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DESIGN, SYNTHESIS, AND STRUCTURAL STUDY OF MONO- AND POLYNUCLEAR Cu(II) IMINODIACETATE COMPLEXES

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Table S1

Bond lengths (Å) and Angles (°) in coordination Cu(II) environment in 1–3.

a) Compound **1**

Bonds	*d, Å*	*Bonds*	*d, Å*	*Bonds*	*d, Å*
Cu(1)–O(1)	1.992(6)	Cu(2)–O(6)	2.437(6)	Cu(3)–O(10)$^{\#2}$	2.231(5)
Cu(1)–O(3)	1.968(6)	Cu(2)–O(7)	1.963(5)	Cu(3)–O(11)	2.665(1)
Cu(1)–O(5)	1.974(6)	Cu(2)–O(9)	1.969(6)	Cu(3)–O(12)	1.983(6)
Cu(1)–N(1)	1.977(6)	Cu(2)–N(2)	2.007(7)	Cu(3)–N(4)	1.987(7)
Cu(1)–O(8)$^{\#1}$	2.251(5)	Cu(2)–O(11)	2.359(6)	Cu(3)–O(13)	1.948(6)
Cu(1)–O(6)	2.699(1)	Cu(2)–N(3)	2.022(7)	Cu(3)–O(15)	1.972(6)
Angles	*ω, °*	*Angles*	*ω, °*	*Angles*	*ω, °*
O(1)Cu(1)O(3)	159.6(2)	O(6)Cu(2)O(7)	88.5(2)	O(10)$^{\#2}$Cu(3)O(11)	150.4
O(1)Cu(1)O(5)	95.2(3)	O(6)Cu(2)O(9)	89.8(2)	O(10)$^{\#2}$Cu(3)O(12)	95.8(2)
O(1)Cu(1)N(1)	83.2(3)	O(6)Cu(2)N(2)	104.8(2)	O(10)$^{\#2}$Cu(3)N(4)	96.8(3)
O(1)Cu(1)O(8)$^{\#1}$	97.4(2)	O(6)Cu(2)O(11)	178.7(2)	O(10)$^{\#2}$Cu(3)O(13)	102.1(2)
O(1)Cu(1)O(6)	86.9	O(6)Cu(2)N(3)	73.4(2)	O(10)$^{\#2}$Cu(3)O(15)	95.1(2)
O(3)Cu(1)O(5)	93.2(3)	O(7)Cu(2)O(9)	177.8(3)	O(11)Cu(3)O(12)	54.7
O(3)Cu(1)N(1)	85.4(3)	O(7)Cu(2)N(2)	92.7(2)	O(11)Cu(3)N(4)	113.1
O(3)Cu(1)O(8)$^{\#1}$	100.7(2)	O(7)Cu(2)O(11)	91.9(2)	O(11)Cu(3)O(13)	81.3
O(3)Cu(1)O(6)	83.8	O(7)Cu(2)N(3)	85.7(2)	O(11)Cu(3)O(15)	88.3
O(5)Cu(1)N(1)	170.2(2)	O(9)Cu(2)N(2)	86.3(3)	O(12)Cu(3)N(4)	167.4(2)
O(5)Cu(1)O(8)$^{\#1}$	93.0(2)	O(9)Cu(2)O(11)	89.8(2)	O(12)Cu(3)O(13)	92.7(3)
O(5)Cu(1)O(6)	54.1	O(9)Cu(2)N(3)	95.2(3)	O(12)Cu(3)O(15)	94.8(3)
N(1)Cu(1)O(8)$^{\#1}$	96.8(2)	N(2)Cu(2)O(11)	76.3(2)	N(4)Cu(3)O(13)	84.7(3)
N(1)Cu(1)O(6)	116.0	N(2)Cu(2)N(3)	177.6(3)	N(4)Cu(3)O(15)	84.0(3)
O(8)$^{\#1}$Cu(1)O(6)	147.3	O(11)Cu(2)N(3)	105.5(2)	O(13)Cu(3)O(15)	160.4(3)

