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Hydrogen bonding and π–π stacking in di-μ-isophthalato-bis[bis(isonicotinamide)copper(II)] trihydrate

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Key indicators

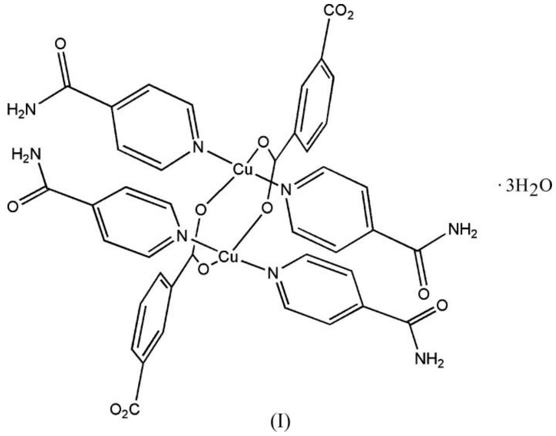
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.096
Data-to-parameter ratio = 15.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $[Cu_2(C_8H_4O_4)_2(C_6H_6N_2O)_4]\cdot 3H_2O$, the Cu^{II} atom exhibits distorted trigonal–bipyramidal geometry and is coordinated by two N atoms of two isonicotinamide (inta) ligands and three O atoms of three isophthalate (ipt) ligands. C—H···O and N—H···O hydrogen bonds, as well as π–π stacking interactions, are observed between.

Comment

In the past decade, the construction of supramolecular architectures has attracted much attention because of their intriguing structural features and potential application in catalysis, separation, gas storage, molecular recognition, magnetic devices and non-linear optical materials (Lehn, 1995; Eddaoudi *et al.*, 2002; Abourahma *et al.*, 2002). Recently, a successful strategy for preparing these materials has been the assembly reaction between a transition metal ion and two types of ligands, one acting as a terminal ligand, while the other acts as a bridging ligand. In this respect, diverse dicarboxylates with various oriented carboxyl groups have been utilized to build coordination polymers. These ligands are able to bridge metal centers in different modes and also produce either linear or zigzag polymeric chains (Groeneman *et al.*, 1999; Chen & Liu, 2002). In addition, organic amides have proved to be useful in self-assembly through hydrogen bonding, and such products have relevance to biological systems (Bhogala *et al.*, 2004; Qin *et al.*, 2003). However, hybrid structures containing dicarboxylate ligands and organic amide-containing ligands have been relatively unexplored. The related structures described by Aakeroy *et al.* (2002), did not contain metals.



(I)

Here we chose the V-shaped dicarboxylate ligand isophthalate (ipt), the terminal ligand isonicotinamide (inta) and the divalent copper ion to explore potential supramole-

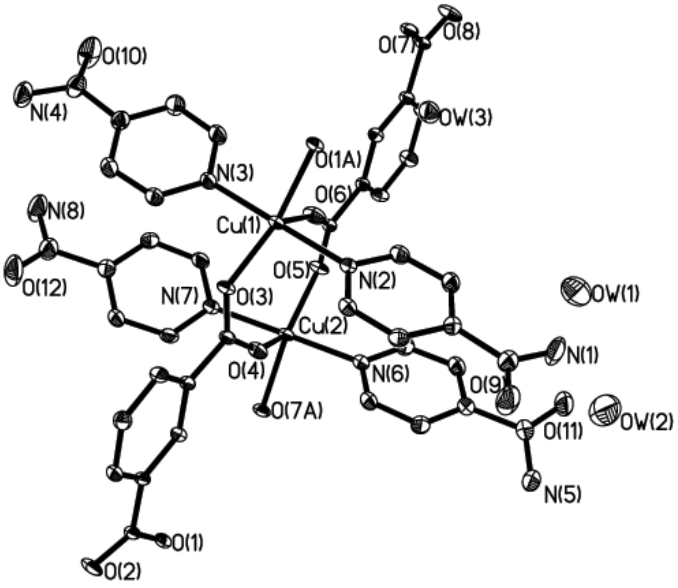


Figure 1
View of the asymmetric unit, shown with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

