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Title: ***Solvatochromism, molecular and electronic structures of trans and cis isomers of a typical styryl pyridinium cyanine dye***

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Abstract:

This paper reports on solvatochromism and molecular and electronic structures of a typical styryl pyridinium cyanine dye, 1-methyl-4-(p-N,N-dimethyl-amino styryl) pyridinium iodide (Cy) in both ground and excited states. There is a hyposchromic shift of the longest absorption band, which is greater than that of the bathochromic shift of the fluorescence band, with decrease of the Stokes shift as the solvent polarity decreases. The results confirm the importance of decreasing the dipole moment of Cy upon excitation and solvent polarity function F(D,n), which describes the orientation polarizability of the solvent, in the energetic stabilization of Cy dye in So and S1 states. Semiempirical molecular orbital calculations using the atom superposition and electron delocalization molecular orbital (ASED-MO) and PM3 methods were also performed. The change of the dipole moment upon excitation was explained on the basis of chanes in the charge redistribution over the whole skeleton of the molecules, whch agree well with the experimental results. Also, the nature and energy of the electronic transitions were elucidated and discussed in relation to the experimental data.