$^{\#1}$ x,-y,z+1/2 $^{\#2}$ x,-y+1,z-1/2

b) Compounds **2** and **3**

Bonds	*d, Å* (**2**)		*Bonds*	*d*, Å (**3**)	
	Cu(1)	Cu(2)		Cu(1)	Cu(2)
Cu–O(1)/O(2)$^{\#2}$	1.953(2)	2.206(3)	Cu–O(1A)/O(1B)	1.937(2)	1.941(3)
Cu–O(3)	2.428(2)	2.742	Cu–O(3A)O(3B)	2.556(1)	2.622(1)
Cu–O(4)	-	1.941(2)	Cu–N(1A)/N(1B)	2.001(3)	2.012(3)
Cu–O(5)	-	1.982(3)			
Cu–N(1)/N(2)	2.010(3)	1.978(3)			
Cu–O(7)	-	1.989(2)			

Angle (2)	*ω, °*		*Angles (3)*	*ω, °*	
O(2)$^{\#2}$CuO(3)	-	141.8			
O(1)/O(2)$^{\#2}$CuO(3)/O(4)	94.08(9)	89.37(10)	O(1)CuO(3)	90.3	82.8
O(1)/O(2)$^{\#2}$CuO(3)$^{\#1}$/O(5)	85.92(9)	109.41(10)	O(1)CuN(1)	85.81(11)	84.50(11)
O(1)/O(2)$^{\#2}$CuN(1)/N(2)	85.58(10)	99.40(11)	O(1)CuO(3)$^{\#1/\#2}$	89.7	97.2
O(1)/O(2)$^{\#2}$CuN(1)$^{\#1}$/O(7)	94.42(10)	90.20(10)	O(1)CuN(1)$^{\#1/\#2}$	94.19(11)	95.50(11)
O(3)CuO(4)	-	53.2	O(3)CuN(1)	72.8	69.8
O(3)CuO(5)	-	84.0	O(3)CuN(1)$^{\#1/\#2}$	107.2	110.2
O(3)CuN(2)	-	117.8			
O(3)CuO(7)	-	85.5			
O(3)/O(4)CuN(1)/N(2)	74.21(10)	170.98(11)			
O(3)/O(4)CuN(1)$^{\#1}$O(7)	105.79(10)	93.62(11)			
O(4)CuO(5)	-	94.78(12)			
O(5)CuN(2)	-	84.37(11)			
O(5)CuO(7)	-	158.71(11)			
N(2)CuO(7)	-	84.28(10)			

2: $^{\#1}$ *x, –y, z*+1/2 $^{\#2}$ *x, –y*+1, *z*–1/2 **3**: $^{\#1}$ *–x*+1, *–y*+2, *–z*+2 $^{\#2}$ *–x, –y*+2, *–z*+1

Table S2

Hydrogen bond distances (Å) and angles (°) in 1 – 3.

