# metal-organic papers

# Aqua(N,N'-ethane-1,2-diylbis{N-[(3-nitro-phenyl)methyl]glycinato})copper(II)

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**Key indicators**

Single-crystal X-ray study
$T = 298$ K
Mean $\sigma$(C–C) = 0.004 Å
Disorder in main residue
$R$ factor = 0.038
$wR$ factor = 0.117
Data-to-parameter ratio = 14.7

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

In the title complex, $[Cu(C_{20}H_{20}N_4O_8)(H_2O)]$, the Cu atom has a distorted trigonal–bipyramidal coordination environment defined by an $N_2O_3$ donor set; the Cu and water O atoms lie on a twofold axis. In the crystal structure, extensive hydrogen bonding links molecules into a two-dimensional network.

## Comment

Previously we have synthesized and characterized the title complex, (I) (Xu *et al.*, 2004). In (I) (Fig. 1), the Cu ion is five-coordinated by two secondary amine N (N2 and N2$^{i}$) and two carboxylate O atoms (O4 and O4$^{i}$) atoms (symmetry code in Table 1), all derived from the tetradentate *N*,*N'*-ethane-1,2-diylbis{*N*-[(3-nitrophenyl)methyl]glycinate ligand, and by an O atom (O5) from a coordinated water molecule. Complex (I) has crystallographic twofold symmetry with atoms Cu and O5 lying on a twofold axis. The coordination geometry is distorted trigonal–bipyramidal and selected bond lengths and angles are given in Table 1.
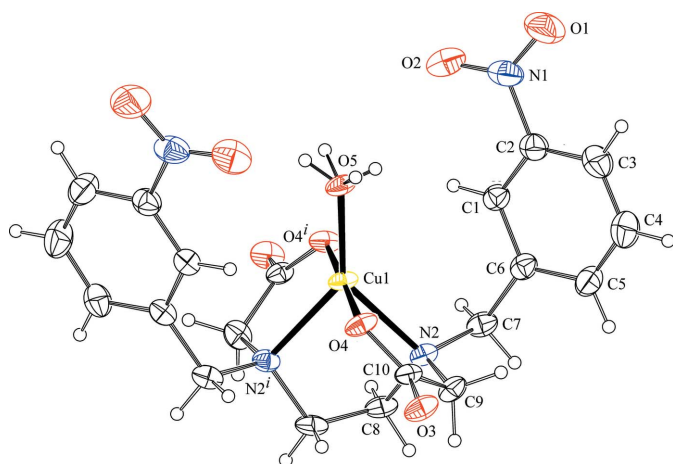


(I)
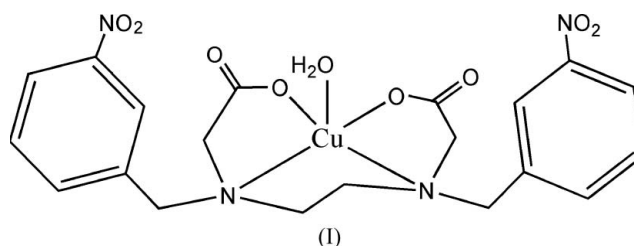
In the crystal structure (Fig. 2), a variety of C—H···O and O—H···O hydrogen bonds (Table 2) consolidate the crystal packing into a two-dimensional array.

## Experimental

Complex (I) was synthesized according to a literature method (Xu *et al.*, 2004). Crystals were obtained by slow evaporation (two weeks) of a methanol solution.

