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TO THE QUESTION OF THE INFLUENCE OF A SILANOL COVER ON THE PROTOLYTIC PROPERTIES OF AMINOPROPYL SILICA GELS

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A method for describing and predicting protolytic and complex-forming properties of the surface of functionalized sorbents based on silica gels with grafted nitrogen-containing groups is proposed. The method is considered on the example of protonation of aminopropyl silica.

Received curves of potentiometric titration of aminopropyl silica gels with hydrochloric acid. They were used to plot the dependences of the surface charge on pH. The obtained points were approximated by an expression relating the surface charge to the concentration of surface ions. In this case, interactions were taken into account:

$$-NH_{2S} + H^{+}s = -NH_{3}^{+}s$$

$$\equiv SiOH_{S} = \equiv SiO^{-}s + H^{+}s$$
(1)
(2)

The above-mentioned expression is:

$$\sigma = \frac{F}{SC_k} \left(\frac{C_{-NH_2s}}{1 + \frac{1}{K[H^+s]}} - \frac{C_{\equiv SiOHs}}{1 + \frac{[H^+s]}{K_s}} \right)$$

K and K_s are equilibrium constants (1) and (2), respectively. C_{-NH_2S} and $C_{\equiv SiOHS}$ are the total concentrations of the corresponding surface groups. The concentration $[H^+S]$ was determined using the diffuse double layer model [1,2]. It was found that the results that are closest to the experiment are obtained when $C_{\equiv SiOHS}$ changes according to a linear law (*a* is the total concentration of amino groups, *b* is the rate of decrease in the concentration of amino groups with a change in the process degree):

 $C_{\equiv SiOHs} = a + bx (4)$

The chosen parameters were the constant K, a and b. Examples of approximation are shown in Figure 1. The average value of log K is 10.55, which is close to the protonation constant of propylamine in an aqueous solution (log $K^0 = 10.5$).

Continuation of the material



Figure 1. Approximation of experimental points of surface charge by calculated lines. 1 - $C_{-NH_2S} = 0.65 \,\mu\text{mol} / \text{m2}, C_{-NH_2S}$ = 0.90 $\mu\text{mol} / \text{m2}, 3 - C_{-NH_2S} = 1.51 \,\mu\text{mol} / \text{m2}.$ © О.В. Филистеев, А.В. Шаров, 2020

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