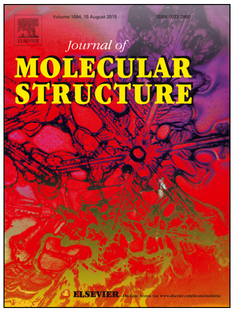

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PII: S0022-2860(18)30196-0

DOI: 10.1016/j.molstruc.2018.02.050

Reference: MOLSTR 24872

To appear in: *Journal of Molecular Structure*

Received Date: 4 September 2017

Revised Date: 15 January 2018

Accepted Date: 12 February 2018

Please cite this article as: K.L. Hayes, E.M. Lasher, J.M. Choczynski, R.R. Crisci, C.Y. Wong, J. Dragonette, J. Deschner, A.J.P. Cardenas, Brooker's merocyanine: Comparison of single crystal structures, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.02.050.

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Brooker’s Merocyanine: Comparison of Single Crystal Structures.

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A R T I C L E I N F O

Article history:
Received 00 December 00
Received in revised form 00 January 00
Accepted 00 February 00

Keywords:
Each keyword to start on a new line

A B S T R A C T

Brooker’s merocyanine and its derivatives are well-studied molecules due to their very interesting optical properties. Merocyanine dyes exhibit different colors in solution depending on the solvent’s polarity, pH, aggregation and intermolecular interactions. The synthesis of 1-methyl-4-[(oxocyclohexadienylidene)ethylidene]-1,4-dihydropyridine (MOED) dye yielded a particularly interesting solid state structure where in one crystal lattice, MOED and its protonated form are bound by hydrogen bonding interactions.

1. Introduction

Merocyanine dyes are a fascinating class of organic molecules due to their optical properties[1-4]. These molecules can absorb different wavelengths of light depending on certain parameters such as solvent polarity, pH, intermolecular interactions, etc.[3, 5, 6] Brooker’s merocyanine or 1-methyl-4-[(oxocyclohexadienylidene)ethylidene]-1,4-dihydropyridine (MOED) is one of the most studied solvatochromic dyes. MOED features a zwittterionic structure that allows it to absorb different wavelength of light depending on the polarity of the solvent (Figure 1)[2, 6]. A non-polar solvent favors the neutral form; A polar solvent, like water, tends to favor zwitterionic form which can be easily distinguished using the C-O bond lengths.[6]

Besides the polarities of solvents, counter ions and aggregation also affect the color of MOED in solution. The effect aggregations either by hydrogen bonding, electrostatic interaction or π-π interactions, on the color, can be utilized as another dimension of modification for photochromic materials.

In 2008, the protonated form of Brooker’s merocyanine was isolated in the form of a dihydrogen phosphate salt (1-methyl-4-[2-(4-hydroxyphenyl)ethenyl]pyridinium dihydrogen phosphate).[7] Similarly, although not in the same extent as the deprotonated form, the protonated form also exhibits interesting optical properties. The aggregation of the salt in solution creates minute changes in the visible spectra of the compound.[7]

In this study, we report an interesting crystal structure containing both the protonated and deprotonated form of MOED. Compounds 1-methyl-4-[2-2(4-hydroxyphenyl)ethenyl]pyridinium iodide (**1**) and 1-methyl-4-[(oxocyclohexadienylidene)ethylidene]-1,4-dihydropyridine dihydrate (**2**) and trihydrate (**3**) were also synthesized and characterized crystallographically for structural comparison.

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Peer review under responsibility of xxxxx.

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http://dx.doi.org/10.1016/j.aebj.2014.10.012