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Self-assembly, binding ability and magnetic properties of dicopper(II) pyrazolenophanes

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Table S1. Selected bond distances (Å) and angles (º) and metal-metal separations for **1**[a]

Cu(1)-N(1)	2.023(2)	Cu(2)-N(5)	2.021(3)
Cu(1)-N(3)	2.026(2)	Cu(2)-N(7)	2.007(2)
Cu(1)-N(9)	1.957(2)	Cu(2)-N(10)	1.962(3)
Cu(1)-N(11)	1.963(2)	Cu(2)-N(12)	1.953(2)
Cu(1)-O(5)	2.473(7)	Cu(2)-O(5)	2.502(6)
		Cu(2)-O(1)	2.705(3)
N(1)-Cu(1)-N(3)	80.17(9)	N(5)-Cu(2)-N(7)	80.4(1)
N(1)-Cu(1)-N(9)	94.6(1)	N(5)-Cu(2)-N(10)	178.5(1)
N(1)-Cu(1)-N(11)	173.7(1)	N(5)-Cu(2)-N(12)	93.0(1)
N(1)-Cu(1)-O(5)	97.2(2)	N(5)-Cu(2)-O(5)	84.9(2)
N(3)-Cu(1)-N(9)	174.5(1)	N(5)-Cu(2)-O(1)	80.6(1)
N(3)-Cu(1)-N(11)	96.0(1)	N(7)-Cu(2)-N(10)	98.2(1)
N(3)-Cu(1)-O(5)	82.2(2)	N(7)-Cu(2)-N(12)	173.3(1)
N(9)-Cu(1)-N(11)	89.4(1)	N(7)-Cu(2)-O(5)	86.5(2)
N(9)-Cu(1)-O(5)	96.6(2)	N(7)-Cu(2)-O(1)	78.9(1)
N(11)-Cu(1)-O(5)	87.2(2)	N(10)-Cu(2)-N(12)	88.4(1)
		N(10)-Cu(2)-O(5)	94.6(2)
		N(10)-Cu(2)-O(1)	99.5(1)
		N(12)-Cu(2)-O(5)	91.6(2)
Cu(1)-O(5)-Cu(2)	83.4(1)	N(12)-Cu(2)-O(1)	101.5(1)
Cu(1)···Cu(2)	3.3076(5)	O(5)-Cu(2)-O(1)	160.9(2)

[a] Only bond distances and angles involving the major component of the disordered bridging perchlorate ion are reported, for clarity.

Table S2. Selected bond distances (Å) and angles (º) and metal-metal separations for **2**[a]

Cu(1)-N(1)	2.025(4)	Cu(1)-N(4)	1.984(3)
Cu(1)-N(2)	2.023(4)	Cu(1)-O(1w)	2.404(3)
Cu(1)-N(3)	1.969(4)	Cu(1)-O(1)	2.740(9)
N(1)-Cu(1)-N(2)	81.0(2)	N(3)-Cu(1)-N(4)	89.9(2)
N(1)-Cu(1)-N(3)	93.1(2)	N(3)-Cu(1)-O(1w)	90.0(2)
N(1)-Cu(1)-N(4)	174.0(1)	N(3)-Cu(1)-O(1)	83.2(2)
N(1)-Cu(1)-O(1w)	96.9(1)	N(4)-Cu(1)-O(1w)	88.4(5)
N(1)-Cu(1)-O(1)	85.7(3)	N(4)-Cu(1)-O(1)	89.4(3)
N(2)-Cu(1)-N(3)	168.5(2)	O(1w)-Cu(1)-O(1)	172.8(2)
N(2)-Cu(1)-N(4)	95.2(2)		
N(2)-Cu(1)-O(1w)	100.4(2)	Cu(1)-O(1w)-Cu(1a)	89.5(2)
N(2)-Cu(1)-O(1)	86.6(2)	Cu(1)···Cu(1a)	3.383(1)

[a] Symmetry transformations used to generate equivalent atoms: (a) *x*, *y*, -*z*+1/2.

Table S3. Selected bond distances (Å) and angles (º) and metal-metal separations for **3**[a,b]

