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Bis(2-amino-4,6-dimethylpyrimidine-κN)bis(isophthalato-κ^2O,O')copper(II) 2-amino-4,6-dimethylpyrimidine disolvate

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Key indicators

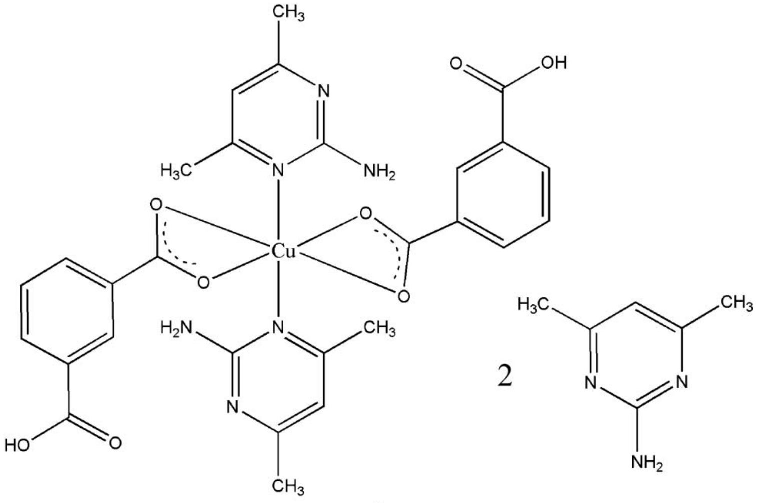
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.118
Data-to-parameter ratio = 12.8

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

The title compound, $[Cu(C_8H_5O_4)_2(C_6H_9N_3)_2]\cdot 2C_6H_9N_3$, is a neutral mononuclear copper(II) complex. The Cu^{2+} cation lies on an inversion centre, coordinated by the N atoms from two 2-amino-4,6-dimethylpyrimidine ligands and four O atoms from two chelating isophthalate ligands, in a distorted octahedral configuration. The asymmetric unit also contains a 2-amino-4,6-dimethylpyrimidine solvent molecule. The crystal structure is stabilized by a network of O—H···N, N—H···O and N—H···N hydrogen bonds and π–π stacking interactions, forming a three-dimensional supramolecular structure.

Comment

In the last decade, aromatic dicarboxylates with carboxylate groups in various orientations have been utilized to build coordination polymers (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). A hybrid structure containing both dicarboxylate and organic amide ligands has been reported by Li *et al.* (2005). We report here the title mononuclear Cu^{2+} complex, (I), formed from a V-shaped dicarboxylate ligand, the isophthalate monoanion acid, (ip^-) and the amine ligand 2-amino-4,6-dimethylpyrimidine (adp) and describe its supramolecular structure (Fig. 1).



(I)

The asymmetric unit of (I) consists of a Cu^{2+} cation, which lies on an inversion centre, a monoanionic isophthalate ligand, a monodentate adp ligand and an uncoordinated adp mol-

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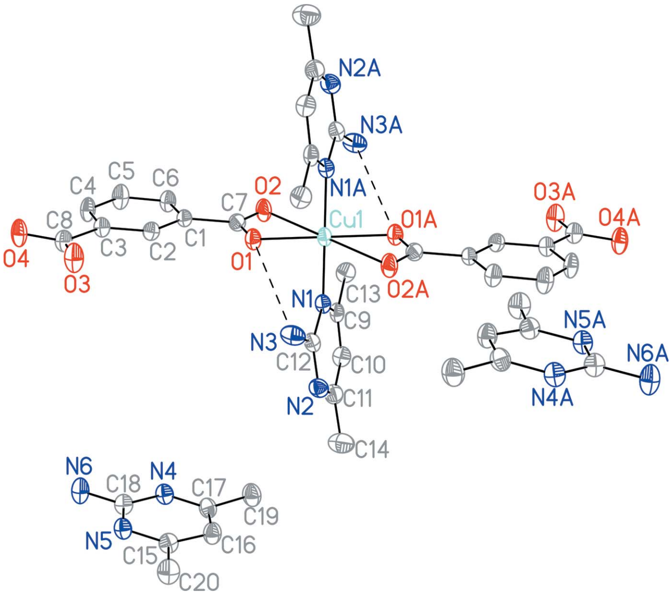

Figure 1
The molecular structure of the title complex with 30% probability displacement ellipsoids. H atoms have been omitted for clarity. Atoms labelled with the suffix A are related to other atoms by the symmetry operation ($-x$, $1 - y$, $2 - z$). Intramolecular hydrogen-bonding interactions are indicated by dashed lines.

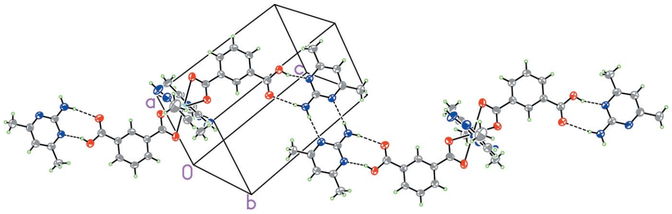

Figure 2
The one-dimensional chain structure of (I). Hydrogen bonds are shown as dashed lines.

ecule. Only one carboxylate group of the isophthalic acid is deprotonated and the resulting monoanion acts as a semi-chelating ligand (Addison *et al.*, 1971; Guilera & Steed, 1999), with Cu1—O1 = 2.002 (2) Å and Cu—O2 = 2.548 (2) Å. This suggests a non-negligible interaction between the copper and the second carboxylate oxygen. The adp ligand is monodentate, binding through a pyrimidine N atom [Cu1—N1 = 2.019 (2) Å]. The overall coordination geometry at Cu is distorted octahedral.

