Supplementary Material (ESI) for *Physical Chemistry Chemical Physics*


Supporting Information for:

# Can the anomalous aqueous solubility of β-cyclodextrin be explained by its hydration free energy alone?

Wensheng Cai, Tingting Sun, Xueguang Shao

*Department of Chemistry*, *Nankai University*, *Tianjin*, *300071*, *P.R. China*

Christophe Chipot

*Equipe de dynamique des assemblages membranaires, UMR CNRS/UHP 7565, Université Henri Poincaré, BP 239, 54506 Vandœuvre-lès-Nancy cedex, France*

**Table S1.** Potential-derived atomic charges of a glucose unit of α-CD at B3LYP/6-311++G(d,p) level of theory.

| Atom | Charges | | Atom | Charges | |
|---|---|---|---|---|---|
| | Gas | Water | | Gas | Water |
| C1 | -0.484198 | -0.469332 | HO2 | 0.475120 | 0.527399 |
| H1 | 0.285803 | 0.299604 | C3 | -0.441343 | -0.369920 |
| O4 | -0.458116 | -0.443527 | H3 | 0.248566 | 0.253638 |
| C5 | -0.672566 | -0.608176 | O3 | -0.658303 | -0.745688 |
| H5 | 0.286465 | 0.300323 | HO3 | 0.520379 | 0.568692 |
| O5 | -0.008618 | -0.039368 | C6 | 0.248543 | 0.224234 |
| C4 | 0.851944 | 0.685303 | H61 | 0.065198 | 0.078961 |
| H4 | 0.027504 | 0.085391 | H62 | 0.065198 | 0.078961 |
| C2 | 0.520476 | 0.554969 | O6 | -0.621108 | -0.707124 |
| H2 | 0.070328 | 0.080054 | HO6 | 0.389264 | 0.448298 |
| O2 | -0.710536 | -0.802691 | | | |

**Table S2.** Diffusion coefficients of CDs in aqueous solution determined from MD simulations using (i)TIP3P and SPC/E water models, (ii)CSFF and B3LYP/6-311++G(d,p) charges (iii) two water boxes containing 1000 and 4000 molecules, characteristic of the water phase. Results are given in unit of $10^{-10}$ $m^2/s$.

| Water model | Charges [a] | Water box | Length /ns | α-CD | β-CD | γ-CD |
|---|---|---|---|---|---|---|
| TIP3P | CSFF | 1000 | 4 | 4.007 | 3.619 | 3.274 |
| TIP3P | CSFF | 4000 | 5 | 3.723 | 3.255 | 3.007 |
| TIP3P | B3LYP | 1000 | 5 | 4.156 | 3.655 | 2.900 |
| SPC/E | CSFF | 1000 | 8 | 2.517 | 2.432 | 2.265 |
| SPC/E [b] | CSFF | 4040 | 5 | 2.535±0.035 | 2.400±0.060 | 2.375±0.070 |
| SPC/E | B3LYP | 1000 | 12 | 2.516±0.046 | 2.252±0.154 | 2.129±0.057 |
| NMR Experimental data [b] | | | | 2.292±0.025 | 2.168±0.015 | 2.097±0.017 |

[a] CSFF: charges in CSFF force field, B3LYP: B3LYP/6-311++G(d,p) charges in water phase from Table S1.
[b] Data from the work of Naidoo *et al*. in ref. 5.