Experimental and Theoretical Determination of Electronic State Energies of Naphthanilides

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Experimental absorption spectra of α- and β-naphthanilide derivatives in the vapour phase and in MCH solution are interpreted on basis of calculations performed using the INDO/S-CI method. The ground state geometries have been optimised with the PM3 parameterisation method. The calculated values of the lowest triplet state T_1 as well as energy differences of the $T_1 \rightarrow T_n$ transitions have been compared with measured data determined from the phosphorescence and picosecond transient absorption spectra. For $S_0 \rightarrow S_n$ and $T_1 \rightarrow T_n$ transitions, a good agreement is noticed between the experimental and calculated energy values. An additional band observed in the total luminescence spectrum at 77 K, is interpreted as due to the emission of the double H-bonded imidol dimer formed in the excited state. – PACS: 31.70 Dk, 33.50 Dg

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