# The use of fuzzy modelling for predicting the values of the classic potential barrier of the reaction phenyl radical with hydrocarbons

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Experimentally reactivity of organic compounds in radical reactions is determined by the activation energy (E) or the value of the classical potential barrier ($E_e$) according to the formula

$$E_e = E - 0.5(hL\nu_i - RT)$$

where $\nu_i$ are vibrational frequencies for stretching bonds, $R$ is the gas constant (J/mol·K), $h$ is the Planck's constant, $L$ is the Avogadro number and $T$ is the reaction temperature (K).

In [1,2] was proposed empirical models of elementary bimolecular radical reactions of abstraction, which allows to build non-linear correlations between the classical potential barrier radical bimolecular reaction and thermochemical properties of reactants.

We consider experimental sample of the reactions:

$$Ph^{\circ} + RH \rightarrow PhH + R^{\circ}$$

The experimental sample of 97 reactions of the phenyl radical with various hydrocarbons is obtained from the database on rate constants of liquid phase radical reactions [3], which 12 were the control sample. The dissociation energy of the C-H bonds are taken from [4]. For this sample $D_f$ = 474 kJ/mol [4] and α = 0.945 are constant. Therefore, the dependence takes the form:

$$E_e = \varphi(D_{ei}, br_e)$$

To approximate the values of the classical potential barrier the Mamdani's fuzzy inference method was used based on the using the matching degree to which they belong to each of the fuzzy rule via membership functions, equal the real number $\alpha_i$, characterizing the degree of membership of input $A_1', A_2', ...., A_n'$ to fuzzy sets $A_{i1}, A_{i2}, ..., A_{in}$ in the background of the i-th rule

$$\alpha_i = \min_{j=1}^{n}\left[\max_{X_i}(A_j'(x_j) \wedge A_{ij}(x_j))\right]$$

where $X_j$ is the domain of the variables ($x_1 = D_{ei}$ и $x_2 = br_e$).

On the example of reactions between substituted phenyl radicals and hydrocarbons an attempt was made to identify the dependence of classical potential barrier of radical reactions by the fuzzy knowledge base built on basis of quantitative and qualitative parameters.

Using a fuzzy knowledge base built by experts, and Mamdani's fuzzy inference method using membership functions

$$\mu^G(x) = \frac{1}{1 + \left(\frac{x-b}{c}\right)^2}$$

produces a good approximation of the values of the classical potential barrier for phenyl radical reactions with hydrocarbons.

**References**

[1] Denisov E T and Tumanov V E 1994 *Russian Journal of Physical Chemistry A* **68** 719
[2] Denisov E T 1997 *Russian Chemical Reviews* **66** 953
[3] Tumanov V and Gaifullin G 2012 *Modern Advances in Intelligent Systems and Tools* **431** 121
[4] Luo Y-R 2007 *Comprehensive Handbook of Chemical Bond Energies*. London - New York: CRC Press, Boca Raton

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