Supplementary Material (ESI) for Chemical Communications

Water Heliacte, $(H_2O)_7$ Hosted by a Diamondoid Metal–Organic Framework

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Electronic Supplementary Information

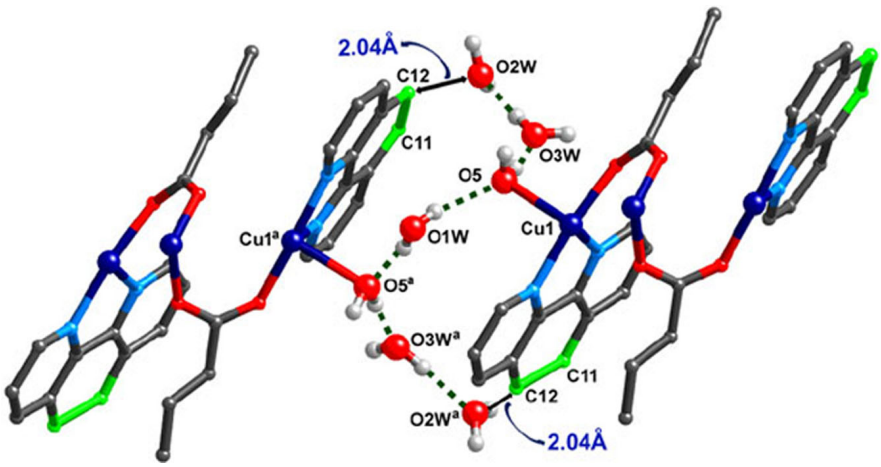

Figure S1. A view showing repulsive interactions between water helicate and phen in the artificial environment. The C-H hydrogens have been omitted for clarity.

Table S1. Hydrogen bond parameters for water helicate in 1

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A	Symmetry
O5-H5A	0.84(2)	1.87(2)	173(4)	2.710(4)	O3W	
O5-H5B	0.84 (2)	2.03(3)	140(4)	2.727(4)	O4	
O1W-H1WA	0.81(2)	2.15(2)	165(4)	2.940(3)	O5	
O2W-H2WA	0.88(2)	1.90(2)	157(4)	2.729(3)	O4	
O2W-H2WB	0.86(2)	1.86(3)	142(4)	2.589(14)	8A	[x, -y+2, z+1/2]
O2W-H2WB	0.86(2)	2.21(3)	147(4)	2.963(14)	O8	[x, -y+2, z+1/2]
O2W-H2WB	0.86(2)	2.62(3)	147(4)	3.369(16)	O7	[x, -y+2, z+1/2]

O3W-H2WA	0.88(2)	2.08(3)	154(4)	2.897(6)	O6	[-x+3/2, -y+3/2, -z+1]
O3W-H3WB	0.85(2)	1.83(2)	177(5)	2.687(5)	O2W	[-x+3/2, -y+3/2, -z+1]

Table S2. Hydrogen bond parameters for cyclic water heptamer in 2

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A	Symmetry
O5-H5A	0.85	1.98(2)	158(6)	2.787(9)	O3W	
O5-H5B	0.85	2.00(3)	152(6)	2.782(6)	O1W	
O1W-H1WA	0.85					
O2W-H2WA	0.85	2.14(5)	147(6)	2.899(6)	O2W	[-x+1, y, -z+1/2]
O2W-H2WB	0.85					
O2W-H2WC	0.85	1.75(5)	164(6)	2.579 (6)	O6	[x, -y+1, z-1/2]
O2W-H2WC	0.85	2.26(5)	164(6)	3.083(6)	O6A	[x, -y+1, z-1/2]
O2W-H2WC	0.85	2.35(5)	144(6)	3.081(6)	O7B	[x, -y+1, z-1/2]
O3W-H3WA	0.85	2.12(4)	142(6)	2.839(2)	O2W	
O3W-H3WB	0.85	1.85(5)	173(6)	2.698(6)	O6B	
O3W-H3WB	0.85	2.07(5)	168(6)	2.913(6)	O9A	
O3W-H3WB	0.85	2.15(5)	156(6)	2.957(6)	O8	

N.B. The atom labels in **2** have been changed as in **1** from the published structure previously for comparison.

