

[μ -1,4-Bis(1,2,4-triazol-1-ylmethyl)-benzene]bis[aqua(pyridine-2,6-dicarboxylato)copper(II)] monohydrate

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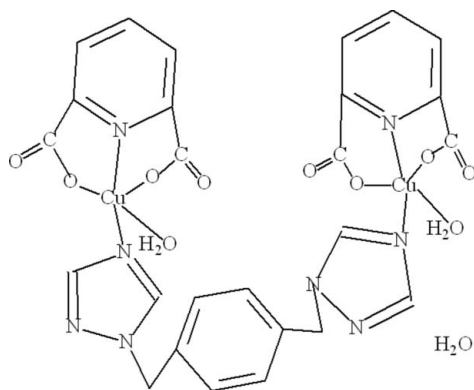
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.161; data-to-parameter ratio = 12.3.

The title compound, $[\text{Cu}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_{12}\text{H}_{12}\text{N}_6)(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$, displays a discrete dinuclear structure, in which the central Cu^{II} atom is five-coordinated in a distorted square-based pyramidal coordination geometry and the flexible ligand 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene adopts a bis-monodentate bridging mode linking the Cu^{II} atoms. It is further assembled by $\text{O}-\text{H} \cdots \text{O}$ hydrogen-bond interactions involving both the coordinated and uncoordinated water molecules. The latter exhibits half-occupancy.

Related literature

For the versatile conformations of the flexible 1,4-bis(1,2,4-triazol-1-yl-methyl)benzene ligand and related complexes, see: Arion *et al.* (2003); Peng *et al.* (2004, 2006); Meng *et al.* (2004); Li *et al.* (2005); Lin & Dong (2007); Ding *et al.* (2009).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_7\text{H}_3\text{NO}_4)_2(\text{C}_{12}\text{H}_{12}\text{N}_6) \cdot (\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$
 $M_r = 751.63$
 Monoclinic, $P2_1/c$
 $a = 4.9017$ (4) Å
 $b = 10.3022$ (9) Å
 $c = 30.178$ (3) Å
 $\beta = 93.541$ (1)°
 $V = 1521.0$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.47$ mm⁻¹
 $T = 298$ K
 $0.20 \times 0.15 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.881$, $T_{\text{max}} = 0.901$
 7340 measured reflections
 2678 independent reflections
 2256 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.161$
 $S = 1.06$
 2678 reflections
 217 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O2W}-\text{H2WA} \cdots \text{O2W}^{\text{i}}$	0.85	2.15	2.920 (5)	151
$\text{O2W}-\text{H2WB} \cdots \text{O2W}^{\text{ii}}$	0.85	1.96	2.807 (5)	179
$\text{O1W}-\text{H1WA} \cdots \text{O4}^{\text{iii}}$	0.83	1.93	2.746 (5)	168
$\text{O1W}-\text{H1WB} \cdots \text{O3}^{\text{iv}}$	0.86	1.86	2.692 (5)	164

Symmetry codes: (i) $-x + 2, -y + 2, -z$; (ii) $-x + 1, -y + 2, -z$; (iii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $x + 1, y, z$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2295).

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supplementary materials

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[μ -1,4-Bis(1,2,4-triazol-1-ylmethyl)benzene]bis[aqua(pyridine-2,6-dicarboxylato)copper(II)] monohydrate

G.-Y. Dong, C.-H. He, L. Tong-Fei, X.-C. Deng and X.-G. Shi

Comment

1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (btx=1,4-bis(1,2,4-triazol-1-ylmethyl)benzene) is a ditriazole-containing bridge ligand, in which the flexible nature of spacers allows the ligands to bend and rotate when coordinating to metal centers so as to conform the coordination geometries of metal ions. (Arion, *et al.*, 2003; Peng, *et al.*, 2004, 2006; Meng, *et al.*, 2004; Li *et al.*, 2005; Lin *et al.* 2007; Ding, *et al.* 2009) To further understand the coordination behavior of this ligand, we report herein the crystal structure of the title compound, (I).

The asymmetric unit of (I) contains one copper^{II}, one 2,6-pyridinedicarboxylato, one half btx ligand, one coordination water molecule and one half free water molecule. The copper center is five-coordinated in distorted square-based pyramidal coordination geometry. As show in Fig. 1, selected geometric parameters see table 1. Each copper^{II} is coordinated by one tridentate dipicolinato ligands *via* their carboxylate and nitrogen donors. (Cu1—N1= 1.908 (3); Cu1—O1=2.007 (3); Cu(1)—O(3)= 2.048 (3) Å) another one (Cu1—N4=1.951 (3) Å) from btx ligand together with one water molecule (Cu1—O1W = 2.217 (4) Å). Two carboxylate oxygen atoms and two nitrogen atoms define a quadrangle equatorial plane, and the water oxygen atom occupies the apical position. Each btx ligand bridges two copper atoms related by a twofold axis into dinuclear structure. The dihedral angle between the imidazole and phenyl rings is 70.0 (4)° in same btx ligand. It is noteworthy that there exist strong hydrogen-bonding interaction (table 2) involving the carboxy group oxygen atoms of dipicolinato ligands as well as coordinated and free water molecules, this may further stabilize the crystal structure.

