

Lei Cao, Ning Li and  
Duan-Jun Xu\*Department of Chemistry, Zhejiang University,  
People's Republic of China

Correspondence e-mail: xudj@mail.hz.zj.cn

## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.021  
 $wR$  factor = 0.052  
Data-to-parameter ratio = 15.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Poly[[ $(1H$ -benzimidazole- $\kappa N^3$ )copper(II)]- $\mu_3$ -oxydiacetato]

In the title compound,  $[\text{Cu}(\text{C}_4\text{H}_4\text{O}_5)(\text{C}_7\text{H}_6\text{N}_2)]_n$ , three oxydiacetate (ODA) dianions and one benzimidazole molecule coordinate to the  $\text{Cu}^{\text{II}}$  atom, resulting in an elongated octahedral coordination geometry. Each ODA links three Cu atoms, chelating one and bridging two, forming a three-dimensional polymeric complex.

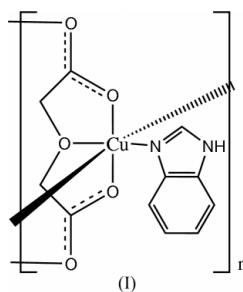
Received 24 June 2004

Accepted 30 June 2004

Online 9 July 2004

## Comment

The versatile coordination modes of dicarboxylate ligands have been revealed in many metal complexes. In the title polymeric compound, (I), the oxydiacetate dianion (ODA) shows a different coordination mode from those found in other transition metal complexes reported previously.



The asymmetric unit of (I) contains a  $\text{Cu}^{\text{II}}$  atom, an  $\text{ODA}^{2-}$  dianion and a benzimidazole molecule. The coordination environment around the Cu atom is illustrated in Fig. 1. The Cu atom assumes an elongated octahedral coordination geometry formed by one benzimidazole and three ODA. One ODA chelates to the Cu atom in the meridional mode and the other two coordinate, in a monodentate fashion, to the Cu atom *via* carboxyl groups in the axial direction. The average Cu–O bond distance in the axial direction is about 0.52 Å longer than that in the equatorial plane (Table 1).

Both five-membered chelate rings of  $\text{ODA}^{2-}$  have the envelope conformation; ether atom O3 is in the flap position and is displaced from the mean planes formed by the other atoms by 0.340 (3) and 0.283 (3) Å, for the O1- and O5-containing rings, respectively.

The carboxy groups of  $\text{ODA}^{2-}$  play the role of bridging ligands in (I). Thus, (I) forms a three-dimensional polymeric structure in the crystal. This is different from the situation found in ODA-bridged complexes of  $\text{Co}^{\text{II}}$  (Wu *et al.*, 2002) and of  $\text{Zn}^{\text{II}}$  (Baggio *et al.*, 2003). In those crystal structures, one carboxy group of ODA bridged neighboring metal atoms but another was uncoordinated.

The benzimidazole molecule in (I) coordinates to the Cu atom in the equatorial plane; the mean plane of the benz-

imidazole is inclined to the equatorial plane of the  $\text{CuO}_5\text{N}$  moiety by a dihedral angle of  $18.89(7)^\circ$ . As well as an  $\text{N}\cdots\text{H}\cdots\text{O}$  hydrogen bond (Table 2),  $\text{C}\text{---}\text{H}\cdots\pi$  interactions occur between the methylene group and a nearby imidazole ring, the  $\text{H12}\cdots\text{Cg}^{\text{iv}}$  distance and  $\text{C12}\text{---}\text{H12}\cdots\text{Cg}^{\text{iv}}$  angle being  $2.85\text{ \AA}$  and  $148^\circ$ , respectively [symmetry code: (iv)  $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ].

## Experimental

An aqueous solution (10 ml) containing ODA (1 mmol) and  $\text{Na}_2\text{CO}_3$  (1 mmol) was mixed with an aqueous solution (5 ml) of  $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$  (1 mmol). The solution was heated for several minutes, then an ethanol solution (5 ml) of benzimidazole (2 mmol) was added. The mixture was refluxed for a further 3 h and then filtered. Blue single crystals were obtained after 2 d.

