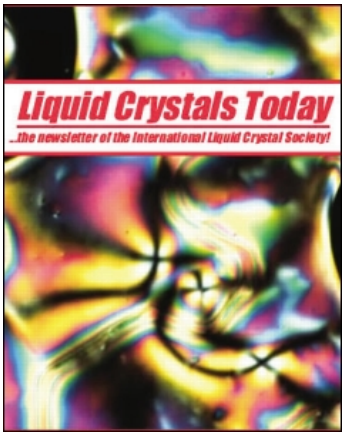


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# Conception and Realization of a Liquid Crystal Database LIQCRYST

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# Conception and Realization of a Liquid Crystal Database LIQCRYST

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**The term liquid crystals covers a wide area of chemical structures, physical properties and technical applications. Thousands of papers contain our knowledge of liquid crystals in words and numbers, but how can we easily access this information, and how can we use the numbers?**

The database LiqCryst documents all recorded physical properties based on the chemical structures of single component thermotropic liquid crystals. Compounds such as biphenyls, soaps, cellulosics, elastomers, cholesterol esters etc. are listed with their transition temperatures, enthalpies and physical properties. Furthermore, all this data can be used to get basic information about structure–property relationships.

The database comprises more than 58000 compounds extracted from 10 000 references [1]. Not only journals and books have been searched, but also patent literature, conference proceedings and PhD theses. Part of the data is published in the Landolt-Bornstein series of liquid crystals [2], and electronic media should be available in the near future [3]. A short overview of the principles, concepts and options of the PC version of LiqCryst is given below.

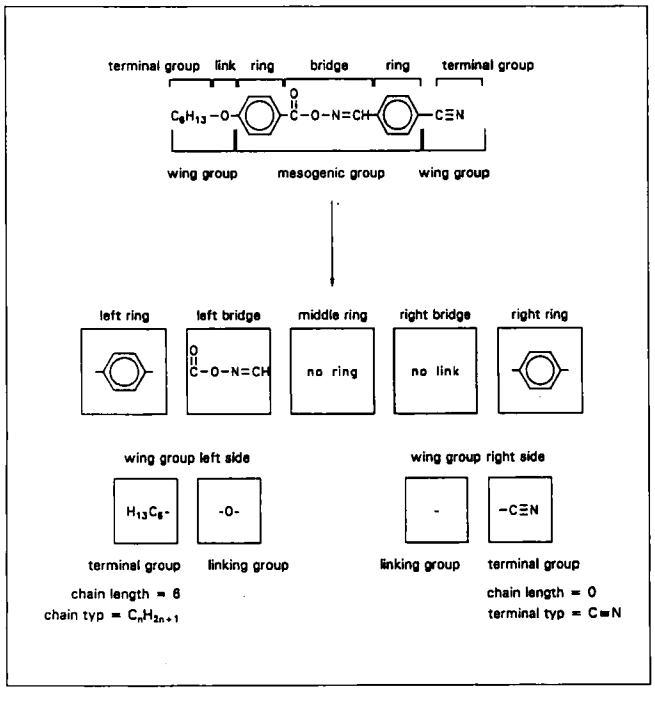


***Figure 1.*** *Fragment system used for structure searching in LiqCryst.*

LiqCryst uses the 'Lego'-model to describe the chemical structure of compounds to be searched (figure 1). The liquid crystal is represented by a linear list of fragments. The main cut is the division of the structure into the mesogenic group and two wing groups. The mesogenic group consists of rings and bridges, while the wing group consists of links and terminal groups. Rings are 1,4-substituted phenyl, 2,6-substituted naphthalene; bridges are –COO–, –CH=N–, –CH=CH–; links are –O–, –CO–; terminal groups are groups such as –CN etc., and various straight or branched alkyl chains. Search is possible by structures, substructures, mesophases, transition ranges, trivial names, authors, sources, chemical elements etc., and additionally all liquid crystals have a set of transition temperatures, which can be searched by numerical values.

Physical properties and chemical structures can be defined by simple numbers, and in setting up LiqCryst, the following questions were considered. Can the compilation of numbers relating to physical properties and structures be used to generate new information? Can laws be identified which define the relationship between the numbers, and can a simple incremental system be established to predict physical properties? LiqCryst supplies the tools for a statistical analysis of the data. It has been shown that it is not possible to develop a simple additive system, and it proves difficult to correlate molecular fragments directly with increments in transition temperatures. However a useful strategy is to compare differences in structure with the differences in transition temperatures. This kind of correlation can give information about mesomorphic sequences, e.g. for the nematic phase the transition temperatures follow the sequence: –COO– < –COS– = –N=N– < –CH=N– < –CH=CH–; the compatibility of fragments by examining deviations from the simple law, the influence of flexibility, and the influence of dipole moments on transition temperatures. The procedures programmed into LiqCryst can be used to predict the

transition temperatures of a new compound or just evaluate the data of a known compound. Figure 2 demonstrates the process: a 'new' structure such as MBBA is created, and the measured clearing temperature was 48°C, what would be the expected transition temperature from a knowledge of other structures? The program first searches for similar structures, e.g. compounds which differ in one fragment. EBBA is such a compound. The clearing temperature is 79.8°C and the structural difference is the replacement of a ethyl group by a methyl group. A single extrapolation to MBBA gives a predicted transition temperature of 58.9°C. Using comparisons with 30 other similar compounds gives a predicted transition temperature for MBBA of 52±6°C. Figure 3 gives more examples of extrapolation including smectic phases and melting temperatures. This method works well with simple structures and for the nematic phase, but much more has to be done to develop this approach to the statistical analysis of liquid crystal data.