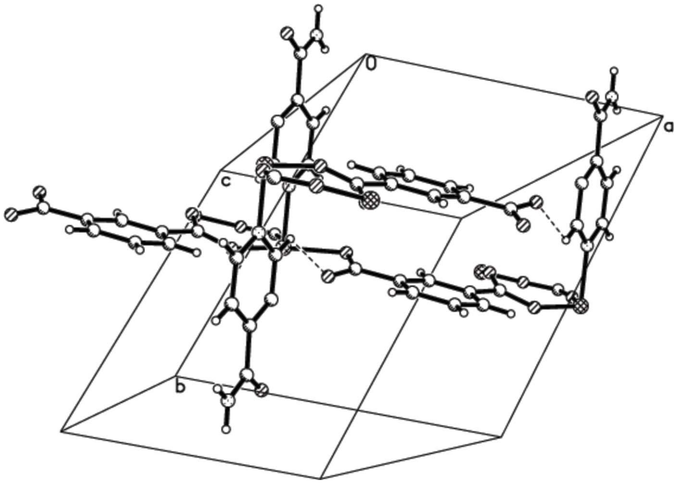


Figure 2
Hydrogen bonds (dashed lines) and π–π stacking interactions between adjacent chains in the title complex.

cular structures. The complex is a metal-organic coordination polymer with a supramolecular structure. The asymmetric unit of the title compound, (I), consists of two divalent copper ions, two isophthalic acid ligands, four isonicotinamide ligands and three uncoordinated water molecules. Both Cu^{II} centers have the same coordination and display a distorted trigonal–bipyramidal coordination geometry, being coordinated by two N atoms of two inta ligands and three O atoms from three different carboxyl groups of three ipt ligands (Fig. 1). One carboxyl group adopts the monodentate mode to coordinate to the Cu^{II} center, and the other carboxyl group from the same ipt ligand acts as a bridge connecting Cu^{II} centers to form a dimeric unit.

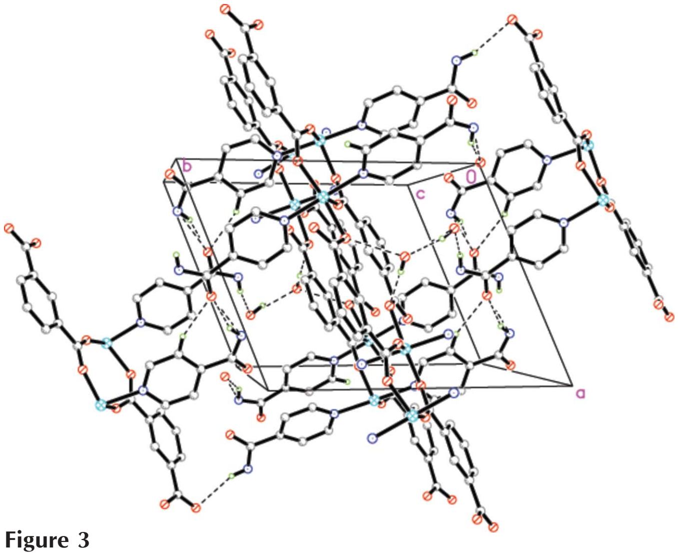


Figure 3
The three-dimensional network, viewed approximately along the *c* axis in the complex. Dashed lines indicate hydrogen bonds.

