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"Photophysical properties of 3MPBA: Evaluation and co-relation between solvatochromism and quantum yield in different solvents"

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ABSTRACT:

The present paper addresses the photophysical properties of 3-Methoxyphenyl boronic acid (3MPBA) by using solvatochromic shift and quantum chemical methods. The absorption and fluorescence spectra of newly synthesized aryl boronic acid derivative (3MPBA) have been recorded in various solvents of different polarities. The dipole moments were estimated using quantum chemical calculations and Solvatochromic correlations. It is observed that the excited state dipole moments (μ_e) are greater than the ground state dipole moment (μ_g) which confirms $\pi \rightarrow \pi^*$ transition. And it is also observed that the ground state and excited state dipole moments are observed to be collinear to each other. The changes in dipole moment ($\Delta\mu$) were also calculated both from solvatochromic shift method and microscopic solvent polarity parameter (E_T^N) and values are compared. The spectral variations were also analyzed by Kamlet-Taft parameters. It is found that HBA (β) influence is more than HBD (α) for $\bar{\nu}_a$ and $\bar{\nu}_f$ in alcohols whereas HBD (α) influence is more than HBA (β) for $\bar{\nu}_a$ and $\bar{\nu}_f$ in non alcohols. Further, the relative quantum yield (Φ), radiative and non-radiative decay constants

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