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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=298 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.006 \AA$
Disorder in solvent or counterion
$R$ factor $=0.037$
$w R$ factor $=0.095$
Data-to-parameter ratio $=12.5$

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

[^0]
## Tetrakis( $\mu$-naphthalene-1-acetato- $\kappa^{2} O: O^{\prime}$ )-bis[(N,N-dimethylformamide- $\kappa$ O)copper(II)] $\mathrm{N}, \mathrm{N}$-dimethylformamide disolvate

The centrosymmetric title compound, $\left[\mathrm{Cu}_{2}\left(\mathrm{C}_{12} \mathrm{H}_{9} \mathrm{O}_{2}\right)_{4}\right.$ $\left.\left(\mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}\right)_{2}\right] \cdot 2 \mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}$, consists of a dinuclear copper paddle-wheel cage structure bridged by four bidentate naphthaleneacetate carboxylate groups. The $N, N$-dimethylformamide molecules at the axial positions complete the octahedral coordination.

## Comment

Naphthalene-1-acetic acid is a plant-growth regulator and our attention is focused on its coordination with the $\mathrm{Cu}^{\text {II }}$ ion. A green crystal of the cupric naphthalene-1-acetate salt, (I), was obtained from an $N, N$-dimethylformamide (DMF) solution. The crystal structure of (I) consists of a centrosymmetric dinuclear cage unit, in which each $\mathrm{Cu}^{\mathrm{II}}$ atom is coordinated by four O atoms $\left[\mathrm{O} 1^{\mathrm{i}}, \mathrm{O} 2, \mathrm{O} 3^{\mathrm{i}}\right.$ and O 4 ; symmetry code: (i) $1-x$, $1-y, 1-z]$ from four different carboxylate groups in equatorial positions and atom O5 from DMF at the axial position (Fig. 1). The dihedral angles of the naphthyl ring planes formed by atoms C3-C12 and atoms C15-C24 with the equatorial plane formed by the four O atoms $\left(\mathrm{O} 1^{\mathrm{i}}, \mathrm{O} 2, \mathrm{O} 3^{\mathrm{i}}\right.$ and O4) are 63.43 (6) and $60.39(6)^{\circ}$, respectively. Selected bond parameters are listed in Table 1.


A dimethyl sulfoxide (DMSO) analogue of (I), viz. (II), has been reported previously (Chen et al., 2004). The coordination environment of the $\mathrm{Cu}^{\mathrm{II}}$ atoms in (II) is similar to that in (I), except that the axial O atoms are from the coordinated DMSO.

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## Experimental

A mixture of naphthalene-1-acetic acid ( 2 mmol ) and $\mathrm{CuCO}_{3}$ ( 1 mmol ) was stirred in water ( 20 ml ); the colour of the resulting precipitate changed from blue to green after about 30 min . The precipitate was washed with water and then dissolved in DMF. Green blocks of (I) suitable for X-ray analysis were obtained by evaporation of this DMF solution at ambient temperature for two months.

## Crystal data

$\left[\mathrm{Cu}_{2}\left(\mathrm{C}_{12} \mathrm{H}_{9} \mathrm{O}_{2}\right)_{4}\left(\mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}\right)_{2}\right]$--
$2 \mathrm{C}_{3} \mathrm{H}_{7} \mathrm{NO}$
$M_{r}=1160.23$
Triclinic, $P \overline{1}$
$a=10.056$ (2) A
$b=11.936$ (2) A
$c=13.636$ (2) $\AA$
$\alpha=73.506(2)^{\circ}$
$\beta=84.991(2)^{\circ}$

$$
\begin{aligned}
& \gamma=65.205(2)^{\circ} \\
& V=1423.7(4) \AA^{3} \\
& Z=1 \\
& D_{x}=1.353 \mathrm{Mg} \mathrm{~m}^{-3} \\
& \text { Mo } K \alpha \text { radiation } \\
& \mu=0.81 \mathrm{~mm}^{-1} \\
& T=298(2) \mathrm{K} \\
& \text { Block, green } \\
& 0.46 \times 0.33 \times 0.21 \mathrm{~mm}
\end{aligned}
$$

## Data collection

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{\text {min }}=0.707, T_{\text {max }}=0.848$

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.037$
$w R\left(F^{2}\right)=0.095$
$S=1.04$
4948 reflections
395 parameters
H -atom parameters constrained

$$
\begin{aligned}
& w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}^{2}\right)+(0.0403 P)^{2}\right. \\
& \quad+0.6167 P] \\
& \text { where } P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3 \\
& (\Delta / \sigma)_{\max }=0.001 \\
& \Delta \rho_{\max }=0.35 \mathrm{e} \AA^{-3} \\
& \Delta \rho_{\min }=-0.27 \mathrm{e}^{-3}
\end{aligned}
$$

Table 1
Selected geometric parameters ( $\AA$, ${ }^{\circ}$ ).

