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SUPPLEMENTARY MATERIAL TO

Binuclear azide-bridged hydrazone Cu(II) complex: Synthesis, characterization and evaluation of biological activity

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ANALYTICAL AND SPECTRAL DATA

Elemental analysis for $C_{14}H_{20}ClN_5O$ (%). Calcd.: C 54.28, H 6.51, N 22.61. Found: C 54.68, H 7.09, N 22.13.

IR (ATR, cm^{-1}) selected peaks: 3377.4 (*m*), 3068.5 (*m*), 3019.4 (*m*), 2976.5 (*m*),1703.4 (*s*), 1618.3 (*w*), 1571.8 (*m*), 1550.4 (*m*), 1491.2 (*m*), 1431.9 (*m*), 1398.4 (*s*), 1333.1 (*m*), 1280.2 (*m*), 1231.0 (*m*), 1164.0 (*m*), 1125.8 (*m*), 987.3 (*m*), 947.3 (*m*), 919.3 (*m*), 858.8 (*w*), 818.5 (*m*), 800.1 (*m*), 710.9 (*m*), 655.4 (*m*), 609.1 (*w*).

^{1}H-NMR (400 MHz, DMSO-d_6), δ (ppm): 11.66 (*s*, 1H, N2-H), 11.50 (*s*, 1H, N4-H), 8.15–7.72 (4H, C1-H, C2-H, C4-H, C5-H),4.91 (*s*, 2H, C11-H), 3.34 (*t*, 9H, C12-H), 2.32 (*s*, 3H, C9-H).

^{13}C-NMR (125 MHz, DMSO-d_6), δ (ppm):167.24 (C10), 161.48 (C8), 156.29–120.21 (C1, C2, C3, C4, C5, C6, C7), 63.21 (C11), 53.74 (C12), 12.73 (C9).

Elemental analysis for $C_{28}H_{38}B_2Cu_2F_8N_{16}O_2$ (%). Calcd.: C 36.11, H 4.11, N 24.06. Found: C 35.74, H 4.25, N 24.58.

IR (ATR, cm^{-1}) selected peaks: 3350.3 (*w*), 3098.4 (*w*), 3044.3 (*w*), 2988.8 (*w*), 2063.4 (*s*), 1583.1 (*s*), 1557.8 (*s*), 1530.8 (*s*), 1501.3 (*m*), 1483.2 (*s*), 1441.4 (*m*), 1400.5 (*m*), 1347.7 (*m*), 1319.7 (*m*), 1296.1 (*m*), 1248.7 (*m*), 1185.3 (*m*), 1118.1 (*m*), 1034.8 (*s*), 997.2 (*m*), 972.1 (*m*), 926.3 (*m*), 910.6 (*m*), 815.7 (*m*), 733.2 (*m*), 655.2 (*w*).

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TABLE S-I. Selected bond lengths (Å) and angles (°) for $[Cu_2\mathbf{L}_2(\mu_{1,3}\text{-}N_3)_2](BF_4)_2$.

Cu1–O1	1.930(3)	O1–Cu1–N6	92.72(13)
Cu1–N1	1.972(3)	O1–Cu1–N1	170.34(13)
Cu1–N3	1.975(3)	N6–Cu1–N1	93.99(14)
Cu1–N6	1.957(3)	O1–Cu1–N3	82.34(13)
Cu1–N8[a]	2.426(4)	N6–Cu1–N3	167.13(14)
N3–C8	1.297(5)	N1–Cu1–N3	89.64(14)
N3–N4	1.391(5)	O1–Cu1–N8[a]	91.62(14)
N4–C10	1.301(5)	N6–Cu1–N8[a]	95.51(14)
O1–C10	1.287(5)	N1–Cu1–N8[a]	94.65(14)
N6–N7	1.188(5)	N3–Cu1–N8[a]	96.49(14)
N7–N8	1.157(5)		

Symmetry code a = *–x*, *–y*, *–z*+1

TABLE S-II. Bridging modes of azido ligands in binuclear Cu(II)-complexes with hydrazone-based NNO-donor ligands.

