COMPUTATION OF DIELECTRIC PROPERTIES OF NANO-PROBE LOCAL SURROUNDING BY SOLVATOCHROMIC SPECTRAL SHIFT MEASUREMENT OF ORGANIC DYE MOLECULE

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Computer modeling of the dielectric properties of the cucurbit [7]uril (CB[7]) cavity based on the Onsager-Liptay model [1] was carried out by analyzing the solvatochromic shift of the absorption spectrum of 1- (3-ammoniumpropyl) -4 - [(E) -2- (3,4-dimethoxyphenyl) ethynyl]pyridinium (D1) upon the formation of the inclusion complex with CB[7] in a water solution. The CB[7] cavity was considered as a polar environment into which the dye chromophore is placed. [2] Positions of the maxima of the dye absorption spectra were measured experimentally in the following solvents: methanol, ethanol, i-propanol, n-butanol and water with known dielectric and optical properties. These values were used for parametrization of the Onsager-Liptay equation. Quantum-chemical method of the combined cluster available in the Gamess-US software package was used to calculate molecular structures, dipole moments of the ground and excited states, and polarizability [2]. Original program that calculate effective molecule volume according to Van der Waals atom radii was developed to calculate the volume of dye molecule.

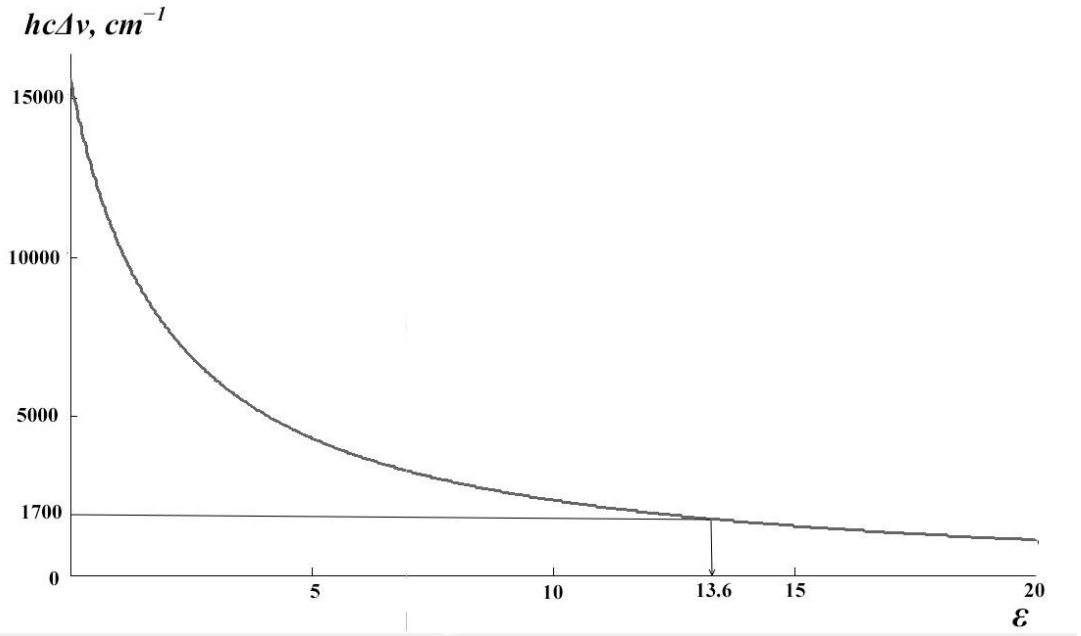

Fig. 1. Determination of the effective permittivity of the cavity of CB [7] based on the theoretical dependence of the solvatochromic shift on ε

Theoretical value of the effective dielectric permittivity of the cavity (≈13.6) is in good agreement with the literature data derived by another method. [4] Thus, we propose a new method for estimating the dielectric properties of a host molecule in a supramolecular inclusion complex according to the experimental shift of the dye molecule optical absorption spectrum due to formation of the inclusion complex with CB[7].

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