Electronic Supplementary Information for Dalton Transactions

Metal coordination and in situ S–C bond cleavage of the bis(2-pyridylthio)methane ligand

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Supplementary material

Table S1. Iodine-iodine bond distances (Å) and angles (º) for the polyiodine network in $[2bpytmH]_2[I_3]_2[I_2]$

Distance (Å)		Angle (º)	
I_2 molecule			
I5–I5$^{\#iii}$	2.786(2)		
I_3^- ion			
I3–I4	2.9509(10)		
I4–I3$^{\#ii}$	2.9509(10)	I3–I4–I3$^{\#ii}$	180.0
I1–I2	2.9136(10)	I1$^{\#i}$–I2–I1	180.000(2)
I1–I2$^{\#i}$	2.9136(10)		
I_2...I_3^- interaction			
I5–I5...I3	3.4591(17)	I5–I5...I3	175.41
I_3^-...I_3^- interaction			
I_3^-... $I_3^{-\#iv}$	3.9524(15)	I4–I3...I3	156.40(4)

#i= –x, –y, –z+1; #ii= 2–x–1, –y, –z; #iii= 3–x, –y+1, –z;
#iv= 1–x, 1–y, 1–z

Table S2. Main hydrogen bond distances (Å) and angles (º).

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)
2bpytm[I_3][I_2]				
N(1)–H(111)...N(11)	0.86	1.88	2.691(11)	158
C(13)–H(13)...I(2)^{i}	0.93	3.08	3.843(10)	140
i = -1+x, y, z				
[$CoBr_2$(2bpytm)].H_2O (1)				
O1–H1...Cl1^{i}	0.97	2.64	3.314(3)	127
C4–H4...O1^{ii}	0.93	2.53	3.359(3)	148
C1–H1A…Cl1^{iii}	0.97	2.85	3.5834(7)	133
C6–H6…S1^{iv}	0.93	2.95	3.859(3)	165
i = x,-1+y,z; ii = ½-x, ½-y,-z; iii = -½+x,- ½+y, z; iv = ½+x, ½+y, z				
[$CoBr_2$(2bpytm)] (2)				
C1–H1B…Br2^{i}	0.97	2.83	3.785(3)	170
C15–H15… Br1^{ii}	0.93	2.88	3.606(4)	136
C14–H14… Br1^{iii}	0.93	2.96	3.664(4)	134
C4–H4… Br1^{iv}	0.93	3.09	3.723(4)	127
i = ½-x,- ½-y,z; ii = ½+x, ½-y.-z; iii = 1-x,2-y,1-z; iv = x,1.5-y, ½+z				
[$NiBr_2$(2bpytm)].H_2O (4)				
O1–H11… Br1	0.96	2.77	3.413(3)	126
C1–H1A…Br1^{i}	0.97	2.88	3.6387(8)	136
C4–H4...O1^{ii}	0.93	2.61	3.454(3)	152
i = ½-x, -½+y, ½-z; ii= -½-x, ½-y, -z				
[$CuBr_2$(2bpytm)]$_2$ (5)				
C15–H15...Br1^{i}	0.93	2.84	3.600(11)	139
C13–H13...Br1^{ii}	0.93	2.97	3.743(10)	142
C4–H4...Br2^{iii}	0.93	3.07	3.703(10)	127
i = 1-x, -½+y, ½-z; ii = x, -1.5-y, ½+z; iii = 2-x. ½+y, ½-z				
[$CuBr_2$(2bpytm)]$_n$.CH_3CN (6)				
C1–H1A…Br2^{i}	0.97	2.85	3.713(5)	149
C4–H4…Br1^{ii}	0.93	3.04	3.725(5)	132
C4–H4…N111^{iii}	0.93	2.61	3.248(8)	127
C5–H5…N111^{iii}	0.93	2.77	3.322(8)	119
i = 1-x, ½+y,½-z; ii = 1+x, y, z; iii = -x, -½+y, ½-z				

Table S3. Torsion angles of the compounds with eight-membered chelate rings (**1**, **2**, **3** and **4**)

	Symmetry	τ_1	τ_2	τ_3	τ_4	τ_5	τ_6	τ_7	τ_8
[2bpytmH]$_2$ [I$_3$]$_2$[I$_2$]	C_1	-84.6	3.6	-44.2(9)	123.6(7)	-77.2(7)	6.1(10)	-7.0	117.8
1	C_2	-35.78(15)	5.0(2)	86.74(18)	-67.67(7)	-67.67(7)	86.74(18)	5.0(2)	-35.78(15)
2	C_1	42.5(3)	–4.4(3)	–89.7(3)	66.2(2)	66.7(2)	–89.9(3)	3.0(3)	22.3(3)
3	C_1	22.6(7)	–4.7(8)	–80.8(6)	68.3(5)	66.7(5)	–89.0(6)	–6.5(7)	48.9(6)
4	C_2	-34.14(17)	-0.8(2)	86.3(2)	-72.17(10)	-72.17(10)	86.3(2)	-0.8(2)	-34.14(17)