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Influence of KIT-6's pore structure on its surface properties evaluated by inverse gas chromatography

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HIGHLIGHTS

- Pore structure effect on KIT-6 surface property was studied by IGC.
- High adsorption free energy and adsorption enthalpy were observed on KIT-6 with microspores.
- Strong dispersive and specific interaction were found on the samples with the relative narrow mesopores.
- The test molecules were believed to partly penetrate into the minor present micropores.

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ABSTRACT

The pore structure of mesoporous silica KIT-6 has been systematically tuned via the variation of calcination temperature (773–1223 K), with the mesopore size ranging from 4.8 to 7.5 nm and micropore volume from 0.000 to 0.078 cm^3/g, respectively. Four *n*-alkanes (C6–C9), cyclohexane, benzene, toluene, trichloroethylene, and tetrachloroethylene were employed as probe molecules in the evaluation of the pore structure effect on KIT-6 surface property using inverse gas chromatography (463.2–493.2 K). High free energy of adsorption and enthalpy of adsorption were observed on the KIT-6 with the micropore volumes. The dispersive interaction parameter γ_S^D, and specific interaction parameter I^{SP}, were found to decrease with the increment of the mesopore size of the samples. These results indicate that the occurrence of micropore contributes the adsorption, while the narrow mesopore of KIT-6 promotes the dispersive and specific interaction.

1. Introduction

During the past decade, the solid material of mesoporous KIT-6 has been intensively investigated in both academics and industry [1–6]. Mesoporous silica KIT-6 has well-ordered (cubic *Ia3d* symmetry) pore structure with high surface area, variable pore diameter (4–12 nm), and large pore volume [3]. Terasaki et al. observed that the complementary micropore (*ca.* 1.8 nm) forms interconnection between the two main pore systems of KIT-6 at a special flat point [4]. Bruce et al. found that the pore structure, including the pore size and micropore volume, can be tuned by simply changing the calcination temperatures [5]. They also synthesized a bimodal porous metal oxide using KIT-6 hard template and proposed that the compensator micropore should partly influence the pore formation of the metal oxide material [5,6]. Although much interest was shed light on the ordered three-dimensional structures of KIT-6 with large pore diameters [1–6], there are no detailed studies about the pore structure effect, especially the compensator micropore bridging the main channels, on its surface properties.

The characteristics of solid surface are generally determined by adsorption of gases and vapors through static or dynamic methods. Compared with conventional gas chromatography, inverse gas chromatography (IGC) has the solid phase of the interested object whereas the vapor of known materials as probes. IGC has been employed in the study of thermodynamics parameters, surface energy, reaction kinetics, and textural parameters of many solid state materials such as polymers [7,8], polymer blends [9], adsorbents [10], fibers [11], catalysts [12,13], and zeolitic imidazolate framework [14]. In our previous work, IGC was firstly employed to study the surface property of Rh/H-Beta and found it has special interaction with benzene [12]. After that, Rh/H-Beta was used to

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