LiqCryst 2019

- Product Information -

Content:

LCI SYSTEMS

Overview

LiqCryst is the world's most comprehensive crystal database and one of the largest numerical material databases at all. Also, LiqCryst enables the user to predict physical properties of chemical compounds by statistical extrapolation of currently known similar compounds.

LiqCryst provides complete documentation of information on currently known liquid crystals.

The aim of LiqCryst is to give insight into the structure-property relationships of liquid crystals by analyzing and comparing the properties of known compounds, and also to enable the prediction of the physical properties of new compounds. LiqCryst is therefore not only a high quality reference work, but also provides the user with a powerful tool for the creation of compounds tailored for specific applications.

With LiqCryst, we offer science and companies a high-quality database and thus an important tool for liquid crystal research with numerous analysis options such as structure comparison, data evaluation and data prediction.

LiqCryst distinguishes between substances, properties and references. Chemical structures can be represented in different notations, e.g. classically by atoms and bonds, as a sequence of fragments (rings, bridges and end groups) or as line notation (single-line structure text description).

In LiqCryst you will find data of liquid crystalline compounds, their structures and physical properties, as well as a multitude of literature references on

- 114.670 Compounds
- 129.753 References
- 448.126 Properties

For all compounds, information is available on phase schemes, phase transition temperatures, elastic constants, spontaneous polarizations and references to literature on spectroscopic properties. Data on the nematic phase can be retrieved for more than 39,000 compounds. In addition to information on 18,000 chiral compounds, LiqCryst also provides data on the ferroelectric smectic C* phase for more than 6,000 compounds.

Functions

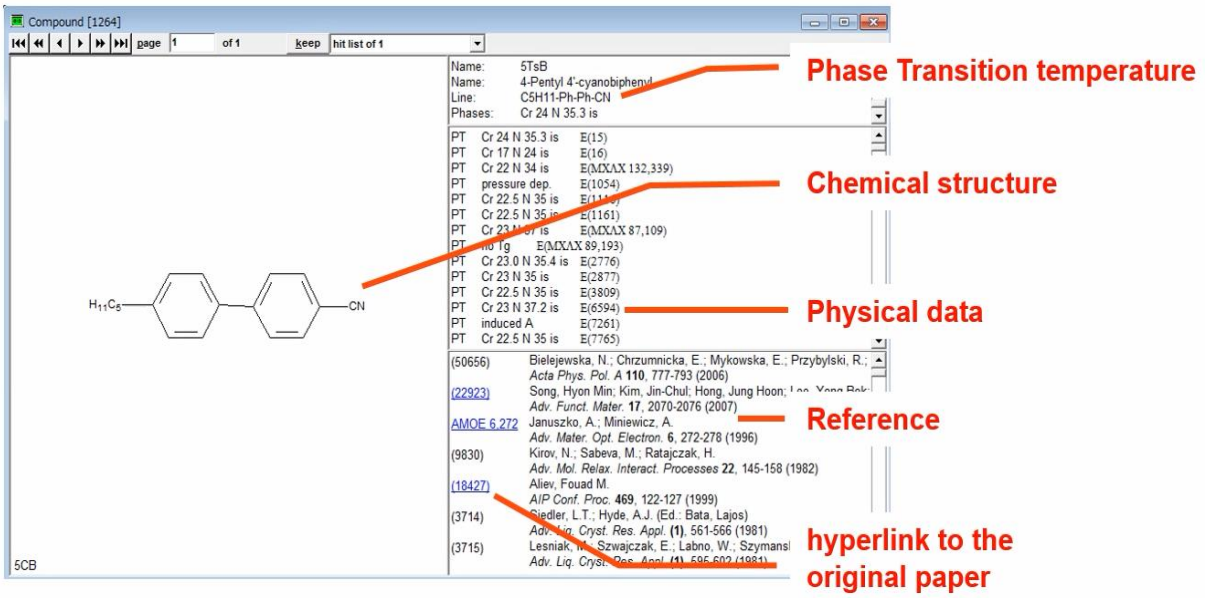
LiqCryst is a Windows-based application that allows easy access to a unique database of structures and properties of liquid crystalline compounds.

The following search parameters can be used:

- structures and substructures
- properties and applications
- similarities
- chemical elements
- phase sequences
- phase transition temperatures
- physical measurements or references.

The search can be performed not only for structures, but also for substructures defined by atoms and bonds or for substructures defined by a list of fragments (ring, bridge, connection, terminal). In addition, physical data such as transition temperatures, mesophases and transition ranges in their numerical values and chemical elements can be used as search queries. A search via trivial names, authors index and specific journals is also possible.

