

Determination of excited state electric dipole moment of the isomeric fluorophenylisocyanates from solvatochromic shift measurements

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Abstract. The excited state electric dipole moments of three isomeric fluorophenylisocyanates are determined using the method of solvatochromic shift measurements recently suggested from our laboratory.

Keywords. Excited state dipole moments; fluorophenylisocyanates; solvatochromic shifts.

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1. Introduction

Ledger and Suppan (1967) had suggested a method to determine the excited state electric dipole moment of a molecule using its solvatochromic shifts from McRae's (1957) equation. This method has since been modified (Suppan 1975; Suppan and Tsiamis 1980; Prabhumirashi *et al* 1983). Recently a new method has been proposed from our laboratory (Ayachit *et al* 1986) and applied for some substituted benzenes. This method has now been applied to the S_1 band of a few more molecules, namely, the three isomeric fluorophenylisocyanates (FPICs).

2. Experimental

The ultraviolet absorption spectra (S_1 band) of pure samples (Aldrich Chemical Co., USA) of the three isomeric FPICs in different solvents of spectroscopic grade purity viz (i) cyclohexane, (ii) tetrahydrofuran, (iii) *n*-propanol, (iv) *iso*-propanol, (v) ether, (vi) hexane, (vii) *t*-butanol and (viii) *n*-heptane were recorded using a ratio recording spectrophotometer (DK-2A) with a cell thickness of 1 cm. The concentration of each of the solute molecules in different solvents was in the range of 0·01 to 0·02 g/litre.

3. Method, results and discussion

In the method suggested earlier (Ayachit *et al* 1986), McRae's equation (McRae 1957) was put in the form of an equation for a straight line (intercept form),

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