INTRODUCING A NEW, SIMPLE AND RAPID METHOD FOR PREFERENTIAL SALVATION STUDY OF PC BY FTIR

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The infrared spectrum of Propylene carbonate, PC, is complex because the molecule is not symmetrical. The strongest band is due to the $\text{-C=O}$ stretch in the carbonyl group attached to the heterocyclic ring. In addition there are important vibrational modes associated with deformation of the ring [1].

Because of the strong dipole-dipole interactions in PC, one finds three bands in the $\text{-C=O}$ stretching region at 1800 cm$^{-1}$. One of these is due to the monomers and the other two to molecular associates in the pure liquid. When PC is a dilute solute in another organic solvent, three bands are still observed in this region and care must be taken to select the one which is due to the monomer [2]. This can be determined by following the intensity and position of each band as a function of PC concentration in dilute solutions.

Preferential solvation which plays an important role in determining changes in thermodynamics of solvation in mixed solvents, have been previously studied by a calorimetric method, using a more complicated solvation theory [3, 4]. A new, simple and rapid spectroscopic method has been introduced to relate the spectroscopic results of the solute in the pure solvents to the degree of preferential solvation in the mixed solvent systems including preferential solvation for the whole molecule and every surfaces of the molecule individually. This is the first time that we have generalized the FTIR results of the solutes in the pure solvents to those of the solutes in the solvent mixtures.

The wave numbers for the $\text{-C=O}$ band of PC in the considered solvents are measured and a correlation with the solvent's acceptor number and solvent’s donor number is found as follow:

$$\omega_1 = 1829.09 - 0.935AN - 0.251DN$$ (8)

With a standard deviation of 0.15 cm$^{-1}$ and a correlation coefficient of 0.9999. Thus, the solvent acidity accounts for 78.84 percent of the variation in $\omega_1$ and solvent basicity for 21.16 percent. The agreement between the experimental values of $\omega_1$ and the estimated values by equation 8 is excellent. In other word, the probability for the solvents to interact with the oxygen atom of $\text{-C=O}$ group of PC is 78.84% and probability for the solvent interaction with other sites on acetonitrile molecule (i.e. $\text{-CH}_3$ group) is 21.16%.

References