



Supporting Information

for

Water inside β -cyclodextrin cavity: amount, stability and mechanism of binding

Stiliyana Pereva, Valya Nikolova, Silvia Angelova, Tony Spassov and Todor Dudev

Beilstein J. Org. Chem. **2019**, *15*, 1592–1600. [doi:10.3762/bjoc.15.163](https://doi.org/10.3762/bjoc.15.163)

Additional data from DFT computations at the M062X/6-311++G(d,p)//M062X/6-31G(d,p) level of theory

Table S1: Enthalpies calculated at the M062X/6-311++G(d,p)//M062X/6-31G(d,p) level of theory in the gas phase (ΔH^1) and water environment (ΔH^{78}) (in kcal mol⁻¹) for the most stable β -CD- n H₂O complex formation ($n = 1-12$).

	ΔH^1	ΔH^{78}
1. β -CD + H ₂ O \rightarrow β -CD - H ₂ O	-2.7	1.9
2. β -CD - H ₂ O + H ₂ O \rightarrow β -CD - 2H ₂ O	-15.7	-9.1
3. β -CD - 2H ₂ O + H ₂ O \rightarrow β -CD - 3H ₂ O	-7.2	-0.3
4. β -CD - 3H ₂ O + H ₂ O \rightarrow β -CD - 4H ₂ O	-7.0	-2.8
5. β -CD - 4H ₂ O + H ₂ O \rightarrow β -CD - 5H ₂ O	-13.3	-5.1
6. β -CD - 5H ₂ O + H ₂ O \rightarrow β -CD - 6H ₂ O	-13.8	-3.6
7. β -CD - 6H ₂ O + H ₂ O \rightarrow β -CD - 7H ₂ O	-11.8	-6.6
8. β -CD - 7H ₂ O + H ₂ O \rightarrow β -CD - 8H ₂ O	-4.7	2.3
9. β -CD - 8H ₂ O + H ₂ O \rightarrow β -CD - 9H ₂ O	-6.1	0.3
10. β -CD - 9H ₂ O + H ₂ O \rightarrow β -CD - 10H ₂ O	-0.2	0.9
11. β -CD - 10H ₂ O + H ₂ O \rightarrow β -CD - 11H ₂ O	-17.0	-9.2
12. β -CD - 11H ₂ O + H ₂ O \rightarrow β -CD - 12H ₂ O	-6.4	3.4

Table S2: Formation energies calculated at the M062X/6-311++G(d,p)//M062X/6-31G(d,p) level of theory (in kcal mol⁻¹) of β -CD- n H₂O ($n = 1-10$) complexes with individual (nonhydrogen)-bonded water molecules.

	ΔH^1	ΔH^{78}
β -CD + 2H ₂ O \rightarrow β -CD - 2H ₂ O	-18.4	-7.1
β -CD + 3H ₂ O \rightarrow β -CD - 3H ₂ O	-25.6	-7.4
β -CD + 4H ₂ O \rightarrow β -CD - 4H ₂ O	-32.6	-10.2
β -CD + 5H ₂ O \rightarrow β -CD - 5H ₂ O	-45.9	-15.3
β -CD + 6H ₂ O \rightarrow β -CD - 6H ₂ O	-59.7	-18.9
β -CD + 7H ₂ O \rightarrow β -CD - 7H ₂ O	-71.5	-25.5
β -CD + 8H ₂ O \rightarrow β -CD - 8H ₂ O	-76.3	-23.3
β -CD + 9H ₂ O \rightarrow β -CD - 9H ₂ O	-82.3	-23.0
β -CD + 10H ₂ O \rightarrow β -CD - 10H ₂ O	-82.6	-22.1