| $\mathrm{Cu} 1-\mathrm{O} 3$ | $1.964(2)$ | $\mathrm{Cu} 1-\mathrm{O} 5$ | $2.1493(18)$ |
| :--- | ---: | :--- | :--- |
| $\mathrm{Cu} 1-\mathrm{O} 4^{\mathrm{i}}$ | $1.965(2)$ | $\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $2.6273(7)$ |
| $\mathrm{Cu} 1-\mathrm{O} 2^{\mathrm{i}}$ | $1.9664(18)$ | $\mathrm{O} 2-\mathrm{Cu} 1^{\mathrm{i}}$ | $1.9664(18)$ |
| $\mathrm{Cu} 1-\mathrm{O} 1$ | $1.9673(18)$ | $\mathrm{O} 4-\mathrm{Cu} 1^{\mathrm{i}}$ | $1.966(2)$ |
|  |  |  |  |
| $\mathrm{O} 3-\mathrm{Cu} 1-\mathrm{O} 4^{\mathrm{i}}$ | $168.46(8)$ | $\mathrm{O} 3-\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $84.86(6)$ |
| $\mathrm{O} 3-\mathrm{Cu} 1-\mathrm{O} 2^{\mathrm{i}}$ | $89.95(9)$ | $\mathrm{O} 4^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $83.62(6)$ |
| $\mathrm{O} 4^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{O} 2^{\mathrm{i}}$ | $89.09(9)$ | $\mathrm{O}^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $81.65(6)$ |
| $\mathrm{O} 3-\mathrm{Cu} 1-\mathrm{O} 1$ | $89.61(9)$ | $\mathrm{O} 1-\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $86.69(5)$ |
| $\mathrm{O} 4^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{O} 1$ | $89.02(8)$ | $\mathrm{O} 5-\mathrm{Cu} 1-\mathrm{Cu} 1^{\mathrm{i}}$ | $172.80(6)$ |
| $\mathrm{O} 2^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{O} 1$ | $168.33(7)$ | $\mathrm{C} 1-\mathrm{O} 1-\mathrm{Cu} 1$ | $119.84(17)$ |
| $\mathrm{O} 3-\mathrm{Cu} 1-\mathrm{O} 5$ | $94.69(8)$ | $\mathrm{C} 1-\mathrm{O} 2-\mathrm{Cu} 1^{\mathrm{i}}$ | $126.02(17)$ |
| $\mathrm{O} 4^{\mathrm{i}}-\mathrm{Cu} 1-\mathrm{O} 5$ | $96.83(8)$ | $\mathrm{C} 13-\mathrm{O} 3-\mathrm{Cu} 1$ | $122.01(19)$ |
| $\mathrm{O} 2^{i}-\mathrm{Cu} 1-\mathrm{O} 5$ | $91.17(8)$ | $\mathrm{C} 13-\mathrm{O} 4-\mathrm{Cu} 1^{\mathrm{i}}$ | $123.40(19)$ |
| $\mathrm{O} 1-\mathrm{Cu} 1-\mathrm{O} 5$ | $100.49(7)$ | $\mathrm{C} 25-\mathrm{O} 5-\mathrm{Cu} 1$ | $120.90(18)$ |

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

Table 2
Hydrogen-bond geometry ( $\AA$, ${ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :---: | :---: | :--- | :--- |
| $\mathrm{C} 26-\mathrm{H} 26 B \cdots \mathrm{O} 1^{\mathrm{ii}}$ | 0.96 | 2.49 | $3.430(4)$ | 165 |
| Symmetry code: (ii) $-x+2,-y+1,-z+1$. |  |  |  |  |

Symmetry code: (ii) $-x+2,-y+1,-z+1$.


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the $30 \%$ probability level. Both disordered DMF components are shown. [Symmetry code: (A) $1-x, 1-y, 1-z$.]


Figure 2
A packing diagram of the title compound, showing the weak intermolecular $\mathrm{C}-\mathrm{H} \cdots \mathrm{O}$ interactions as dashed lines. The DMF solvent molecules have been omitted for clarity. [Symmetry codes: (i) $x, y, z$; (ii) $2-x, 1-y, 1-z]$.


Figure 3
A packing diagram of (I). The DMF solvent molecules have been omitted for clarity.

## metal-organic papers

All H atoms were located in difference Fourier maps. H atoms bonded to C atoms were treated as riding atoms, with $\mathrm{C}-\mathrm{H}=0.93$ (aromatic, formyl), 0.97 (methylene) and $0.96 \AA$ (methyl), and with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ (aromatic, formyl, methylene) or $1.5 U_{\mathrm{eq}}(\mathrm{C})$ (methyl). The methyl groups bonded to N of the solvent DMF were found to be disordered over two sites. The coordinates of these two sites were refined with the occupancies tied to sum to unity. The site occupancies for $\mathrm{C} 28-\mathrm{C} 30$ with attached H atoms and $\mathrm{C} 28^{\prime}-\mathrm{C} 30^{\prime}$ with attached H atoms refined to 0.554 (7) and 0.446 (7), respectively.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL and MERCURY (Macrae et al., 2006).

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