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Energy of Carbon (IV) Oxide Adsorpation on Ca_5Na_3AZeolithic

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ABSTRACT: The differential heat, isotherm, differential entropy, and thermokinetics of carbon dioxide adsorption on Ca_5Na_3A zeolite were measured at 303 K. Based on the results obtained, the mechanism of water adsorption from Ca_5Na_3A in zeolite from initial filling to Caturation is described in detail.

KEYWORDS: Isotherm, adsorption heat, entropy, thermokinetics, ion-molecular complexes, Ca_5Na_3A zeolite, H_2O, adsorption calorimeter.

I. INTRODUCTION

Up to date, the acceleration of production processes in the world has led to the release of large amounts of carbon monoxide into the environment, resulting in ecological imbalances. To prevent this, a lot of research is being done on obtaining detergents from harmful gases.

In particular, one of the most important tasks is to obtain selective microporous adsorbents, taking into account the size of the gas molecules.In Uzbekistan, the purification of exhaust gases from carbon monoxide is very important for the manufacturing industry. To do this, it is adviCable to use NaA and CaA zeolites using the adsorption method [1-2]. Cations in the cavities of type A zeolites form complex compounds with carbon monoxide [3]. Initially, the laws of water adsorption on NaA zeolite were considered in the study [4].

It was found that water molecules are adsorbent in the b-space, the molecular size of carbon monoxide is slightly larger than the water (2,7 Å) molecule, Ca it cannot enter the b-space through six-membered oxygen glasses and ion-molecular clusters with metal cations located here. forms. However, cations in the β-space can migrate to the a-space. [5]

In type A zeolites, cubic octahedrons form a simple cubic lattice [6-7].Each cubic octahedrons is connected by six adjacent four-membered oxygen bridges. The gaps between the eight cubic octahedrons form large pores [8-9].

II. SIGNIFICANCE OF THE SYSTEM

The differential heat, isotherm, differential entropy, and thermokinetics of carbon dioxide adsorption on Ca_5Na_3A zeolite were measured at 303 K.The study of literature survey is presented in section III, methodology is explained in section IV, section V covers the experimental results of the study, and section VI discusses the future study and conclusion.

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III. METHODOLOGY

The structural formula of Ca_5Na_3A zeolite obtained as the object of study is as follows: $Ca_5Na_3[(AlO_2)_{12}(SiO_2)_{12}]$. The adsorption properties of carbon dioxide molecules on the adsorbent Ca_5Na_3A zeolite were studied in the high-vacuum adsorption differentiated DAK-1-1 calorimetric device [10-11]. Initially, Ca_5Na_3A zeolite was purified at 4500C for 8 h in a vacuum pump and in a diffusion pump to a pressure state of 1*10-6 Pa. The carbon dioxide obtained as the adsorbate was alCa purified by appropriate methods, i.e., it was passed through various adsorbents purified through a glass tube and prepared for experimentation in the dry gas state. The study was carried out in a volumetric manner in a high-vacuum adsorption device

IV. EXPERIMENTAL RESULTS

The adsorption isotherm of CO_2 molecules to Ca_5Na_3A zeolite was measured by volume in a high vacuum adsorption device.On the adsorption isotherm of the CO_2 molecule in Ca_5Na_3A zeolite (ln (P/P^0)) at 303K (Caturation vapor pressure P^0-54806 torr, Caturation pressure of P^0- CO_2 at 303K, calculated at 1 atm. 760 mm.sim.ust. calculated. The adsorption isotherm obtained as a result of the study is shown in Figure 1 and the adsorption amount is N, CO_2/e.ya. are expressed.At the initial Caturation, the adsorption isotherms start from ln (P/P^0)= -11,40, and the adsorption is N=0,36 CO_2/e.ya. It can be seen from the isothermal lines that as they Caturate with CO_2 molecules, they gradually approach the adsorption axis.At the intersection of the isotherm lines on the adsorption axis, the isotherm value is ln (P/P^0) = -4,61, and the adsorption is N=9,02 CO_2/e.ya. forms. At initial Caturation, CO_2 molecules form mono- and dicomplexes on the Na^+ and Ca^{2+} cations in the zeolite cavities. Since chemical adsorption occurs, the adsorption isotherm values are very small.

