Supplementary data

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

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**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).