Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

A Line Notation for Thermotropic Liquid Crystal Phase Transitions

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Version of record first published: 21 Mar 2007.

To cite this article: Lawrence Verbit (1971): A Line Notation for Thermotropic Liquid Crystal Phase Transitions, Molecular Crystals and Liquid Crystals, 15:1, 89-93

To link to this article: http://dx.doi.org/10.1080/15421407108083226

Molecular Crystals and Liquid Crystals. 1971. Vol. 15, pp. 89–93

Printed in Great Britain

A Line Notation for Thermotropic Liquid Crystal Phase Transitions†

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Received November 23, 1970, *in revised form January* 15, 1971

The recent upsurge of activity in the field of liquid crystals is undoubtedly a prelude to the synthesis of new mesomorphic compounds of varied structures. Liquid crystals are characterized typically by two parameters; the structure of the various phases, e.g. smectic, nematic, etc., and by the transition temperatures between these phases.

The discussion on nomenclature which took place at the 1965 International Conference on Liquid Crystals(1) pointed out the need for an unambiguous system for recording the thermal and structural phase data. However, a look at the recent liquid crystal literature indicates that varied, cumbersome, and sometimes confusing methods of data presentation are in use.

The purpose of this communication is to suggest a unified approach for presenting liquid crystal phase transition data for single component systems. It should be stressed at this point that we are concerned with a method for communicating in as clear and unambiguous a manner as possible the results of thermal and structural phase data; the system which is described does *not attempt to classify* liquid crystal phases.

The proposed method is built on existing notation(2) and entails only slight departures from present usage.

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† Presented at the Third International Liquid Crystal Conference, Berlin, August 24–28, 1970.

The following symbols are used:

Symbol	*Phase*
K (from German, Kristall)	Solid
S	Smectic
N	Nematic
C†	Cholesteric†
I	Isotropic

The following general rules apply:

1. All phase transitions not otherwise specified are to be regarded as enantiotropic.
2. All liquid-liquid transitions, whether mesomorphic or isotropic, are regarded as subject to negligible supercooling. On the other hand, liquid–solid transitions are considered as always subject to supercooling; monotropic transitions are possible.
3. Monotropic transitions are indicated in the notation by parentheses.
4. The line notation begins with the lowest energy modification, usually the solid, and proceeds through the highest energy transition, followed by all monotropic phases written in order of their normal occurrence upon cooling. In other words, the notation is in the form of a heating and cooling cycle.
5. Polymorphism and polymesomorphism are accommodated by appropriate numbering of the phase followed by a comma, with the highest temperature transition receiving the lowest number,(1) e.g.,

   $K2$, $K1$, $S5$, $S4$, $S3$, $S2$, $S1$, $N2$, $N1$, etc.

   Other symbols may be numbered as appropriate.‡

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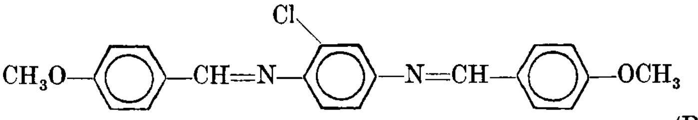
† The cholesteric phase has been shown by several investigators to have a twisted nematic structure. An alternative symbol to C would be N^*. However, it seems clear that the term " cholesteric " will continue to be used albeit with its new meaning.

‡ It is appropriate to emphasize again that numbering of the mesomorphic phases is used to indicate the fact that polymesomorphism exists in a given compound. The numbering is not to be construed as conforming to any *classification* scheme as, for example, Sackmann's classification of smectic phases as Smectic *A*, *B*, and *C* (Arnold, H. and Sackmann, H., *Z. Elektrochem. Ber. Bunsenges. physik. Chem.* **63**, 1171 (1959); Sackmann, H. and Demus, D., *Mol. Cryst.* **2**, 81 (1966)). See also Arora, S. L., Taylor, T. R., Fergason, J. L. and Saupe, A., *J. Amer. Chem. Soc.* **91**, 3671 (1969) for evidence of additional smectic phases which have not yet been classified.

