Chemical Databases from Springer Verlag

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Chemical databases offered by Springer Verlag are described. The databases include ChemReact, a file of 370 000 organic reactions, and LiqCryst, a file of data on some 60 000 liquid−crystalline compounds.

CHEMREACT41 WITH INFOCHEM CD-ROM

The original source of ChemReact is the VINITI/ZIC structural database which was developed jointly by the All-Union Institute of Scientific and Technical Information of the Academy of Sciences of the USSR (VINITI) in Moscow and the German Zentrale Informationsverarbeitung Chemie (ZIC) in Berlin. This database encompasses information on 3.3 million organic and organometallic compounds published in the worldwide literature between 1975 and 1991. From this structural database, a reaction database of 2.5 million reaction was developed.

ChemReact is a subset of this large database with currently 370 000 reaction types out of the full data set. These reaction types have been selected by grouping all reactions with identical reaction centers and identical environments under one type. Each different reaction type is represented only once and by one example but with reference to the total number of published examples. Additional examples can be displayed offline from the InfoChem CD-ROM containing the complete set of 2.5 million reactions.

ChemReact41 with **InfoChem CD-ROM** is a chemical reaction search system consisting of a database of about 41 000 high-yielding organic reaction types from key journals, search software, and the InfoChem CD-ROM for display of the complete InfoChem Reaction Database with 2.5 million reactions.

Reactions were selected from the InfoChem Reaction Database containing some 2.5 million reactions.

ChemReact41 allows for sophisticated reaction substructure searches in the database including atom−atom mapping and marking of reactive centers.

Either ISIS/Draw from MDL or STN Express from STN International is required (not contained in this package) to display reaction graphics and textual information.

Hardware Requirements

 IBM PC or compatible, CPU 80486

 8 MB RAM

 Mouse

 VGA monitor or higher resolution

 50 MB free disk space

 DOS 3.1 or higher

 CD-ROM player (for InfoChem CD-ROM only)
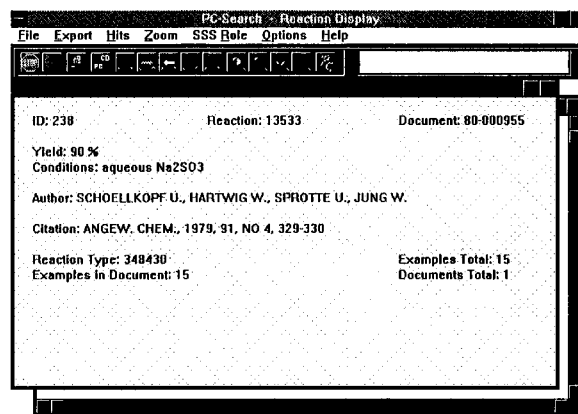
 MS Windows 3.1, Windows95

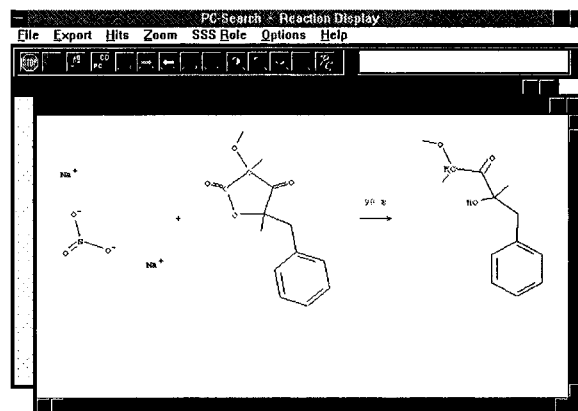**Figure 1.** ChemReact41: Data display for a reaction.

Figure 2. ChemReact41: Reaction graphics for a reaction.

Additional software: ISIS/Draw 1.01 or higher (MDL Information Systems, Inc.) or STN Express 3.12 or higher (STN International).

LIQCRYST

LiqCryst is a database of critically selected and evaluated data on more than 60 000 liquid−crystalline compounds with citations including patents on CD-ROM. The liquid−crystalline phases and states are characterized, and the transition temperatures and heats of transition are given.

Liquid−crystalline research encompases three major fields: physics, chemistry, and the biological sciences. Over the years an interdisciplinary research effort has generated fascinating interactions and developments both basic and applied research; and this research has resulted in an increasing number of liquid−crystalline compounds—from 14 000 in 1982 to more than 50 000 in 1992. The physical,

CHEMICAL DATABASES FROM SPRINGER VERLAG

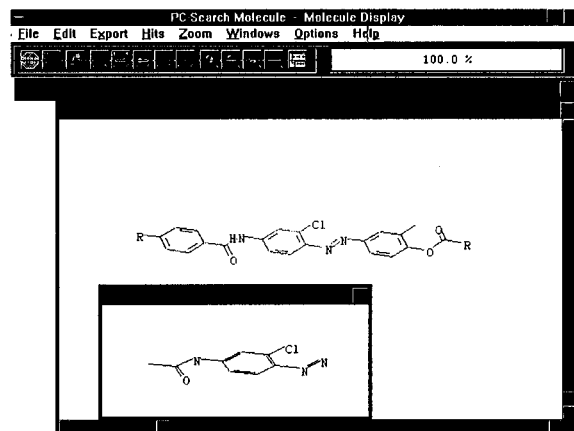*J. Chem. Inf. Comput. Sci., Vol. 37, No. 1, 1997* **155**

Figure 3. Data Search Screen.

chemical, and biochemical properties for each of these compounds have been extensively investigated.

Displays in all sorts of equipment and machines that are in daily use are dependent on liquid−crystalline phases and their technical use. An area of rapidly growing interest and research is concerned with how membranes are formed, their stability, and their molecular−molecular interactions. Liquid− crystalline phenomena are also associated with detergents, lipids, and steroids. Recently polymeric materials with liquid−crystalline properties have proved to be valuable in such "high tech" areas as space research and household equipment.

LiqCryst provides an overall picture of the liquid− crystalline field between 1850 and today. This allows a ready comparison of corresponding data and the elucidation of structure-function relationships.

LiqCryst comes with InfoChem's Windows search software PC-Search. PC-Search allows for sophisticated structure/substructure searches in LiqCryst. Either ISIS/Draw from MDL or STN Express is required for structure input. Queries are then copied to PC-Search via the Windows clipboard.

Figure 4. Hit Display Screen, data window.

Search options:

Structure/substructure
Property data
Bibliograhpic and patent information
Combined searches
Hitlists can be combined with Boolean operators

Display:

Structure (if a substructure search was performed, the substructure is highlighted)
Data, bibliography and source
Field order in the display definable by user
Export:
into an Excel worksheet

The data can also to be found in the Handbook Landolt-Börnstein, New Series, Group IV: Macroscopic and Technical Properties of Matter, Volume 7: Liquid Crystals, Subvolumes a−f.

System Requirements:

IBM PC or 100% compatible 80486 CPU
Mouse
8 MB RAM
VGA or higher resolution
80 MB free disk space
CD-ROM player (for installation)
MS-Windows, version 3.1, or Windows 95

Additional software:

For single user or LAN version: ISIS/Draw 1.01 or later (MDL Information Systems, Inc.) or STN Express 3.12 or later (STN International)

optional:
Microsoft Excel, version 4.0 or later for data export

Substructure Search:
substructure search screen