STRUCTURAL FEATURES AND MECHANISMS OF GAS ADSORPTION IN THE METAL-ORGANIC FRAMEWORK ZIF-8

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Abstract. This paper examines the structural features of the metal-organic framework ZIF-8 and the physicochemical mechanisms of carbon dioxide (CO_2) and methane (CH_4) adsorption. Particular attention is paid to the effects of pore structure, imidazolate linker flexibility, and the nature of intermolecular interactions on adsorption capacity and gas separation selectivity. The roles of molecular sieving, dispersion forces, and electrostatic interactions in gas adsorption processes are analyzed. The effects of temperature, pressure, and diffusion limitations on the separation efficiency of CO_2/CH_4 mixtures are discussed. The necessity of a comprehensive analysis of equilibrium, kinetic, and thermodynamic characteristics is emphasized to ensure a reliable assessment of the adsorption properties of ZIF-8 and its potential for practical applications.

Keywords: ZIF-8, microporosity, CO_2, CH_4, selectivity, adsorption.

Introduction. The development of selective adsorbents for natural gas purification, carbon dioxide capture, and the separation of process gas mixtures is a pressing challenge in chemical engineering. Zeolitic imidazolate frameworks (ZIFs) occupy a special place among modern porous materials, combining the coordination chemistry of metal-organic frameworks with the topological characteristics of zeolite-like structures. The most extensively studied member of this family is ZIF-8, in which Zn^{2+} ions are linked by 2-methylimidazolate ligands. Owing to its controllable synthesis, well-developed microporosity, and relatively high chemical stability, this material is of interest for the adsorption of CO_2, CH_4, and other gases [1-3].

Structure and characteristics of the pore system. The crystalline framework of ZIF-8 has sodalite (SOD) topology: cavities are interconnected by narrow windows formed by organic linkers. The nominal aperture size is commonly estimated at approximately 3.4 Å, whereas the internal cavities are considerably larger. When interpreting adsorption behavior, it is important to recognize that the nominal window geometry is not completely rigid: rotation and vibration of imidazolate fragments may alter pore accessibility for individual molecules. Consequently, a simple comparison between the kinetic diameter of a gas and a single geometric parameter does not always reliably predict actual permeability and sorption rates [1, 2].

Influence of synthesis conditions. The physicochemical properties of ZIF-8 depend on the solvent, concentrations of the zinc salt and 2-methylimidazole, reactant ratio, temperature, and crystallization time. Changes in these parameters affect crystallite size, aggregation, defect concentration, and surface accessibility. For powder samples, washing and activation are particularly important: residual solvent or unreacted ligands can block micropores and reduce the measured sorption capacity. Therefore, comparisons of materials synthesized by different routes are valid only when sample preparation and degassing protocols are comparable [3, 4].

Mechanisms of interaction with gas molecules. CO_2 adsorption in ZIF-8 is governed by a combination of dispersion and electrostatic interactions with the internal framework surface. The quadrupole moment of CO_2 promotes interactions with local variations in the electric field. For CH_4, dispersion forces and geometric accessibility of micropores are more significant. At low pressures, the interaction energy between molecules and the most favorable surface sites plays the primary role; as pressure increases, pore-volume filling becomes more important. Unlike certain MOFs containing open metal sites, the zinc nodes in ZIF-8 are predominantly coordinatively saturated. Thus, strong CO_2 binding at open Zn sites should not be attributed to this material without additional evidence [1-3].

Adsorption selectivity and kinetics. The selectivity of ZIF-8 cannot be reduced to the ratio of pure-gas adsorption capacities. For a binary mixture, competition between components, differences in diffusion coefficients, feed composition, and operating pressure and temperature must be considered. Equilibrium selectivity can be assessed using experimental binary adsorption data or the ideal adsorbed solution theory, provided that the fitted isotherms are suitable. However, the time required to reach equilibrium and the possibility of regeneration are also critical in real processes. A material exhibiting high equilibrium selectivity does not necessarily deliver optimal performance in a cyclic adsorber [3, 5].

Characterization methods. Establishing a reliable synthesis-structure-adsorption relationship requires a combination of techniques. X-ray diffraction confirms the formation of the crystalline ZIF-8 phase; infrared spectroscopy reveals characteristic vibrations of the organic ligand; and scanning electron microscopy characterizes particle morphology and aggregation. N_2 adsorption at 77 K is used to assess textural properties, although the results must be interpreted in view of possible diffusion limitations. CO_2 and CH_4 adsorption isotherms measured at several temperatures provide information about equilibrium and interaction energetics.

Evaluating practical applicability requires mixed-gas tests, adsorption–desorption cycling, and verification of structural stability following exposure to moisture [1-4].

Application prospects. ZIF-8 is of interest as an independent powder adsorbent, a membrane component, and a functional phase in hybrid materials. Moving from laboratory measurements to technological applications requires consideration of powder shaping, mass-transfer resistance, mechanical strength, and stability in the presence of water vapor and impurities. In particular, studies of competitive CO_2/CH_4 adsorption under varying humidity and temperature, combined with the evaluation of thermal effects, are promising. Direct measurement of the differential heat of adsorption could complement isotherm data and help identify energetic heterogeneity among active sites [2, 3, 5].

Conclusion. An analysis of the literature indicates that the properties of ZIF-8 are governed not only by nominal pore dimensions but also by organic linker mobility, activation conditions, structural defects, and molecular transport kinetics. Assessing its potential for gas separation requires the combined investigation of adsorption equilibrium, diffusion, thermodynamics, and cyclic stability. Such an integrated approach enables informed selection of ZIF-8 modification strategies and helps avoid overstated conclusions based on individual pure-gas isotherms.

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