CALCULATION OF pKa OF PHENOLS AND THIOLS AS A MODEL TO EVALUATE THE ACIDITY OF CATALYSTS ON ACTIVATED CHARCOAL

One of the most perspective carriers for making solid acid-base catalysts is activated carbon (AC). Halogenated activated carbons (AC–Hal, Hal=F, Br and Cl) used as precursors were functionalized with SO_3H groups to prepare (AC–Hal–S) solid acid catalysts. Such ACs were shown high catalytic activity in the propan-2-ol dehydration reaction.

For modeling the surface of activated carbon was chosen polycyclic aromatic hydrocarbons such coronene $C_{24}H_{12}$. Techniques of modification of activated carbon include receiving conventional compounds $C_{24}H_{11}SH$, or $C_{24}H_{11}SHX$ (X = Br, CF_3, CCl_3, H, OH etc) with the $C_{24}H_{10}SO_3H$ as final product. To study the properties of these catalysts, evaluation of their catalytic activity would be interesting to calculate, or at least evaluate their acidity.

It was chosen a method which uses the correlation between experimental pK_a values and calculated one in a presence of solvent. $pK_a = -\lg K_a = \frac{\Delta G_r}{2{,}303RT} = a_f \Delta E_{el}^{aq} + b_f$ *, where a and b - parameters are defined by least squares method (they contain systematic errors of quantum-chemical and solvating models, entropy effects, etc.), f - define a class of compounds (for functions), and* $\Delta E_{el}^{aq} = E_{A^-} - E_{AH}$ *is the difference between the electronic energy of the anion and the electronic energy of a molecule. This method was applied using the software package ORCA.*

When it was calculated a pK_a values for set of the phenols and thiols. The pK_a values don't deviate from its experimental values more than one unit. Such deviations are less noticeable for thiols than for phenols. There were salient deviations for compounds with nitro- and amino-groups. It can be seen that there is an error in the calculation of pK_a for compounds which has lone pairs. With the increase of the size of atom, this effect is not so sharp. This is illustrated by pK_a values of thiols. Tested method can be applied to theoretical predication of the acidity of activated charcoal catalyst with different functional groups on its surface.

Key words: activated charcoal, acidity, catalysis.