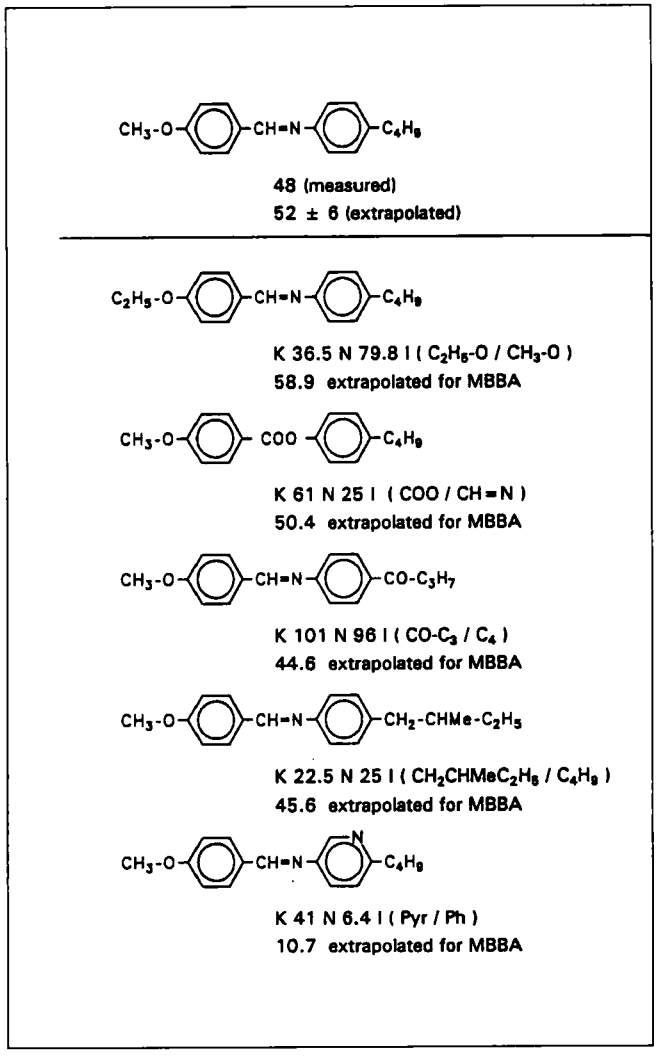


*Figure 2. Extrapolated nematic–isotropic transition temperatures for MBBA based on various parent structures.*

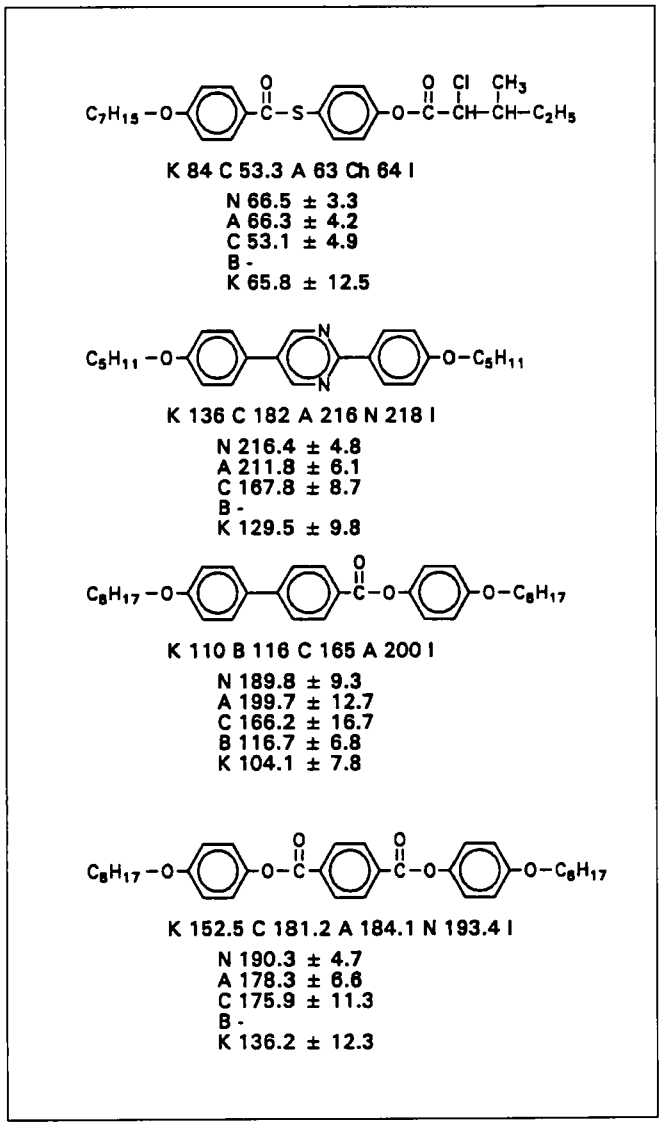


*Figure 3. Extrapolated transition temperatures derived from related structures.*

## References

[1] Vill, V., 1994, *Adv. Mater.* 6, 527.
[2] Landolt–Börnstein, New Series, Vol. IV/7 *Liquid Crystals*, V. Vill (Springer-Verlag, Berlin, 1992-1995).
[3] Vill, V., *LiqCryst - Liquid Crystal Database*, in preparation.

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