THEORY OF ADSORPTION COMPLEXES OF N-HEXANE MOLECULES AND VOLUMETRIC FILLING OF MICROPORES IN NAL ADSORBENT

Turabov Bahodir Alikul ugli
Andijan State Technical Institute, Andijan Uzbekistan
https://doi.org/10.5281/zenodo.21218914

ARTICLE INFO

Received: 01st July 2026
Accepted: 04th July 2026
Online: 06th July 2026

KEYWORDS

Ion-molecular complexes, NaL adsorbents, n-hexane, adsorption calorimetry

ABSTRACT

Isotherm and differential heats of n-hexane adsorption in the NaL adsorbents were measured at 303K. The isotherm of adsorption was quantitatively reproduced on the basis of VOM theory. The detailed mechanism of ammonia adsorption in NaL adsorbents from zero filling to saturation was discovered.

Adsorbent L of the shells diameter (entry window to the size of correct comes) 7.2Å, ZLMOF of the shells diameter and of ligands thiomethyl groups by 7.55Å [1]. Both adsorbent L and ZLMOF have a hexagonal pore array along the c axis; moreover, for the prepared materials, the pores also contain clusters of water molecules [2].

At the same time, a thorough theoretical study of the structural arrangement of water in adsorbent L may be relevant for improving adsorbent-L-based compositions and their applications. Interestingly, high-pressure overhydration experiments conducted on adsorbent L recently showed a sharp increase in the amount of water up to 31 H_2O molecules compared to the initial value of 18 (at ~6GPa). increase confirmed [3]. Such growth (pressure since being released later The adsorption capacity (recyclable) is significantly higher than that of other aluminosilicate adsorbents [4] and indicates a special affinity of water for adsorbent L.

The differential heat of adsorption was measured in a DAK 1-1 calorimeter of the Tian-Calve model. Adsorption isotherm was determined using volumetric method. The convenience of this method is that it helps to enrich the theoretical knowledge of adsorption based on thermodynamic laws. This device is adapted only for the determination of adsorption quantities. Adsorption isotherm has an accuracy of 0.1% and a heat of 1% [5].

The n-hexane obtained as adsorbate was purified and dried under vacuum conditions before use in sorption. The dissolved gases were removed until its vapor pressure was the same as the vapor pressure data given in the tables for pure n-hexane. NaL in the adsorbent n-hexane adsorption 303 K also take It's gone.

The isotherm of n-hexane adsorption on the adsorbent has the same logarithmic value as benzene adsorption at initial saturation, ln(P/P 0)=-5.92. The initial adsorption amount of n-hexane molecules is 0.01 mmol/g, and the subsequent adsorption of n-hexane molecules is The isotherm lines are gradually observed towards the adsorption axis. The sorbed n-hexane molecules 0.30 mmol/g isotherm logarithmic value ln(P/P^0)=-0.50 In this part, the

adsorbates are localized on the sodium cations located at the active centers on the adsorption surfaces of the NaL adsorbent. The adsorbent obtained in this way the sodium cations located in the pores are filled with a small amount of n-hexane molecules. In this process, the methyl radicals of n-hexane and the sodium cations in the pores of the adsorbent form weak hydrogen bonds. N-Hexane Adsorption quantity 0.36mmol/g to when it arrives isotherm value $\ln(P/P^0)$=-0.37 to equal becomes and tends to the direction of the adsorption axis when the next n-hexane molecules are absorbed and reaches the saturation level of n-hexane when it reaches 0.72mmol/g. The saturation vapor pressure of N-hexane molecules in adsorbates at 303 K is equal to 119.35mmHg.