There are π–π stacking interactions and hydrogen bonds in the complex between adjacent one-dimensional chains which run parallel to the *a* axis (Fig. 2). The face-to-face distance between the adjacent ipt rings, in an offset fashion, is about 3.607 (3) Å, indicating significant interlayer π–π stacking interactions (Janiak, 2000). The C—H proton of one inta ligand forms a hydrogen bond to an O atom of an ipt ligand on an adjacent one-dimensional chain [C22$\cdots$O2 = 3.130 (2) Å and C—H$\cdots$O = 120.95 (1)°]. In addition, there are also three kinds of hydrogen bonds between other chains, mainly involving the N and O atoms of the inta ligands and water molecules (Fig. 3). Hydrogen-bond interactions play an important role in generating a three-dimensional network (Fig. 3). The O$\cdots$N distances vary from 2.801 (1) to 3.090 (2) Å and the C$\cdots$O distance is 3.372 (2) Å (Qin *et al.*, 2001; Burrows *et al.*, 2004). Finally, the presence of the π-π stacking and various hydrogen bonds lead to the supramolecular structure of the title complex.

Experimental

A mixture of $CuSO_4$ (0.5 mmol), isophthalic acid (0.5 mmol) and isonicotinamide (1 mmol) was heated in H_2O (20 ml) and stirred continuously for 30 min at 333 K. The pH was adjusted to about 7 with sodium hydroxide. The mixture was filtered and the filtrate was allowed to stand. One month later, blue block-shaped crystals suitable for X-ray structural analysis were obtained. Elemental analysis calculated for $C_{40}H_{38}Cu_2N_8O_{15}$: C 48.1, H 3.8, N 11.2%; found: C 48.3, H 3.6, N 11.5%.

Crystal data

$[Cu_2(C_8H_4O_4)_2(C_6H_6N_2O)_4]\cdot 3H_2O$
M_r = 997.86
Triclinic, $P\overline{1}$
a = 10.0909 (7) Å
b = 12.7898 (9) Å
c = 17.5601 (12) Å
α = 95.6425 (12)°
β = 99.8511 (13)°
γ = 109.6652 (11)°
V = 2072.8 (2) Å^3

Z = 2
D_x = 1.599 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10290 reflections
θ = 1.7–28.3°
μ = 1.11 mm^{-1}
T = 293 (2) K
Block, blue
0.43 × 0.19 × 0.13 mm

m1706 Li *et al.* • $[Cu_2(C_8H_4O_4)_2(C_6H_6N_2O)_4]\cdot 3H_2O$ *Acta Cryst.* (2005). E**61**, m1705–m1707

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.801$, $T_{\max} = 0.838$
12901 measured reflections
9109 independent reflections
6542 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.039$
$\theta_{\max} = 28.3°$
$h = -11 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -23 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.096$
$S = 1.02$
9109 reflections
592 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.021P)^2 + 0.9P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.77$ e Å^{-3}
$\Delta\rho_{\min} = -0.43$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···O2	0.93	2.55	3.130 (?)	121
C40—H40···O10$^{\rm i}$	0.93	2.49	3.372 (?)	161
N5—H5*A*···O2$^{\rm ii}$	0.86	2.27	3.090 (?)	159
N8—H8*B*···O10$^{\rm iii}$	0.86	1.93	2.801 (?)	157
O*W*2—H*W*2···O*W*3	0.85	1.90	2.713 (?)	160
O*W*3—H*W*5···O7	0.85	2.00	2.839 (?)	177
N1—H1*B*···O*W*1$^{\rm iv}$	0.86	2.05	2.850 (?)	155
N4—H4*B*···O*W*2$^{\rm v}$	0.86	2.21	3.043 (?)	163

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

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso} = 1.2U_{\rm eq}$(C,N). Water H atoms were found in a difference Fourier map (O—H = 0.85 Å) and assigned riding isotropic displacement parameters of $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm O})$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2005). E**61**, m1705–m1707 Li *et al.* • $[{\rm Cu_2(C_8H_4O_4)_2(C_6H_6N_2O)_4}]\cdot 3{\rm H_2O}$ **m1707**

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In the original report by Li, Liu, Gao & Che [*Acta Cryst.* (2005), E**61**, m1705–m1707], the hydrogen-bond $D\cdots A$ parameters were published without their associated s.u. values. The correct Table is given below.

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
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OW3—HW5$\cdots$O7	0.85	2.00	2.839 (1)	177
N1—H1$B\cdots$OW1^{iv}	0.86	2.05	2.850 (2)	155
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