ON THE ORIENTATION OF SUBSTITUENTS IN N-METHYL- and N, N-DIMETHYL- ANILINES IN THE EXCITED STATES

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The orientation of amino group in aniline was considered to change to 180 degrees in the excited state from 38 degrees in the ground state by Suppan[1], to determine the excited electric dipole moment using solvent shifts. Ayachit[2] freed the problem of assumption of considering the orientation in the excited state. This method led to not only to the better calculation of excited state dipole moments also gave a novel method of calculating the orientation of substituents in mono substituted benzenes in their excited states. This method was shown to work successfully in some other cases [3, 4]. In this paper the method has been applied to N-methyl- and N, N-dimethyl-anilines and the orientation of the substituents in the excited state seems to follow the same changes as in amino group in aniline. (References:1. P. Suppan, Chemical Physics Letters 94, 272(1983): 2. N. H. Ayachit, Chemical Physics Letters 164, 272(1989).; 3. N. H. Ayachit, D. K. Deshpande, M. A. Shashidhar & K. Suryanarayana Rao, Spectrochimica Acta, 42A, 585, 1405(1986); 4. N. H. Ayachit & G. Neeraja Rani, Physics and Chemistry of Liquids, 45, 41(2007))