Experimental

A mixture of Cu(NO₃)₂·3H₂O (120.5 mg, 0.5 mmol), 2,6-Pyridinedicarboxylic acid (167 mg, 1 mmol), NaOH (80 mg, 2 mmol), btx (60 mg, 0.5 mmol) and water (12 ml) was sealed in a 25 ml teflon-lined stainless steel reactor and heated to 413 K for 72 h. The reaction was cooled to room temperature over a period of 24 h. Blue prism crystals of 1 suitable for X-ray diffraction analysis were obtained with a yield of 37% (based btx)

Refinement

H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$. Water H atoms were located in Fourier difference maps and isotropically.

Figures

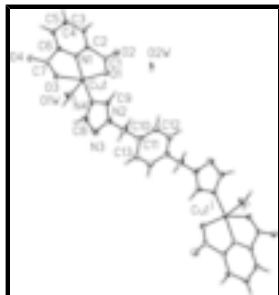


Fig. 1. Fig. 1. The part molecular structure of (I), showing displacement ellipsoids at the 30% probability level for atoms [symmetry code: (i) $-x, -y + 3, -z$]

[μ -1,4-Bis(1,2,4-triazol-1-ylmethyl)benzene]bis[aqua(pyridine-2,6-dicarboxylato)copper(II)] monohydrate

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Hall symbol: $-P\ 2ybc$

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$b = 10.3022\ (9)\ \text{\AA}$

$c = 30.178\ (3)\ \text{\AA}$

$\beta = 93.541\ (1)^\circ$

$V = 1521.0\ (2)\ \text{\AA}^3$

$Z = 2$

$F(000) = 764$

$D_x = 1.641\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3568 reflections

$\theta = 22.3\text{--}3.6^\circ$

$\mu = 1.47\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Prism, blue

$0.20 \times 0.15 \times 0.11\ \text{mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.881$, $T_{\max} = 0.901$

7340 measured reflections

2678 independent reflections

2256 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -5 \rightarrow 5$

$k = -12 \rightarrow 12$

$l = -35 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.161$

$S = 1.06$

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1045P)^2 + 1.8845P]$

2678 reflections
217 parameters
0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 1.40 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	0.08344 (10)	0.98034 (5)	0.149509 (16)	0.0318 (2)	
O3	-0.1809 (6)	0.9403 (3)	0.19769 (10)	0.0376 (7)	
O1	0.3528 (6)	0.9508 (3)	0.10311 (10)	0.0392 (7)	
N1	0.1905 (7)	0.8071 (3)	0.16460 (11)	0.0300 (8)	
C7	-0.1409 (9)	0.8318 (4)	0.21771 (14)	0.0328 (9)	
O4	-0.2555 (7)	0.7960 (3)	0.25024 (11)	0.0469 (8)	
N4	-0.0779 (7)	1.1422 (3)	0.12697 (12)	0.0346 (8)	
C2	0.3801 (9)	0.7519 (4)	0.14164 (14)	0.0335 (9)	
C3	0.4592 (10)	0.6261 (4)	0.15103 (16)	0.0419 (11)	
H3	0.5917	0.5859	0.1350	0.050*	
C6	0.0697 (8)	0.7462 (4)	0.19736 (13)	0.0309 (9)	
O2	0.6818 (8)	0.8113 (4)	0.08671 (12)	0.0565 (10)	
C11	-0.1952 (9)	1.4310 (5)	0.02197 (15)	0.0415 (11)	
C1	0.4833 (9)	0.8436 (4)	0.10695 (14)	0.0358 (10)	
C5	0.1422 (10)	0.6216 (4)	0.20832 (16)	0.0417 (11)	
H5	0.0613	0.5787	0.2312	0.050*	
C12	-0.0882 (11)	1.3819 (5)	-0.01557 (17)	0.0486 (12)	
H12	-0.1473	1.3016	-0.0266	0.058*	
C4	0.3384 (10)	0.5605 (5)	0.18465 (17)	0.0453 (11)	
H4	0.3890	0.4754	0.1914	0.054*	
O1W	0.3552 (8)	1.0793 (4)	0.20033 (14)	0.0698 (13)	
N2	-0.2780 (8)	1.2853 (4)	0.08451 (13)	0.0439 (10)	
C13	-0.1072 (11)	1.5492 (5)	0.03729 (17)	0.0492 (12)	
H13	-0.1788	1.5841	0.0625	0.059*	
C10	-0.4037 (11)	1.3552 (6)	0.04620 (19)	0.0576 (15)	
H10A	-0.5411	1.4144	0.0562	0.069*	
H10B	-0.4942	1.2936	0.0259	0.069*	
C9	-0.1903 (11)	1.1643 (5)	0.08746 (16)	0.0465 (12)	

