An Anchor in the Flood of Data

As an avid liquid crystal scientist, I find the following scenario happens more frequently than one might think. I am traveling and suddenly realize I need the phases and transition temperatures of some liquid crystal (LC) material. With a connection to the internet, this problem can often be solved by a visit to Liqcryst Online, a web-based "teaser" for the powerful (and expensive) Liqcryst liquid crystal database, now in version 4.0. The full database is legendary, giving the structure of and a large amount of useful data on over 80000 thermotropic liquid crystals; about 50000 of these records were input by Volkmar Vill himself (the living Liqcryst) and about 5000 of the compounds are reported only in theses which Vill has searched for otherwise unpublished information. The database also includes powerful tools for visualization and manipulation of the data, allowing the development of useful insights into structure–property relationships. While the full database is clearly required by well-healed LC scientists, I find that the free web version, while providing only a small subset of the data included in the full Liqcryst, is still extremely useful. Through a web-based interface, searches can be accomplished by registry number, literature, line notation, SMILES strings, abbreviations, and chemical-structure drawing by means of a Java applet. It is in beta testing but works fine on my Mac. It took me only a minute to draw benzoic acid; with no hydrogen counts this yields 27882 matches in a sub-structure search. Search results are returned almost instantaneously due to the efficient structure storage and retrieval approach developed by Vill. Matches are collected in lists which can be displayed, manipulated, and combined. The structure of any of the compounds in the list can be displayed.

Liqcryst Online kindly notifies me of the internal registry number and molecular mass, then frequently states "No further information. Structure is not in the free set." The free database is still very useful. Every search I have done in the database (for about the past three years) is preserved on the Liqcryst server, and can be reviewed in a "history" section. When I feel the need, I can go back to the search I did in the literature tool for all records listing myself as an author. This type of search can be quite entertaining. A search on "Goodby" as an author provided a list of 1181 structures, each of which can be viewed in the free database. Only for the classic LC material *p*-*n*-octyl-*p*'-cyanobiphenyl (8CB), there is a great amount of free useful information. This information is also readily available by typing "8CB" in an abbreviation search. Instead of the dreaded "no further information" the free record for 8CB provides over 200 literature citations (!) on 8CB in addition to the CAS registry number, date of the first publication, and the kind message "Even More Data". A quick click on that link provides the structure, phases, and transition temperatures, an apparently comprehensive list of transition temperatures taken from other literature citations (this can be embarrassing!), the enthalpy and volume changes of the various transitions, the density, refractive indices, dielectric anisotropy and constants, dipole moments, and much, much more from several sources. Each physical property is associated with a reference, and many more physical properties are not given but referenced.

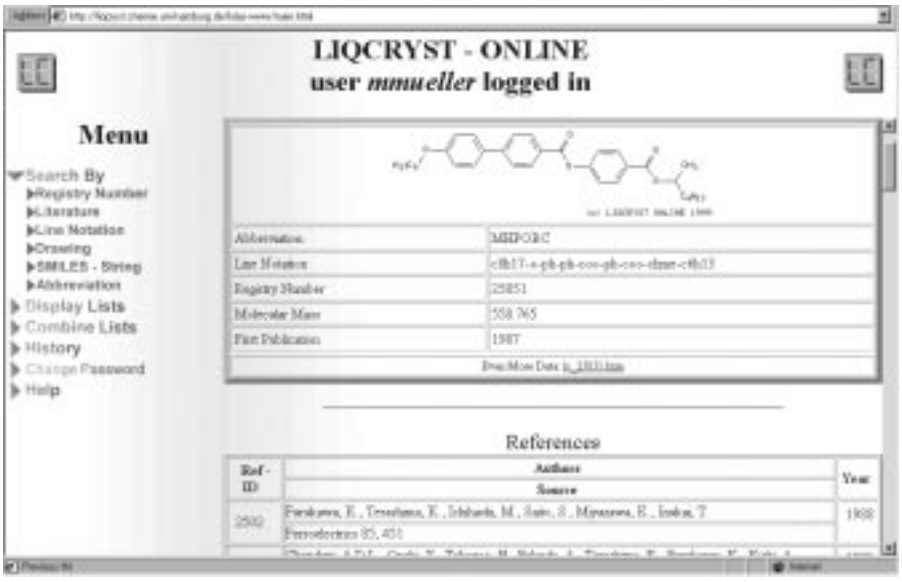

Figure 1. The first screen of information after a search for "mhpobc".

Suggest a web site or submit a review:
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So, the next time you're on the road, or just sitting at your desk, and you have a burning desire to know the phase sequence and transition temperatures of the famous liquid crystal material MHPOBC (at least up to 1997), you can have an answer in a few seconds from Liqcryst Online (Figure 1).

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For further information visit:
http://liqcryst.chemie.uni-hamburg.de/lolas-www/main.html
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