Table S3. Cartesian Coordinates (in Å) of B3LYP/6-31+G** optimized geometries[a]

$(H_2O)_7\cdots(ClO_4^-)_2$				$(H_2O)_7$ in constrained environment of 2 Cu^{2+} and 2 ClO_4^-			
O	7.34093	-0.40710	-0.69958	Cu	4.00195	1.04060	3.40452
H	7.94717	-0.96596	-0.17833	O	3.40144	-0.62853	2.69398
H	7.94097	0.31690	-0.94872	H	2.49149	-0.97092	2.94050
O	2.30043	0.18756	-0.96322	H	4.02261	-1.36540	2.77953
H	3.20826	0.19144	-0.58766	O	3.79301	-0.31380	-0.29055
H	2.03840	-0.74035	-0.97286	H	3.23997	-0.59742	0.45330
O	0.02577	1.66952	0.23608	H	3.25824	0.28880	-0.82948
H	0.79357	1.23112	-0.17267	O	1.04709	-1.53390	3.54366
H	-0.72560	1.06020	0.12614	H	0.61431	-1.50553	4.40834
O	4.81779	0.03134	0.23862	H	0.62174	-2.24306	2.99714
H	4.94570	0.59118	1.01247	Cl	-3.36580	3.81229	0.12745
H	5.72113	-0.12078	-0.13587	O	-3.72830	3.68007	1.49438
Cl	-10.70997	-0.03152	0.09690	O	-2.93043	5.09209	-0.14029
O	-11.76100	-0.95128	0.63047	O	-2.30150	2.89103	-0.19353
O	-9.91980	-0.73745	-0.98506	O	-4.40853	3.47669	-0.70485
O	-9.75737	0.34995	1.21219	O	0.08505	-3.39539	1.89655
O	-11.33846	1.20256	-0.46618	H	0.15288	-4.34043	2.09912
O	-7.28140	-0.71849	0.19927	H	-0.73063	-3.28002	1.38027
H	-7.92701	-0.93637	-0.49643	Cu	4.07905	-1.08997	-3.48429
H	-7.86225	-0.26774	0.83927	O	3.40300	0.64136	-3.01426
O	-2.24183	-0.21300	0.30809	H	2.47037	0.94791	-3.20791
H	-3.15576	-0.04678	-0.01157	H	3.99880	1.39384	-3.13101
H	-2.32563	-0.30880	1.26388	O	0.98263	1.48506	-3.63139
O	-4.86416	0.34418	-0.47330	H	0.54238	1.46977	-4.49376
H	-5.06031	1.25027	-0.73542	H	0.58214	2.20313	-3.07640
H	-5.73263	-0.06396	-0.23069	Cl	-3.36861	-3.82556	-0.16884
Cl	10.72266	-0.08723	0.15961	O	-3.70609	-3.69303	-1.54114
O	11.85401	-0.63052	-0.65325	O	-2.94002	-5.10618	0.10771
O	9.79602	-1.21956	0.55644	O	-2.30900	-2.90602	0.17238
O	9.93502	0.90679	-0.66621	O	-4.42579	-3.48864	0.64540
O	11.24398	0.58411	1.38966	O	0.06778	3.37853	-1.97053
				H	0.17077	4.32103	-2.17148
				H	-0.75483	3.29692	-1.45662

[a] For all optimizations, the convergence criteria were set to tight. The optimized structures were confirmed to have all real vibrational frequencies, which represent a local energy minimum on the potential energy surface.

