INTERNAL ROTATION POTENTIAL FUNCTION CALCULATION AND THE INTRAMOLECULAR HYDROGEN BOND ENERGY ESTIMATION IN 2-METHOXYPHENOL

Valiev E. V., Sheikh-Zade M. I.

State Budget Educational Institution of Higher Education of the Republic of Crimea "Crimean Engineering and Pedagogical University.", Simferopol, Crimea, Russian Federation
E-mail: envervaliyev@ukr.net

If the bands of *cis*- and *trans*- forms are observed for molecules with intramolecular hydrogen bond (IHB) in IR spectra, then by measuring the absolute or relative populations of *cis*- and *trans*- states in a certain temperature range, it is possible to make a direct determination of the IHB energy. For 2-methoxyphenol (2-MPh), which we selected as the

object of investigation, only the band corresponding to the *trans*- form is observed in the IR spectra in the region of νOH. The heating of a solution of 2MPh in various inert solvents to boiling temperatures of these solvents shows that the band corresponding to the *trans*- form does not appear in the IR spectrum. This means that for 2-MPh it is impossible to apply the above method of direct determination of the IHB energy by IR spectra.

The task of this paper was to estimate the IHB energy of the 2-MP by determining the parameters V_1, V_2 of the internal rotation potential function (IRPF),

$$V(\alpha) = \sum_{k=1}^{2} \frac{V_k}{2} \cdot (1 - \cos(k \cdot б)), \quad (1)$$

where α is the angle of internal rotation.

This problem was solved by calculation using the frequency values τ_1, τ_2 of the torsion transitions 0→1 in the *cis*- and *trans*- potential wells and the value of the reduced inertia I_r calculated from the geometric parameters of the 2-MPh molecules that were adopted as for phenol. The obtained values of V_1, V_2 are equal: $V_1 = 685$ cm^{-1}, $V_2 = 2088$ cm^{-1}. These data make it possible to reconstruct the IRPF (1), and also to calculate the values of the energy levels in the *cis*- and *trans*- potential wells.

If, under the IHB energy, we understand the difference ΔE between zero energy levels in *trans*- and *cis*- potential wells, then for 2-MPh the energy is equal to $\Delta E = 666$ cm$^{-1} = 1.90$ kcal/mol.

Keywords: intramolecular hydrogen bond, energy, internal rotation, potential energy.

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