BASIC PROPERTIES OF A NUMBER OF ORGANIC LIGANDS. QUANTUM-CHEMICAL CALCULATIONS AND MODELLING THE STRUCTURE–PROTONATION CONSTANT RELATIONSHIPS

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We have previously quantitatively discussed the protonation ability of antipyrine – a weak base and bioactive ligand [1]. With the aim of estimating the protonation ability which can be considered as well as the ability of complex formation, the protonation energy values have been calculated by the DFT method ("Priroda" program package, exchange-correlational functional PBE, 3z-basis) [2] for a number of organic ligands with different composition and structure. It has been demonstrated that relative compounds are characterized by the close values of protonation constants while transition to compounds of other classes is accompanied by their change which may serve as the criterion of complex formation (or non-formation).

In addition, on the basis of the *Wolfram Mathematica* 8 program package a number of models of the type "structure–property" has been obtained for the protonation constant (K) for some organic ligands. These models are represented by the linear equations $\log K = a_1x_1+\ldots+a_nx_n+a_0$, where $x_1,\ldots,x_n$ – are the molecule structural parameters, such as the number of H atoms, the ratio of the number of C atoms to that of the non-hydrogen ones, the Wiener index, etc. [3], and $a_0,\ldots,a_n$ – parameters, obtained on the basis of the "teaching" sample of compounds. The best 300 models from the constructed 4000 ones were used for estimation of protonation constants for two compounds for which experimental data are unknown.

Литература

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