Elucidating the Structures and Binding of Halide ions bound to Cucurbit[6]uril, Hemi-Cucurbit[6]uril and Bambus[6]uril using Density Functional Theory Calculations

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SUPPLIMENTARY INFORMATION

Table S1. Calculated Mulliken charges (e^-) using B3LYP functional.

	$(H_2O)_6$	CB-6	hm-CB-6	BU-6
Desolvated				
Cl^-	-1	-0.853	-0.714	-0.732
Br^-	-1	-0.880	-0.773	-0.788
I^-	-1	-0.897	-0.802	-0.808
Solvated				
Cl^-	-0.661	-0.717	-0.682	-0.708
Br^-	-0.715	-0.877	-0.728	-0.768
I^-	-0.808	-0.897	-0.773	-0.807

Table S2. Structural parameters (Å) of bare CB-[6], hm-CB-[6] and BU-[6]. Refer figure 1 for captions

	Calculated			Experimental		
	CB-6	hm-CB-6	BU-6	CB-6	hm-CB-6	BU-6
a	6.27	-	9.0	9.1	-	10.70
b_1, b_2, b_3	7.25	5.20, 5.59, 5.73	5.59, 5.65, 5.85	5.8	4.55, 4.88, 5.28	4.75, 4.75, 4.79
c_1, c_2, c_3	10.15	8.10, 8.38, 8.54	10.06, 10.28, 10.43	-	8.70, 8.75, 9.06	7.46, 7.49, 7.81
c_4, c_5, c_6			8.00, 8.01, 8.21			8.82, 8.86, 8.90

Table S3. Calculated hydrogen bonding distances (Å) between halide ions and methylene carbons of hm-CB-[6] and BU-[6]

	Calculated			Experiment
	Cl^-	Br^-	I^-	Cl^-
hm-CB-6	6×2.64-2.65 6×3.17-3.19	4×2.84-2.87 4×2.93-2.97 2×3.09-3.11 2×3.16-3.18	2×3.03 4×3.07-3.10 4×3.18-3.20 2×3.28	6×2.9 2×3.0 2×3.2 2×3.3
BU-6	2×2.70 2×2.84 4×3.11-3.14 4×3.22-3.23	2×2.95 2×3.06 4×3.13-3.16 4×3.21-3.23	2×3.22 2×3.23 4×3.27-3.29 4×3.30-3.31	6×2.9 2×3.0 4×3.1

Table S4: Calculated Local Topological Properties of the Electronic Charge Density Distribution at BCPs in *CB6-X*

BCP	CB6-Cl		CB6-Br		CB6-I	
	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
X-N	0.0009881	0.0007108	0.0012390	0.0008649	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012390	0.0008649	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N	0.0009881	0.0007108	0.0012389	0.0008648	0.0016672	0.0010200
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012250	0.0008757	0.0016398	0.0010327
X-N			0.0012250	0.0008757	0.0016672	0.0010200
X-N			0.0012250	0.0008757	0.0016398	0.0010326
X-N			0.0012250	0.0008757	0.0016398	0.0010326
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016731	0.0010264
X-N			0.0012440	0.0008696	0.0016710	0.0010264
X-N			0.0012251	0.0008757	0.0016398	0.0010330
X-N			0.0012251	0.0008757	0.0016398	0.0010330
X-N			0.0012251	0.0008757	0.0016397	0.0010326
X-N			0.0012251	0.0008757	0.0016398	0.0010326
Cl-C	0.0009960	0.0007163				
Cl-C	0.0009960	0.0007163				
Cl-C	0.0009960	0.0007163				
Cl-C	0.0009960	0.0007163				

Table S5: Calculated Local Topological Properties of the Electronic Charge Density Distribution at BCPs of hydrogen bonding interactions in *hm-CB6-X*

BCP	hm-CB6-Cl		hm-CB6-Br		hm-CB6-I	
	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
X-H	0.01180	0.00949	0.00995	0.00711	0.00933	0.00645
X-H	0.00481	0.00375	0.00585	0.00407	0.00630	0.00444
X-H	0.01157	0.00932	0.00962	0.00693	0.00848	0.00593
X-H	0.00488	0.00377	0.00651	0.00459	0.00712	0.00502
X-H	0.01160	0.00935	0.00807	0.00577	0.00738	0.00520
X-H	0.00495	0.00384	0.00870	0.00624	0.00879	0.00612
X-H	0.01178	0.00947	0.01001	0.00715	0.00930	0.00643
X-H	0.00479	0.00373	0.00595	0.00415	0.00636	0.00448
X-H	0.01158	0.00932	0.00958	0.00690	0.00835	0.00584
X-H	0.00480	0.00373	0.00664	0.00469	0.00719	0.00507
X-H	0.01161	0.00936	0.00803	0.00574	0.00736	0.00519
X-H	0.00491	0.00381	0.00869	0.00625	0.00881	0.00614

