

Acta Crystallographica Section C

**Crystal Structure
Communications**

ISSN 0108-2701

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

Daniel E. Lynch and Helen L. Duckhouse

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site provided that this cover page is retained. Republication of this article or its storage in electronic databases or the like is not permitted without prior permission in writing from the IUCr.

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

Daniel E. Lynch* and Helen L. Duckhouse

School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England

Correspondence e-mail: apx106@coventry.ac.uk

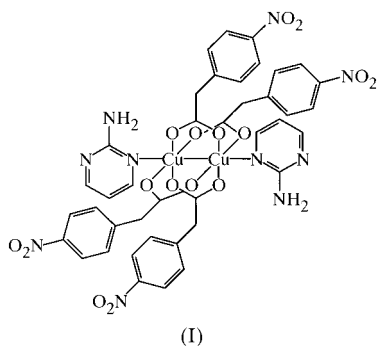
Received 31 August 2000

Accepted 14 November 2000

The structure of the title compound, $[\text{Cu}_2(\text{C}_8\text{H}_6\text{NO}_4)_4(\text{C}_4\text{H}_5\text{N}_3)_2]$, 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



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

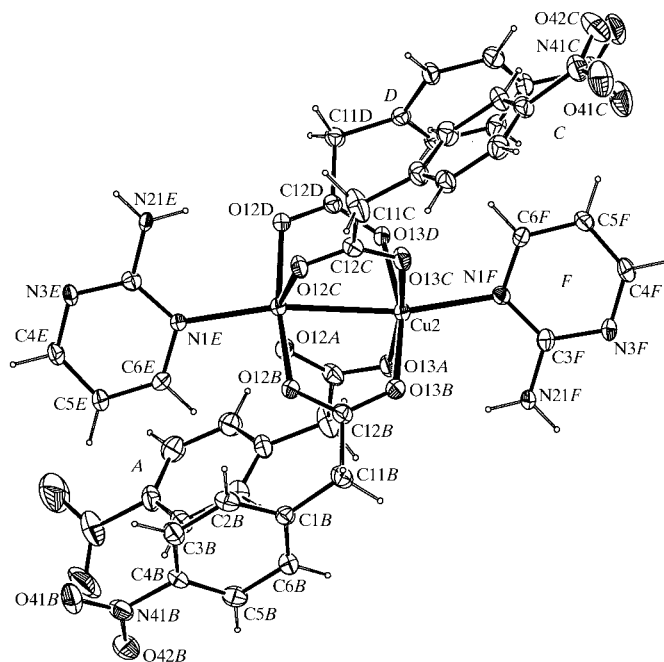


Figure 1
The molecular configuration and atom-numbering scheme for (I) showing 30% probability ellipsoids.

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.

Experimental

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

Crystal data

$[\text{Cu}_2(\text{C}_8\text{H}_6\text{NO}_4)_4(\text{C}_4\text{H}_5\text{N}_3)_2]$
 $M_r = 1037.85$
 Monoclinic, $P2_1/c$
 $a = 17.134$ (5) Å
 $b = 18.9575$ (8) Å
 $c = 14.0859$ (6) Å
 $\beta = 111.159$ (3)°
 $V = 4266.9$ (13) Å³
 $Z = 4$

$D_x = 1.616$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8113 reflections
 $\theta = 2.91$ – 27.48°
 $\mu = 1.083$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.127$
 $\theta_{\max} = 27.48^\circ$
 $h = -21 \rightarrow 21$
 $k = -24 \rightarrow 24$
 $l = -18 \rightarrow 18$

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, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
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 (CH₂) 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: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON97* (Spek, 1997); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support from the School of Natural and Environmental Sciences (Coventry) and thank the EPSRC National Crystallography Service (Southampton).

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.

References

- Blessing, R. H. (1995). *Acta Cryst. A* **51**, 33–37.
 Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
 Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Smith, G., O'Reilly, E. J., Carrell, H. L., Carrell, C. J. & Kennard, C. H. L. (1996). *Polyhedron*, **15**, 1995–2001.
 Spek, A. L. (1997). *PLATON97*. Version of May 1997. University of Utrecht, The Netherlands.