COMBINED COMPUTATIONAL AND EXPERIMENTAL STUDIES OF THE DUAL FLUORESCENCE IN DIMETHYLAMINOBENZONITRILE (DMABN)

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The dual florescence of dimethylaminobenzonitrile (DMABN) has been investigated since the 1960s. Despite more than 50 years of previous research, the spatial configuration of the excited state causing the dual fluorescence is still controversial. We have performed excited state calculations of DMABN in a variety of solvents of varying hydrogen-bonding affinity and polarity using implicit solvation (COSMO-PCM) at the M06-HF level of theory, and we have also collected steady-state absorption and fluorescence spectra of DMABN in these solvents. Our experimental spectra are broadly consistent with previous work, and the computational results show a significant solvent dependence.