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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.030
 wR factor = 0.090
Data-to-parameter ratio = 16.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.A dinuclear copper complex with a *p*-amino-
benzoate anion

In the title compound, bis(μ -*p*-aminobenzoato- $\kappa^2O:O$)bis-[(*N,N*-dimethylformamide- κO)copper(II)], $[\text{Cu}_2(L)_4(\text{DMF})_2] \cdot 2\text{DMF}$ (*HL* is *p*-aminobenzoic acid, $\text{C}_7\text{H}_6\text{NO}_2$, and DMF is *N,N*-dimethylformamide, $\text{C}_3\text{H}_7\text{NO}$), two Cu^{II} cations are bridged by four L^- anions to form a dinuclear complex that lies on a center of inversion. The Cu^{II} cation is coordinated by four carboxylate O atoms from four L^- anions and one O atom from a DMF molecule. A free DMF molecule is present in the asymmetric unit. The L^- anions and the uncoordinated DMF molecules are linked through hydrogen bonds to form a one-dimensional structure along the *c* axis.

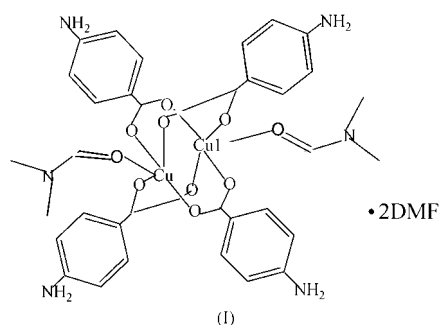
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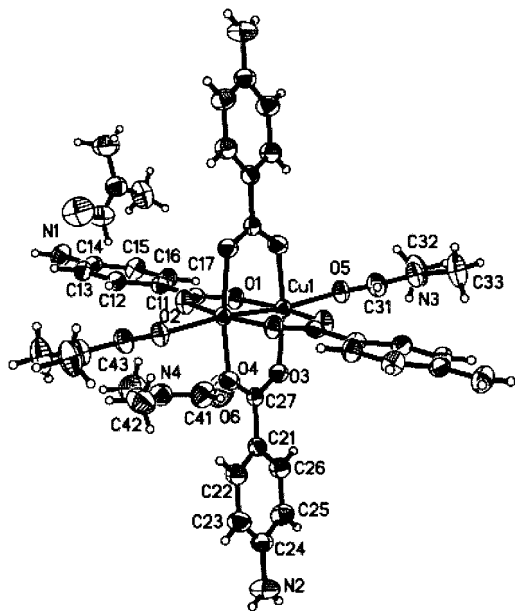
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Comment

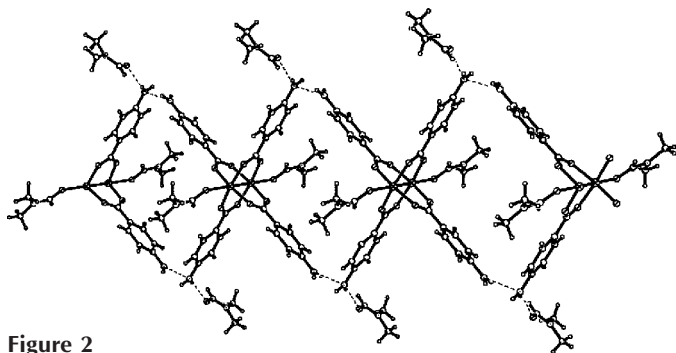
In recent years, divalent transition metal complexes with molecules having biochemical properties, such as amino acids, have been studied in considerable detail for their use as models in biological systems (Wang *et al.*, 2002). Related to these aminoacetates are the aminobenzoates, and a number of studies on transition metal complexes with the *o*-aminobenzoate and *p*-aminobenzoate anions have been carried out (Hu *et al.*, 2003). In order to extend the study on *p*-aminobenzoate complexes, we present here a new dinuclear copper complex with the *p*-aminobenzoate anion, $[\text{Cu}_2(L)_4(\text{DMF})_2] \cdot 2\text{DMF}$, (I) (*HL* is *p*-aminobenzoic acid and DMF is *N,N*-dimethylformamide), which is a centrosymmetric dinuclear compound (Fig. 1).



