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Electronic Supplementary Information

Interaction of 2,4,6-tris(2-pyrimidyl)-1,3,5-triazine (TPymT) with CoX_2 (X = Cl, Br) in water: Trapping of new self-assembled water-chloride/bromide clusters in a $[Co(bpca)_2]^+$ host (bpca = bis(2-pyrimidylcarbonyl)amidate anion)

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Table S1. Selected bond lengths (Å) and angles (°) for **$[Co(bpca)_2]Cl·7.5H_2O$**

Bond lengths					
Co(1)–N(1)	1.895(4)	Co(1)–N(9)	1.930(5)	N(1)–C(1)	1.369(7)
Co(1)–N(2)	1.929(5)	O(1)–C(1)	1.219(6)	N(1)–C(6)	1.376(7)
Co(1)–N(4)	1.947(5)	O(2)–C(6)	1.216(6)	N(6)–C(11)	1.364(8)
Co(1)–N(6)	1.890(4)	O(3)–C(11)	1.215(7)	N(6)–C(16)	1.379(7)
Co(1)–N(7)	1.940(5)	O(4)–C(16)	1.206(6)		
Bond angles					
N(1)–Co(1)–N(2)	83.26(19)	N(2)–Co(1)–N(4)	166.18(18)	N(4)–Co(1)–N(7)	92.25(19)
N(1)–Co(1)–N(4)	82.98(19)	N(2)–Co(1)–N(6)	98.18(19)	N(4)–Co(1)–N(9)	91.29(19)
N(1)–Co(1)–N(6)	178.33(19)	N(2)–Co(1)–N(7)	90.42(19)	N(6)–Co(1)–N(7)	83.2(2)
N(1)–Co(1)–N(7)	96.0(2)	N(2)–Co(1)–N(9)	89.36(18)	N(6)–Co(1)–N(9)	83.0(2)
N(1)–Co(1)–N(9)	97.91(19)	N(4)–Co(1)–N(6)	95.60(19)	N(7)–Co(1)–N(9)	165.99(19)

Table S2. Selected bond lengths (Å) and angles (°) for **$[Co(bpca)_2]Br·7.5H_2O$**

Bond lengths					
Co(1)–N(1)	1.895(2)	Co(1)–N(9)	1.945(3)	N(1)–C(1)	1.368(4)
Co(1)–N(2)	1.934(3)	O(1)–C(1)	1.212(4)	N(1)–C(6)	1.377(4)
Co(1)–N(4)	1.948(3)	O(2)–C(6)	1.211(4)	N(6)–C(11)	1.367(4)
Co(1)–N(6)	1.899(2)	O(3)–C(11)	1.210(4)	N(6)–C(16)	1.369(4)
Co(1)–N(7)	1.940(3)	O(4)–C(16)	1.206(4)		
Bond angles					
N(1)–Co(1)–N(2)	83.11(10)	N(2)–Co(1)–N(4)	166.08(10)	N(4)–Co(1)–N(7)	91.09(11)
N(1)–Co(1)–N(4)	82.99(10)	N(2)–Co(1)–N(6)	98.07(11)	N(4)–Co(1)–N(9)	92.45(11)
N(1)–Co(1)–N(6)	178.62(11)	N(2)–Co(1)–N(7)	90.05(11)	N(6)–Co(1)–N(7)	83.09(11)
N(1)–Co(1)–N(7)	97.65(11)	N(2)–Co(1)–N(9)	89.72(11)	N(6)–Co(1)–N(9)	83.25(11)
N(1)–Co(1)–N(9)	96.06(11)	N(4)–Co(1)–N(6)	95.84(11)	N(7)–Co(1)–N(9)	166.17(11)

