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Tuning the Emission Colour of Phenothiazine by Introduction of Withdrawing Electron Groups

Authors : Andrei Bejan, Luminita Marin, Dalila Belei

Abstract : Phenothiazine with electron-rich nitrogen and sulfur heteroatoms has a high electron-donating ability which promotes a good conjugation and therefore low band-gap with consequences upon charge carrier mobility improving and shifting of light emission in visible domain. Moreover, its non-planar butterfly conformation inhibits molecular aggregation and thus preserves quite well the fluorescence quantum yield in solid state compared to solution. Therefore phenothiazine and its derivatives are promising hole transport materials for use in organic electronic and optoelectronic devices as light emitting diodes, photovoltaic cells, integrated circuit sensors or driving circuits for large area display devices. The objective of this paper was to obtain a series of new phenothiazine derivatives by introduction of different electron withdrawing substituents as formyl, carboxyl and cyanoacryl units in order to create a push pull system which has potential to improve the electronic and optical properties. Bromine atom was used as electrono-donor moiety to extend furthermore the existing conjugation. The understudy compounds were structural characterized by FTIR and 1H-NMR spectroscopy and single crystal X-ray diffraction. Besides, the single crystal X-ray diffraction brought information regarding the supramolecular architecture of the compounds. Photophysical properties were monitored by UV-vis and photoluminescence spectroscopy, while the electrochemical behavior was established by cyclic voltammetry. The absorption maxima of the studied compounds vary in a large range (322-455 nm), reflecting the different electronic delocalization degree, depending by the substituent nature. In a similar manner, the emission spectra reveal different color of emitted light, a red shift being evident for the groups with higher electron withdrawing ability. The emitted light is pure and saturated for the compounds containing strong withdrawing formyl or cyanoacryl units and reach the highest quantum yield of 71% for the compound containing bromine and cyanoacrilic units. Electrochemical study show reversible oxidative and reduction processes for all the compounds and a close correlation of the HOMO-LUMO band gap with substituent nature. All these findings suggest the obtained compounds as promising materials for optoelectronic devices.

Keywords : electrochemical properties, phenothiazine derivatives, photoluminescence, quantum yield
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