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Supplementary materials

Synthesis, Crystal Structures and Catalytic Activities of Two Copper Coordination Compounds Bearing an N,N′-dibenzylethylenediamine Ligand

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Table 1. Selected bond lengths (Å) and angles (°) of compounds **(1)** and **(2)**.

Compound **(1)**									
Cu1—O2	1.976(5)	Cu1—O3	2.178(5)	Cu1—O5	1.980(5)	Cu1—O1(ii)	1.989(5)		
Cu1—O6(ii)	1.977(5)	Cu2—O4	1.976(5)	Cu2—N1	2.007(5)	Cu2—O4(i)	1.976(5)		
Cu2—N1(i)	2.007(5)								
O2—Cu1—O3	97.1(2)	O2—Cu1—O5	88.1(2)	O1(ii)—Cu1—O2	169.1(2)	O2—Cu1—O6(ii)	90.6(2)		
O3—Cu1—O5	93.58(19)	O1(ii)—Cu1—O3	93.68(19)	O3—Cu1—O6(ii)	97.12(19)	O1(ii)—Cu1—O5	89.8(2)		
O5—Cu1—O6(ii)	169.3(2)	O1(ii)—Cu1—O6(ii)	89.4(2)	O4—Cu2—N1	94.7(2)	O4—Cu2—O4(i)	93.5(2)		
O4—Cu2—N1(i)	158.1(2)	O4(i)—Cu2—N1	158.1(2)	N1—Cu2—N1(i)	85.1(2)	O4(i) —Cu2—N1(i)	94.7(2)		
Compound **(2)**									
Cu1—Cl4	2.2643(7)	Cu1—Cl1	2.2529(7)	Cu1—Cl2	2.2199(7)	Cu1—Cl3	2.2648(7)		
Cl3—Cu1—Cl4	91.80(2)	Cl1—Cu1—Cl4	98.22(2)	Cl1—Cu1—Cl2	96.54(2)	Cl1—Cu1—Cl3	135.02(2)		
Cl2—Cu1—Cl3	102.21(2)	Cl2—Cu1—Cl4	141.65(2)						

Symmetry codes: (*i*)1-x,y,3/2-z; (*ii*)1/2-x,3/2-y,1-z for compound **(1)**.

Table 2. Hydrogen bonding parameters for compounds **(1)** and **(2)**.

Compound	D—H···A	D—H (Å)	H···A(Å)	D···A(Å)	D—H···A(°)
(1)	N1—H1···O5	0.98	2.25	3.136(7)	150
(2)	N1—H1A···Cl1(*iii*)	0.89	2.37	3.217(2)	158
	N1—H1B···Cl4(*iv*)	0.89	2.51	3.196(2)	134
	N2—H2A···Cl3	0.89	2.41	3.187(2)	146
	N2—H2B···Cl3(*v*)	0.89	2.37	3.246(2)	168
	C16—H16B···Cl4(*v*)	0.97	2.82	3.531(2)	131

Symmetry codes: (*iii*) 1−x,−y,1−z; (*iv*) 1+x,y,z; (*v*) 1−x,1−y,1−z for compound **(2)**.

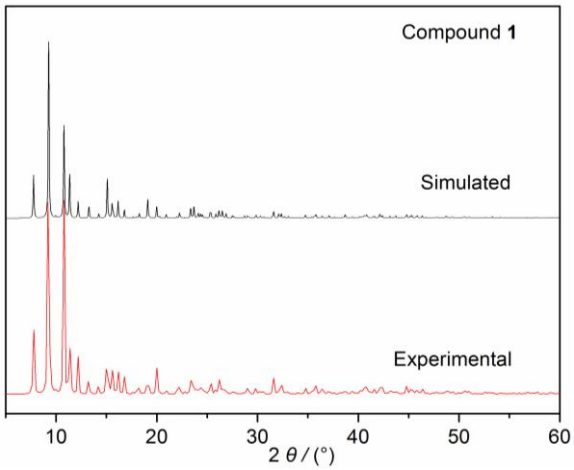

Figure 1. PXRD patterns of compound **(1)**.

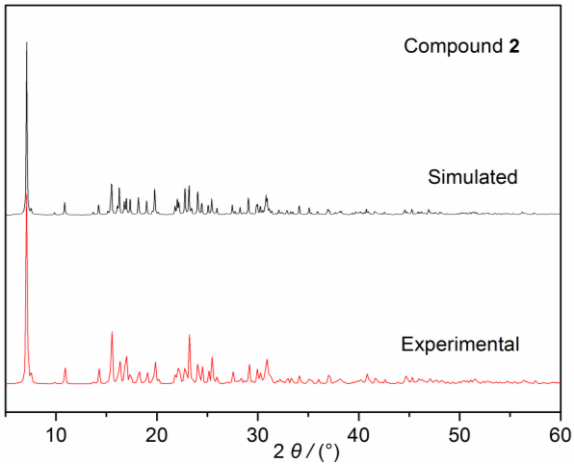

Figure 2. PXRD patterns of compound **(2)**.