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Tetrakis[μ-(4-nitrophenyl)acetato-*O*:*O*′]bis[(2-aminopyrimidine-N^1)-copper(II)]

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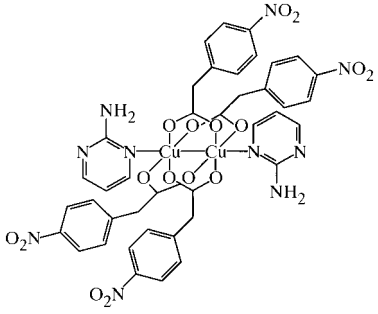
The structure of the title compound, $[Cu_2(C_8H_6NO_4)_4(C_4H_5N_3)_2]$, comprises individual units of tetra-μ-carboxylato-*O*:*O*′-dicopper(II) end-capped with two 2-aminopyrimidine molecules. These pyrimidines then form dimers across a typical N—H···N association, thus producing linear hydrogen-bonded polymer chains.

Comment

Complexes of the copper(II) acetate monohydrate type prepared by the addition of 2-aminopyrimidine are expected to produce arrays of alternating tetra-μ-carboxylato-*O*:*O*′-dicopper(II) and 2-aminopyrimidine units linked by axial Cu—N bonds (Smith *et al.*, 1996). However, the structure of the title compound, (I), comprises individual units of tetra-μ-carboxylato-*O*:*O*′-dicopper(II) end-capped with two 2-aminopyrimidine molecules, which form a hydrogen-bonded polymer chain *via* the pyrimidines. The hydrogen-bonding geometry is listed in Table 1. The eight Cu—O distances are in the range 1.943 (4)–2.012 (4) Å, with an average of 1.969 (4) Å, while the two Cu—N distances are 2.154 (4) and 2.150 (4) Å. The hydrogen-bonding patterns in these types of molecules usually consist of associations from the two amino H atoms to two adjacent carboxylate O atoms. This is the case



(I)

in (I) for the two inwardly facing NH groups but the two outward amino H atoms bind to an adjacent outward pyrimidine N atom, thus forming pyrimidine dimers. With like binding to like (*i.e.* *E*–*E* and *F*–*F*), the structure forms a hydrogen-bonded polymer with individual groups of alternating direction. All structures of the copper(II) acetate type made with 2-aminopyrimidine have the potential to exhibit packing similar to (I), but this is the first reported example.

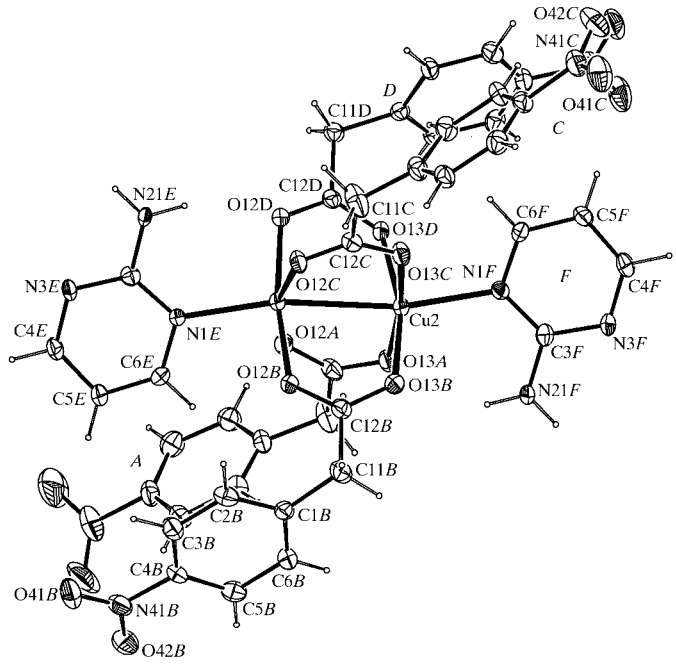


Figure 1
The molecular configuration and atom-numbering scheme for (I) showing 30% probability ellipsoids.

Experimental

Complex (I) was prepared as per the literature procedure of Smith *et al.* (1996).

Crystal data

$[Cu_2(C_8H_6NO_4)_4(C_4H_5N_3)_2]$
M_r = 1037.85
Monoclinic, $P2_1/c$
a = 17.134 (5) Å
b = 18.9575 (8) Å
c = 14.0859 (6) Å
β = 111.159 (3)°
V = 4266.9 (13) Å^3
Z = 4
D_x = 1.616 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8113 reflections
θ = 2.91–27.48°
μ = 1.083 mm^{-1}
T = 150 (2) K
Plate, green
0.50 × 0.10 × 0.02 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.613, T_{max} = 0.979
21389 measured reflections
9074 independent reflections
3921 reflections with $I > 2\sigma(I)$
R_{int} = 0.127
θ_{max} = 27.48°
$h = -21 \rightarrow 21$
$k = -24 \rightarrow 24$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.149
S = 0.918
9074 reflections
613 parameters
H atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N21E—H21E···O12D	0.88	2.41	3.121 (6)	139
N21E—H22E···N3E^{i}	0.88	2.10	2.971 (7)	168
N21F—H21F···O13A	0.88	2.47	3.190 (6)	139
N21F—H22F···N3F^{ii}	0.88	2.08	2.958 (7)	176

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

All H atoms were included in the refinement at calculated positions as riding models with C—H set to either 0.95 (Ar-H) or 0.99 Å (CH_2) and N—H set to 0.88 Å.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1163). Services for accessing these data are described at the back of the journal.

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