bis(pyrazolate)(aquo)-bridged units			
Cu(1)-N(1)	2.042(5)	Cu(2)-N(3)	2.019(7)
Cu(1)-N(2)	2.039(5)	Cu(2)-N(4)	2.050(8)
Cu(1)-N(5)	1.977(5)	Cu(2)-N(6)	1.978(6)
Cu(1)-N(7)	1.968(6)	Cu(2)-N(8)	1.971(7)
Cu(1)-O(1w)	2.382(5)	Cu(2)-O(1w)	2.468(5)
Cu(1)-O(1)	2.789(7)	Cu(2)-O(2w)	2.66(1)
		Cu(2)-O(5)	2.67(2)
N(1)-Cu(1)-N(2)	80.8(2)	N(3)-Cu(2)-N(4)	80.6(4)
N(1)-Cu(1)-N(5)	95.2(2)	N(3)-Cu(2)-N(6)	95.5(2)
N(1)-Cu(1)-N(7)	168.6(3)	N(3)-Cu(2)-N(8)	174.7(3)
N(1)-Cu(1)-O(1w)	98.0(2)	N(3)-Cu(2)-O(1w)	90.3(2)
N(1)-Cu(1)-O(1)	82.3(2)	N(4)-Cu(2)-N(6)	175.9(4)
N(2)-Cu(1)-N(5)	175.4(2)	N(4)-Cu(2)-N(8)	94.3(4)
N(2)-Cu(1)-N(7)	93.3(2)	N(4)-Cu(2)-O(1w)	93.8(3)
N(2)-Cu(1)-O(1w)	93.4(2)	N(6)-Cu(2)-N(8)	89.6(3)
N(2)-Cu(1)-O(1)	90.4(2)	N(6)-Cu(2)-O(1w)	87.0(2)
N(5)-Cu(1)-N(7)	90.3(2)	N(8)-Cu(2)-O(1w)	91.4(2)
N(5)-Cu(1)-O(1w)	89.3(2)	O(2w)-Cu(2)-N(3)	90.8(4)
N(5)-Cu(1)-O(1)	86.9(2)	O(2w)-Cu(2)-N(4)	94.0(4)
N(7)-Cu(1)-O(1w)	92.1(2)	O(2w)-Cu(2)-N(6)	85.2(3)
N(7)-Cu(1)-O(1)	88.0(3)	O(2w)-Cu(2)-N(8)	88.3(4)
O(1w)-Cu(1)-O(1)	176.2(2)	O(2w)-Cu(2)-O(1w)	172.2(3)
		O(5)-Cu(2)-N(3)	71.6(7)
		O(5)-Cu(2)-N(4)	71.3(7)
		O(5)-Cu(2)-N(6)	106.7(7)
Cu(1)-O(1w)-Cu(2)	87.6(2)	O(5)-Cu(2)-N(8)	105.7(7)
Cu(1)···Cu(2)	3.357(1)	O(5)-Cu(2)-O(1w)	157.9(7)
bis(pyrazolate)(perchlorate)-bridged unit			
Cu(3)-N(9)	2.026(5)	Cu(3)-N(12)	1.964(5)
Cu(3)-N(10)	2.024(5)	Cu(3)-O(10)	2.704(8)
Cu(3)-N(11)	1.965(5)	Cu(3)-O(13)	2.478(2)
N(9)-Cu(3)-N(10)	81.0(2)	N(10)-Cu(3)-O(13)	96.5(4)
N(9)-Cu(3)-N(11)	175.1(2)	N(11)-Cu(3)-N(12)	89.7(2)
N(9)-Cu(3)-N(12)	93.5(2)	N(11)-Cu(3)-O(10)	95.6(3)
N(9)-Cu(3)-O(10)	80.9(3)	N(11)-Cu(3)-O(13)	88.5(5)
N(9)-Cu(3)-O(13)	95.2(5)	N(12)-Cu(3)-O(10)	86.0(2)
N(10)-Cu(3)-N(11)	95.3(2)	N(12)-Cu(3)-O(13)	91.3(4)
N(10)-Cu(3)-N(12)	170.9(2)	O(10)-Cu(3)-O(13)	175.0(4)
N(10)-Cu(3)-O(10)	85.9(2)	Cu(3)-O(13)-Cu(3a)	86.3(2)
		Cu(3)···Cu(3a)	3.382(1)

[a] Only bond distances and angles involving the major component of the disordered perchlorate ions are reported, for clarity. [b] Symmetry transformations used to generate equivalent atoms: (a) *x*, -*y*+1/2, *z*.

Table S4. Selected bond distances (Å) and angles (º) and metal-metal separations for **4**

Cu(1)-N(1)	2.033(6)	Cu(2)-N(3)	2.050(6)
Cu(1)-N(2)	2.034(6)	Cu(2)-N(4)	2.033(6)
Cu(1)-N(5)	1.992(7)	Cu(2)-N(6)	1.968(6)
Cu(1)-N(7)	1.953(7)	Cu(2)-N(8)	2.000(7)
Cu(1)-N(1S)	2.218(8)	Cu(2)-N(2S)	2.204(9)
Cu(1)···Cu(2)	3.098(1)		
N(1)-Cu(1)-N(2)	80.2(3)	N(3)-Cu(2)-N(4)	80.2(3)
N(1)-Cu(1)-N(5)	94.6(3)	N(3)-Cu(2)-N(6)	91.2(3)
N(1)-Cu(1)-N(7)	168.0(3)	N(3)-Cu(2)-N(8)	148.6(3)
N(1)-Cu(1)-N(1S)	93.7(3)	N(3)-Cu(2)-N(2S)	108.8(3)
N(2)-Cu(1)-N(5)	146.9(3)	N(4)-Cu(2)-N(6)	167.9(3)
N(2)-Cu(1)-N(7)	91.2(3)	N(4)-Cu(2)-N(8)	95.2(3)
N(2)-Cu(1)-N(1S)	113.7(3)	N(4)-Cu(2)-N(2S)	90.7(3)
N(5)-Cu(1)-N(7)	88.1(3)	N(6)-Cu(2)-N(8)	87.7(3)
N(5)-Cu(1)-N(1S)	99.2(3)	N(6)-Cu(2)-N(2S)	100.1(3)
N(7)-Cu(1)-N(1S)	97.4(3)	N(8)-Cu(2)-N(2S)	102.3(3)