The Cu^{II} cation is coordinated by four carboxylate O atoms from four L^- anions and one O atom from a DMF molecule in a square pyramidal geometry; the Cu^{II} cations are bridged by the four L^- anions. The distance between the two Cu^{II} cations is 2.6270 (7) Å, which is similar to that in a related Cu^{II} complex (Gao *et al.*, 2003). The average $\text{Cu}-O_{\text{carboxylate}}$ distance is also similar to that in other Cu^{II} complexes (Ma *et al.*, 2003), as is the $\text{Cu}-O_{\text{DMF}}$ distance (Eddaoudi *et al.*, 2001). In (I), the amine groups of the L^- anions are pyramidal and are not involved in coordination; however, in a related


Figure 1

View of the structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation in Table 1.


Figure 2

The one-dimensional structure of (I), running along the *c* axis. Dashed lines indicate hydrogen bonds.

compound the amine groups coordinate to the copper(II) cation (Hu *et al.*, 2003).

The molecules of (I) are held together through hydrogen bonds to form a one-dimensional structure (Fig. 2); two H atoms are available for hydrogen bonding from each anion and the O atoms of the uncoordinated DMF molecules serve as acceptors.

Experimental

Crystals of (I) were prepared by diffusing an ethanol solution containing $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (0.0342 g, 2 mmol) into a DMF solution of *p*-aminobenzoic acid (0.548 g, 4 mmol) in a vertical glass tube at room temperature. After about three weeks, blue crystals were obtained (79% yield based on Cu). Calculated for $\text{C}_{40}\text{H}_{52}\text{Cu}_2\text{N}_8\text{O}_{12}$: C 49.79, H 5.39, N 11.62%; found: C 49.47, H 5.51, N 11.52%. IR (cm^{-1} , KBr): 3407 (*m*), 3055 (*w*), 2361 (*w*), 1622 (*w*), 1559 (*vs*), 1514 (*m*), 1493 (*w*), 1450 (*m*), 1387 (*s*), 1340 (*w*), 1269 (*w*), 1223 (*w*), 1144 (*w*), 1100 (*w*), 992 (*w*), 849 (*s*).

Crystal data

$[\text{Cu}_2(\text{C}_7\text{H}_6\text{NO}_2)_4(\text{C}_3\text{H}_7\text{NO})_2] \cdot 2\text{C}_3\text{H}_7\text{NO}$
 $M_r = 963.98$
 Monoclinic, $P2_1/c$
 $a = 12.513$ (3) Å
 $b = 15.918$ (3) Å
 $c = 12.122$ (2) Å
 $\beta = 115.32$ (3)°
 $V = 2182.5$ (9) Å³
 $Z = 2$

$D_x = 1.467$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 17 677 reflections
 $\theta = 1.8$ – 27.5 °
 $\mu = 1.05$ mm⁻¹
 $T = 296$ (2) K
 Block, blue
 $0.50 \times 0.33 \times 0.21$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scan
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.587$, $T_{\max} = 0.803$
 20 168 measured reflections

4992 independent reflections
 3586 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$
 $\theta_{\text{max}} = 27.5$ °
 $h = -16 \rightarrow 14$
 $k = -20 \rightarrow 0$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.090$
 $S = 0.96$
 4992 reflections
 300 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0462P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.67$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9627 (15)	Cu1—O4 ⁱ	1.9639 (16)
Cu1—O2 ⁱ	1.9792 (15)	Cu1—O5	2.2074 (15)
Cu1—O3	1.9724 (16)		
O1—Cu1—O2 ⁱ	168.43 (6)	O2 ⁱ —Cu1—O4 ⁱ	91.28 (7)
O1—Cu1—O3	89.52 (7)	O2 ⁱ —Cu1—O5	91.08 (6)
O1—Cu1—O4 ⁱ	88.81 (7)	O3—Cu1—O4 ⁱ	168.51 (6)
O1—Cu1—O5	100.49 (6)	O3—Cu1—O5	101.10 (6)
O2 ⁱ —Cu1—O3	88.10 (7)	O4 ⁱ —Cu1—O5	90.37 (6)

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Table 2

Hydrogen-bond 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>
N1—H1A...O6 ⁱⁱ	0.864 (10)	2.122 (11)	2.982 (3)	174 (3)
N2—H2A...N1 ⁱⁱⁱ	0.858 (10)	2.43 (2)	3.165 (4)	143 (3)

Symmetry codes: (ii) $-x + 2, y - \frac{1}{2}, -z + \frac{3}{2}$; (iii) $-x + 2, -y + 1, -z + 2$.

The H atoms of amine groups were located from difference Fourier maps and refined isotropically, with N—H distances restrained to 0.85 (2) Å. The methyl H atoms were refined as members of rigid groups with C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{parent atom})$, allowing for rotation about the C—N bonds. Other H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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