*Crystal data*

$[Cu(C_{20}H_{20}N_4O_8)(H_2O)]$
$M_r = 525.96$
Monoclinic, $C2/c$
$a = 11.5227\ (11)$ Å
$b = 9.1244\ (9)$ Å
$c = 20.782\ (2)$ Å
$\beta = 96.757\ (2)°$
$V = 2169.8\ (4)$ Å$^3$

$Z = 4$
$D_x = 1.610$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 1.07$ mm$^{-1}$
$T = 298\ (2)$ K
Prism, blue
$0.23 \times 0.20 \times 0.20$ mm

**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids. Both positions of the disordered water H atoms are shown. [Symmetry code: (i) $1 - x$, $y$, $\frac{3}{2} - z$.]
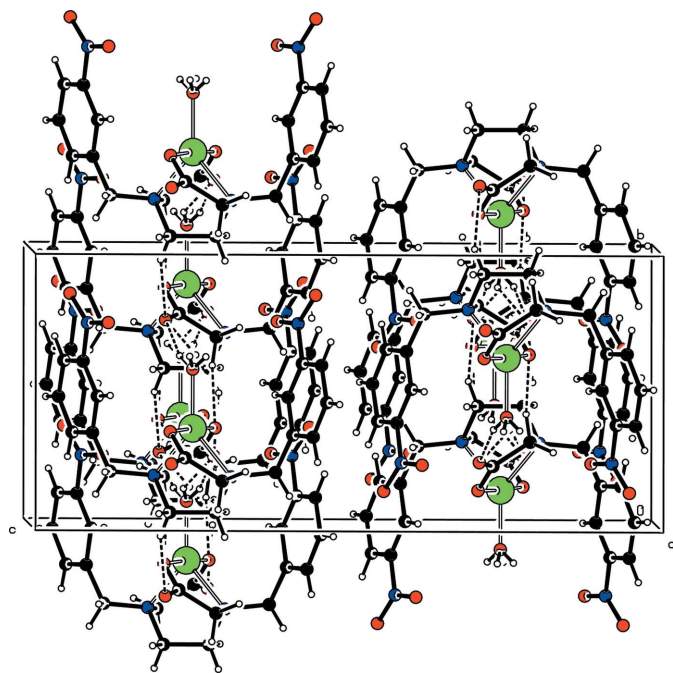


**Figure 2**
Packing diagram for (I), viewed approximately down the $c$ axis. Dashed lines denote hydrogen bonds.

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 7022 measured reflections |
| $\varphi$ and $\omega$ scans | 2360 independent reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001) | 2090 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.769$, $T_{max} = 0.850$ | $R_{int} = 0.027$ |
| | $\theta_{max} = 27.0°$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.483P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.117$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.13$ | $\Delta\rho_{max} = 0.43$ e Å$^{-3}$ |
| 2360 reflections | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| 161 parameters | |
| H atoms treated by a mixture of independent and constrained refinement | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—O4 | 1.9253 (16) | Cu1—N2 | 2.1601 (18) |
| Cu1—O5 | 1.956 (2) | | |
| O4$^i$—Cu1—O4 | 176.97 (9) | O5—Cu1—N2$^i$ | 136.95 (5) |
| O4$^i$—Cu1—O5 | 91.51 (4) | O4$^i$—Cu1—N2 | 94.14 (7) |
| O4—Cu1—O5 | 91.52 (4) | O4—Cu1—N2 | 83.64 (7) |
| O4$^i$—Cu1—N2$^i$ | 83.64 (7) | O5—Cu1—N2 | 136.95 (5) |
| O4—Cu1—N2$^i$ | 94.14 (7) | N2$^i$—Cu1—N2 | 86.09 (10) |

Symmetry code: (i) $-x + 1$, $y$, $-z + \frac{3}{2}$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C8—H8$A\cdots$O3$^{ii}$ | 0.97 | 2.54 | 3.457 (3) | 157 |
| C9—H9$B\cdots$O4$^{ii}$ | 0.97 | 2.54 | 3.443 (3) | 155 |
| O5—H5$C\cdots$O3$^{iii}$ | 0.818 (10) | 1.91 (3) | 2.696 (2) | 161 (7) |
| O5—H5$C\cdots$O3$^{iii}$ | 0.818 (10) | 1.91 (3) | 2.696 (2) | 161 (7) |

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

Water H atoms were modeled as disordered over two sites with fixed occupancies of 0.5 and refined so that O—H = 0.818 (10) Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The remaining H atoms were included in the riding-model approximation, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

### References

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