A Polyaromatic Capsule Solid as a Vapor Adsorbent for Benzene Derivatives

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Porous materials, such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs), are useful solids for adsorption, separation, and storage of molecules.[1] Most of these materials possess infinite cavities and windows in subnanometer to nanometer size. In contrast, polyaromatic capsule **1**, composed of eight anthracene panels and two metal ions, provides a finite, large cavity with four small windows.[2] Here we report that capsule solid $(\mathbf{1})_n$ displays adsorption ability for benzene derivatives as a new vapor adsorbent.

Capsule solid $(\mathbf{1})_n$ was put in a sealed vessel including benzene (**BN**), toluene (**TL**), and *o*-xylene (**oXL**) without direct host-guest and guest-guest contact (Figure 1a). After standing at r.t. for 1 h, the resultant solid $(\mathbf{1})_n\bullet(\mathbf{BN})_x\bullet(\mathbf{TL})_y\bullet(\mathbf{oXL})_z$ was subjected to reduced pressure and dissolved in CD_3CN. ^{1}H NMR analysis of the product solution revealed that 3.3 equivalent of the benzene derivatives (based on **1**) are bound by solid $(\mathbf{1})_n$, with >80% **oXL** selectivity (Figure 1b, left). In the same way, solid $(\mathbf{1})_n$ bound **oXL** from a mixture of three xylene isomers with 53% selectivity (Figure 1b, right). The volatilization of the adsorbed molecules was suppressed by solid $(\mathbf{1})_n$ even at 100 ºC for 1 h (Figure 1c). Furthermore, solid $(\mathbf{1})_n$ could be reused at least five times with the same adsorption ability for three xylene isomers (Figure 1d).

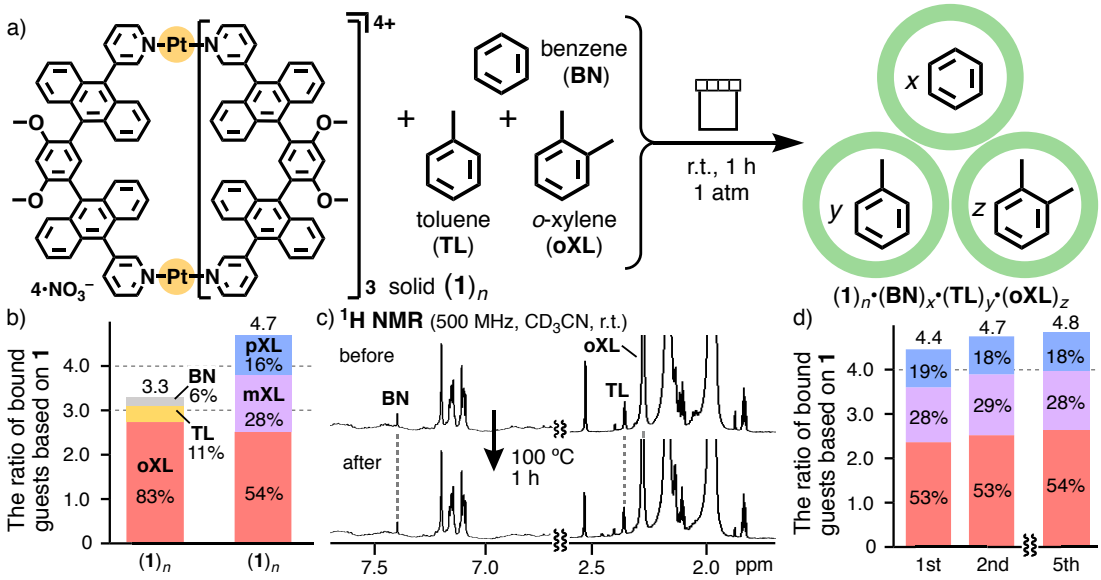

Figure 1. a) Selective vapor adsorption by solid $(\mathbf{1})_n$. b) Guest ratios and % after binding experiments. c) ^{1}H NMR spectra of $(\mathbf{1})_n\bullet(\mathbf{BN})_x\bullet(\mathbf{TL})_y\bullet(\mathbf{oXL})_z$ before/after heating. d) Reusability of solid $(\mathbf{1})_n$.

[1] G. Zhang, B. Hua, A. Dey, M. Ghosh, B. A. Moosa, N. M. Khashab, *Acc. Chem. Res.* **2021**, *54*, 155–168. [2] N. Kishi, Z. Li, K. Yoza, M. Akita, M. Yoshizawa, *J. Am. Chem. Soc.* **2011**, *133*, 11438–11441.