CCDC numbers of binuclear Cu(II)-azido complexes with NNO donor hydrazone ligands	Bridging modes of azido ligands	Cu(II)-ligand chelate ring-system	References
$[Cu_2\mathbf{L}_2(\mu_{1,3}\text{-}N_3)_2](BF_4)_2$	double EE[a] (di-$\mu_{1,3}$-N_3)	6-5	this work
978363	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[1]
843830	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[2]
615282	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[3]
704271	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[4]
649737	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[5]
1920797	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[6]
1886535	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[7]
902698	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[8]
1569840	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[9]
797642	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[10]
1945216	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[11]
1983984	double EO[b] (di-$\mu_{1,1}$-N_3)	5-5	[12]

[a]EE = end-to-end; [b]EO = end-on

TABLE S-III. Hydrogen-bond parameters for $[Cu_2\mathbf{L}_2(\mu_{1,3}\text{-}N_3)_2](BF_4)_2$

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symm. Operation on A
N2–H2N···F3	0.92(4)	2.48(4)	3.390(8)	167(5)	2-*x*,1-*y*,1-*z*
C4–H4···F4A	0.93	2.39	3.249(12)	154	
C4–H4···F4B	0.93	2.50	3.418(16)	167	
C5–H5···N8	0.93	2.52	3.369(7)	151	1+*x*,1+*y*,*z*
C11–H11A···F2	0.97	2.48	3.350(11)	149	1-*x*,-*y*,1-*z*
C11–H11B···F2	0.97	2.38	3.316(10)	163	*x*,*y*,1+*z*
C14–H14A···F1	0.96	2.55	3.460(9)	159	-1+*x*,*y*,1+*z*

C14–H14B···F4A	0.96	2.48	3.181(10)	129	1-*x*,*1*-*y*,1-*z*
Intra C9–H9A···N4	0.96	2.26	2.675(8)	105	
Intra C13–H13B···O1	0.96	2.58	3.162(6)	119	

TABLE S-IV. Intermolecular π···π interaction parameters for complex **1**

Cg(*I*)[a]	Cg(*J*)[a]	Cg(*I*)···Cg(*J*)[b] (Å)	α[c] (°)	β[d] (°)	γ[e] (°)	Slippage[f] (Å)	Sym. code on (*J*)
Cg(1)	Cg(1)	3.460(3)	0.0(2)	4.0	4.0	0.240	1−*x*,1 −*y*, 1−*z*

[a] Labels of aromatic rings: (1) = N(2),C(5),C(4),C(3),C(7),C(6).
[b] Cg(*I*)···Cg(*J*) = Distance between ring centroids (Ang.).
[c] α = Dihedral angle between planes (*I*) and (*J*) (Deg).
[d] β = Angle between Cg(*I*)–Cg(*J*) vector and normal to plane (*I*) (Deg).
[e] γ = Angle between Cg(*I*)–Cg(*J*) vector and normal to plane (*J*) (Deg).
Slippage = Distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring (*I*) (Ang).

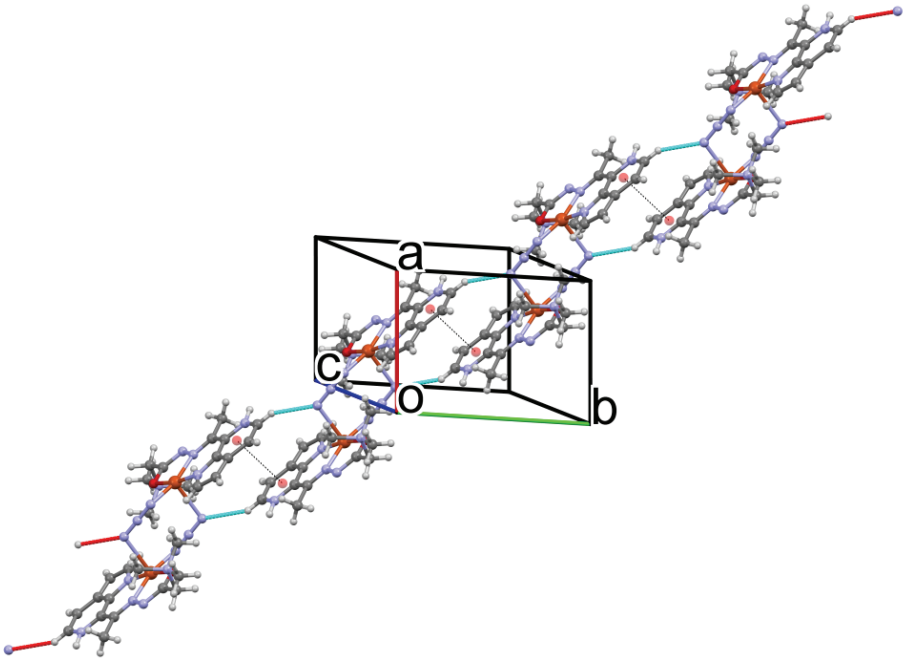

Fig. S-1. Crystal packing, showing intermolecular π···π and C–H···N contacts between dimeric complex cations extending in [110] direction.

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