Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Infrared Multiple Photon Dissociation Spectroscopy and Density Functional Theory (DFT) Studies of Protonated Permethylated β-Cyclodextrin-Water Noncovalent Complexes

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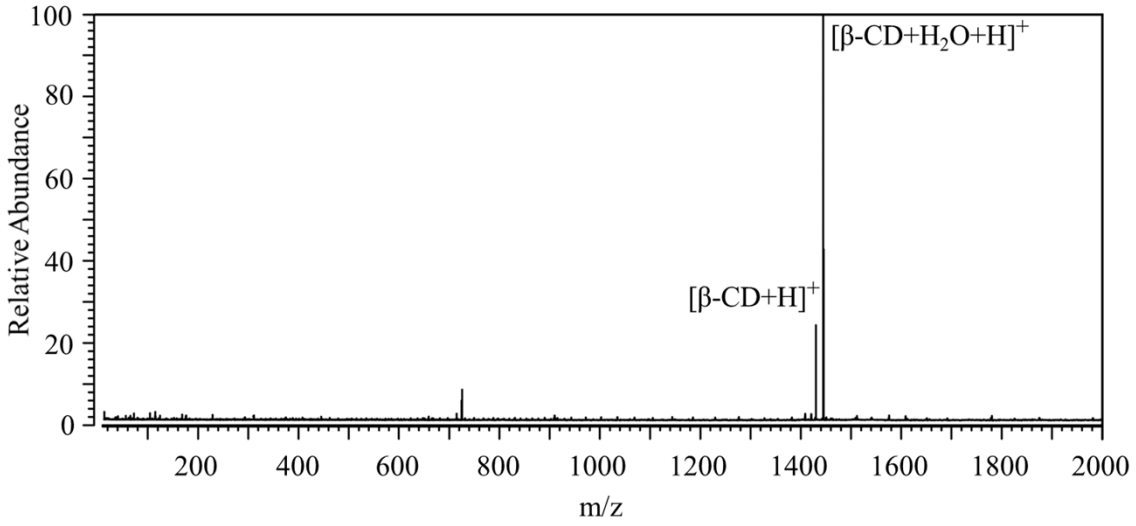

Figure S1. ESI-MS spectrum showing the abundant formation of protonated permethylated β-cyclodextrin-wate r non-covalent complexes.

Table S1. Electronic energies, zero-point energies, relative electronic energies, and relative Gibbs free energies at 298 K of two permethylated β-CD conformers.

	E (Hartee)	ZPE (kcal/mol)	Δ*E* (kcal/mol)	ΔG_{298K} (kcal/mol)
Conformer I	-5098.95478	1131.19	0	0
Conformer II	-5098.93754	1130.81	10.82	12.21