Vapor–Liquid Equilibrium Database

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It has been said that the most ubiquitous process in the chemical industry is separations. This combination of book, database, and retrieval software deals with the underlying data behind the most common type of separation, distillation. The fact that almost 9000 references to vapor–liquid equilibrium (VLE) data on over 12 000 systems are covered attests to the practical importance of this class of data. The references cover the period from 1900 to 1991, and an update is promised for 1994. Both organic and inorganic compounds are covered, including aqueous solutions of electrolytes. Mixtures of up to nine components are included.

The book contains 724 pages of literature citations and indexes. The basic index, arranged by molecular formula, allows one to locate a desired multicomponent system; a reference code then leads to the pertinent citations. Since molecular formulas for more complex molecules can require some effort to work out, a separate alphabetical index to compound names and synonyms is given. With this index one can quickly find the molecular formula, as well as the Chemical Abstracts Service Registry Number (CAS RN), for each component. Since all commonly encountered synonyms are included in this index, it is not necessary to know the systematic name in order to locate a compound.

While the book alone constitutes a valuable reference source, the diskette which accompanies it adds another dimension. The program on the diskette allows one to specify each component of a mixture of interest by name (trivial or systematic), formula (written in any order), or CAS Registry Number. Different components may be specified in different ways. Fragments of a name or synonym may be entered, and the program returns a list of names from which the user can select the desired compound. After building up the list of components in the mixture, the user can order a search and obtain all the citations to vapor–liquid equilibrium data on that mixture. There is an option of returning only the references for the precise mixture specified or all references for systems with those components and other constituents as well. For complex multicomponent mixtures the electronic search is certainly more efficient than using the indexes in the book alone. Also, the electronic search returns all the citations in one batch, which is a convenience if the number of citations is large. When using the book alone, it is necessary to copy the reference codes and look up each one separately.

The program on the diskette also permits one to search for references on the basis of author, journal, and/or time period.

This is convenient if one remembers that a particular author worked on certain systems of interest but does not recall the details. After locating the relevant citations, the systems reported in each reference can be displayed. More complex searches can be done in which restrictions are placed on both the systems and the references. After any search is completed, the results can be printed or written to an ASCII file with a simple command.

The software requires DOS 3.3, 640 kbytes of RAM, and 7 Mbytes of hard disk space. It is supplied in packed form on a single high-density diskette. All searches tried by the reviewer ran in a few seconds or less on a 486 machine. The book contains very detailed instructions on how to carry out various types of searches, and on-screen help messages are provided. However, the software is highly intuitive, and the reviewer was able to pick up the basic search procedures very quickly without studying the instructions.

The software appears to be very robust and has many features that should serve as a model for user-friendly chemical databases, such as the ability to search on any name without worrying whether it is systematic or trivial and the ability to enter H_2SO_4 without converting it to a proper molecular formula in the Hill convention. There are nice touches such as error checking of CAS Registry Numbers and ISSN designations for journals; if there is no hit on a CAS RN, the user is told whether the entry is invalid or whether the compound is simply not in the database. In fact, the software could be useful even to those who have limited interest in VLE data. It provides a very convenient way to get CAS Registry Numbers from names or formulas, systematic names from synonyms, and other permutations of these items. Over 2200 chemical substances are covered, all of industrial importance.

It will be interesting to see how the concept of a combined electronic–hard copy product is accepted. Such products are becoming more common, both for scientific information and consumer items like dictionaries. Perhaps this approach will improve the sales of chemical databases, which frequently have been disappointing.

REFERENCES AND NOTES

(1) Vapor–Liquid Equilibrium Bibliographic Database is available from ELDATA, 81–83 rue Michelet, 93100 Montreuil, France (Phone: 33-1-4988-3046. Fax: 33-1-4988-3045). The list price is French Francs 2750, approximately $490 (includes book and diskette); educational institutions receive a 10% discount. The authors are I. Wichterle, J. Linek, Z. Wagner, and H. V. Kehiaian.

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IUPACSEARCH 1.0 (for DOS)

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IUPACSEARCH (version 1.0) is a bibliographic database that provides summaries of nomenclature and symbol recommendations, as well as technical reports, published in *Pure and Applied Chemistry* from 1960–1992. References to basic IUPAC nomenclature books are also included.

Searching the database is analogous to CD-ROM products in that, after selecting an appropriate option (e.g. IUPAC Body/Year or Keywords), one is offered a list of categories. Selection of a particular category then allows one to enter a term of interest, and, if found, the number of occurrences is displayed. As an aside, the number of occurrences (count) often does not agree with the number of retrieved records. Selecting the term then retrieves the relevant records, which are displayed in chronological order.

Options available under IUPAC Body/Year include the following: Division/Section, Commission, Standing Committee, Division + Commission, Access Number, and Year of Recommendation. Options available under Keywords include the following: Abstract + Title, Title and Author.

Selecting Mercury, for example, in the Keyword/Title category retrieves 10 records of which three are the successively updated procedures for the determination of mercury content of foodstuffs published in 1965, 1979, and 1984.

Superseded records do not consistently note that updated recommendations are available and also do not include direct references to the most recent version. For example, there are entries for the 1970 and 1979 editions of the *Manual of Symbols and Terminology for Physicochemical Quantities and Units*. While there is a note in the record for the 1979 edition, "superseded 1988 book form", it omits mention that the title has changed to *Quantities, Units and Symbols in Physical Chemistry*. As an aside, the current version was published in 1993.

The product is obviously useful, and the cost is also very reasonable in that "IUPAC grants to the purchaser/user of IUPACSEARCH the right to copy the diskette and make it available to others for scientific purposes". Hopefully future editions will eliminate the outdated recommendations or, at the least, give direct references to the current version.

IUPACSEARCH is an executable program with the following minimum hardware and software requirements: IBM PC or equivalent, high-density disk drive, computer RAM of 640 kbytes or greater, DOS 3.30 or later, hard disk with 4.5 Mbytes of memory available, a printer connected to a parallel port; color monitor desirable.