Determinants of the host-guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study

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Supplementary Information

Experimental structural data from $[Mg(H_2O)_2(15\text{-crown-}5)]^{2+}$ cation of $[Mg(H_2O)_2(15\text{-crown-}5)]_3[NO_3]_6$ complex have been used to calibrate the theoretical method employed. An averaged experimental distance of 2.190 Å was calculated from the experimental Mg-O_{crown} distances of the X-ray structure determined by Junk and Steed[S1] (Figure S1):

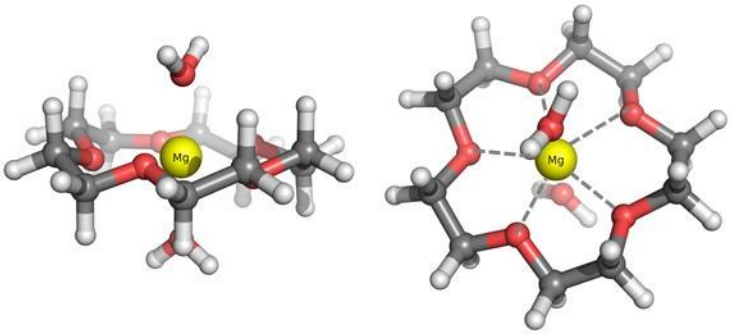

Figure S1.

Table S1. Experimental and calculated mean Mg^+-O_{crown} distances in $[Mg(H_2O)_2(15\text{-crown-}5)]^{2+}$ cation of $[Mg(H_2O)_2(15\text{-crown-}5)]_3[NO_3]_6$ complex.

	Mg-O_{crown} distance, Å	Exp. – calc., Å
Exp.[S1]	2.190	
M062X/6-31G(d,p)	2.179	0.011
M062X/6-31+G(d,p)	2.178	0.012
M062X/6-31+G(2d,p)	2.176	0.014
M062X/6-311G(d,p)	2.174	0.016
M062X/6-311+G(d,p)	2.173	0.017
B3LYP/6-31G(d,p)	2.207	-0.017
B3LYP/6-31+G(d,p)	2.205	-0.015
B3LYP/6-31+G(2d,p)	2.204	-0.014
B3LYP/6-311G(d,p)	2.203	-0.013
B3LYP/6-311+G(d,p)	2.202	-0.012

[S1] P. C. Junk, J. W. Steed, *J. Chem. Soc., Dalton Trans.* **1999**, 407-414.