The adsorption isotherm of CO_2 to Ca_5Na_3A zeolite was redefined using the equation of the Caturation theory of two-dimensional micropores (*VOM*) [6-7].

$$N=5,653\exp[(A/21,98)^4]+4,583\exp[(A/16,38)^3],$$

Here, the amount of adsorption in N-micropores is CO_2/e.ya., A=RTln (P°/P) - free energy work (kJ/mol).

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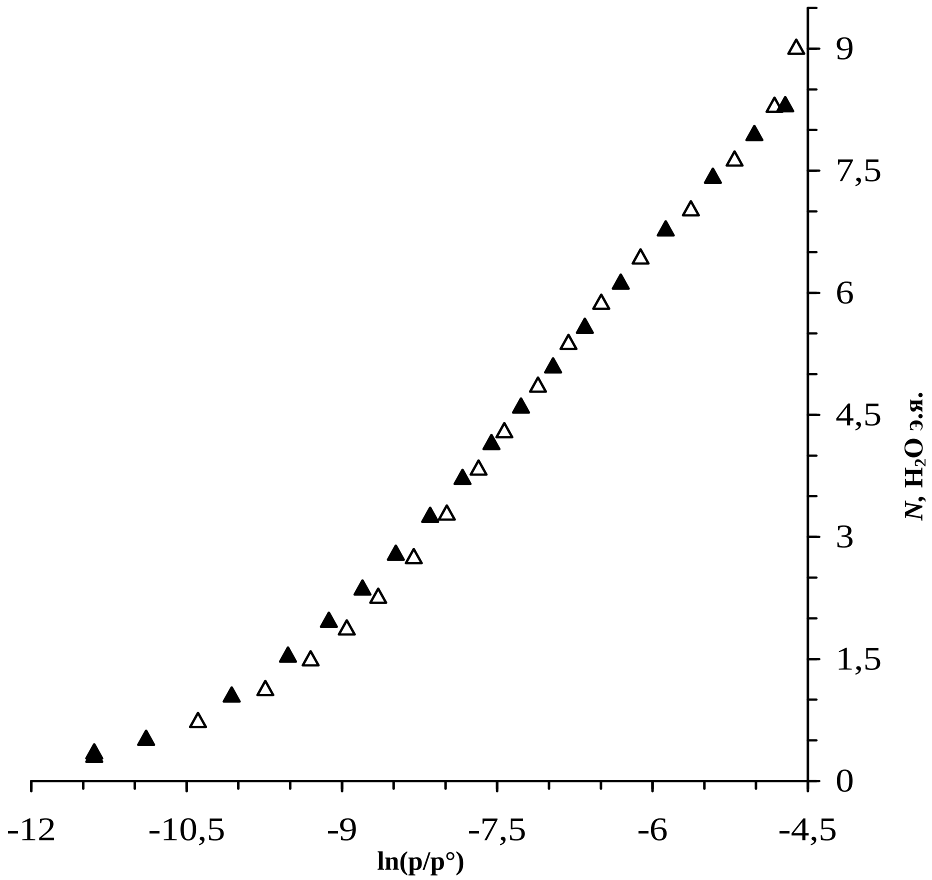

Figure 1. experimental value of CO_2 adsorption isotherm in Ca_5Na_3A zeolite at 303 K; Points calculated by the equation ▲-VOM

Figure 2 shows the differential heat (Q_d) of CO_2 adsorption on Ca_5Na_3A zeolite at 303K. The condensing heat of carbon (IV) oxide at 303 K *(ΔHv* = 27 kJ/mol) is given by the continuous straight lines.