In the following illustrative examples the phase data are presented under the structural formulae using arrows between transitions in order to facilitate comparison with the proposed notation.

Example A—Enantiotropic transition

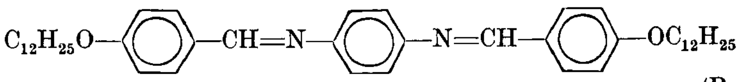


(Ref. 3)

Solid $\overset{131^\circ}{\rightleftarrows}$ Nematic $\overset{275.5^\circ}{\rightleftarrows}$ Isotropic Liquid

Proposed Notation: *K*131 *N*275.5 *I*

Example B—Polymesomorphism



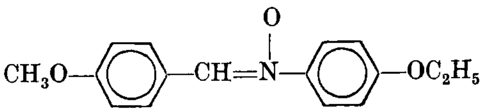
(Ref. 3)

Solid $\overset{122^\circ}{\rightleftarrows}$ Smectic 4 $\overset{131^\circ}{\rightleftarrows}$ Smectic 3 $\overset{134^\circ}{\rightleftarrows}$ Smectic 2 $\overset{157^\circ}{\rightleftarrows}$ Smectic 1 $\overset{204^\circ}{\rightleftarrows}$ Nematic $\overset{205^\circ}{\rightleftarrows}$ Isotropic Liquid

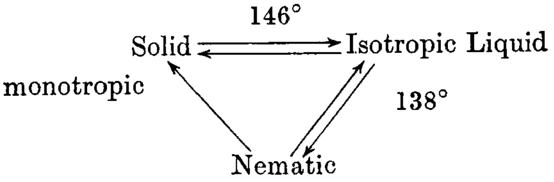
Proposed Notation:

*K*122 *S*4, 131 *S*3, 134 *S*2, 157 *S*1, 204 *N*205 *I*

Example C—Monotropic transition

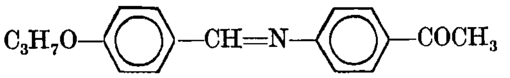


(Ref. 4)



Proposed Notation: *K*146 *I* (138*N*)

Example D—Monotropic polymesomorphism



(Ref. 5)

$$\begin{tikzcd}
\text{Solid} \arrow[r, shift left, "92.0^\circ"] & \text{Nematic} \arrow[l, shift left] \arrow[r, shift left, "101.7^\circ"] \arrow[d, shift left, "90.9^\circ"] & \text{Isotropic Liquid} \arrow[l, shift left] \\
\text{Smectic 2} \arrow[u, "\text{monotropic}"] \arrow[r, shift left, "67.6^\circ"] & \text{Smectic 1} \arrow[l, shift left] \arrow[u, shift left] &
\end{tikzcd}$$

Proposed Notation: $K92.0\ N101.7\ I\ (90.9\ S1,\ 67.6\ S2)$

The proposed notation may be characterized as possessing the following advantages:

1. Simplicity of form and economy of space.
2. The linear form of the notation make it ideal for computer usage; an application which will be more important in the future.(6)
3. The flexibility inherent in the system. For example, the discovery of a fundamentally new type of liquid crystalline phase can be accommodated simply by adding a symbol to represent the new phase.

In conclusion, the line notation system will handle the vast majority of thermotropic liquid crystal phase transition data. One recognizes, however, that the notation is by no means complete. In its present form it does not deal with multi-component systems or, for example, with polymorphic compounds where two solid modifications may each give the same mesophase.(7) As research in liquid crystals progresses, the notation will be further developed.

Acknowledgement

I would like to thank Professor Glenn H. Brown, Kent State University, Professor George W. Gray, University of Hull, Dr. Hans Kelker, Farbwerke Hoechst, and Professor K. Keith Innes, SUNY at Binghamton for valuable discussions.

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