

A GENUINE MOLECULAR RECOGNITION BY INCLUSION WITH MACROCYCLIC HOSTS

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Specific features of guest inclusion by calixarenes and beta-cyclodextrin were found, which may be used for selective discrimination of volatile guests in one-component vapors and even in complex mixtures using only one receptor. These features include a cooperativity of guest binding by solid host and clathrate decomposition, partial binding reversibility, multi-step formation and decomposition of clathrates, guest exchange in solid host phase, host polymorphism with a memory of eliminated guest structure, and cooperative hydration effect for hydrophilic hosts with guest encapsulation upon host drying. Some effects are extremely selective being observed only for one guest irrespective of its ability for key-to-lock binding, e.g. Figure 1.

The clathrate properties were studied using gas chromatographic headspace analysis, simultaneous thermogravimetry and differential scanning calorimetry combined with mass-spectrometry, and quartz crystal microbalance (QCM) sensors. Thus, the vapor sorption isotherms, Gibbs energy of clathrate formation, clathrate stoichiometry, temperatures and enthalpies of guest elimination and of host collapse were determined.

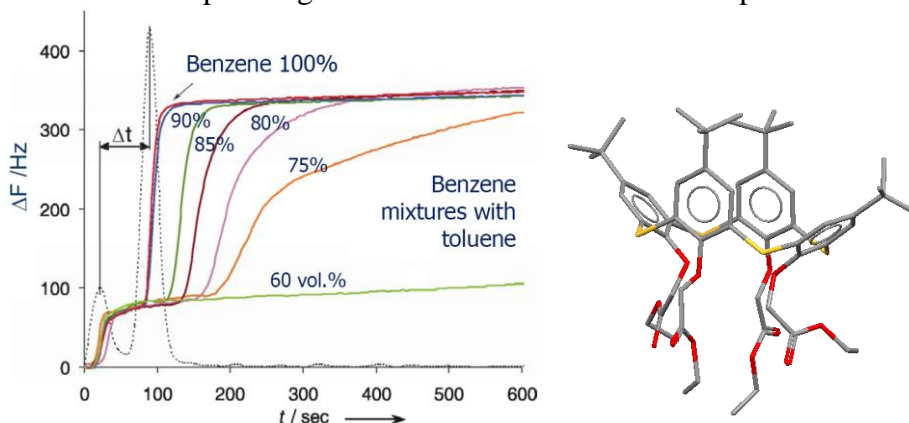


Figure 1. Molecular recognition of benzene in its mixture with toluene by a stepwise response of QCM sensor with a layer of thiocalix[4]arene derivative [1].

The clathrate parameters were observed to depend much on the host molecular structure and on the related type of guest encapsulation or interstitial binding. Hence, several new approaches were offered to boost a molecular recognition capability of a receptor for determination of single vapors and components of complex mixtures [1-4].

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