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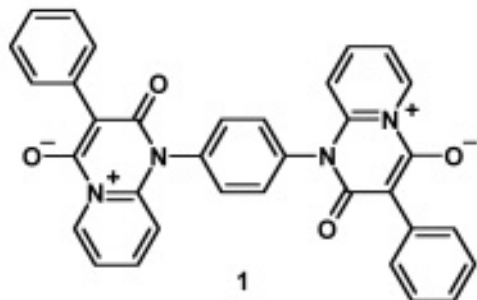
Mesoionic fluorescent organic yellow pigment

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Mesoionic ("zwitterionic") compounds are molecules with both positively and negatively charged atoms [1]. They have recently been synthesized as organic pigments. They show bright yellow colours and strong solid state fluorescence [2]. Because of their poor solubility no crystal structures were known.



Compound **1** has been crystallized out of a mixture of hot N-methyl-2-pyrrolidone and 2-propanol giving yellow fluorescent crystals with sizes up to 0.8 mm. The compound crystallizes in $P\bar{1}$, $Z = 1$, $a = 8.7737(10)$ Å, $b = 10.4982(11)$ Å, $c = 11.7877(12)$ Å, $\alpha = 98.463(8)^\circ$, $\beta = 101.314(8)^\circ$, $\gamma = 104.750(8)^\circ$, $V = 1007.07(19)$ Å³.

The central phenylene moiety is almost perpendicular to the other parts of the molecule (dihedral angle 84.5°).

[1] C. Plüg, B. Wallfisch, H. Gade Andersen, P. V. Bernhardt, L.-J.-Baker, G. R. Clark, M. W. Wong, C. Wentrup, J. Chem. Soc., Perkin Trans. 2, 2000, 2096-2108.

[2] C. Plüg, T. Metz, Internat. Patent WO 2005/070928 A1.

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4-Bromo-2--[4-(3-metistyl-3-methyl-cyclobutyl)thiazol-2-yl]hydrazono-methyl}phenol, with N-H...N, C-H... π and π ... π interactions

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Keywords: azomethine, graph-set, ring-ring interaction

The title compound contains the thiazole, cyclobutyl, hydrazono moieties. Hydrazine is a highly reactive base and reducing agent. Its primary uses are as a high-energy rocket propellant, as a reactant in military fuel cells, in nickel plating, in the polymerization of urethane, for removal of halogens from wastewater, as an oxygen scavenger in boiler feed water to inhibit corrosion and in photographic development. Hydrazones have been widely studied as chelating ligands for the spectrophotometric and fluorimetric determination of trace metal ions.

The title compound, $C_{24}H_{26}BrN_3OS$, crystallizes in the triclinic space group $P\bar{1}$, with two independent molecules in the asymmetric unit. The molecules adopt an E geometry about the azomethine C=N double bond. The structure is stabilized as dimers by N-H...N hydrogen bonding. C-H... π and π ... π interactions are also effective in the crystal packing.