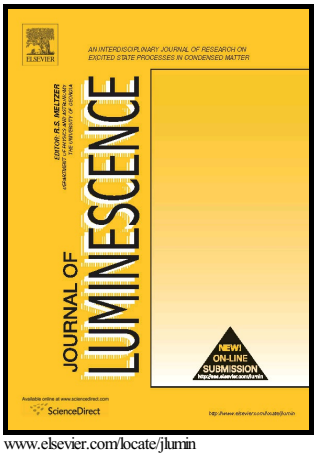

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Abstract

We report the synthesis and spectroscopic studies of two novel 6-substituted fluorine (FMPPQX) and chlorine (ClMPPQX) derivatives of 1-Methyl-3-phenyl-1*H*-pyrazolo[3,4-*b*]quinoxaline (MPPQX) core. The spectroscopic measurements have been performed in solvents of different polarity. Steady state and time-resolved spectroscopy provide photophysical characterization of FMPPQX and ClMPPQX dyes. The fluorescence transition moments exhibit evidently lower values compared to relevant absorption transition moments what apparently is related with formation of instantly twisted molecular conformations in the excited state due to rotation of the phenyl group singly bonded to pyrazolo-quinoxaline moiety. The optical absorption and fluorescence emission transition energies are compared with results of quantum-chemical calculations. Quantum-chemical modeling employs the density functional theory (DFT/TDDFT methods) basing on re-parameterized LRC-BLYP ($\omega = 0.231$ Bohr^{-1}) or CAM-B3LYP xc-functionals and is combined with self consistent reaction field models with linear response (LR) and two different state-specific (IBSF and CLR) solvation models. Re-parameterized functional LRC-BLYP in combination with CLR solvation exhibits the best performance providing most accurate prediction of both excitation and emission transition energies. Relevant quantum-chemical technique may be therefore of interest for chemical engineering dealing with design and synthesis of novel organic dyes. Newly synthesized 6-substituted