Synchrotron Radiation Linear Dichroism (SRLD) and Time Dependent Density Functional Theory (TD-DFT) Calculations on Dihydroxy-Anthraquinones

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Introduction
Dihydroxy derivatives of 9,10-anthraquinone are widely used as intermediates for dyes, pigments, photographic chemicals, paints and as catalysts in paper industry to improve fiber strength, and also used in manufacturing drugs, for example, stimulant laxatives. But they are no longer used in some countries (USA, UK, ...) because they can cause cancer [1]. Their structures are shown below:

Anthrarufin  Chrysazin  Quinizarin

Of particular importance in the application of dichroic dyes and in optical studies of drug-substrate interactions is precise information of the transition moment directions of the electronic transitions. Linear dichroism (LD) spectroscopy can provide experimental information on molecular transition moment directions, and quantum calculations can predict electronic transitions and transition moments, providing more precise assignment of observed electronic states [2].

Materials and Method
Low density polyethylene (LDPE) is used as an anisotropic solvent. Solute molecules can be partially aligned by uniaxial stretching of the polymer.

The linear dichroism (LD) spectra were obtained by using a traditional spectrophotometer with Glan prism polarizers for the visible and near ultraviolet region (13000-47000 cm⁻¹) and synchrotron radiation linear dichroism (SRLD) spectroscopy for the far ultraviolet region (47000-57000 cm⁻¹). The SRLD measurements were performed at Faculty of Science, Institute for Storage Ring Facilities, Arhus University (ISA). The LD spectra were analyzed by the TEM method [2].

Time-dependent density functional theory (TD-DFT) is used to predict and assign the electronic transitions. This calculational method was applied with success in previous studies [3] on hydroxy derivatives of 9,10-anthraquinone.

Conclusion
SRLD spectroscopy provides additional information on the transition moment directions of the electronic transitions in high energy region. And TD-DFT calculations is a very useful tool in the prediction and assignment of the electronic transitions for these dihydroxy derivatives of anthraquinone.

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References