Supplementary Material for Chemical Communications

Supplementary data

Guest exchange in dimeric capsules of tetraurea calix[4]arene in the solid state

Marat A. Ziganshin,[a] Ludmila S. Yakimova,[a] Khasan R. Khayarov,[a] Valery V. Gorbatchuk,*[a] Myroslav O. Vysotsky[b] and Volker Böhmer*[b]

[a] Institute of Chemistry, Kazan State University, Kremlevskaya 18, Kazan, 420008, Russia; Fax: +7 843 2927418; Tel: +7 843 2315309; E-mail: Valery.Gorbatchuk@ksu.ru

[b] Fachbereich Chemie, Pharmazie und Geowissenschaften, Abteilung Lehramt Chemie, Johannes Gutenberg-Universität, Duesbergweg 10-14, D-55099 Mainz, Germany; E-mail: vboehmer@mail.uni-mainz.de

Supplemental figure for Guest exchange in dimeric capsules of tetraurea calix[4]arene in the solid state

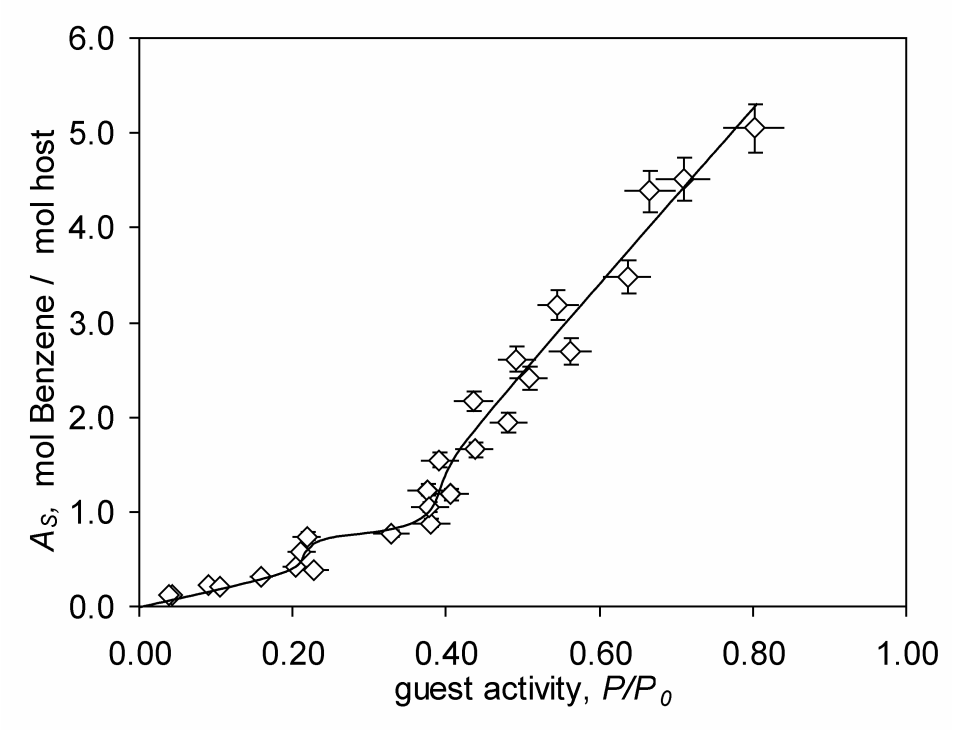

Figure S1. The vapor sorption isotherm of benzene by material **C** obtained by (re)crystallization of **1** from methanol/chloroform and drying, T = 298 K, after 3 days of equilibration between the host powder and guest vapor at the same temperature in hermetically closed vials. Guest uptake A_S (mol per mol of host monomer) is plotted *vs.* guest relative vapor pressure, or activity, P/P_0. The line was drawn to guide the eye.

The first step of guest uptake on the sorption isotherm below $P/P_0 = 0.37$ corresponds to the formation of relatively stable 1:1 inclusion compound with benzene probably bound inside calixarene bowls. Here, P is the benzene vapor pressure in the studied system, and P_0 is the saturated vapor pressure of benzene over its pure liquid. Above $P/P_0 = 0.37$, a phase transition takes place with formation of unstable clathrate having near 5 benzene molecules per 1 host monomer, where benzene may be bound mostly outside host bowls (See Ref.12 in the paper).