Improved Eco-Friendliness of a Common Flame Retardant through Inclusion Complexation with Cyclodextrins

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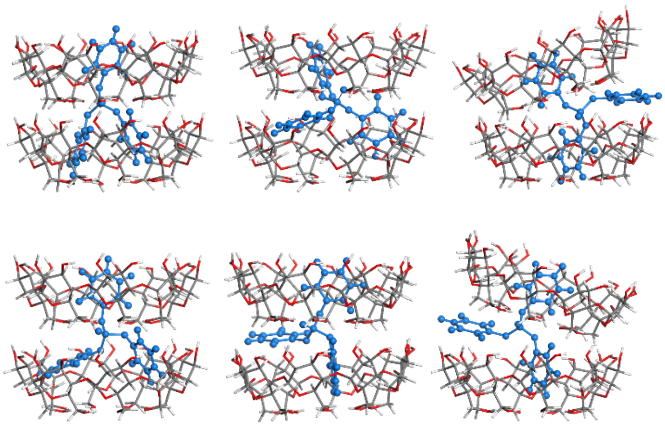
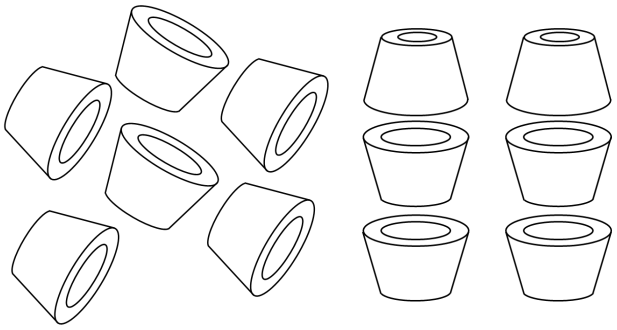


Figure S1. Six different initial structures constructed for 1:2 models of TPP:γ-CD ICs in the head-to-tail (HT) configuration.



(a) (b)

Figure S2. Types of crystal structures that CDs commonly form: (a) cage herringbone crystal, and (b) head-to-head; tail-to-head; tail-to-tail columnar-type (3-γ-CD repeating unit).

Table S1. Energies calculated from the PM6 calculations for the structures given in Figure 2. Graphs of these values are also given in Figure 3.

		ΔH_f (kcal/mol)	E_{inter} (kcal/mol)	$E_{complex}$ (kcal/mol)	E_{conf}(CD) (kcal/mol)	E_{conf}(TPP) (kcal/mol)
α	TT	-2871.15	-267.98	-148.52	42.64	7.97
	HT	-2900.18	-278.96	-177.55	28.29	5.54
	HH	-2913.23	-270.71	-190.60	20.47	2.04
β	TT	-3362.79	-327.01	-196.85	25.64	7.56
	HT	-3384.92	-339.05	-218.98	19.27	5.74
	HH	-3407.12	-333.82	-241.18	11.31	3.38
γ	TT	-3778.41	-401.53	-242.40	29.54	6.85
	HT	-3808.82	-412.84	-272.81	24.11	3.44
	HH	-3816.80	-405.21	-280.79	20.57	1.16

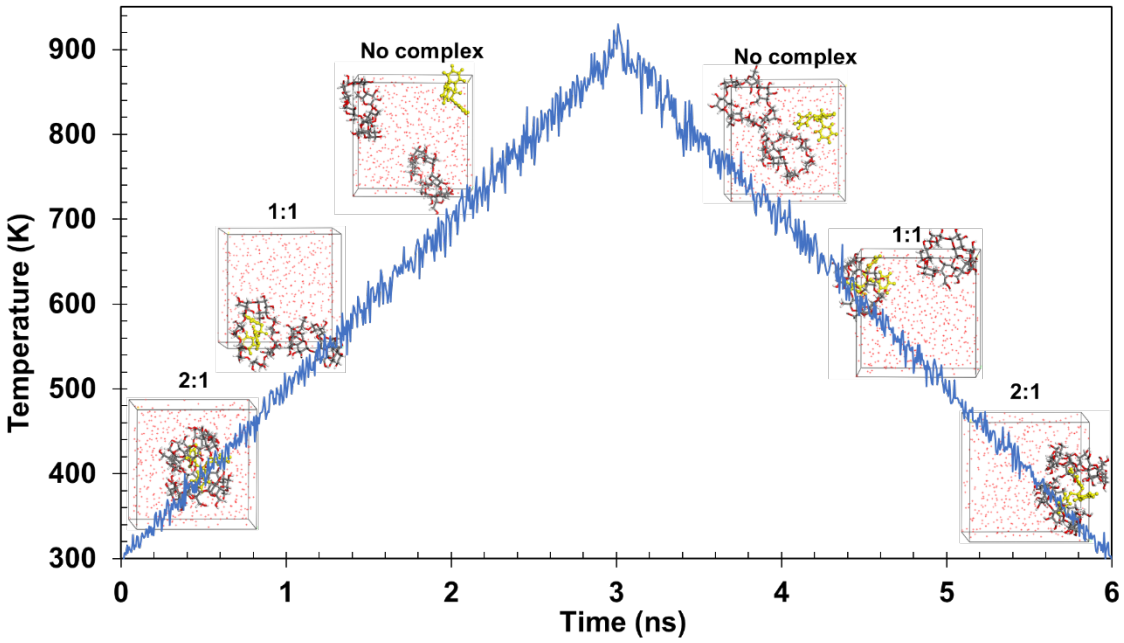


Figure S3. Snapshots along an MD simulation trajectory of 1:2 TPP:β-CD IC complexes in water being heated and then cooled.