Electronic supplementary information

SUPRAMOLECULAR COMPLEXES OF CUCURBITURILS WITH SECOND GROUP METAL SALTS AND HYDRATES AND HISTAMINE

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Table S1. Results of the computational study of the complexes of cucurbiturils with second group metal salts and hydrates using DFT B3LYP/6-31G* and DFT B3LYP/LanL2DZ methods

Compound	$-E_{tot}$, a. u.	$-E_{zpve}$, a. u.	$-E_G$, a. u.	S, cal/K
6-31G(d) basis				
Q8	4814.0026	4812.8901	4812.9983	377.3
Q7	4212.2517	4211.2785	4211.3803	345.3
Q6	3610.4968	3609.6627	3609.7511	298.4
H_2O	76.4090	76.3878	76.4055	45.1
$CaCl_2$	1598.1063	1598.1044	1598.1316	69.2
Q7_Be^{2+}	4226.5654	4225.5853	4225.6786	326.3
Q7_ Be^{2+} –W_1	4303.1017	4302.0941	4302.1858	325.2
Q7_ Be^{2+} –W_2	4379.5820	4378.5482	4378.6405	329.6
Q7_ Be^{2+} –W_3	4456.0397	4454.9831	4455.0797	344.3
Q7_ Be^{2+} –W_4	4532.4878	4531.4047	4531.5051	357.3
Q7_ Be^{2+} –W_5	4608.9369	4607.8236	4607.9231	359.1
Q7_ Be^{2+} –W_6	4685.3399	4684.2042	4684.3071	371.7
Q7_ Be^{2+} –W_7	4761.7481	4760.5899	4760.6934	377.7
Q7_ Be^{2+}–W_8	4838.2909	4837.0997	4837.2037	381.1
Q6_Be^{2+}	3624.8096	3623.9674	3624.0451	271.7
Q6_2Be^{2+}	3638.7663	3637.9187	3637.9953	270.7
Q6_$CaCl_2$	5208.6796	5207.8398	5207.9290	309.8
Q6_2$CaCl_2$ (**I**)	6806.8580	6806.0130	6806.1071	330.6
Q6_2$CaCl_2$ (**II**)	6806.8874	6806.0427	6806.1358	328.1
LanL2DZ basis				
Q8	4813.1127	4812.0061	4812.1085	363.0
Q7	4211.4760	4210.5076	4210.6000	323.3
Q6	3609.8342	3609.0039	3609.0852	280.9
Q7_Ba^{2+}	4236.4445	4235.4719	4235.5630	323.3
Ba^{2+}	24.6518	–	–	–
H_2O	76.4143	76.3936	76.4112	45.1
BaI_2	48.1340	48.1334	48.1673	84.9
Q7_Ba^{2+} –W_1	4312.9249	4311.9260	4312.0219	338.7
Q7_Ba $^{2+}$ –W_2	4389.3976	4388.3716	4388.4678	342.5
Q7_ Ba^{2+} –W_3	4465.8547	4464.8023	4464.8989	346.2
Q7_ Ba^{2+} –W_4	4542.3163	4541.2384	4541.3382	359.8
Q7_ Ba^{2+} –W_5	4618.7620	4617.6597	4617.7624	370.3
Q7_ Ba^{2+} –W_6	4695.2182	4694.0894	4694.1945	381.2
Q7_Ba^{2+} –W_7	4771.6720	4770.5156	4770.6194	380.7
Q7_Ba^{2+} –W_8	4848.1031	4846.9228	4847.0293	389.8

Q6_Ba^{2+}	3634.8274	3633.9933	3634.0784	292.6
Q6_2Ba^{2+}	3659.5186	3658.6808	3658.7638	289.5
Q7_BaI_2	4259.7200	4258.7481	4258.8510	358.9
Q6_BaI_2	3658.0953	3657.2614	3657.3530	316.0
Q6_2BaI_2 (**I**)	3706.2895	3705.4539	3705.5579	349.4
Q6_2BaI_2 (**II**)	3706.3649	3705.5266	3705.6306	355.5
Q6_$BaCl_2$	3665.2206	3664.3859	3664.4723	304.8
Q6_2$BaCl_2$	3720.5644	3719.7268	3719.8238	337.0
Q6_CaI_2	3669.3995	3668.5643	3668.6537	310.2
Q6_2CaI_2	3728.9237	3728.0871	3728.1865	340.2
Q8_BaI_2	4861.3455	4860.2358	4860.3493	400.5

Table S2. Results of the computational study of the complexes of Q7 with HA and Ca^{2+} in water at the B3LYP-D3 or wB97xD (in parentheses) level using the 6-31G* basis and SMD solvation method

