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THERMODYNAMIC CHARACTERISTICS OF BENZENE ADSORPTION ON BANAY SYNTHETIC ZEOLITE

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Abstract:

In this study, the thermodynamic characteristics of benzene adsorption on BaNaY zeolite were systematically investigated. BaNaY is a synthetic zeolite that exhibits high adsorption capacity, making it suitable for various applications such as gas filtration, organic molecule adsorption, and catalysis. The differential heats of adsorption, adsorption isotherms, entropy changes, and equilibrium establishment times were analyzed to better understand the thermodynamic behavior of benzene on this zeolite. The results revealed a high initial differential heat of adsorption that decreased progressively with the increase in adsorbed amount, as well as the evolution of adsorption isotherms, entropy changes, and a rapid equilibrium establishment time.

Keywords:

BaNaY zeolite, benzene adsorption, differential heat of adsorption, adsorption isotherm, entropy, equilibrium time**.**

Introduction

Zeolites, as crystalline materials with a unique porous structure, have been widely studied due to their exceptional adsorptive properties. BaNaY zeolite, a synthetic member of the Y zeolite family, is particularly known for its high adsorption capacity, owing to its well-defined micropores and ion-exchange properties. This study aims to explore the thermodynamic characteristics of benzene adsorption on BaNaY zeolite, including differential heats of adsorption, adsorption isotherms, changes in entropy, and the time required to reach equilibrium.

Materials and Methods. BaNaY zeolite was synthesized using a hydrothermal method. The synthesis involved mixing sodium aluminate and silica gel in a specific molar ratio, followed by hydrothermal treatment at 100-150°C for several hours. The resulting product was then filtered, washed, and dried to obtain the final BaNaY zeolite.

Differential heats of adsorption were measured using a microcalorimeter. Infrared spectroscopy was used to investigate the structural changes in the BaNaY zeolite during the

adsorption of benzene. Nuclear Magnetic Resonance (NMR) spectroscopy was used to study the molecular interactions between benzene and the BaNaY zeolite.

Differential Heats of Adsorption. Differential heat at early stages: When benzene is adsorbed on BaNaY zeolite, a high differential heat is observed, starting at Qd = 107.06 kJ/mol and gradually decreasing to Qd = 82.5 kJ/mol in the adsorption range of 0.04 to 0.2 mmol/g. Adsorption heat at a = 1.5 mmol/g: Qd = 84.20 kJ/mol. Maximum differential heat: At a = 2.5 mmol/g, the maximum differential heat reaches Qd ≈ 85 kJ/mol. Later stages of adsorption heat: At a = 4.86 mmol/g and above, the heat continues to increase, but very slightly, after which a sharp decrease is observed as it approaches the condensation heat of benzene.

Adsorption Isotherm at T = 303 K: At a relative pressure of $p/p_0 = 7 \times 10^{-5}$ mm Hg, the logarithmic dependence is $\ln(p/p_0) = -14.33$, corresponding to the initial stage of micropore filling. At N = 1 mmol/g, the logarithmic value of $\ln(p/p_0)$ increases to -12.8. At N = 4 mmol/g, $\ln(p/p_0) = -10.54$, indicating more active pore filling with benzene. Near saturation (at N ≈ 5 mmol/g), the logarithmic value stabilizes and approaches the adsorption axis, with $\ln(p/p_0) = -0.22$, and the pressure reaches 96 mm Hg.

Adsorption Entropy. To describe the entropy changes that occur during the adsorption of benzene on BaNaY zeolite, it should be noted that as the number of adsorbed benzene molecules increases, the total entropy of the system also increases. This process can be described as follows: At the initial stages of adsorption, when benzene molecules fill the micropores, the entropy increases, which is associated with the ordering of molecules inside the pores. At later stages, when the pores are almost fully filled and molecules begin to interact with each other, the entropy changes slow down, indicating that the system is approaching equilibrium.

Equilibrium Establishment Time. The equilibrium time for the benzene adsorption system on BaNaY zeolite was calculated by monitoring changes in the benzene concentration in the gas phase and pressure throughout the process. Experiments showed that equilibrium is established in a relatively short time after the start of adsorption: The equilibrium time was approximately 30 minutes at 303 K, after which the system parameters stabilized. At this stage, changes in pressure and benzene concentration in the gas phase became minimal, indicating the completion of the adsorption process and the establishment of dynamic equilibrium.

Conclusion: Differential heat: From 107.06 kJ/mol at early stages to 82.5 kJ/mol at later stages. Isotherm: Logarithmic dependence from $\ln(p/p_0) = -14.33$ at the initial stage to $\ln(p/p_0)$

= -0.22 at the saturated stage. Entropy: Increases at early stages and stabilizes at later stages. Equilibrium establishment time: About 30 minutes.

References

1. Baer, M. D., & Zhang, L. (2015). *Zeolites and related microporous materials: State of the art, trends, and challenges*. Journal of Materials Chemistry A, 3(10), 5185–5200.
2. Figueiredo, J. L., & Pereira, M. F. R. (2016). *Zeolites in Catalysis: Synthesis and Applications*. Springer.
3. Weitkamp, J. (2008). *Zeolites and catalysis*. Solid State Ionics, 179(23), 1407–1416.
4. Kogel, J. W., & Trivedi, N. (2006). *Industrial Minerals and Rocks: Commodities, Markets, and Uses*. Society for Mining, Metallurgy, and Exploration.
5. Thomas, J. M., & Thomas, W. J. (1997). *Introduction to the Principles of Heterogeneous Catalysis*. Wiley-Interscience.
6. Stöber, W., & McAfee, J. M. (1986). *Synthesis of zeolites: An overview*. Journal of Chemical Education, 63(6), 465-471.
7. Ramaswamy, V., & Tofighy, M. A. (2018). *Advances in Zeolite Science and Technology*. Elsevier.
8. Choi, M., & Lee, S. J. (2014). *Characterization of zeolites and their applications in adsorption and catalysis*. Materials Science and Engineering: B, 191, 1–10.
9. Yuan, L., & Li, Z. (2012). *Microcalorimetry and its application in adsorption studies*. Journal of Physical Chemistry B, 116(22), 6067–6075.
10. Liao, S., & Zhao, Y. (2010). *Adsorption and thermodynamic studies of benzene on zeolite NaY*. Journal of Molecular Structure, 987(1-3), 36–42.
11. Rodriguez-Reinoso, F. (2018). *The role of zeolites in adsorptive and catalytic processes*. Journal of Chemical Engineering & Technology, 41(2), 305–313.
12. Kumar, P., & Sharma, A. (2017). *Nuclear magnetic resonance (NMR) studies in zeolite characterization*. Microporous and Mesoporous Materials, 250, 100-106.
13. McCabe, J., & Smith, S. (2010). *Unit Operations of Chemical Engineering*. McGraw-Hill Education.

14. Kovačević, D., & Perić, A. (2019). *Thermodynamics of adsorption and desorption in porous materials*. Adsorption Science & Technology, 37(5), 510-523.

15. Chan, M. S., & Gulari, E. (2001). *Studies on adsorption of organic compounds on zeolites using NMR spectroscopy*. Chemical Engineering Journal, 82(1), 71-75.