

# Estimation of the free energy of the supramolecular effect on host-guest complex formation between solid tert-butylcalix[4]arene and vapors of organic compounds

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## Abstract

The free energy of the supramolecular effect was estimated by the difference of the free energy of the solid host-guest complex formation between the vapor guest and the solid tert-butylcalix[4]arene (1) and the free energy of the guest solvation in toluene. These thermodynamic parameters were obtained from the vapor sorption isotherms of the guests with various molecular structure by solid 1 and limiting activity coefficients of the guests in toluene determined by headspace gas chromatographic analysis. The supramolecular effect was found to decrease slightly with the increase of the guest molecular size.

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## Keywords

Headspace gas chromatographic analysis, Solid macrocyclic calixarene, Thermodynamics of molecular recognition, Vapor sorption isotherms