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catena-Poly[[tetrakis[μ-(3-methoxyphenyl)acetato-*O*:*O*′]dicopper(II)]-μ-2-aminopyrimidine-N^1:N^3]

Lynch and Duckhouse

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catena-Poly[[tetrakis[μ-(3-methoxyphenyl)acetato-*O*:*O*′]dicopper(II)]-μ-2-aminopyrimidine-N^1:N^3]

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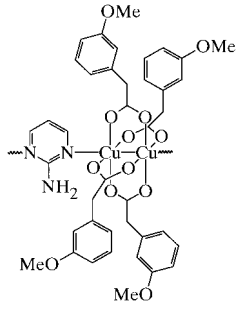
The structure of the title compound, $[Cu_2(C_9H_9O_3)_4(C_4H_5N_3)]$, comprises a zigzag polymer of alternating tetrakis(carboxylato-*O*:*O*′)dicopper(II) and 2-aminopyrimidine units linked by axial Cu—N bonds, and the non-centrosymmetric structure has four unique (3-methoxyphenyl)acetate moieties.

Comment

In the structure of the title compound, (I), one of the methoxy groups (O9) is disordered with two methyl groups (C36 and C37) of equal occupancy. Hydrogen-bonding associations are recorded from the pyrimidine 2-amino group (N3) to the



(I)

carboxylate O3^{i} [N···O 2.868 (7) Å and angle at H 154°; symmetry code: (i) $\frac{3}{2}-x, y-\frac{1}{2}, \frac{1}{2}+z$] and O5 atoms [N···O 2.964 (7) Å and angle at H 157°].

Experimental

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

Crystal data

$[Cu_2(C_9H_9O_3)_4(C_4H_5N_3)]$
M_r = 882.84
Orthorhombic, $Pna2_1$
a = 27.981 (6) Å
b = 15.523 (3) Å
c = 8.9366 (18) Å
V = 3881.7 (13) Å^3
Z = 4
D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8113 reflections
θ = 2.91–27.48°
μ = 1.164 mm^{-1}
T = 150 (2) K
Plate, green
0.10 × 0.10 × 0.01 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.879, T_{max} = 0.989
36 035 measured reflections
7250 independent reflections
4441 reflections with $I > 4\sigma(I)$
R_{int} = 0.106
θ_{max} = 27.50°
$h = -32 \rightarrow 32$
$k = -20 \rightarrow 20$
$l = -7 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.096
S = 0.891
7250 reflections
528 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0460P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.008
$\Delta\rho_{max}$ = 0.335 e Å^{-3}
$\Delta\rho_{min}$ = −0.380 e Å^{-3}
Absolute structure: Flack (1983), 3447 Friedel pairs
Flack parameter = −0.002 (12)

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*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97.

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