The adsorption heat of CO_2 to Ca_5Na_3A zeolite starts from Q_d ~69,57 kJ/mol, where the adsorption is *N*=0,18 CO_2 e.ya. then decreases to 47,01 kJ/mol and the adsorption is *N*=0,77 CO_2 e.ya. In previous studies, the initial adsorption differential temperatures were higher than Q_d~65 kJ/mol [12].

In this zeolite, the adsorption heat is alCa higher than Q_d~65 kJ/mol. When type A zeolites were only Na^+ cations, the maximum rate of adsorption differential temperatures would be Q_d ~60 kJ/mol. [13].

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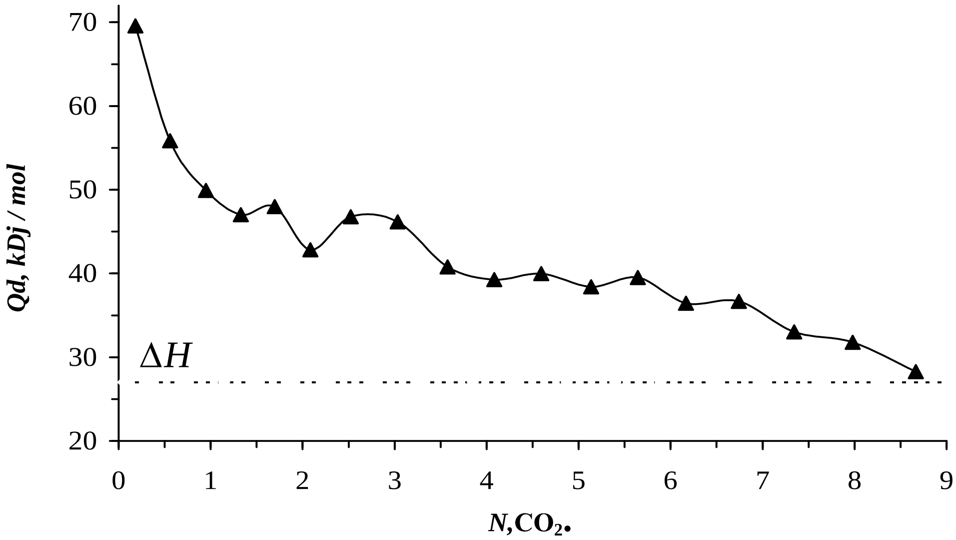

Figure 2. Differential heat of CO_2 adsorption on Ca_5Na_3A zeolite at 303K temperature. Horizontal ring line condensing heat

Adsorption produces 42,84 kJ/mol of heat when it reaches N=2,08 CO_2 e.ya.

Adsorption N=2,08 CO_2/e.ya. and 3,57 CO_2/e.ya. differential heat values in the range of 42,84 kJ/mol to 40,77 kJ/mol.In this heat range, the adsorption heat generates the maximum heat in the zeolite supercollectors, where the differential heat rises and falls to Q_d~46,76 kJ/mol.

Then the adsorption is N=3,57 CO_2/e.ya. and N = 5,13 CO_2/e.ya. s in the range of differential temperatures with small changes and decreases to 38,40 kJ/mol. This adsorption is N=2,08 CO_2/e.ya. and N=3,57 CO_2/e.ya. intervals in cations in the zeolite supercolumns, this small-wave adsorption goes with the Sorption in differential heat Na^+cations. Adsorption N = 5,13 Ca_2/e.ya to 6,17 Ca_2/e.ya. when differential heat goes in the form of small waves and varies from 38,40 to 36,45kJ/mol. After this process, the amount of heat decreases from 36,45 kJ/mol to 33,03 kJ/mol when the differential heat reaches 6,17 Ca_2/e.ya. to 7,34 Ca_2/e.ya in two stages, and in the next stage 7,34 Ca_2/e.ya. from 8,67 Ca_2/e.ya., the differential temperatures decrease from 33,03 kJ/mol to 28,27 kJ/mol to the condensing heat.Differential adsorption temperatures are in the form of waves and are divided into 7 stages: (I) from 0,18 to 1,32 CO_2/CO_2/ (1,14 CO_2/CO_2/ e.ya.), (II) from 1,327 to 2,08 CO_2/CO_2/(0,75 CO_2/CO_2/ e.ya.), (III) from 2,08 to 3,57 CO_2/CO_2/ (1,49 CO_2/CO_2/ e.ya.), (IV) from 3,57 to 5,13 CO_2/CO_2/ (1,56 CO_2/CO_2/ e.ya.), (V) from 5,13 to 6,17 CO_2/CO_2/. (1,03 CO_2/CO_2/ e.ya.), (VI) from6,17 to7,34 CO_2/CO_2/ e.ya. (1,17 CO_2/CO_2/ e.ya.). and(VII)from7,34 to8,67 CO_2/CO_2/ (1,33 CO_2/CO_2/ e.ya.).

