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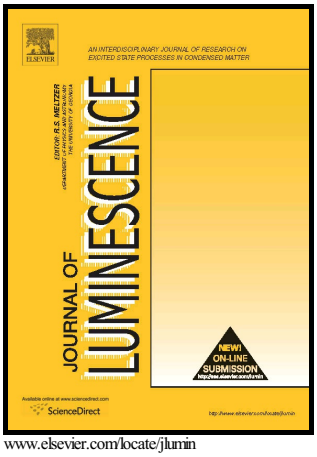

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D-π-A type Barbituric Derivatives: Aggregation induced emission, mechanofluorochromic and solvatochromic properties

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Abstract

Four new barbituric derivatives that bears the furan and thiophene and the 1,3-dimethyl barbituric acid moiety, has been synthesized. These D-π-A type conjugated compounds showed obvious intramolecular charge transfer (ICT) properties, which were evidenced by theoretical calculations and spectral analysis. The compounds exhibited Aggregation induced emission (AIE) characteristic. **TOB-1** and **FTB-1** were quite weakly emission in pure THF, while a significant AIE effect was observed in water/THF (f_w = 70% and 90%) mixtures with a large AIE factor of 40.5 and 46.8. Barbituric acid derivatives with thiophene electron donating group possess the distinct mechanofluorochromic (MFC) behavior. The original powder of **FTB-1**, **BFTB-2** and **TFTB-4** could emit strong orange-yellow (614 nm), orange-red (663 nm) and yellow (571 nm) light under UV irradiation, while the fluorescence color changed into orange (629 nm), red (691 nm) and orange yellow (583 nm) emission after grinding, respectively, a red shift of 15, 28 and 12 nm was observed, respectively. Among them, the emission color of compound **BFTB-2** can be observed by naked eyes. Such mechanochromism was reversible upon the treatment of grinding and fuming with CH_2Cl_2. The XRD studies of the powders showed that the MFC