The role of ring substituents on hydrogen bonding of 5-cyano-2-hydroxyacetophenone and 2-hydroxy-4-methoxy-5-nitroacetophenone in the ground and excited states.

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The crystal structures of two *ortho*-hydroxyacetophenones (5-cyano-2-hydroxyacetophenone and 2-hydroxy-4-methoxy-5-nitroacetophenone) were determined by X-ray diffraction at 100 K. These experimental values are compared with quantum mechanical DFT calculations (B3LYP/6-311++G(d,p)). DFT calculations have resulted in potential energy surfaces for the ground state (GSPES). The effect of intramolecular interactions, in particular of intramolecular hydrogen bonds, on steady-state fluorescence spectra in non-polar solvents and solid state at room temperature show interesting results. Excited state intramolecular proton transfer (ESIPT) was evidenced by a large Stokes shifted fluorescence (~11,000 cm^{-1}). Intensive fluorescence was observed in the solid state of 5-cyano-2-hydroxyacetophenone.

Słowa kluczowe

Intramolecular hydrogen bonds, Ortho-Hydroxyacetophenones, Excited state intramolecular proton transfer, B3LYP/6-311++G(dp), Fluorescence spectroscopy

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