCO, ONN, ONO, OOO, OSO, or SCS triad molecules. They would learn from the beginning that "HH" (as drawn by Slossen in 1919 and by Josiah Parsons Cooke for Harvard College students 100 years ago!) is a true picture of the molecule, whereas "H2" reflects the early 19th century formula "parts lists" that need subscripts (originally superscripts) unavailable on standard keyboards. *Letters* are searching *signals*, and the advanced character set in AWLN is like in infrared-to-ultraviolet spectrum with some 88 sharply quantized "colors".

Graphically direct descriptions like OCO also are very concise connection tables that provide exhaustive atom-by-atom searching and reflect the symmetry of molecules. Thus a pictorial "ONN" istantly provides a deeper understanding than the blindly copied "N2O" marks. It would become obvious even to the young online users that the smartest way to use their enormous computer powers in educational "hunting, fishing, or browsing" games is to describe molecules with the simplest possible linear sequences of chemical symbols like those Berzelius devised in 1813, because these are instant search signals. Berzelius truly became the organizer of chemistry when he said that "The chemical signs ought to be letters, for the greater facility of writing, and not to disfigure a printed book".[51] A truly advanced notation system should be like a work of art as defined by poet John Keats: "A thing of beauty and a joy forever".

The game-playing introduction to the WLN is limited to nine very frequently cited atomic symbols; it begins with "BC", has "I" in the middle, like "hurricane", and appropriately ends with a "PS", as shown in the very easily remembered tic-tac-toe

B	C	F
H	I	N
O	P	S

Figure 2. The Berzelian beginning of AWLN.

A	D	E	L
G	J	K	M
Q	R	T	V
W	X	Y	Z

Figure 3. Advancing the Berzelian beginning with 12 WLN letter symbols and 4 AWLN symbols: D for unbranched CH, L for CH2, T for T-branched =C<, and J for a similar junction —N<.

(Figure 1). B is for *boron*, named after ancient Arabian-desert *borax*. C is for *carbon*, from "*carbo*", the Roman name for *charcoal*. I is for *iodine*, named after its violet vapor. P is for *phosphorus*, which glows in air. S is for *sulfur*, spelled with "F" (not "PH") by the Romans. Now the puzzle-solving challenge to this elementary 3 × 3 set is to fill in the four remaining blanks with similar single-letter symbols (all well-known in grade-school chemistry) for four important gaseous elements—in an alphabetic sequence that begins (BC) and ends (PS) with two pairs of symbols for the nonmetallic solids (Figure 2).

Now, what equally important "glorious green gas" in group 7 deserves that *seventh* single-letter symbol, a virtual fusion of its 150-year-old marks? Berzelius firrst denoted it with the single-letter "M", for the "Muriatic" radical.[51] What companion halogen, Extracted from the "sEa", can have an "Equal aim" letter Extracted from the front of its 154-year-old mark? The guiding "least effort" aim of the WLN is that the simplest symbols are the best *signals*.

EXPANDING THE WLN LETTERS TO THE AWLN LETTER SET

The WLN start of the AWLN symbol story echoes an ancient Egyptian rope trick that Pythagoras popularized: "magic" squares of 3 × 3 and 4 × 4 add up to 5 × 5. The 3 × 3 WLN set shows a long-overlooked teaching aid: it associates the *nine non*metals that have one-letter symbols and are so important that each should retain its ideal "signal".

Next, the 4 × 4 square (Figure 3) shows how four AWLN letters (D, J, L, T) perfect the 1949 WLN set with "3-D" interrelations: "AD" appropriately matches the "BC" above it; E is under pictorially related F, J is under I, Q is under O, and R is under P. In AWLN, A is for Any Alkyl, and D is for the Dehydrogenated Diatomic CH group (suggesting a reversed C with a closing H line). E is for a bromine atom (in sEa). G is for an atom of Green "Glorine" Gas. J is for the Junction –N< of tertiary amiNes. K is for the "Kationic" >N<(+) of "Kwat" salts. Corner-fiLLing L is for the aLLyL :CH_2 group, L shaped with H atoms above and to the right of the holding C atom. M is for the Mid-aMIDo (aMino/iMIDo/iMino) NH group, seen as N atom with an H prop. Q is for an OH group, picturing an O atom with an H tail. R is for the Resonating Regular-hexagonal Ring, pictured with ortho-bonding legs. T is for a T-branched :C< atom, as in Thioketo S:C< groups, while V is for the Very common di-

Valent carbonyl O:C< connectiVe that also incorporates a ternary :C< atom. W is for the two branched dioxygen atoms, Whispered as "double U" in the traditional DOUBLy-Unsaturated $-NO_2$ and $-SO_2-$ groups. X is for the X-branched quaternary >C< atom, and Y is for the related Y-branched –CH< group. Z is for the end-NH2 groups in hydraZine, seen as "an N on end" when rotated 90°. Thus ends the A, B, C's of the WLN and AWLN single-letter sets.