The high differential heat of adsorption is observed as a result of the contact of carbon (IV) oxide molecules with Ca_5Na_3A zeolite through the entrance window to the zeolite supercolors by touching the oxygen atoms that bind silicon and aluminum. This is the first stage of adsorption heat.

In the second to sixth stages, Ca_5Na_3A zeolite is adsorbent in the S_{II} cavity, in which (7,67-1.327 = 5,66) 6,343 carbon (IV) oxide molecules are adsorbent. In this zeolite, 3.35 molecules of carbon monoxide are adsorbent on Ca^{2+} cations and 3,05 molecules of carbon monoxide on Na^+ cation.

In the first and seventh stages, a total of 2,657 molecules of carbon monoxide are adsorbent on the Ca^{+2} cations of this zeolite in the S_I cavities. Thus, a total of 8,67 CO_2/e.ya to Ca_5Na_3A zeolite. a molecule of carbon monoxide gas is adsorbent.Carbon monoxide gases are sorbent into 0,8375 Ca^{+2} and 1 Na^+ in the S_{II} super-cavities of each zeolite and 0,66 Ca^{+2} cations in the S_I cavity.

Differential entropy of CO_2 adsorption (ΔS_d) to Ca_5Na_3A zeolite at 303K was shown. The Gibbs-Helmholtz equation was used to calculate the differential entropy of adsorption based on the differential heat of adsorption and isotherm values.

Adsorption N=0,36 to 1.50 CO_2/e.ya. The cations located inside the cube form adCarb CO_2 molecules until they enter a large super void.This therefore leads to high differential heat and entropy values. In the last stage, Sorption of cations in the S_I space is are observed, in which case the cations rise to a positive value in entropy due to Caturation with carbon monoxide gas.

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In the second to seventh stages, the differential heat and entropy of adsorption in the form of a curvilinear wave on the adsorption of Ca_2 molecules on Ca_5Na_3A zeolite rises from -25,77 J/mol*K to -10,02 J/mol*K and then reaches the maximum values in the last section, where entropy the value rises to 45,33 J/mol*K. In the final stage, strong localization of four-dimensional clusters of CO_2 molecules to 2,657 carbon (IV) oxides to 0,6 Ca^{+2} cations is observed.

