metal-organic papers

## *catena*-Poly[[[aqua(2-amino-4,6-dimethyl-pyrimidine-κN^1)copper(II)]-μ-benzene-1,3-dicarboxylato-$\kappa^2O^1:O^3$] 2-amino-4,6-dimethyl-pyrimidine solvate]

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In the title polymer, $\{[Cu(C_8H_4O_4)(C_6H_9N_3)(H_2O)]\cdot C_6H_9N_3\}_n$, the Cu^{II} ion approximates a distorted square-pyramidal geometry defined by an NO$_4$ donor set. Adjacent Cu^{II} ions are bridged by isophthalate dianions to form a one-dimensional chain. Chains interact through π–π stacking interactions of 2-amino-4,6-dimethylpyrimidine rings and hydrogen bonds, to build a three-dimensional crystal structure.

Comment

Two types of interactions, namely coordinate covalent bonds and non-covalent intermolecular forces, such as hydrogen bonding and π–π stacking interactions, play a key role in building and stabilizing polymers, which have important applications in the areas of magnetism, optics, electronics and catalysis (Ye *et al.*, 2005; Janiak, 2000; Steiner, 2002). Considering the coordination properties of 2-amino-4,6-dimethyl-pyrimidine (abbreviated ADP hereafter) and the bridging character of isophthalate, these ligands were used to construct the title polymer, (I).


(I)
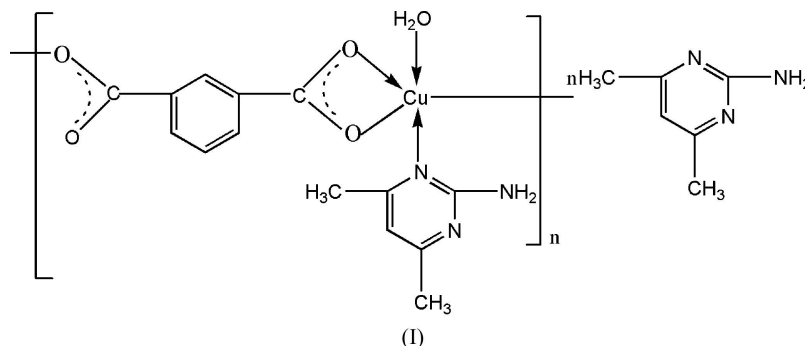
As shown in Fig. 1, the Cu^{II} ion may be described as five-coordinated by three O atoms (O1, O2 and O4) of isophthalate ligands (Billing *et al.*, 1970), one N atom belonging to an ADP ligand and one O atom of a water molecule, giving a distorted square-pyramidal geometry (Table 1). As shown in Fig. 2, Cu^{II} ions are bridged by isophthalate dianions to form a one-dimensional chain. There is one uncoordinated ADP molecule completing the asymmetric unit.

Coordinated and uncoordinated ADP molecules are linked by hydrogen bonds (Table 2, entries 1 and 2). The one-dimensional chains are interlaced *via* free ADP molecules; coordinated and symmetry-related uncoordinated ADP molecules (symmetry code: $2 - x, -y, 1 - z$) have offset face-to-face π–π stacking interactions, the centroid-to-centroid separation being 3.807 Å (Janiak, 2000). The hydrogen bonds together with π–π interactions build the three-dimensional structure of $[Cu(C_6H_9N_3)(H_2O)(C_8H_4O_4)]_n(C_6H_9N_3)_n$.
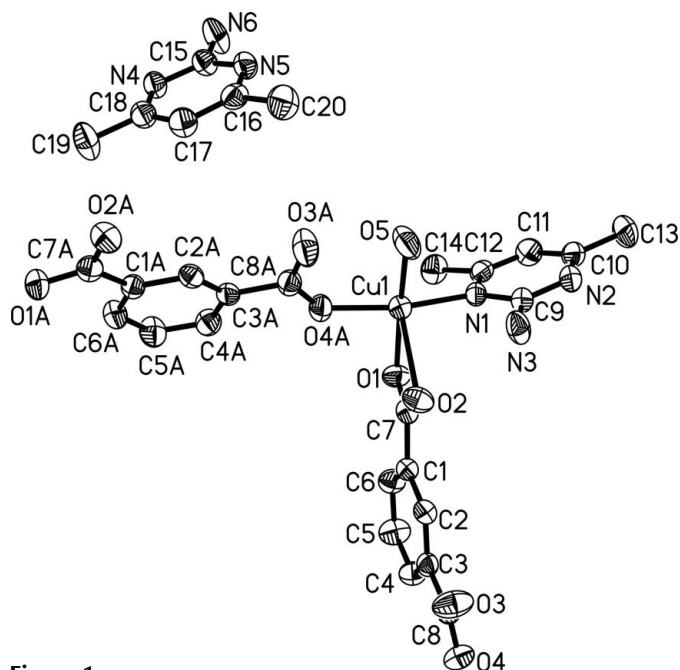
Figure 1
Part of the structure of the title complex, showing the coordination geometry and the uncoordinated ADP molecule. Displacement ellipsoids are drawn at the 50% probability level. For clarity, H atoms have been omitted. [Symmetry code: (A) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.]
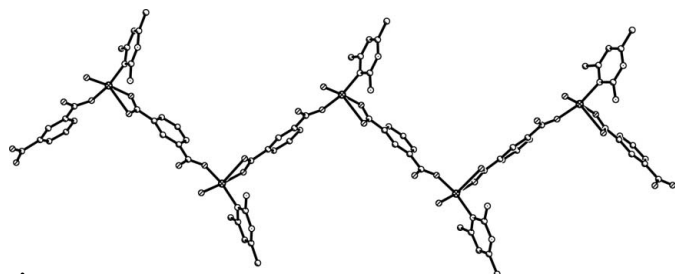
Figure 2
A one-dimensional polymeric chain in the crystal structure of (I). All H atoms have been omitted for clarity.
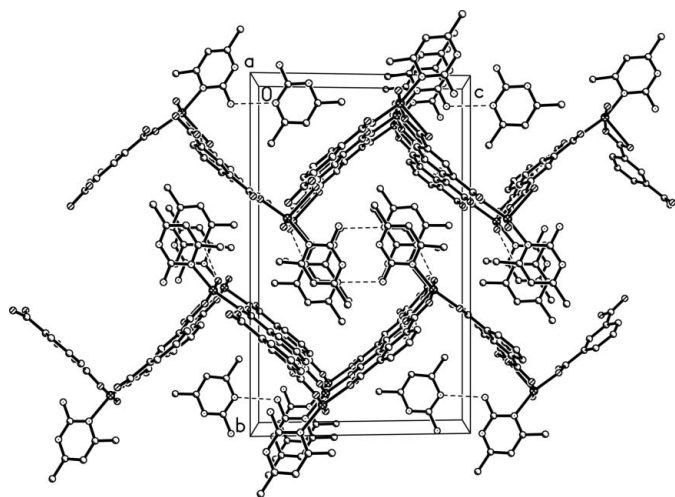
Figure 3
The packing arrangement of the title compound viewed along [100]. Dashed lines represent hydrogen bonds. All H atoms have been omitted for clarity.

