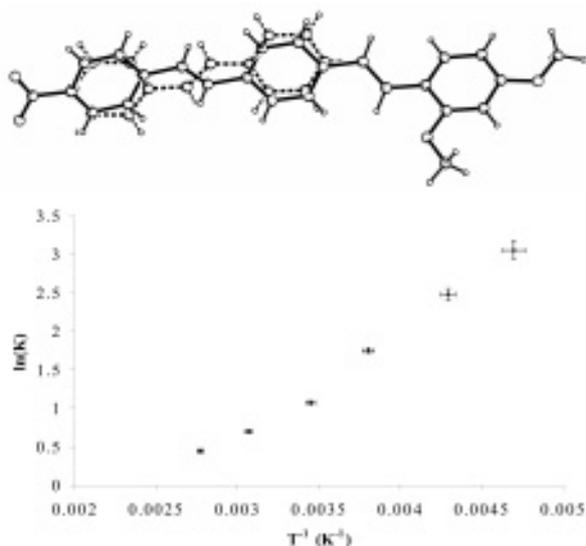


m43.p01**The conformational landscape of stilbenes: a reassuring observation**Roeland De Borger, Alain Collas,
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Keywords: organic phase transitions, thermodynamic properties, organic semiconductors

The pedal-like motion of stilbenes and stilbene-like compounds has recently received some attention [1,2,3]. The disorder of the central double bond is reported to be dynamic, and this disorder or large-amplitude librational motion are invoked to explain the uncharacteristically short observed distances in ethenyl fragments in these types of compounds. We have synthesised an asymmetrically substituted donor-acceptor-type distyrylbenzene which contains a stilbene moiety that is unsubstituted in the four *ortho*-positions. Quantum chemical calculations on the free molecules indicate that the two possible conformers (*syn* and *anti*, see Figure) are quasi equal in energy, providing an objective basis with which to compare the influence of the crystal environment. Measurement of the structure at six different temperatures yields a van 't Hoff plot which is not linear.



This nonlinearity is *not* due to "freezing in" of states, yielding a non-equilibrium state, but, on the contrary, to a change in the entropic and enthalpic contributions to the equilibrium. A report on a benzylideneaniline [3] yields a van 't Hoff plot which is linear from low temperature to room temperature, but does *not*, exactly like the plot above, pass through the origin. Since this is physically impossible (the entropic contribution *has* to become 0 for the maximum amount of disorder at infinite T), we suggest that at higher temperatures a similar non-linearity in the van 't Hoff plot, i.e. a phase transition, could be observed for this compound.

[1] Harada, J., Ogawa, K., *J. Am. Chem. Soc.*, 2001, 123, 10884-10888.[2] Harada, J., Ogawa, K., *J. Am. Chem. Soc.*, 2004, 126, 3539-3544.[3] Harada, J., Harakawa, M., Ogawa, K. *Acta Cryst. B*60, 589-597.**m43.p02****10 Years of small molecule crystallography at the SRS - A users perspective**

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Keywords: synchrotron, calixarenes, supramolecular

We have been using the UK's synchrotron source at Daresbury Laboratory for 10 years. We first collected data during the commissioning phase and have obtained beam time regularly ever since. We wish to present a users perspective on the development of the small molecule crystallography stations, our experiences of using the facility as a whole, and some key results including those most recently obtained.

Key aspects will be:

- Detector advances and effects on data collection.
- Computing developments (hardware and software).
- The opening of the second station 16.2 SMX.
- Key structures and publications in the fields of calixarene chemistry and supramolecular structures.
- Countdown to closure in 2008.
- Looking forward to the UK's new synchrotron - Diamond.