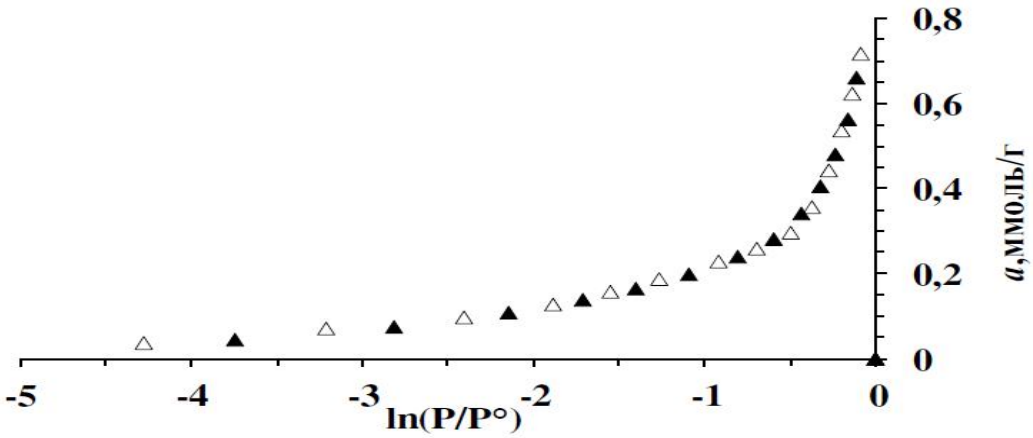

Figure1. 303K also NaL in the adsorbent n-hexane adsorption isotherm.

The adsorption isotherm of n-hexane molecules on the NaL adsorbent obtained from local angren kaolin and alumina was described using the equation of the two-state micropore saturation theory (MSTT).

a=0.365exp[(A/4.47)^1]+0.578exp[(A/0.45)^1]

a- the amount of adsorption in the mixture C_6H_{14}, A=RTln(P°/P)-free energy work (kJ/mol).

The adsorption isotherm is linear in the BET equation coordinates over the relative pressure range $0.021<P/P^o<0.42$. The surface are (a_m) of the NaL adsorbent was 129.2 mkmol/g, and the energy constant was 1.0. Natural in the state NaL of the adsorbent n-hexane for comparison surface area 37.2 m^2/g will be.

The adsorption of n-hexane molecules on the NaL adsorbent obtained from local angren kaolin and alumina occurs mainly by forming molecular complexes with sodium cations located at the entrance of the pores. Therefore, the differential heat initially increases. With subsequent adsorption of n-hexane molecules, a decrease in the differential heat is observed. The reason for the wavy stepwise decrease in the adsorption of n-hexane on the adsorbent is the presence of inlet windows of different sizes in the adsorbent.

Conclusion.

The heat of adsorption in initial fillings is 53.26 kJ/mol. The differential heat of adsorption decreases in a wavy stepwise fashion. The heat of adsorption was studied in five parts. Adsorption isotherms on the surfaces of micropores were described using the equation of the volume saturation theory of micropores. Based on the isotherm values of adsorbent surface areas with respect to benzene and n-hexane, their specific surface area was determined using BET and Langmuir equations.

References:

1.Noh, T. H.; Jang, J.; Hong, W.; Lee, H.; Jung, O.-S. Truncated Trigonal Prismatic Tubular Crystals Consisting of a Zeolite L-Mimic Metal-Organic Framework. Chem. Commun. 2014, 50 (56), 7451–7454.

2.Gigli, L.; Arletti, R.; Quartieri, S.; Di Renzo, F.; Vezzalini, G. The High Thermal Stability of the Synthetic Zeolite K–L: Dehydration Mechanism by in Situ SRXRPD Experiments. Microporous Mesoporous Mater. 2013, 177, 8–16.

3.Gigli, L.; Vezzalini, G.; Quartieri, S.; Arletti, R. Compressibility Behavior and Pressure-Induced over- Hydration of Zeolite K–AlSi-L. Microporous Mesoporous Mater. 2019, 276, 160–166.

4.Comboni, D.;Gatta, G.D.;Lotti, P.;Merlini, M.;Hanfland, M.Crystal-Fluid Interactions in Laumontite. Microporous Mesoporous Mater. 2018, 263, 86-95.

5.Mentzen B.F., Rakhmatkariev G.U. Host/Guest interactions in zeolitic nonostructured MFI type materials: Complementarity of X-ray Powder Diffraction, NMR spectroscopy, Adsorption calorimetry and Computer Simulations. // Uzbek. chemical magazine, 2007. -No.6. -S. 10- 31.