D–H···A	*d(H···A)*	*d(D···A)*	*∠(DHA)*	*Symmetry transformations for acceptor*
		1		
N(1)–H(1N)···O(13)	2.19	2.895(9)	142	*x, –y, z+1/2*
N(2)–H(2N)···O(16)	2.02	2.799(9)	158	*x, y–1, z*
N(3)–H(3N)···O(2)	2.17	2.935(9)	160	*x, y+1, z*
N(4)–H(4N)···O(3)	2.22	2.912(9)	138	*x, –y+1, z–1/2*
C(11)–H(11B)···O(4)	2.59	3.536(11)	166	*x, –y, z–1/2*
C(14)–H(14A)···O(7)	2.66	3.588(11)	161	*x, y+1, z*
C(15)–H(15A)···O(2)	2.58	3.530(10)	167	*x, y+1, z*
O(1W)–H(1W1)···O(5)	2.06	3.87(2)	154	*x, y, z*
O(1W)–H(2W1)···O(8)	2.05	3.78(2)	175	*x, y, –z+1/2*
N(1D)–H(8)···O(15)	2.18	2.988(12)	149	*–x–1/2, –y+3/2, –z*
C(2D)–H(13)···O(10)	2.40	3.08(3)	128	*–x–1/2, y+1/2, –z+1/2*
O(4W)–H(1W4)···O(3W)	2.48	3.11(2)	130	*–x–1/2, y+1/2, –z+1/2*
O(4W)–H(2W4)···O(12)	2.18	3.01(2)	172	*–x–1/2, –y+3/2, –z*
N(2D)–H(3)···O(10)	2.08	2.858(7)	145	*x, y+1, z*
C(3D)–H(6)···O(1W)	2.43	3.33(2)	155	*x, –y+1, z–1/2*
C(3D)–H(6)···O(2W)	2.64	3.51(8)	151	*–x, y+1/2, –z+1/2*
N(3D)–H(5D)···O(1)	2.18	3.05(2)	163	*x, y+1, z*
O(2W)–H(1W2)···O(8)	1.99	2.81(10)	152	*x, –y+1, z+1/2*
		2		
N(1)–H(1N)···O(8)	2.00	2.866(4)	173	*x, y+1, z*
N(2)–H(2N)···O(5)	2.32	3.097(4)	144	*–x+3/2, y–1/2, –z+1*
O(6)–H(1O)···O(1W)	1.99	2.857(5)	175	*–x–3/2, –y+1/2, –z+1/2*
C(2)–H(2B)···O(3W)	2.57	3.518(10)	167	*x, y, z*
C(2)–H(2B)···O(4W)	2.46	3.36(2)	154	*x, y, z*
C(6)–H(6B)···O(4)	2.59	3.376(5)	139	*–x+3/2, y–1/2, –z+1*
C(7)–H(7A)···O(1)	2.48	3.353(5)	150	*–x+3/2, –y+1/2, –z+1/2*
C(7)–H(7A)···O(5)	2.61	3.237(5)	123	*–x+3/2, y–1/2, –z+1*
C(7)–H(7A)···O(3)	2.51	3.287(4)	137	*–x+3/2, –y+1/2, –z+1/2*
O(1W)–H(1W1)···O(2)	2.38	2.922(4)	120	*x+1, –y+1, –z*
O(1W)–H(1W1)···O(3W)	2.40	3.038(9)	130	*x, y, z*
O(1W)–H(2W1)···O(8)	2.13	2.817(4)	140	*x, y, z*
O(2W)–H(1W2)···O(2)	2.07	2.95(2)	174	*–x+1, –y+1, –z*
O(3W)–H(1W3)···O(4)	2.40	3.150(9)	169	*–x+1, y, –z+1/2*

Continuation of Table 2

D–H···A	*d(H···A)*	*d(D···A)*	*∠(DHA)*	*Symmetry transformations for acceptor*
O(3W)–H(2W3)···O(1W)	2.22	3.017(9)	177	*x, y, z*
O(4W)–H(2W4)···O(2)	2.32	2.95(2)	127	*–x+1, –y+1, –z*
O(4W)–H(2W4)···O(4)	2.37	2.95(2)	122	*–x+1, y, –z+1/2*
O(5W)–H(1W5)···O(7)	2.21	2.79(2)	125	*x, y, z*
3				
N(1A)–H(1N)···O(2A)	2.10	2.911(4)	139	*x, y–1, z*
N(1B)–H(2N)···O(4B)	2.12	3.094(4)	170	*x, y+1, z*
O(4A)–H(1O)···O(4B)	1.70	2.481(4)	159	*x, y, z*
C(2A)–H(2A)···O(2A)	2.45	3.383(4)	162	*–x+1, y–1/2, –z+5/2*
C(2A)–H(2A)···O(2B)	2.62	3.573(5)	167	*x, y+1/2, –z+3/2*
C(2B)–H(2D)···O(4B)	2.51	3.392(4)	151	*–x, y–1/2, –z+3/2*
C(3B)–H(3C)···O(4A)	2.58	3.285(4)	130	*– x, y+1/2, –z+3/2*
O(1M)–H(2O)···O(3B)	1.96	2.719(7)	171	*x, y, z*
C(1M)–H(1B)···O(4B)	2.60	3.500(6)	157	*x, y–1, z*
C(1M)–H(1C)···O(4A)	2.65	3.369(6)	132	*x, y, z*