Trends and deviations within homologous series can be displayed graphically.



Data prediction

LiqCryst enables the prediction of phase transition temperatures of new compounds by statistical extrapolation from known similar compounds.

Data analysis

One of the most important functions of LiqCryst is the statistical analysis of structures/ property relationships, e.g. two substructures can be compared by their transition temperatures. Herefore a multitude of comparison tools can be applied to molecules as well as to fragments. This is possible also for named compounds and fragments as well as for structure drawings, which can be created or imported using the structure editor (see below). The same applies to rings or homologous series.

Search functions

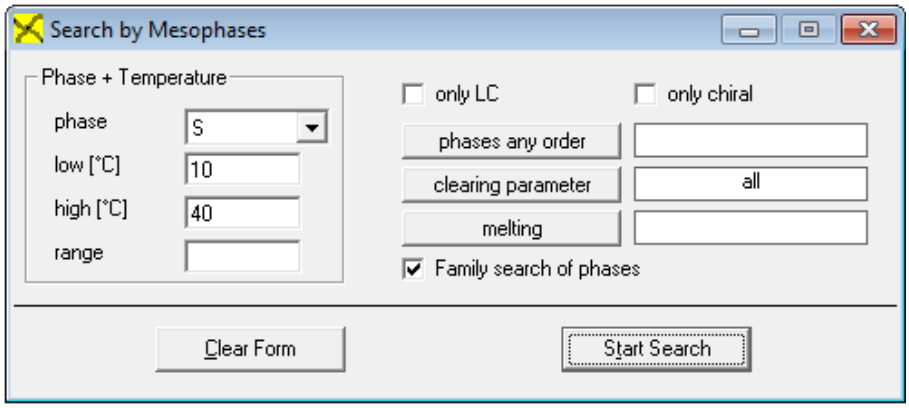
In addition to data analysis, the extensive search options are one of the most important functions of LiqCryst. In addition to the quick search, the following search functions are available:

- Search by substances / compounds
- Search by properties
- Search by references
- Search by (sub)structure drawing

Search by substances /compounds
The search by substances / compounds is based on the name, formula or mass. The following search parameters are also possible:

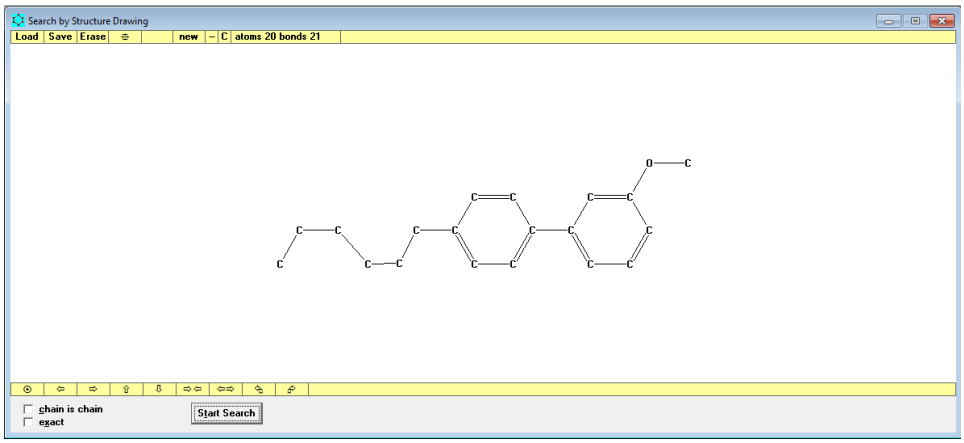
- Mesophases: Search for liquid crystals with identical or similar phase behavior.

  A "search by mesophase" is usually based on a certain phase behavior, so that a list of compounds is created that all have similar phase transition temperatures. The search can be performed around a specific phase transiton temperature with or without temperature limits (these can be in the form of a temperature range and/or high and low temperature values).

