E- Global Congress
Hosted online from Dubai, U. A. E., E - Conference.
Date: 19th February, 2023
Website: https://eglobalcongress.com/index.php/egc
ISSN (E): 2836-3612

DIFFERENTIAL HEATS OF ORTA-XYLENE IN ZEOLITE AgZSM-5

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Annotation
This paper presents the differential heat of adsorption of o-xylene on zeolite AgZSM-5 at a temperature of 303 K, obtained by the microcalorimetric method. A correlation between the adsorption-energy characteristics was found and the molecular mechanism of o-xylene adsorption in AgZSM-5 zeolite was revealed in the entire filling region. A stepwise nature of the heat of adsorption of o-xylene was revealed. The adsorption of the o-xylene molecule forms by the intersection of straight and zigzag channels and the formation of ion/molecular complexes of various multiplicity in them.

Keywords: adsorption, adsorption heat, thermodynamics, enthalpy, adsorption isotherm, entropy, thermo kinetics, calorimeter, o-xylene.

Using the atom–atom approximation, the adsorption energies of m-xylene, o-xylene, p-xylene, toluene, and benzene were calculated at different positions of the porous structure of the MFI zeolite for several variants of the topological structure of the adsorbent [1]. The calculation results strongly depend on the accepted structural model of the zeolite synthesized under different conditions. The X-ray diffraction spectra for these synthetic zeolites were also calculated. By comparing the obtained results with experimental values, the most probable type of structure of zeolites and adsorbate was determined. The theoretically calculated heats of adsorption agree with the experimentally obtained values of the differential heats. It has been shown that the results of theoretical calculations provide valuable information on the location and mobility of different molecules adsorbed on different zeolites [2].

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To describe the adsorption of aromatic hydrocarbons in silicalites [3], it is proposed to use a lattice model with three types of sites; in straight channels, sinusoidal and channel intersections. The statistical approximation was used for calculations. By changing the set of model parameters, the adsorption of both benzene and xylene in ZSM-5 zeolites is described. In [4], calculations were carried out and presented in the form of potential maps for various cross sections along the pore axis for the CH_4-LiZSM-5 and CH_4-CsZSM-5 systems. For each of the systems, good agreement was obtained between the experimental adsorption and that calculated from the potential energy.

The differential heats of adsorption of o -xylene on AgZSM-5 have a rather complex form (Fig. 1). In the initial region, the heats fall linearly from ~150 kJ/mol to 95 kJ/mol and form a step at adsorption of 0.3 mmol/g. The initial section of elevated heats of adsorption is apparently associated with the adsorption of o -xylene at the crossroads of channels with Ag^+ cations. The linear section of the differential heat of adsorption and the resulting stepped part fully correspond to the amount of Ag^+ cations included in the zeolite (~0.3 mmol/g). In this section, we observe the stoichiometric interaction of

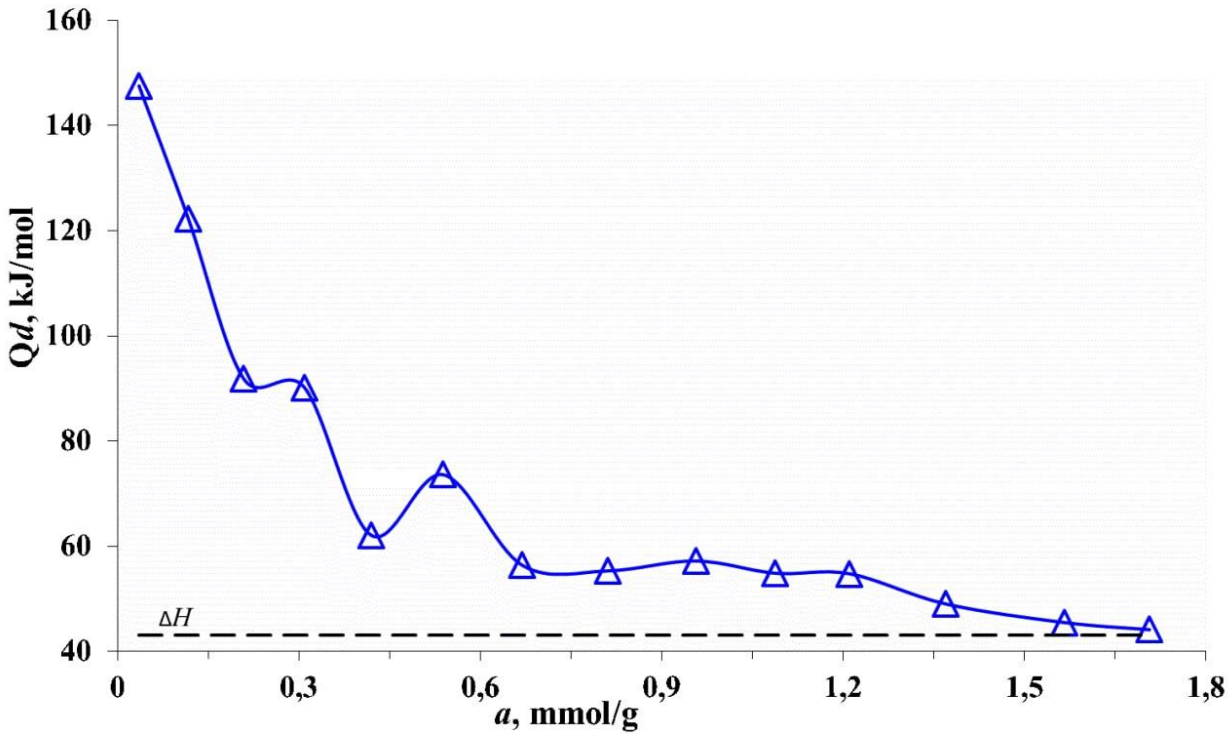

Figure 1. Differential heats of adsorption of o-xylene in Ag ZSM-5 zeolite at 303 K. The horizontal dotted line is the heat of condensation of o-xylene at 303 K.

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o-xylene with the Ag^+ cation with the formation of the o-xylene/Ag^+ mono complex.

The area with constant adsorption energy indicates the adsorption of o-xylene on the homogeneous sections of the ZSM-5 zeolite channels. These sections can be either straight or zigzag channels. Taking into account that the dispersion potential in zigzag channels is higher, it can be assumed that adsorption first proceeds in

zigzag channels. After zigzags, p-xylene is adsorbed in straight channels, but due to steric hindrances, it fills them only halfway. The drop in heat is caused by adsorption in the remaining unfilled sections of straight channels and crosshairs. The mechanism of filling AgZSM-5 zeolite with o-xylene at different stages of this process is different. From the first stage to the fourth, adsorption occurs due to the formation of nC_8H_{10}/Ag^+ complexes by silver ions in the cross channels of the zeolite and by o-xylene molecules. The process of filling the remaining stages, it can be assumed that this occurs due to the physical bond between the zeolite and adsorbate molecules.

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