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Steady-State Spectroscopy and Ultrafast Dynamics of Flavylum Derivatives in the Red and Near-Infrared Spectral Region

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Abstract

In an effort to enhance the absorption and fluorescence of flavylum in the red and near-infrared (NIR) spectral region, we synthesized a 2'-hydroxyflavylum derivative (FLV-OH) with a rigid electron donating julolidine group attached to position 7 and examined its ground and excited states spectroscopy by absorption, fluorescence, ultrafast dynamics, and by density functional theory (DFT). The precursor compound without the hydroxyl group (FLV) was also synthesized and characterized in order to clarify the role of the intramolecular hydrogen bond on the spectroscopy of FLV-OH. The $S_1 \leftarrow S_0$ absorption peaks at 540 nm and extends to 620 nm, whereas the corresponding fluorescence has two peaks and extends to 900 nm. The ability of the flavylum moiety to undergo ring opening to form chalcone is observed in basic solution. The presence of the hydroxyl group in FLV-OH promotes the formation of a quinonoidal base which was not possible in FLV. Femtosecond fluorescence upconversion and transient absorption measurements reveal the solvation dynamics within the initial 1-2 ps after photexcitation, followed by molecular relaxation to the ground state. The latter was measured to be 505 ps in FLV-OH and 164 ps in FLV. The longer lifetime of FLV-OH in the excited state is correlated to the presence of a hydrogen bond (OH---O) that tends to stabilize the excited molecule. The current results indicate that FLV-OH has spectroscopic properties that make it suitable for many applications such as a potential light harvesting dye in solar cell

Fig. 1: Transient absorption profiles of FLV-OH and FLV dissolved in MeOH

Keywords: Flavylum; Red, Near-infrared, Absorption; Fluorescence; Ultrafast dynamics

Reference:

- [1] Ismail, A. H., Khyasudeen, M. F., Husband, J., Ibrahim, A. R., Baqi, Y., & Abou-Zied, O. K., Steady-state spectroscopy and ultrafast dynamics of flavylum derivatives in the red spectral region, *Journal of Luminescence*, **223**,117261 (2020).