THERMOKINETICS OF META- AND ORTA-XYLENE ADSORPTION IN ZEOLITE Cu^{2+}ZSM-5

Bakhronov Kh.N.[1], Yunusova R.G.[2]

[1]Institute of General and Inorganic Chemistry, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan

[2]Bukhara State Medical Institute named after Abu Ali ibn Sina

Email: baxronov@mail.ru

Among the aromatic hydrocarbons, benzene, toluene and p-xylene are the most easily adsorbed on ZSM-5 type zeolites (all of them have a kinetic diameter of 0.58 nm). The studies of the adsorption of benzene, toluene, and paraxylene in silicalite are the subject of works [1–4]. Adsorption on the acid sites of zeolites proceeds according to the usual mechanism of physical adsorption. It was noted that aromatic hydrocarbon molecules move freely over the outer surface of the zeolite before they reversibly attach to OH groups, enter micropores, or desorb. Molecules capable of entering micropores (benzene, toluene, n-xylene) adsorb faster on SiOHA1 groups than on SiOH groups. For o-xylene molecules, whose entry into the pores is sterically hindered, the rate of adsorption on the remaining SiOH groups increases significantly. The study of the adsorption properties of zeolites provides useful information about the structural characteristics and possibilities of practical application. Using adsorption measurements, one can obtain data on various factors (for example, channel sizes, pore volume, cation localization, etc.) associated with the structure of a particular zeolite.

The main thermodynamic parameters of ortho- and meta-xylenes in Cu^{2+}ZSM-5 zeolite were studied by the adsorption-calorimetric method. A correlation between the adsorption-energy characteristics was found and the molecular mechanism of metaxylene adsorption in Cu^{2+}ZSM-5 zeolite was revealed in the entire filling area. A stepwise nature of the heat of adsorption of meta- and

ortho-xylene was revealed. It has been established that the cations in the Cu^{2+} zeolite are located in screened positions of the ZSM-5 zeolite crystal lattice. The adsorption of a meta- and ortho-xylene molecule leads to the migration of Cu^{2+} cations from the zeolite lattice to the crosshairs formed by the intersection of straight and zigzag channels and the formation of ion/molecular complexes of various multiplicity in them [5, 6].

Of interest is the course of the curve of the dependence of the time of establishment of adsorption equilibrium on the filling of the adsorption of orta-xylene on zeolite CuZSM-5 (Figure 1). Before adsorption of 0.15 mmol/g, the establishment of equilibrium slows down (from ~5 to ~10 hours). The content of copper cations, according to the chemical composition of the unit cell, is 0.3 mmol/g, i.e. the amount of adsorbed ortho-xylene upon adsorption of 0.15 mmol/g corresponds to the C_8H_{10}:2Cu^{2+} scheme. At higher fillings, the time for establishing adsorption equilibrium is sharply accelerated. This fact also indicates the diffusion of cations in the zeolite lattice, which leads to such a sharp slowdown in the sorption process. With an increase in the amount of adsorption, redistribution of copper cations occurs, and the amount of adsorbed meta-xylene corresponds to the C_8H_{10}:Cu^{2+} scheme (0.3 mmol/g).

The content of copper cations, according to the chemical composition of the unit cell, is 0.3 mmol/g.

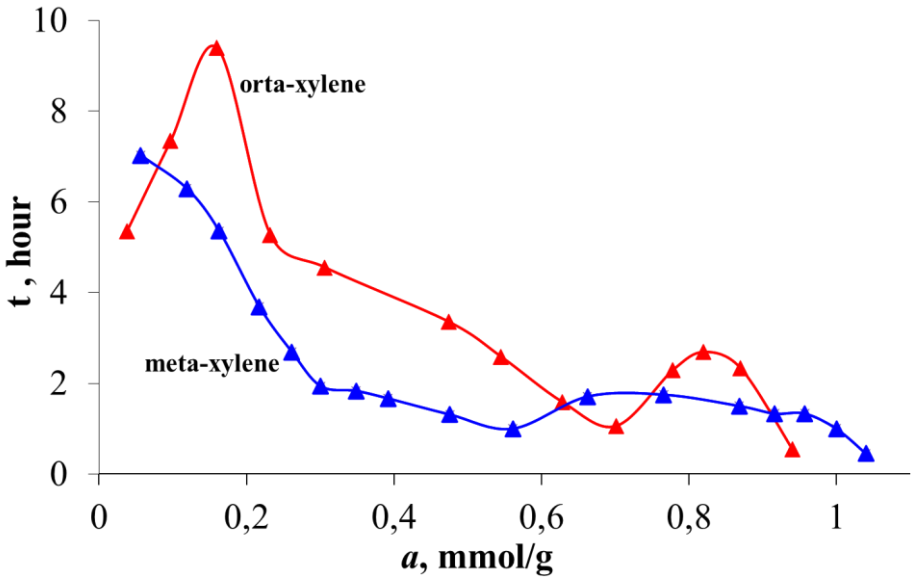

Figure 1. Thermokinetics of adsorption of meta-xylene and orta-xylene on zeolite Cu^{2+}ZSM-5.

Starting from a filling of 0.3 mmol/g, the adsorption process accelerates and equilibrium is established in 2 hours at an adsorption of 0.7 mmol/g. Further, the adsorption rate, forming a small growth, decreases to 0.5 hours at an adsorption of 0.94 mmol/g.

The thermokinetics of meta-xylene adsorption correlates with the thermokinetics of ortho-xylene. It forms a small step at 0.15 mmol adsorption and then decreases linearly to 2 hours at 0.3 mmol/g adsorption. Further, forming a step, the thermokinetics decreases to 1 hour at an adsorption of 0.6 mmol/g. With adsorption of 1.1 mmol/g, the time of adsorption equilibrium is set in 0.5 hours.

Literature

1. Jentys A., Tanaka H., Lercher J. A. Surface processes during sorption of aromatic molecules on medium pore zeolites //J. Phys. Chem., 2005, N6, -v.109, -P.2254-2261

2. Xomeritakis G., Nair S., Tsapatsis M. Microporous Mesoporous Mater. The Location of o- and m-Xylene in Silicalite by Powder X-ray Diffraction//- 2000. – Vol. 38. -P. 61-73.

3. Nair S., Tsapatsis. The Location of o- and m-Xylene in Silicalite by Powder X-ray Diffraction // J. Phys. Chem. -2000. -Vol. 104. -P. 8982-8988.

4. Kh.Bakhronov, O.Ergashev, Kh.Karimov, T.Abdulkhaev, Y.Yakubov, A.Karimov, Thermodynamic Characteristics of Paraxylene Adsorption in LiZSM-5 and CsZSM-5 Zeolites, AIP Conference Proceedings 2432, 050056 (2022); Published Online: 16 June 2022, https://doi.org/10.1063/5.0090039

5. Bakhronov X.N., Sobirjonova S.T. Moral differential entropy of adsorption meta-xylene in zeolite CuZSM-5 International Conference on Advance Research in Humanities, Sciences and Education Hosted from Istanbul, Turkey https://confrencea.org July 15th 2022, pp.222-224

Bakhronov Kh.N., Ruzimova G.Kh. Heats and entropy of ortho-xylene adsorption in CuZSM-5 //International Conference on Advance Research in Humanities, Sciences and Education, Hosted from Sydney, Australia https://confrencea.org August 15th 2022, pp.110-111