Supporting Information

The structural variations influenced by ligand conformation and counter anions in copper(II) complexes with flexible bis-triazole ligand

Bin Ding [a,b], Yuan-Yuan Liu,[a,b] Yong-Quan Huang,[a] Wei Shi,[a] Peng Cheng,*[a] Dai-Zheng Liao,[a] Shi-Ping Yan[a]

[a]*Department of Chemistry, Nankai University, Tianjin 300071, P. R. China.*
[b]*College of Chemistry and Life Science, Tianjin Normal University, Tianjin 300074, P. R. China*

Table S1. Selected Bond Length (Å) and Bond Angle (°) for **1-4** [a]

1			
Cu(1)-N(1)	2.038(3)	Cu(1)-O(1)	2.411(3)
Cu(1)-N(7)	2.023(3)		
N(7)-Cu(1)-N(7)#1	180.0(0)	N(7)-Cu(1)-N(1)	92.07(11)
N(7)-Cu(1)-N(1)#1	87.93(11)	N(1)-Cu(1)-O(1)#1	93.35(11)
N(7)-Cu(1)-O(1)#1	91.35(11)	N(1)-Cu(1)-O(1)	86.65(11)
2			
Cu(1)-N(3)	2.014(3)	Cu(1)-N(6)#2	2.022(3)
Cu(1)-N(6)#3	2.022(3)	Cu(1)-O(1)	2.412(5)
Cu(1)-O(2)	2.391(5)		
N(3)#1-Cu(1)-N(6)#2	89.32(14)	N(3)#1-Cu(1)-N(6)#3	90.89(14)
N(6)#2-Cu(1)-O(1)	87.47(11)	N(3)#1-Cu(1)-O(1)	92.37(11)
N(3)-Cu(1)-N(3)#1	175.3(2)		
3			
Cu(1)-N(1)#1	2.017(2)	Cu(1)-N(5)	2.0315(19)
Cu(1)-Cl(1)	2.840(3)		
N(1)#1-Cu(1)-N(5)	91.31(8)	N(1)#1-Cu(1)-N(5)#3	88.69(8)
4			
Cu(1)-N(1)	2.006(3)	Cu(1)-N(4)	2.006(3)
N(1)-Cu(1)-N(1)#1	180.0(2)	N(1)-Cu(1)-N(4)	87.97(12)
N(1)-Cu(1)-N(4)#1	92.03(12)		

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

Table S2 Selected hydrogen bond lengths (Å) and angles (°) in **1**-**4**.

Donor-H···Acceptor	D-H	H···A	D···A	D-H···A
1				
O(1)-H(1A)···O(5)	0.854	1.895	2.737	168.01
O(1)-H(1B)···O(6)	0.851	1.980	2.824	171.36
O(5)-H(5A)···N(6)	0.848	1.969	2.806	169.12
O(5)-H(5B)···O(2)	0.853	2.012	2.841	163.40
O(6)-H(6A)···O(4)	0.854	2.158	2.966	157.73
O(6)-H(6B)···N(5)	0.850	2.128	2.968	169.49
C(1)-H(1)···O(5)	0.930	2.347	3.252	164.32
C(2)-H(2)···O(1)	0.930	2.609	3.081	147.33
C(13)-H(13)···O(3)	0.930	2.436	3.203	139.81
C(15)-H(15A)···O(3)	0.970	2.424	3.282	147.33
2				
O(1)-H(1A)···O(3)	0.847	1.948	2.777	165.46
O(2)-H(2A)···O(4)	0.849	1.997	2.778	152.53
O(6)-H(6B)···N(2)	0.871	2.591	3.294	138.50
C(11)-H(11)···O(4)	0.930	2.532	3.438	164.70
3				
C(1)-H(1)···Cl(1)	0.9300	2.6788	3.534	153.21
C(11)-H(11)···Cl(1)	0.9300	2.7206	3.344	125.15
C(12)-H(12)···Cl(1)	0.9300	2.8123	3.434	125.25
4				
C(7)-H(7)···F(1)	0.9300	2.5302	3.056	116.14
C(8)-H(8)···F(4)	0.9300	2.5324	3.394	154.14
C(1)-H(1)···F(2)	0.9300	2.4520	3.258	145.08
C(2)-H(2)···F(2)	0.9300	2.2811	3.079	143.51
C(3)-H(3B)···F(4)	0.9700	2.4415	3.406	172.69