Table S3. Hydrogen bond lengths (Å) and angles (°) for **$[Co(bpca)_2]Cl·7.5H_2O$** and **$[Co(bpca)_2]Br·7.5H_2O$**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
$[Co(bpca)_2]Cl·7.5H_2O$[a]	O(5)–H(5B)···Cl(1)	0.96	2.25	3.208(5)	176
	O(5)–H(5C)···Cl(1)$^{\#1}$	1.00	2.22	3.197(5)	165
	O(6)–H(6A)···O(7)	0.96	1.91	2.849(7)	166
	O(6)–H(6B)···O(5)	1.01	1.87	2.821(7)	157
	O(7)–H(7A)···O(6)	0.96	2.41	2.849(7)	107
	O(7)–H(7A)···N(8)$^{\#2}$	0.96	2.57	3.032(7)	110
	O(7)–H(7B)···O(10)$^{\#3}$	1.00	2.28	2.815(7)	112
	O(8)–H(8B)···Cl(1)	0.96	2.38	3.130(6)	135
	O(8)–H(8C)···O(9)	1.00	1.87	2.713(8)	140
	O(9)–H(9B)···O(11)$^{\#4}$	0.96	1.85	2.658(7)	141
	O(9)–H(9C)···Cl(1)$^{\#5}$	1.00	2.29	3.114(6)	139
	O(10)–H(10B)···O(6)	0.96	1.90	2.812(7)	157
	O(10)–H(10C)···O(7)$^{\#3}$	1.00	1.94	2.815(7)	144
	O(11)–H(11B)···O(10)$^{\#6}$	1.00	2.34	2.878(7)	113
	O(12)–H(12A)···N(8)	0.96	2.41	3.182(10)	138
	O(12)–H(12B)···O(4)$^{\#2}$	1.00	2.04	2.948(9)	149
$[Co(bpca)_2]Br·7.5H_2O$[b]	O(5)–H(5B)···Br(1)	0.96	2.39	3.338(3)	172
	O(5)–H(5C)···Br(1)$^{\#1}$	1.00	2.35	3.307(3)	159
	O(6)–H(6B)···O(5)	0.96	1.94	2.816(5)	151
	O(6)–H(6C)···O(10)$^{\#2}$	1.00	1.84	2.824(5)	165
	O(7)–H(7B)···Br(1)	0.96	2.44	3.351(4)	159
	O(7)–H(7C)···O(8)	1.00	1.77	2.692(12)	151
	O(8)–H(8B)···O(7)	0.96	2.17	2.692(12)	113
	O(8)–H(8C)···Br(1)$^{\#3}$	1.00	2.24	3.142(8)	148
	O(9)–H(9B)···O(3)$^{\#2}$	0.96	2.12	2.964(4)	146
	O(9)–H(9C)···O(1)$^{\#3}$	1.00	2.31	2.927(4)	118
	O(9)–H(9C)···O(2)$^{\#3}$	1.00	2.45	3.386(4)	154
	O(10)–H(10B)···N(10)	0.95	2.03	2.959(4)	164
	O(10)–H(10C)···O(7)$^{\#2}$	1.00	1.83	2.760(5)	153
	O(11)–H(11A)···O(6)$^{\#4}$	0.96	1.99	2.763(12)	136
	O(11)–H(11B)···O(10)	1.00	2.04	2.726(13)	123
	O(11)–H(11C)···O(6)$^{\#4}$	0.80	1.97	2.763(12)	172
	O(11)–H(11D)···O(12)	1.00	1.82	2.297(15)	105

[a] Symmetry transformations used to generate equivalent atoms: #1: x, 3/2 – y, 1/2 + z; #2: 1 – x, 2 – y, –z; #3: –x, 2 – y, –z; #4: x, y, –1 + z; #5: x, 3/2 – y, –1/2 + z; #6: –x, 2 – y, 1 – z.

[b] Symmetry transformations used to generate equivalent atoms: #1: x, 1/2 – y, –1/2 + z; #2: 1 – x, –y, 1 – z; #3: x, 1/2 – y, ½ + z; #4: –1 + x, y, z.