Poster

Piezosolvatochromic insights into solvent-solute interactions

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Molecular interactions formed between solute and solvent can profoundly affect the optical spectra of solutions, altering the position, intensity, and shape of absorption and emission bands. Solvatochromic dyes, which are particularly sensitive to the physicochemical nature of the surrounding medium, manifest a strong, visible changes in their solution colour [1]. This phenomenon, known as solvatochromism, not only provides a visual representation of dye-solvent interactions, including hydrogen bonds, dipole-dipole, and van der Waals interactions but also offers deep insights into the electronic structure of the dye.

In this study, we employ high-pressure in-situ crystallization and high-pressure UV-vis spectroscopy to investigate the structure-property relationships of solvatochromic effects in the simplest pyridinium N-betaine dye (Figure 1), 4-(2,4,6-triphenyl-1-pyridinio)phenolate, thereafter referred to as ET(1) [2]. Our comprehensive examination of ET(1) in various solvent environments—methanol, ethanol, and acetone—under high pressure, reveals a close correlation between solvatochromism and solvatomorphism. We demonstrate that ET(1) preferentially crystallizes in the form of solvates, with the crystal colour reflecting that of the solutions. The observed piezosolvatochromic effects may be associated to the intricate interplay between solvent polarity, hydrogen bonding, molecular conformation, and crystal packing.

Our findings pave the way for the development of pressure-sensitive photonic materials and molecular sensors, leveraging solvatochromic shifts to design devices capable of optical modulation under varied environmental conditions. This work not only advances our understanding of the solvatochromism process but also highlights the correlation between crystal structure and solute-solvent interactions, marking a significant step towards the practical application of solvatochromic compounds in materials science and nonlinear optoelectronics.

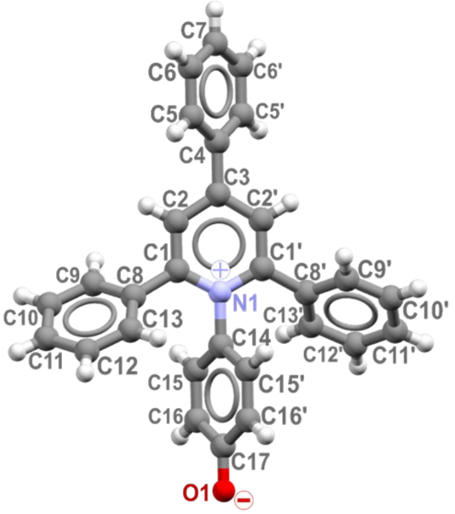

Figure 1. Zwitterion of 4-(2,4,6-triphenylpyridinium-1-yl)-phenolate, ET(1), investigated at high-pressure.

[1] Reichardt, C. & Welton, T. (2010). *Solvents and Solvent Effects in Organic Chemistry* Wiley.

[2] Dimroth, K., Reichardt, C., Siepmann, T. & Bohlmann, F. (1963). *Justus Liebigs Ann. Chem*. **661**, 1–37.

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