

The Retrieval & Dissemination of Chemical Information. II. The Wiswesser Line Notation

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In a previous editorial in this series⁽¹⁾ I noted that *Wiswesser Line Notation (WLN)* is the coding system we use for the *Index Chemicus Registry System® (ICRS®)* and that *ICRS* makes chemical-compound substructure data available in a form that can be searched by computer.

Many manual searches can be made simply by referring to the printouts provided as part of the *ICRS* system and available separately as the *ICRS Substructure Index*. You don't have to master every detail of *WLN* to understand these printouts for retrieving information from *Current Abstracts of Chemistry and Index Chemicus*.^{T.M.} A basic grasp of the notation symbolism will suffice⁽²⁾. To formulate complex searches in the *ICRS* system a more detailed knowledge of *WLN* is helpful⁽³⁾

WLN was introduced in 1950 by W.J. Wiswesser. He published an excellent account of the system in 1954⁽⁴⁾ which has now been supplanted by the recently published Manual⁽³⁾. *WLN* uses the ten numerals, 26 capital letters, three punctuation marks (&, -, and /) and the blank space. Thus, *WLN* can be used on any computer or punched-card accounting machine that handles alphabetic information.

WLN uses most of the standard symbols for chemical elements, but

single letters of the alphabet represent the most frequent elements and groups. Much of the popularity of *WLN* is due to the simplicity of the notation.

WLN was chosen for *ICRS* because it is an *operationally practical* and tested system. Well over 2,000,000 compounds have been encoded in *WLN* by members of the Chemical Notation Association, an international group formed to control *WLN* rules. The *WLN* system produces a detailed, definitive description of each compound. It is compact and minimizes computer storage.

Unlike atom-by-atom connectivity tables, *WLN* is readily used in systems for selective dissemination of information, as well as for retrospective search. For example, in ISI's *RADICAL*.^{T.M.} software the "Floating Stem" question is used to search the *WLN* for any desired string of characters defining a given substructure.

ICRS will be briefly summarized in the next part of this series. If you would like more detailed information immediately, please do not hesitate to let us know, or to request a reprint of an excellent paper by Wiswesser and Barnard⁽⁵⁾.

1. Garfield, E. The retrieval & dissemination of chemical information. *Current Contents*, No. 28, July 15, 1970, pp. M1-2.
2. A brief description of the notation with samples of its use is available on request to ISI.
3. Smith, Elbert G. *The Wiswesser Line-Formula Chemical Notation*. McGraw-Hill, New York, 1968, 309 pp.
4. Wiswesser, William J. *A Line Formula Chemical Notation*. Thomas J. Crowell, New York, 1954, 149 pp.
5. Wiswesser, W.J. & Barnard, A.J. Jr. The retrieval of chemical structure information. *Brit. Soc. Rheology Bulletin* No. 2, 1968.