supplementary materials

H9	-0.2064	1.1037	0.0646	0.056*	
N3	-0.2233 (16)	1.3460 (5)	0.12323 (17)	0.092 (2)	
C8	-0.1028 (17)	1.2542 (6)	0.14744 (19)	0.080 (2)	
H8	-0.0398	1.2672	0.1768	0.096*	
O2W	0.746 (3)	0.9295 (7)	0.0049 (2)	0.092 (4)	0.50
H2WA	0.9152	0.9472	0.0077	0.137*	0.50
H2WB	0.5966	0.9714	0.0018	0.137*	0.50
H1WA	0.3201	1.1370	0.2183	0.137*	
H1WB	0.5177	1.0475	0.2023	0.137*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0373 (4)	0.0240 (3)	0.0348 (4)	0.0079 (2)	0.0068 (2)	0.00618 (19)
O3	0.0425 (17)	0.0334 (16)	0.0376 (16)	0.0129 (14)	0.0083 (13)	0.0073 (14)
O1	0.0469 (18)	0.0330 (16)	0.0390 (17)	0.0053 (14)	0.0130 (14)	0.0077 (13)
N1	0.0351 (19)	0.0255 (17)	0.0296 (18)	0.0040 (14)	0.0026 (14)	0.0005 (14)
C7	0.037 (2)	0.030 (2)	0.033 (2)	0.0001 (18)	0.0042 (18)	0.0012 (17)
O4	0.063 (2)	0.0381 (18)	0.0418 (18)	0.0049 (16)	0.0205 (16)	0.0073 (15)
N4	0.042 (2)	0.0274 (18)	0.035 (2)	0.0085 (15)	0.0039 (15)	0.0055 (15)
C2	0.038 (2)	0.030 (2)	0.032 (2)	0.0025 (18)	0.0025 (17)	-0.0045 (17)
C3	0.047 (3)	0.031 (2)	0.048 (3)	0.013 (2)	0.009 (2)	-0.003 (2)
C6	0.036 (2)	0.026 (2)	0.030 (2)	0.0017 (17)	-0.0005 (17)	0.0018 (17)
O2	0.063 (2)	0.054 (2)	0.056 (2)	0.0176 (18)	0.0296 (18)	0.0073 (17)
C11	0.043 (3)	0.038 (3)	0.043 (3)	0.010 (2)	-0.006 (2)	0.015 (2)
C1	0.044 (3)	0.031 (2)	0.033 (2)	0.0020 (19)	0.0056 (19)	-0.0015 (17)
C5	0.051 (3)	0.030 (2)	0.044 (3)	0.004 (2)	0.008 (2)	0.008 (2)
C12	0.062 (3)	0.031 (2)	0.051 (3)	0.004 (2)	-0.003 (2)	-0.003 (2)
C4	0.056 (3)	0.024 (2)	0.056 (3)	0.010 (2)	0.008 (2)	0.006 (2)
O1W	0.049 (2)	0.074 (3)	0.083 (3)	0.026 (2)	-0.0229 (19)	-0.046 (2)
N2	0.046 (2)	0.041 (2)	0.045 (2)	0.0095 (18)	-0.0008 (17)	0.0148 (18)
C13	0.066 (3)	0.045 (3)	0.037 (3)	0.013 (3)	0.007 (2)	-0.003 (2)
C10	0.049 (3)	0.060 (3)	0.063 (3)	0.010 (3)	-0.004 (2)	0.034 (3)
C9	0.068 (3)	0.031 (2)	0.040 (3)	0.005 (2)	-0.005 (2)	0.006 (2)
N3	0.173 (6)	0.051 (3)	0.049 (3)	0.057 (4)	-0.007 (3)	0.000 (2)
C8	0.155 (7)	0.043 (3)	0.039 (3)	0.042 (4)	-0.015 (3)	-0.001 (2)
O2W	0.235 (12)	0.026 (4)	0.017 (3)	0.038 (5)	0.034 (5)	0.010 (3)

Geometric parameters (\AA , $^\circ$)

Cu1—N1	1.908 (3)	C11—C10	1.510 (7)
Cu1—N4	1.950 (3)	C5—C4	1.384 (7)
Cu1—O1	2.006 (3)	C5—H5	0.9300
Cu1—O3	2.048 (3)	C12—C13 ⁱ	1.389 (7)
Cu1—O1W	2.217 (4)	C12—H12	0.9300
O3—C7	1.280 (5)	C4—H4	0.9300
O1—C1	1.278 (5)	O1W—H1WA	0.8301
N1—C2	1.322 (5)	O1W—H1WB	0.8599

