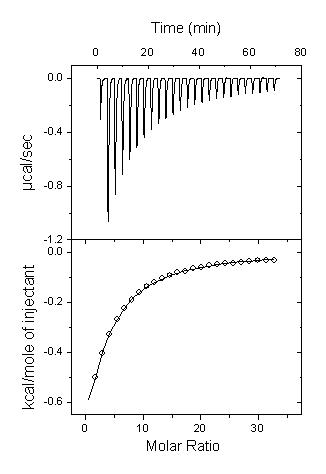
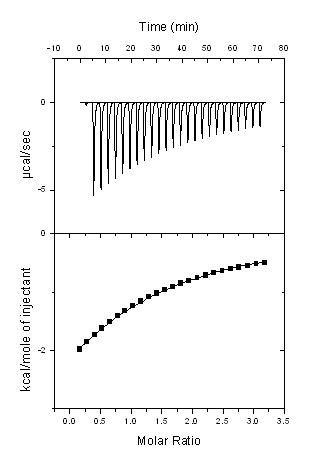
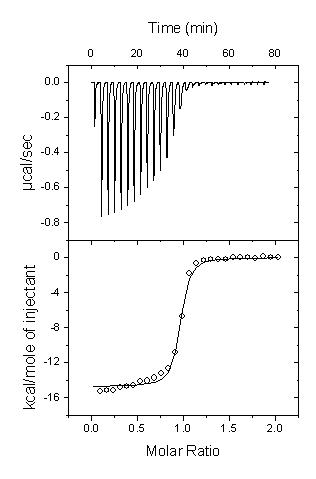
**Supporting Information**

**Inclusion of Neutral Guests by Water-Soluble Macrocyclic Hosts – A Comparative Thermodynamic Investigation with Cyclodextrins, Calixarenes, and Cucurbiturils**

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a.b.c.

**Figure S1.** ITC isotherm for the titration of 7.91, 9.63 and 0.15 mM DBN into 0.045 mM *β-*CD (a), 0.56 mM CX4 (b) and 0.015 mM CB7 (c) aqueous solution, respectively.

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**Figure S2.** 1H NMR spectra of a) free and complexed DBO with CB7, b) free and complexed DBN with CB7.

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**Figure S3.** Distribution functions of free host diameter; see Figure S4 for the diameter definition.

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**Figure S4.** Definition of the diameters used to determine the flexibility of the free hosts.

**Table S1.** Water-guest intermolecular Hydrogen bond analysis[a], obtained from the MD trajectories.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Number** | **free** | **@*β*-CD** | **@CX4** | **@CB7** |
| DBH | 0.70 | 0.53 | 0.85 | 0.53 |
| DBO | 0.70 | 0.59 | 0.90 | 0.68 |
| DBN | 0.70 | 0.59 | 1.02 | 0.79 |

[a]A hydrogen bond cut distance ≤ 2.8 Å and an angle ≥ 120° were used.