A combined experimental and computational study of anthraquinone dyes as guests within nematic liquid crystal hosts

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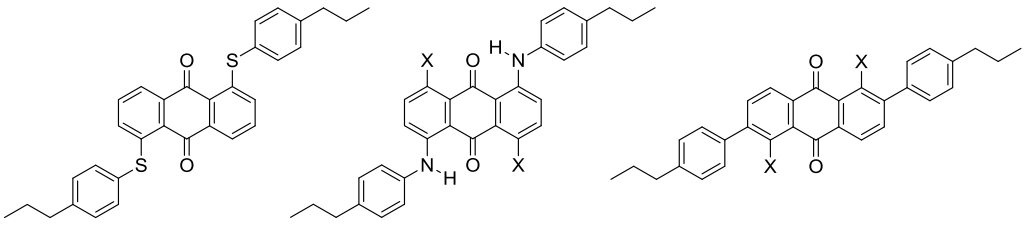
The use of dye molecules within a liquid crystal host has been studied in the past for a wide variety of different dyes and host mixtures, and explored for the development of a range of practical devices. The possible applications of such systems are widespread, with the focus often being on guest-host display devices, which may offer benefits over traditional liquid crystal displays.

For guest-host applications, the alignment of guest dye molecules within a liquid crystal host is important for the development of practical devices, and other factors such as the dye colour, absorption strength, and stability also need to be considered. Hence, it is desirable to obtain a detailed knowledge of the structure and properties of dye molecules proposed for such applications, and the factors affecting their behaviour in liquid crystal hosts.

We have been studying anthraquinone dyes with a range of colours, including some 1,5-disubstituted systems drawn from a class which have been relatively widely studied, and some recently synthesised 2,6-substituted systems,[1] as shown by the structures below.



X = H or OH

Our UV-visible absorption studies of these dyes in a nematic host have provided experimental dichroic ratios of the dyes that give significant differences in their observed order parameters. We have also been carrying out computational studies, including density functional theory calculations on the dyes. The calculated structures of the dyes quantify the molecular shapes, giving aspect ratios that may relate to the geometric alignments of the dyes within a host system, and how this alignment may differ between the dyes. The calculated electronic transitions provide energies for comparison with experimental wavelengths, and also elucidate the orbital nature of the transitions and hence the basis for the variation in colour between the dyes. In addition, these calculations provide transition dipole moments of the dyes that give vectors which, in combination with the calculated shapes, may offer an insight into the significant differences in observed order parameters for these dyes within a liquid crystal host; for example, the host mixture E7.

In summary, a combination of experimental and computational studies on a set of anthraquinone dyes has provided an approach for rationalising the observed differences in behaviour between the dyes, and hence their relative suitability for application as guests within liquid crystal hosts.

References:

[1] S. J. Cowling, C. Ellis, and J. W. Goodby, *Liquid Crystals,* **38**: 1683–1698 (2011).

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