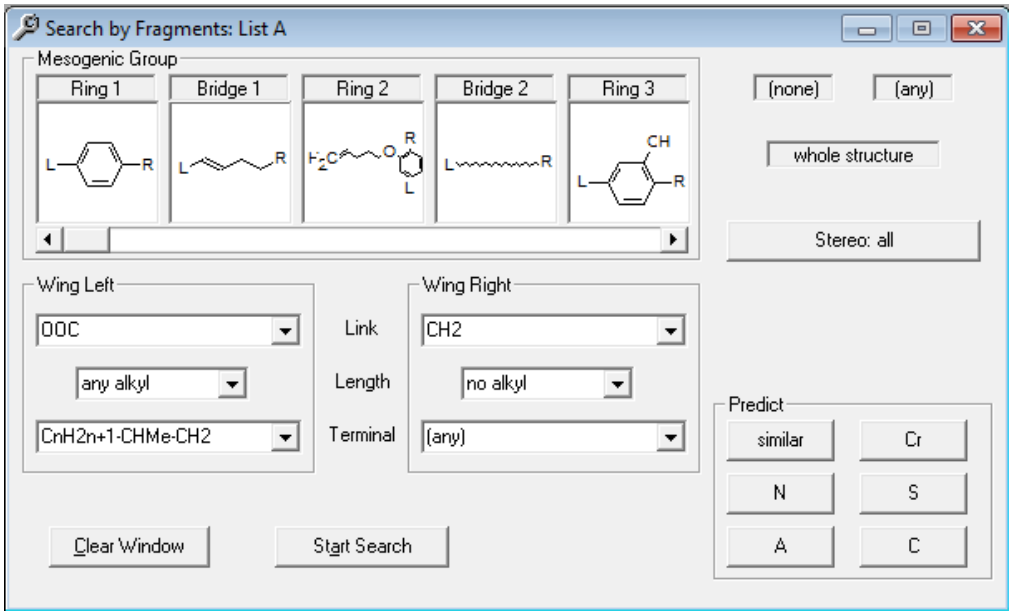


- Line notation: Search by substances or (sub-)structures using a line notation.

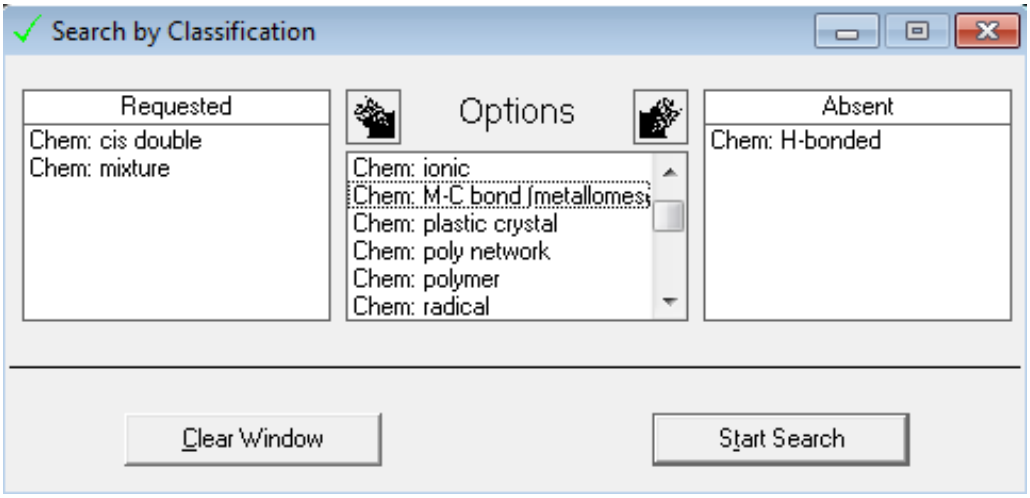
  The "Search by Structure Drawing" is based on the drawing of a liquid crystal molecule. Using this search option you can either edit a previously saved molecule or draw a new one.



- “Search by Fragments": With this search option a chemical substructure is created by selecting substructures for the various sections of the molecule.



- “Search Compounds by Classification" involves the selection of key features of liquid crystal molecules as an advanced search option. To narrow down the search criteria, properties can be requested or excluded to ensure that either all or none of the molecules found in the search have the selected characteristics.



Search by properties
The "Search by Properties" enables the search based on physical properties, e.g. density or phase transition temperature. Numbers, number ranges or text fragments can be used as search parameters.

