ESTIMATION OF INFLUENCE OF FRAGMENTS C_1–OH AND OCH_3-GROUPS GEOMETRIC PARAMETERS AT THE MOLECULE 2-METHOXYPHENOL REDUCED INERTIA MOMENT

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When finding the form of the internal rotation potential function of molecules according to their IR spectra it is necessary to calculate the reduced moment of inertia I_r molecules. I_r value can be calculated directly for molecules with certain elements of symmetry as described using the molecules geometric parameters. In this case, it becomes important authenticity and uniqueness of molecular geometry data.

The task of this study is estimation of which geometric parameters of C_1–OH and OCH_3–fragment groups in the molecule 2-methoxyphenol (2-MPh) have a preferential effect on this molecule I_r.

To solve this problem was used the method of factorial experiment, which allows to obtain a mathematical model of influence of geometrical parameters on I_r as a regression equation. The calculations were performed for the *cis*-form 2-MPh. In this study we considered only linear model of these parameters influence on the I_r. The resulting regression equation is as follows:

$$\hat{y} = (7372{,}0 - 9{,}2 \cdot x_1 - 1088{,}0 \cdot x_2 + 9{,}5 \cdot x_3 + 1445{,}5 \cdot x_4 + 2{,}7 \cdot x_5 + 1{,}3 \cdot x_6 + 0{,}6 \cdot x_7) \cdot 10^{-4}$$

where by x_1, x_2, ..., x_7 are designated $\angle\alpha$ – the angle between the C_1–O_1 bond and axis z, passing through atoms C_1 and C_4, $\angle C_1O_1H_7$, $r(C_1 - O_1)$, $r(O_1 - H_7)$, $\angle C_2O_2C_7$, $r(C_2 - O_2)$, $r(O_2 - C_7)$, respectively, $y = I_R$.

From this equation it follows that because of the considered factors to have a predominant influence by factors x_2 and x_4, i.e. the geometry of the top (OH-group); the influence of other factors is much less significant.

Keywords: factor analysis, regression equation, the molecule, geometric parameters, the reduced moment of inertia.

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