Hydrogen bond geometries are shown in Table 2. The packing arrangement of the title polymer is shown in Fig. 3.

Experimental

All reagents were of analytical grade from commercial sources and used without further purification. A mixture of ADP (0.0246 g, 0.2 mol), isophthalic acid (0.0166 g, 0.1 mol), copper(II) nitrate (0.0187 g, 0.1 mol) and water (7 ml) was stirred in air for 5 min and sealed in a 10 ml Teflon-lined stainless steel Parr bomb, which was heated to 423 K for 36 h and then cooled to room temperature. Green block single crystals were separated and washed with deionized water (yield 45%, based on Cu).

Crystal data

$[Cu(C_8H_4O_4)(C_6H_9N_3)(H_2O)]\cdot C_6H_9N_3$	$V = 2194.07\ (10)$ Å^3
$M_r = 491.99$	$Z = 4$
Monoclinic, $P2_1/n$	$D_x = 1.489$ Mg m^{-3}
$a = 7.8409\ (2)$ Å	Mo $K\alpha$ radiation
$b = 21.4009\ (7)$ Å	$\mu = 1.04$ mm^{-1}
$c = 13.1791\ (3)$ Å	$T = 296\ (2)$ K
$\beta = 97.195\ (2)°$	Block, green
	$0.38 \times 0.25 \times 0.13$ mm

Data collection

Bruker SMART APEX-II area-detector diffractometer	9167 measured reflections
φ and ω scans	3900 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2923 reflections with $I > 2\sigma(I)$
$T_{min} = 0.693$, $T_{max} = 0.877$	$R_{int} = 0.030$
	$\theta_{max} = 25.1°$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.045$	
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0981P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	
3900 reflections	$(\Delta/\sigma)_{max} = 0.001$
301 parameters	$\Delta\rho_{max} = 0.41$ e Å^{-3}
	$\Delta\rho_{min} = -0.54$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O5	1.926 (3)	Cu1—N1	2.011 (3)
Cu1—O1	1.950 (2)	Cu1—O2	2.530 (3)
Cu1—O4^i	1.955 (2)		
O5—Cu1—O1	171.91 (15)	O4^i—Cu1—N1	164.05 (11)
O5—Cu1—O4^i	91.88 (12)	O5—Cu1—O2	114.60 (15)
O1—Cu1—O4^i	89.34 (11)	O1—Cu1—O2	57.32 (9)
O5—Cu1—N1	88.67 (13)	O4^i—Cu1—O2	96.94 (10)
O1—Cu1—N1	92.35 (11)	N1—Cu1—O2	97.31 (10)

Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$A\cdots$N4^{ii}	0.86	2.14	2.994 (4)	175
N6—H6$A\cdots$N2^{iii}	0.86	2.25	3.109 (4)	175
N3—H3$B\cdots$O2	0.86	2.16	2.944 (4)	152
O5—H5$E\cdots$N5^{iv}	0.843 (10)	1.98 (4)	2.712 (4)	144 (6)
O5—H5$F\cdots$O3^i	0.846 (10)	1.76 (3)	2.507 (4)	145 (5)

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

metal-organic papers

All C- and N-bonded H atoms were placed geometrically and refined with bond lengths constrained to 0.93 (aromatic CH), 0.96 (methyl CH_3) or 0.86 Å (amine NH_2), and $U_{iso}(H) = 1.2U_{eq}$(carrier atom) for aromatic CH and NH_2 group, or $U_{iso}(H) = 1.5U_{eq}$(carrier C) for methyl groups. H atoms of the water molecule were located in a difference map, and refined with O—H distances restrained to 0.85 (1) Å and free isotropic displacement parameters.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*(Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

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