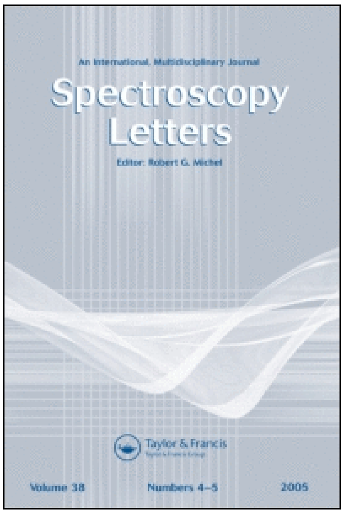

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Spectroscopic Studies of Some Organic Compounds: Aprotic Solvent Effects on Electronic Absorption Spectra of Nicotinamide

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Spectroscopic Studies of Some Organic Compounds: Aprotic Solvent Effects On Electronic Absorption Spectra Of Nicotinamide

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Abstract:

The electronic absorption spectra of nicotinamide were measured in seventeen aprotic solvents. The solvatochromic method is used to unravel solvent polarity and hydrogen bonding effects on $\pi - \pi^*$ transition. Solvent effects are rationalized in terms of the solvatochromic parameters : π^* , δ , α , and β .

Correlation of these type has been the subject of extensive studies which were so far reported[4-8].

The present work is concerned with the application of the solvatochromic equation (1) to resolve solvent effects on the electronic transition spectra of nicotinamide.

Table (1) Electronic Spectral Data Of Nicotinamide in Various Solvents And Solvents Parameters.[a]

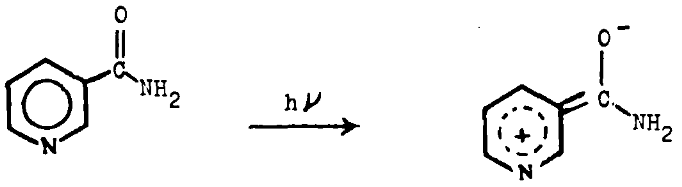
Solvent	$\nu_{max.}$ 10^3 cm^{-1}	π^*	β	α
n-hexane	39.68	-0.08	0.0	0.0
c-hexane	39.52	0.0	0.0	0.0
Ph H	35.97	0.59	0.1	0.0
Ph Me	35.08	0.54	0.11	0.0
Ph CL	34.72	0.71	0.07	0.0
Ph Br	34.60	0.79	0.06	0.0
CCL_4	38.16	0.29	0.0	0.0
$CHCL_3$	38.46	0.76	0.0	0.38
CH_2CL_2	38.61	0.82	0.0	0.3
Dioxane	38.46	0.55	0.37	0.0
DEE	38.91	0.29	0.47	0.0
THF	38.31	0.58	0.55	0.0
THP	37.73	0.51	0.54	0.0
EtAC	38.02	0.55	0.45	0.0
MeCN	38.61	0.76	0.31	0.24
DMF	37.17	0.88	0.69	0.0
DMSO	37.31	1.00	0.76	0.0

a - Values traken from references (1-7).

Result and Discussion:

The maximum of the absorption band is usually well defined position; it correspond to the $\pi - \pi^*$ electronic transition of nicotinamide in seventeen aprotic solvents, the data are assembled in table (1) to gether with the solvents parameters.

Electronic spectral transition from a ground state which is more like canonical structure (1) to an excited state more like (2), charge is generated in the electronic excited state, such structures are stabilized by solvent polarity in accord with simple electrostatic theory[9]. Hence the polar solvent facilitates excitation and results in a bathochromic shift as compared to the nonpolar solvent.



(1) (2)

Experimental:

The solvents used in this study were of spectroscopic grade whenever posible, while the commercial solvents were purified by standared methods[10]. All solvents were fractionally distilled and middle fractions were used for this study. The following solvents were used; n-hexane, cyclohexane (c-hexane), benzene (PhH), chlorobenzene (PhCl), bromobenzene (PhBr) , toluene (PhMe), CCL_4 , $CHCL_3$, CH_2CL_2, dioxane, tetrahydropyrane (THP), diethylether (DEE), tetrahydrofurane (THF) , acetonitrile (MeCN), dimethylformamide (DMF), ethylacetate (EtAC), and dimethylsulfoxide (DMSO).

Solutions of nicotinamide ($4x10^{-5}$ M) were prepared by diluting astock ($1x10^{-4}$ M) solution in the desired solvent. The spectral measurements were preformed on a Pye-Unicam SP 800 double beam U.V.-Vis. spectrophotometer.

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