### Crystal data

$[\text{Cu}(\text{C}_4\text{H}_4\text{O}_5)(\text{C}_7\text{H}_6\text{N}_2)]$   
 $M_r = 313.75$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 7.2693(3)\text{ \AA}$   
 $b = 9.5506(3)\text{ \AA}$   
 $c = 16.6714(4)\text{ \AA}$   
 $V = 1157.43(7)\text{ \AA}^3$   
 $Z = 4$   
 $D_x = 1.801\text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 10 407 reflections  
 $\theta = 2.8\text{--}25.0^\circ$   
 $\mu = 1.91\text{ mm}^{-1}$   
 $T = 295(2)\text{ K}$   
 Prism, green  
 $0.33 \times 0.22 \times 0.18\text{ mm}$

### Data collection

Rigaku R-Axis RAPID diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.53$ ,  $T_{\text{max}} = 0.71$   
 11 325 measured reflections

2655 independent reflections  
 2576 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -12 \rightarrow 12$   
 $l = -21 \rightarrow 21$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.021$   
 $wR(F^2) = 0.052$   
 $S = 1.07$   
 2655 reflections  
 172 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 0.3325P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.28\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.26\text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983), 1101 Friedel pairs  
 Flack parameter = 0.020 (10)

**Table 1**

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

|                                      |             |                     |             |
|--------------------------------------|-------------|---------------------|-------------|
| Cu—O1                                | 1.9504 (13) | Cu—O4 <sup>ii</sup> | 2.4410 (14) |
| Cu—O2 <sup>i</sup>                   | 2.5263 (15) | Cu—O5               | 1.9549 (14) |
| Cu—O3                                | 1.9814 (12) | Cu—N3               | 1.9478 (15) |
| O1—Cu—O3                             | 81.76 (5)   | N3—Cu—O1            | 101.52 (6)  |
| O1—Cu—O5                             | 163.58 (6)  | N3—Cu—O3            | 176.58 (6)  |
| O2 <sup>i</sup> —Cu—O4 <sup>ii</sup> | 175.46 (5)  | N3—Cu—O5            | 94.47 (6)   |
| O3—Cu—O5                             | 82.20 (5)   |                     |             |

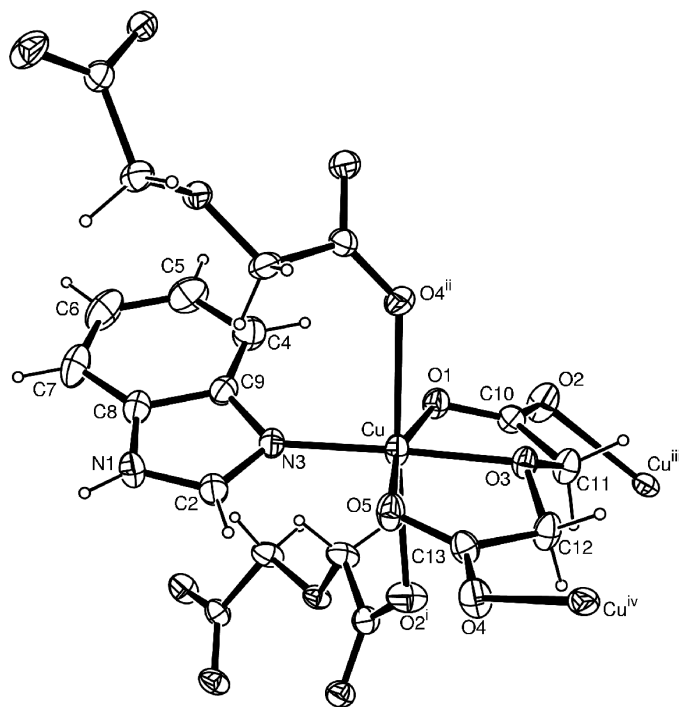
Symmetry codes: (i)  $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$ ; (ii)  $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$ .

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

| $D\text{---}H\cdots A$                          | $D\text{---}H$ | $H\cdots A$ | $D\cdots A$ | $D\text{---}H\cdots A$ |
|---|----------------|-------------|-------------|------------------------|
| $\text{N1}\text{---}\text{H1}\cdots\text{O4}^v$ | 0.86           | 1.89        | 2.746 (3)   | 177                    |

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



**Figure 1**

Fragment of (I), showing the Cu-atom environment [40% displacement ellipsoids; symmetry codes: (i)  $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$ ; (ii)  $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (iii)  $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$ ; (iv)  $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$ ].

H atoms were placed in calculated positions, with  $\text{C}\text{---}\text{H} = 0.93$  (aromatic) or  $0.97\text{ \AA}$  (methylene) and  $\text{N}\text{---}\text{H} = 0.86\text{ \AA}$ , and were included in the final cycles of refinement in the riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Natural Science Foundation of Zhejiang Province (No. 202033), China.

## References

- Altomare, A., Casciaro, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.  
 Baggio, R., Garland, M. T. & Perec, M. (2003). *Acta Cryst.* **C59**, m30–m32.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku/MSK (2002). *CrystalStructure*. Version 3.00. Rigaku/MSK, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.  
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.  
 Wu, Z.-Y., Xu, D.-J., Wu, J.-Y. & China, M. Y. (2002). *Acta Cryst.* **E58**, m634–m635.