Solvent Effect on the Electronic Polarizability of Benzonitrile

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In this study, the static and dynamic electronic polarizability of benzonitrile is reported. This property was determined using refraction index measurements of neat benzonitrile and CCl_4, THF, C_6H_{12} and CH_3CN diluted solutions. The real refractive index of pure benzonitrile was obtained by refractometry, FTIR transmission spectroscopy and Kramers-Krönig transform. These results indicate that the vibrational contribution to the visible refraction is very small, and the electronic polarizabilities calculated with these values agree with reported values. In binary mixtures, the polarizability of benzonitrile was obtained with the refractometric method proposed by Singer and Garito at five frequencies to obtain the dispersion curve. The local field effects were tested within the Onsager and Lorentz local field approach. The static properties in each solvent was obtained by extrapolation of the Cauchy-type dispersion curve to zero frequency, which gave a monotonic increased as a function of the squared frequency. The polarizabilities obtained in this work agree well with theoretical and experimental data, reported by other authors. The static and dynamic electronic polarizability of benzonitrile was found to be little affected by the dielectric nature of the solvent, and the electric deformability is similar to that of the benzene molecule. The effect of the replacement of the C—H group by N in 4-cyano-pyridine and benzonitrile molecules is discussed.

Key words: Benzonitrile; Polarizability; Solvent Effect.