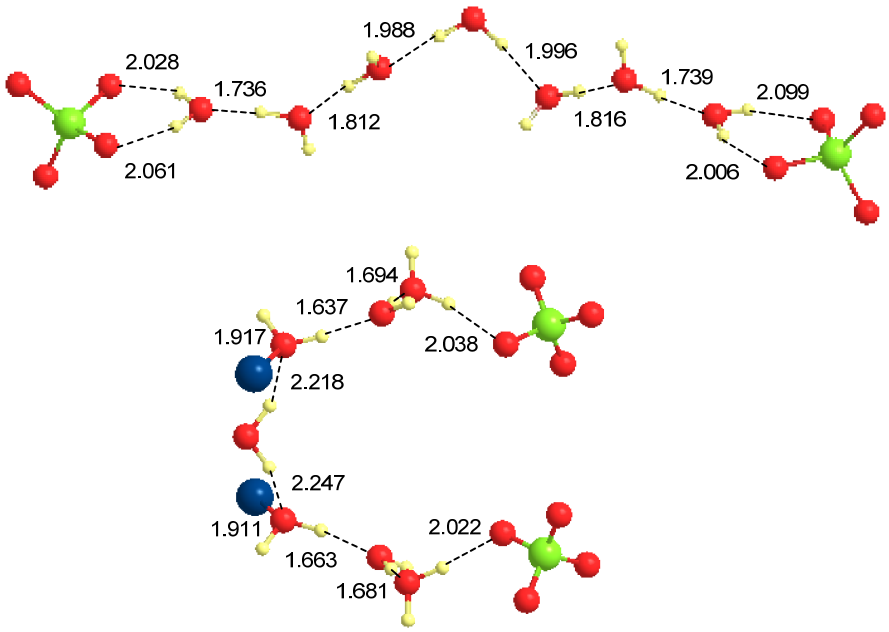

Figure S2. Optimized (B3LYP/6-31+G**) geometries of $(H_2O)_7\cdots(ClO_4^-)_2$ (top) and $(H_2O)_7$ in constrained environment of 2 Cu^{2+} and 2 ClO_4^- (bottom). Bond distances are given in Å.

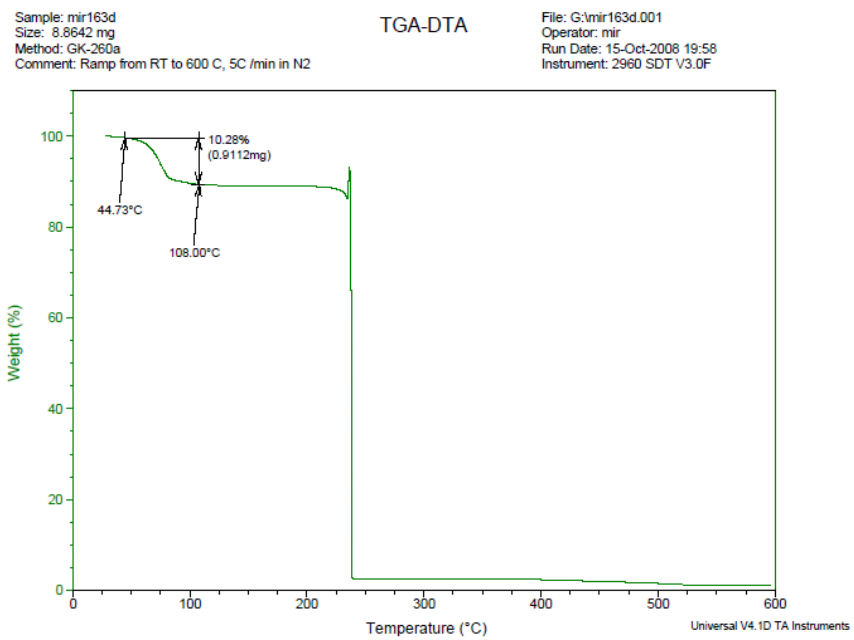

Figure S3. Thermogravimetry of 1 showing the loss of all the water molecules below 110ºC.