Compound	**$-E_{tot}$, a. u.**	**$-E_{zpve}$, a. u.**	**$-E_G$, a. u.**	**S, cal/K**
Q7–HA	4573.1268 (4571.5044)	4571.9946 (4570.3562)	4572.0946 (4570.4542)	356.1 (349.5)
Q7–W_8	4824.4202 (4822.7276)	4823.1559 (4821.5250)	4823.3392 (4821.6292)	385.6 (380.5)
Q7	4212.8383 (4211.354)	4211.8585 (4210.3629)	4211.9500 (4210.4494)	320.6 (306.5)
HA	360.2341 (360.07893)	360.0792 (359.9307)	360.1206 (359.9630)	87.1 (85.7)
W_8	611.5033 (611.3089)	611.2857 (611.1065)	611.3506 (611.1515)	136.8 (135.5)
Q7–HA–2Ca^{2+}	5928.1880	5926.9781	5927.1487	359.029
Q7–HA–H^+	4573.6205	4572.4040	4572.5729	355.6
Q7–HA–2H^+	4574.0896	4572.928	4573.0266	352.1
Q7–HA–H^+–Ca^{2+}	5251.1466	5249.9976	5250.0976	357.4
Q7–HA–2H^+–Ca^{2+}	5251.6126	5250.3784	5250.5478	356.5
H_3O^+	76.8362	76.803572	76.8220	46.8
H_2O	76.4227	76.401707	76.4194	45.2
W_6	458.6179	458.4689	458.5072	111.7
Ca^{2+}–W_6	1136.1240	1135.9786	1136.0216	127.4

Table S3. Results of the computational study of the complexes of Q7 with HA, 2Ca^{2+}, and water in the explicit form at the wB97xD level using the 6-31G* basis

Reaction		**ΔG, kcal/mol**	**ΔH, kcal/mol**
1	Q7–HA–2Ca^{2+} + W → Q7–HA–2Ca^{2+}–W_1	–16.1	–26.9
2	Q7–HA–2Ca^{2+}–W_1 + W → Q7–HA–2Ca^{2+}–W_2	–13.3	–26.2
3	Q7–HA–2Ca^{2+}–W_2+ W → Q7–HA–2Ca^{2+}–W_3	–2.8	–15.4
4	Q7–HA–2Ca^{2+}–W_3+ W → Q7–HA–2Ca^{2+}–W_4	–0.1	–10.5

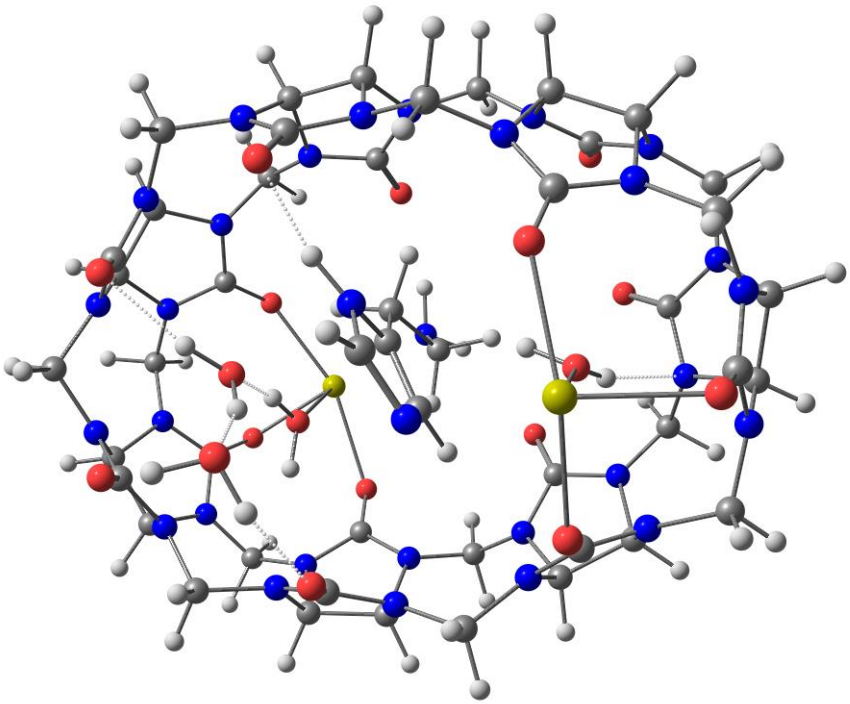

Fig. S1. Structure of complex Q7–HA–2Ca^{2+}–W_4.