HOW AWLN ADVANCES THE WLN

The AWLN lower case letters alone achieve spectacular reductions in unwanted search "hits", apart from their educational desirability. Thus in a WLN file of 30 000 herbicide-tested compounds, the 590 boron records are buried in the 13 000 "B"-containing records, because most of these are spaced-B locants. In AWLN as in the 1949 WLN, LOwer CAse letTErs LOCATE all ring positions, so the "B for boron", "C for carbyl carbon", and "A for alkyl" are easily separated letter signals. Only 33 of 5300 A-containing WLN records are alkyl A; about 5000 are a locants, and some alkyls can be lost in deleting all a-locant items. Similarly overloaded WLN letters D–F provide more discriminating online searching with lower case distinctions. At the other side of the lower case usage, locants cited for rarer ring structures like bridged or perifused points are not lost among frequently cited atomic group symbols, even when these are not prefixed by blank spaces. Thus the cited last locant in perifused systems is prefixed by a uniquely distinctive comma in AWLN. Branched locants are suffixed by a rarely used single prime, instead of the overworked WLN hyphen. The nearly 20 000 benzene ring symbols are immediately recognized as "C6H5" if "R&" or terminal, "o-C6H4" if "R b", "m-C6H4" if "R c", "p-C6H4" if "R d", branched "C6H3" if "R*", "C6H2" if "R#", "C6H" if "R%", and completely substituted "C6" rings if "R$"; these same priming marks are used to show corresponding connectivities of –Mt atoms, as explained briefly below, with the single- and double-prime starters. The meanings of WLN digits also are sharpened: arabic numerals in the AWLN symbol set are restricted to alkyl ends or links, because D, L, and T symbols more sharply define :CH, :CH2, or noncarbonyl :C< groups. Eight "online" punctuation marks very sharply define connectivities of P, R, S, and rarer symbols in this order: ' " * # % $ < @. The 1- or 2-connected R and S, 3-connected B, and 4-connected P are the most commonly met types of these groups, so have no AWLN prime marks: SHPO&R&BHH thus denotes HS-P(:O) (C6H5)-BH2; QR d1 denotes HO-C6H4-4-CH3.

AWLN ring systems are readily recognized because they use the "ring-closing" parentheses of 1949 WLN's. Saturated systems have a suggestive $ATURATION $ mark, and in mixed sets, the @-mark tallies @ROM@TIC rings: tetralin thus is denoted distinctively as (66@$).

Polycyclic *ring analysis* begins with the elucidating equation for the number of rings (n) in any path of atoms having extra bonds (e) beyond the two needed to get into the loop: $n = 1 + e/2$. That is, each *pair* of ends can connect in any way whatever to add another ring to the first one. This fundamental analysis continues with the recognition of just 2 bicyclic types: "YY" points in the fused or bridged and an equivalent "X" point in spiro, 8 basic tricyclic types—ending with 5- and 6-connected (chelate) patterns, and 43 tetracyclic types, as I explained in the 1963 Airlie House conference.[43] In AWLN, 2-connected locants that appear in more than *one* ring are cited after a spaced ditto (") mark, 3- and 4-connected locants that appear in more than *two* rings are cited after discriminating spaced * (for 3) or # (for 4) marks, 5- and 6-connected locants that appear in more than *three* rings are cited after % (for 5) or $ (for 6) marks, and 7- and 8-connected locants that appear in more than *four* rings are cited after spaced < (for 7) or @ (for 8) marks. These measures are for the ring system itself and not for the substituted ring descriptions. Even though such "chelate" structures were not in Patterson's Ring Index, these are important polycyclic forms that demand fully extended systematic symbols.

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Chemical Supply Catalog Indexing: Now and the Future. An Ideal Place for Use of the Wiswesser Line Notation†

MURRAY D. ROSENBERG,* MARIAN Z. DEBARDELEBEN, and JOHN F. DEBARDELEBEN‡
Research and Development Department, Philip Morris Research Center, Richmond, Virginia 23261

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This paper covers the traditional indexes found in single-source catalogs, complied catalog listings, and approaches to improve access to a chemical supplier. The approach by Fraser Williams Ltd. in their originally called "Index to Commercially Available Chemicals" (CAOCI) in compiling the listings of many chemical supply catalogs in one source, with frequent and accurate updates, and the use of Wiswesser line notation (WLN) as an additional index, now called "The Fine Chemicals Directory", are recommended.

INTRODUCTION

As the basic source for the starting materials or building blocks for practically all research and many development projects, chemicals (organic, inorganic, etc.) serve many masters in industry, government, and academia. The user of chemicals at these institutions and organizations must at one time or another resort to a chemical supply listing or catalog or, as in most cases, to many listings or catalogs to find a source or sources at a reasonable price. Significant savings are to be made by ensuring that a chemist uses a readily available starting material to prepare a compound by the most practical synthetic route. To reach this goal, chemists should have access to files of internally prepared compounds as well as commercial sources.

For those compounds prepared within a company, manual or automated systems are usually available to provide information. On the other hand, access to commercially available compounds is somewhat limited. Until recently there have been only two types of sources. We have had the individual supplier catalogs, either of a specialist nature (e.g., Alfa Products'[1] phosphonic acids listing or Pyrazine Specialties[2] catalog) or a general nature (e.g., Eastman's[3] organic chemicals catalog, Aldrich's[4] handbook of fine chemicals, and catalogs by companies like Takeda Chemical Industries,[5] Hopkin & Williams,[6] and Fluka[7]). We have also had such compilations as Chem Sources-USA,[8] Chem Sources-Europe,[9] Chemical Week's[10] Buyer's Guide, Chemical Marketing Reporter's OPD[11] (Oil, Paint, and Drug) Chemical Buyers Directory, Stanford Research Institute's[12] Chemical Economics Handbook, etc.

In February 1979, Fraser Williams (Scientific Systems) Ltd.[14] offered to make a set of the Index of Commercially Available Chemicals (CAOCI) available to the Technical

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‡ Richmond Organics, Inc., Ashland, VA 23005.

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