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Synthesis, spectral properties and DFT quantum chemical calculations of some rhodamine 6G derivatives. Preparation and characterization of the vapour deposited OLED structures

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Three Rhodamine 6G derivatives have been synthesis by replacement of ester group with different aromatic hydrazine/amines containing electron withdrawing (EW) or electron donating (ED) groups. The optimized molecular geometry was computed at DFT/ B3LYP 6-31+G(d,p) level of theory in vacuo. The NBO analysis was performed to evaluation the charge transfers (CT) and resonance energy on molecular backbone. The electron transitions spectra and excitation energies of the dyes were computed by TD-DFT in vacuo in order to understand the electron transitions, which are referred to the experimental excitation spectra of nanosized films of the dyes [1].

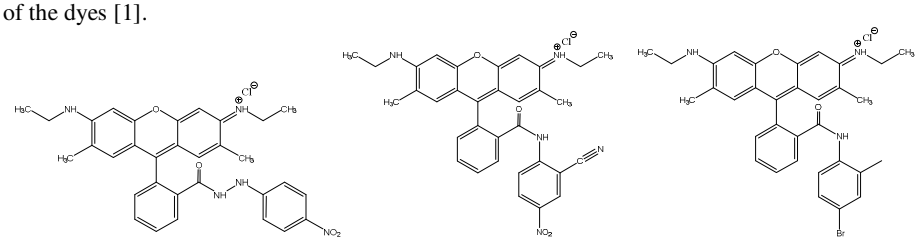

Fig. 1. Structures of Rhodamine 6G derivatives.

Rhodamine 6G and its derivatives are widely used laser dyes. The organic light emitting diode (OLED) structures were obtained by vapour deposition on glass in following order ITO\DPP\ Rhodamine 6G derivatives\Al, ware hole transporting layer (TPD) and emissive layer Rhodamine 6G derivatives. The structures were investigated trough electrical (I\V curves) and luminescence measurements [2].

Keywords: rhodamine 6G derivatives; OLED; DFT quantum chemical calculations

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References

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