Table S6: Calculated Local Topological Properties of the Electronic Charge Density Distribution at BCPs of hydrogen bonding interactions in *BU6-X*

BCP	**BU6-Cl**		**BU6-Br**		**BU6-I**	
	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
X-H	0.00849	0.00672	0.00698	0.00476	0.00672	0.00443
X-H	0.00510	0.00380	0.00594	0.00397	0.00622	0.00405
X-H	0.00424	0.00302	0.00548	0.00361	0.00606	0.00393
X-H	0.00511	0.00374	0.00618	0.00413	0.00636	0.00414
X-H	0.004565	0.00348	0.00543	0.00362	0.00597	0.00388
X-H	0.01650	0.00854	0.00834	0.00582	0.00684	0.00451
X-H	0.00834	0.00661	0.00697	0.00476	0.00672	0.00443
X-H	0.00518	0.00387	0.00594	0.00397	0.00622	0.00405
X-H	0.00425	0.00303	0.00547	0.00361	0.00606	0.00393
X-H	0.00508	0.00371	0.00618	0.00413	0.00636	0.00415
X-H	0.00466	0.00350	0.00542	0.00362	0.00596	0.00388
X-H	0.01071	0.00860	0.00834	0.00582	0.00683	0.00451

Figure S1. Structures of bare CB-[6], hm-CB-[6] and BU-[6] (Color code: yellow=Oxygen, bright blue=Carbon, green=Nitrogen, pale white=Hydrogen)