N1—C6	1.339 (5)	N2—C9	1.319 (6)
C7—O4	1.218 (5)	N2—N3	1.338 (6)
C7—C6	1.517 (6)	N2—C10	1.466 (6)
N4—C9	1.302 (6)	C13—C12 ⁱ	1.389 (7)
N4—C8	1.318 (7)	C13—H13	0.9300
C2—C3	1.377 (6)	C10—H10A	0.9700
C2—C1	1.520 (6)	C10—H10B	0.9700
C3—C4	1.382 (7)	C9—H9	0.9300
C3—H3	0.9300	N3—C8	1.313 (7)
C6—C5	1.367 (6)	C8—H8	0.9300
O2—C1	1.226 (5)	O2W—H2WA	0.8500
C11—C13	1.364 (8)	O2W—H2WB	0.8482
C11—C12	1.374 (7)		
N1—Cu1—N4	169.43 (16)	O2—C1—C2	118.8 (4)
N1—Cu1—O1	80.88 (13)	O1—C1—C2	114.4 (4)
N4—Cu1—O1	99.00 (14)	C6—C5—C4	118.7 (4)
N1—Cu1—O3	79.57 (13)	C6—C5—H5	120.6
N4—Cu1—O3	99.15 (13)	C4—C5—H5	120.6
O1—Cu1—O3	159.60 (14)	C11—C12—C13 ⁱ	120.7 (5)
N1—Cu1—O1W	96.92 (16)	C11—C12—H12	119.7
N4—Cu1—O1W	93.53 (15)	C13 ⁱ —C12—H12	119.7
O1—Cu1—O1W	99.18 (15)	C3—C4—C5	120.0 (4)
O3—Cu1—O1W	88.91 (16)	C3—C4—H4	120.0
C7—O3—Cu1	115.2 (3)	C5—C4—H4	120.0
C1—O1—Cu1	114.5 (3)	Cu1—O1W—H1WA	129.9
C2—N1—C6	122.9 (4)	Cu1—O1W—H1WB	112.7
C2—N1—Cu1	118.0 (3)	H1WA—O1W—H1WB	117.2
C6—N1—Cu1	119.1 (3)	C9—N2—N3	109.6 (4)
O4—C7—O3	125.5 (4)	C9—N2—C10	129.6 (5)
O4—C7—C6	120.6 (4)	N3—N2—C10	120.7 (4)
O3—C7—C6	113.9 (3)	C11—C13—C12 ⁱ	120.6 (5)
C9—N4—C8	103.3 (4)	C11—C13—H13	119.7
C9—N4—Cu1	127.5 (3)	C12 ⁱ —C13—H13	119.7
C8—N4—Cu1	129.2 (3)	N2—C10—C11	111.8 (4)
N1—C2—C3	119.7 (4)	N2—C10—H10A	109.2
N1—C2—C1	111.6 (4)	C11—C10—H10A	109.2
C3—C2—C1	128.7 (4)	N2—C10—H10B	109.2
C2—C3—C4	118.9 (4)	C11—C10—H10B	109.2
C2—C3—H3	120.6	H10A—C10—H10B	107.9
C4—C3—H3	120.6	N4—C9—N2	110.2 (4)
N1—C6—C5	119.9 (4)	N4—C9—H9	124.9
N1—C6—C7	111.7 (3)	N2—C9—H9	124.9
C5—C6—C7	128.5 (4)	C8—N3—N2	102.0 (5)
C13—C11—C12	118.7 (5)	N3—C8—N4	114.9 (5)
C13—C11—C10	120.4 (5)	N3—C8—H8	122.5
C12—C11—C10	120.9 (5)	N4—C8—H8	122.5
O2—C1—O1	126.7 (4)	H2WA—O2W—H2WB	137.0

Symmetry codes: (i) $-x, -y+3, -z$.

supplementary materials

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—H2WA \cdots O2W ⁱⁱ	0.85	2.15	2.920 (5)	151.
O2W—H2WB \cdots O2W ⁱⁱⁱ	0.85	1.96	2.807 (5)	179.
O1W—H1WA \cdots O4 ^{iv}	0.83	1.93	2.746 (5)	168.
O1W—H1WB \cdots O3 ^v	0.86	1.86	2.692 (5)	164.

Symmetry codes: (ii) $-x+2, -y+2, -z$; (iii) $-x+1, -y+2, -z$; (iv) $-x, y+1/2, -z+1/2$; (v) $x+1, y, z$.

Fig. 1