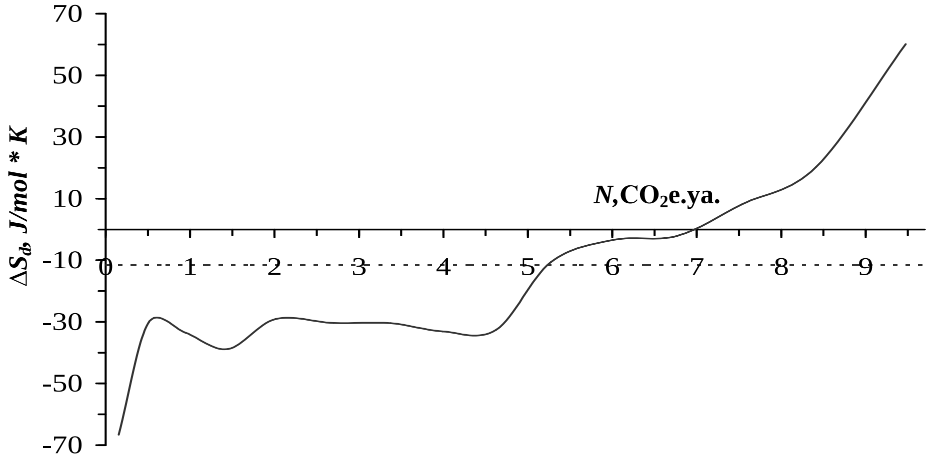
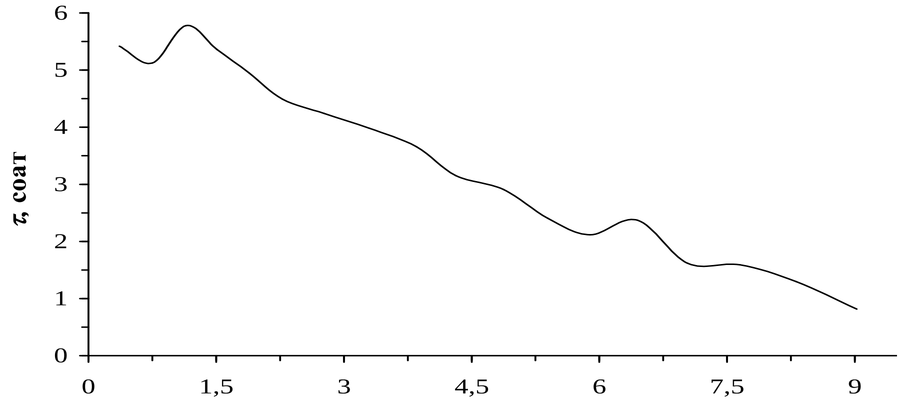


Figure 3. Differential entropy of CO_2 adsorption on Ca_5Na_3A zeolite at 303K temperature. Horizontal bar lines are average integral entropy.

Ca_5Na_3A the average integral entropy to zeolite is -16,78 Dj/mol*K, indicating that the motion of adsorbent carbon (IV) oxide molecules is much higher than that of carbon dioxide in the liquid state.

The graph of adsorption of carbon (IV) oxide molecules on Ca_5Na_3A zeolite is given. It is initially observed that the equilibrium time is high. Initially, the balance is decided over a period of 6 hours. The adsorption amount is from 0,3 CO_2/e.ya to 2 CO_2/e.ya. The adSorption equilibrium time is high.This is because it initially takes longer for the carbon monoxide molecules to reach equilibrium for distribution to the cations in the zeolite matrices. Subsequently, the equilibrium time is gradually reduced from 4 hours to 2,76 hours in a wavy manner, and in these cases the amount of adsorption is 2CO_2/e.ya. and – 5,5CO_2/e.ya. corresponds to a range of values from.

Then a sharp drop in equilibrium time to an hour is observed. The equilibrium time graph shows that 0,77 CO_2/e.ya. and 7,3 CO_2/e.ya. The equilibrium time also gradually decreases as the equilibrium time lines go in a wavy pattern.



***N*, H_2O э.я.**

Figure 4. Equilibrium time of CO_2 adsorption on Ca_5Na_3A zeolite at 303 K.

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V. CONCLUSION AND FUTURE WORK

Ca_5Na_3A zeolite to a total of 8,67 CO_2/e.ya. carbon (IV) oxide gas adsorption was observed. Adsorption differential heats occur in 7 stages in a wavy form. In the Ca_5Na_3A zeolite matrix, the carbon monoxide gas is in a stationary state, indicating the entropy of the liquid state.

Due to the presence of Ca^{+2} and Na^{+} cations in this zeolite, the adsorption heat at initial saturations is higher than 60 kJ/mol. While the initial equilibrium time was high, it was then observed that the equilibrium time gradually decreased. Adsorption isotherms were described using the equations of the volumetric saturation theory of two-dimensional micropores.

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