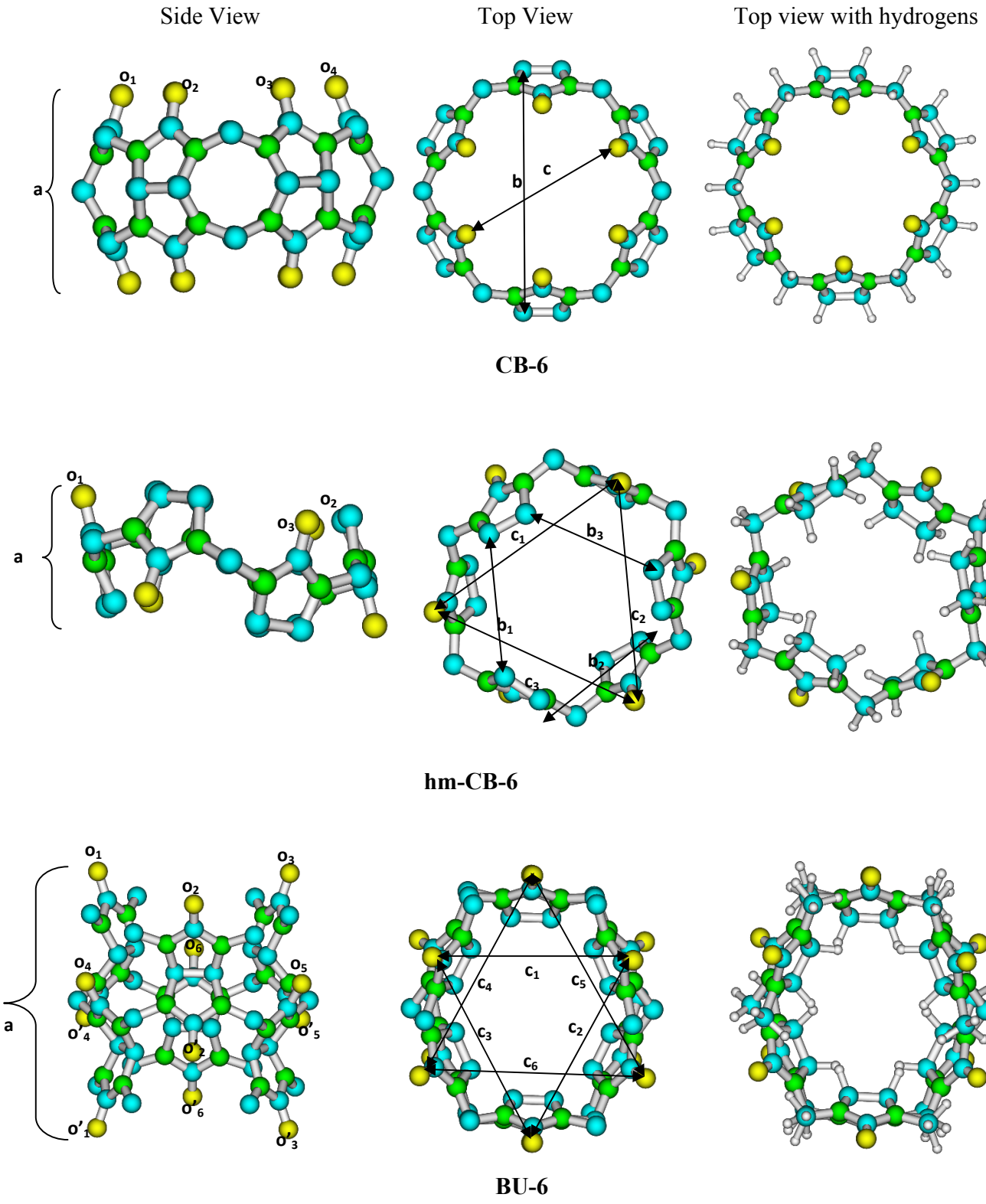

Figure S2. Bond critical points of bare and halide encapsulated (i) CB-[6], hm-CB-[6] and (iii) BU-[6]