In the crystal structure, atoms N5 and N6 of an uncoordinated adp molecule form N—H···O and O—H···N hydrogen bonds to atoms O3 and O4 of the protonated carboxylate group from an ip ligand, forming an $R_2^2(8)$ ring motif (Bernstein *et al.*, 1995) (Fig. 2). In addition, N—H···N hydrogen bonds connect adjacent non-coordinating adp molecules which, in turn, link to the Cu complex, forming a one-dimensional chain. The hydrogen-bonding network is completed by N—H···O interactions between neighboring chains, forming a two-dimensional network (Fig. 3).

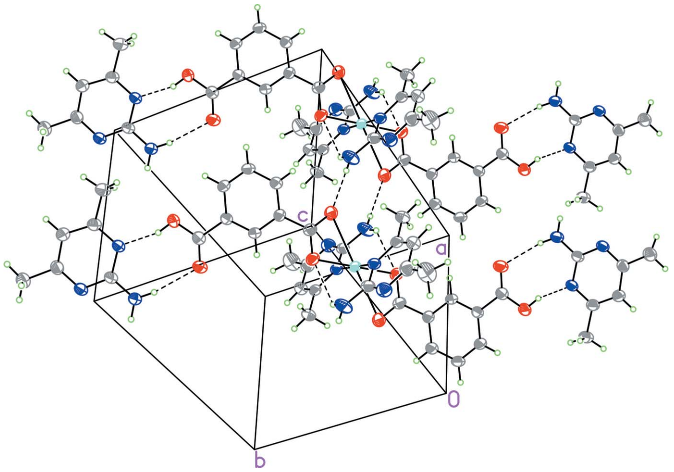

Figure 3
The two-dimensional sheet structure of (I). Hydrogen bonds are shown as dashed lines.

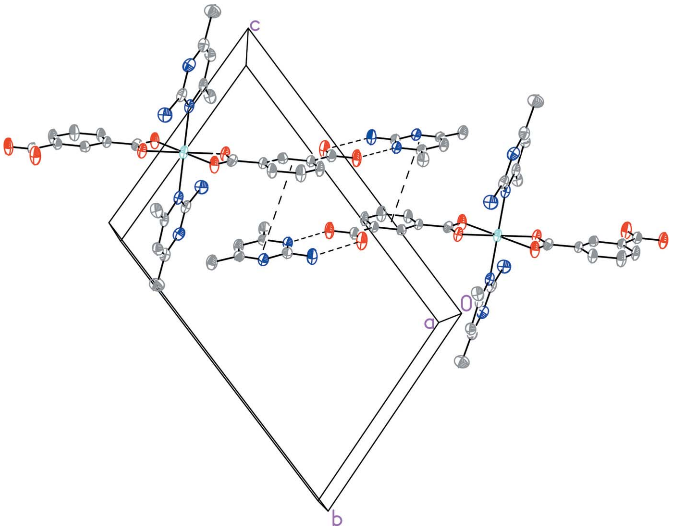

Figure 4
π–π Stacking interactions in (I), with centroid–centroid interactions shown as dashed lines.

Offset π–π stacking interactions between the adp and ip rings of complex molecules in adjacent parallel planes further stabilize the structure. The face-to-face distance between the centroids of adjacent adp and ip rings is 3.693 Å (Fig. 4). These combine with the hydrogen-bonding interactions to give the three-dimensional supramolecular structure of (I).

Experimental

The title compound was obtained as the main product of the hydrothermal reaction of copper(II) nitrate trihydrate, 2-amino-4,6-dimethylpyrimidine and isophthalic acid in the molar ratio 1:2:2 in a Teflon-lined stainless steel Parr bomb at 413 K over a period of 3 d. After cooling slowly to room temperature, green single crystals of (I) were obtained.

Crystal data

$[Cu(C_8H_5O_4)_2(C_6H_9N_3)_2]\cdot 2C_6H_9N_3$
$M_r = 886.43$
Triclinic, $P\overline{1}$
$a = 7.4010$ (2) Å
$b = 9.3811$ (3) Å
$c = 15.2889$ (5) Å
$\alpha = 101.819$ (2)°
$\beta = 93.013$ (2)°
$\gamma = 93.547$ (2)°
$V = 1034.69$ (5) Å^3
$Z = 1$
$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.60$ mm^{-1}
$T = 273$ (2) K
Block, green
0.33 × 0.21 × 0.15 mm

Data collection

Bruker SMART APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.828$, $T_{max} = 0.916$
8817 measured reflections
3600 independent reflections
2933 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.118$
$S = 1.07$
3600 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0029 (5)

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···N5^{i}	0.82	1.80	2.585 (3)	160
N3—H3A···O2^{ii}	0.86	2.11	2.921 (3)	157
N3—H3B···O1	0.86	2.37	2.992 (3)	129
N6—H6A···N4^{iii}	0.86	2.28	3.116 (3)	165
N6—H6B···O3^{i}	0.86	2.25	3.099 (3)	170

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C) for aromatic, C—H = 0.96 Å and U_{iso}(H) = $1.5U_{eq}$(C) for methyl, N—H = 0.86 Å and U_{iso}(H) = $1.2U_{eq}$(N) for amine and O—H = 0.82 Å and U_{iso}(H) = $1.5U_{eq}$(O) for carboxy H atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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