

DFT Investigation on the Complexation of β -Cyclodextrin and Hydroxypropyl- β -Cyclodextrin as Recognition Hosts with Trichloroethylene

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Table S1. HOMO-LUMO gaps (eV) for different considered configurations in both Modes A and B

HOMO-LUMO gap (eV)									
TCE@HP- β -CD									
	-8	-6	-4	-2	0	2	4	6	8
Mode A	3.78	3.78	3.79	3.52	3.52	3.53	3.66	3.71	3.68
Mode B	3.70	3.53	3.55	3.55	3.71	3.46	3.59	3.72	3.84
TCE@ β -CD									
	-8	-6	-4	-2	0	2	4	6	8
Mode A	3.40	3.25	3.25	3.25	3.51	3.49	3.55	3.34	3.39
Mode B	3.29	3.25	3.25	3.31	3.33	3.39	3.50	3.61	3.74