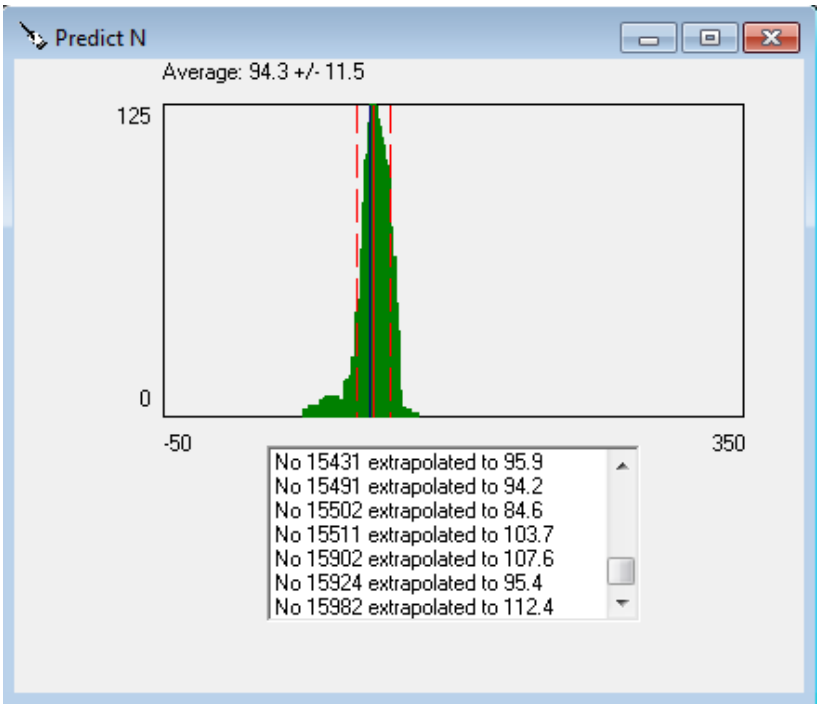
Search by references
"Search by References" refers to literature sources, years, periods, volumes or authors.

Analyses and predictions

Prediction of phase behavior and similarities
The function "Predict by Similarity" shows similarities between molecules and predicts values for the phase.

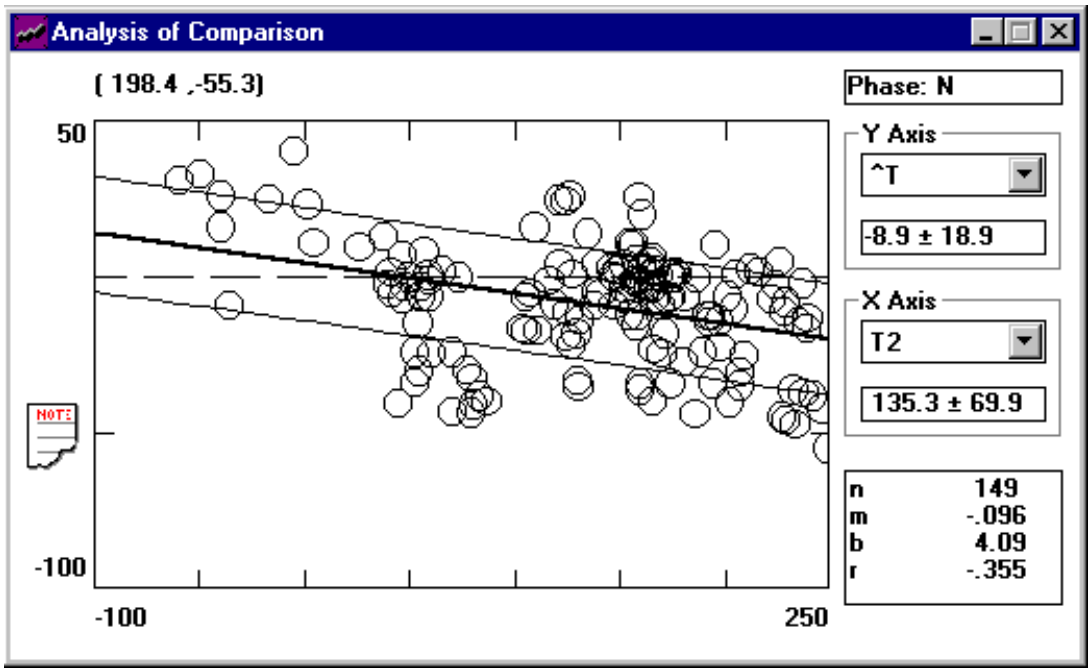
Transitions:
Cr: melting point

- N: Nematic phase transition temperature
- S: Smectic phase transition temperature
- A: Smectic A phase transition temperature
- C: Smectic C-phase transition temperature



Analysis of Comparison

With the function "Analysis of Comparison" LiqCryst enables simple statistical analysis of structure-property relationships, e.g. two substructures can be compared by their transition temperatures. This option allows the investigation of pairs in relation to phase behavior.



Structure editor

The structure editor allows the graphical representation of molecules or single fragments. Various functions are available to simplify the construction of such structures; finished structure fragments can also be inserted into existing structures by drag & drop.

In addition, the structure editor is also able to convert a line notation into a structure drawing - three variants of line notations are supported: LiqCryst line notation, protein three-letter peptide and protein one-letter peptide. The graphical data of the structure editor can also be used for data analysis.

Questions? Ask us!

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