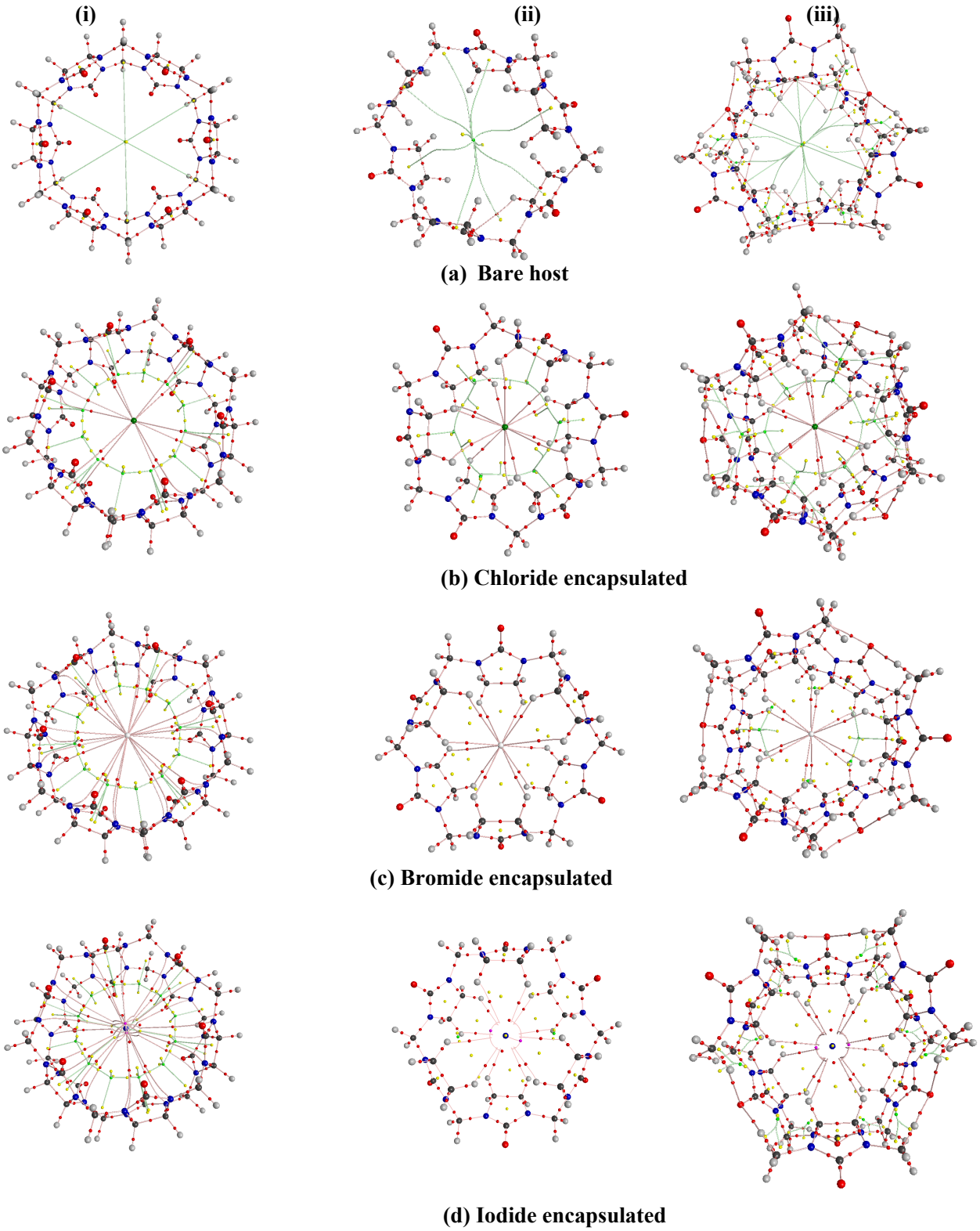

Figure S3. The electron density at the BCP of hydrogen bonds H---Cl, H---Br and H---I present in the hm-CB-[6]-Cl, hm-CB-[6]-Br and hm-CB-[6]-I complexes respectively.

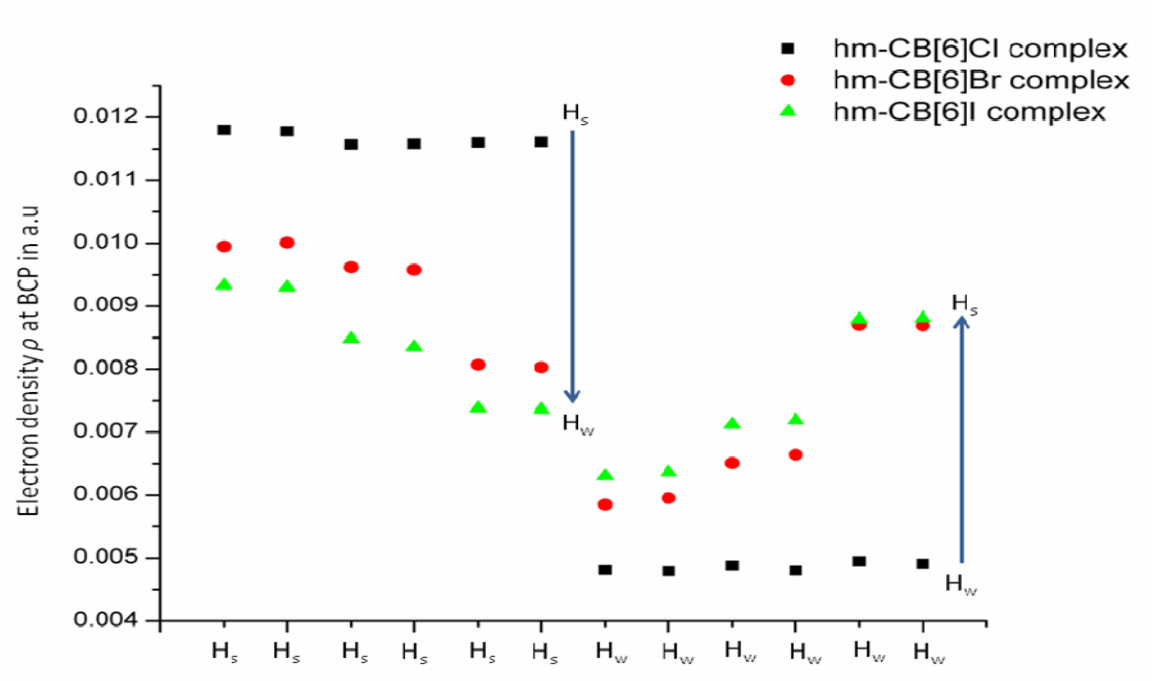

Figure S4. The electron density at the BCP of hydrogen bonds H---Cl, H---Br and H---I present in the BU-[6]-Cl , BU-[6]-Br and BU-[6]-I complexes respectively.