Poster

Shedding a new light on nitro compounds: NIR-emitting quadrupole-structured dyes

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Near-infrared (NIR) emission is of significant importance despite its relative scarcity. It finds numerous applications, particularly in the fileds of optoelectronics and biological imaging, owing to the weak absorption of near-infrared by tissues, commonly referred to as the 'biological window'. In this study, we synthesized and characterized 1,2,4,5-tetraaryl-1,4-dihydropyrrolo[3,2-b]pyrroles (TAPPs) containing strongly electron-withdrawing moieties. By reducing the energy level of the lowest unoccupied molecular orbital, we successfully shifted the emission maxima to the deep red range and even achieved near-infrared emission in the solid state. Having investigated crystal structures we found the correlation of absorption maxima and cosine of torsion angle between donor and acceptor parts. Theoretical calculations matched with experimental results in the range of angles we observed in crystal structures.

Combining UV-Vis measurements in solution, we could analyse only shifts in absorption maxima between solution and the solid state. In solutions however, due to excited-state symmetry breaking characteristic for quadrupolar dyes, we observed strong solvatofluorochromism, especially in polar solvents. In such cases shift in maximum of emission was followed by fluorescence quantum yield decay.

Finding from these research allows for the prediction of the optical properties of dyes in the solid state, basing on data from solutions and theoretical calculations.

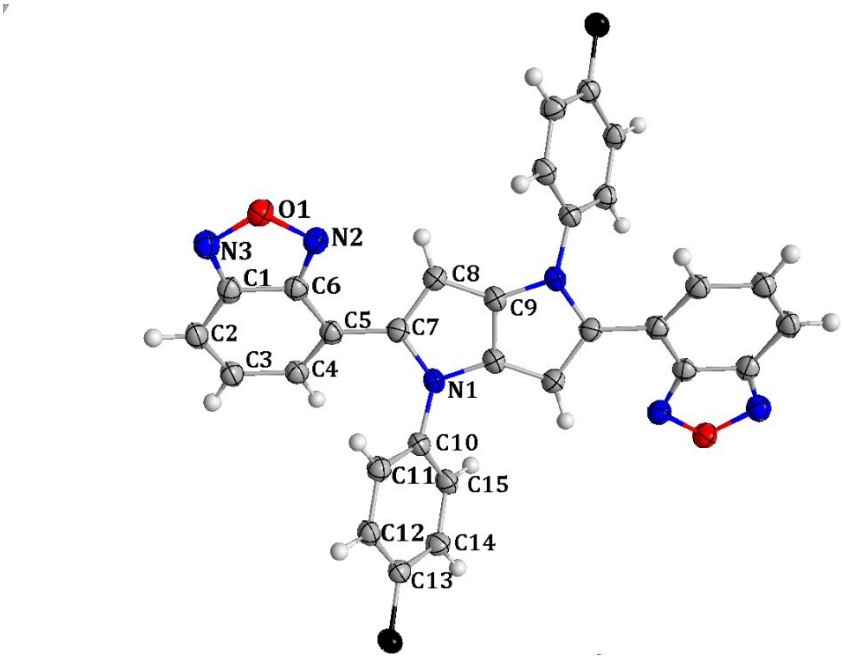

Figure 1. ORTEP structure of synthesized quadrupolar dye. The analysed torsion angle is C8-C7-C5-C6 dihedral angle. In this quadrupolar system, pyrrolopyrrole core is a donor and benzoxadiazole moiety is an acceptor, yielding acceptor-donor-acceptor system.

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