

## Tetra- $\mu$ -acetato- $\kappa^8$ O:O'-bis[(2-phenoxy-pyrimidine- $\kappa$ N<sup>1</sup>)copper(II)](Cu—Cu)

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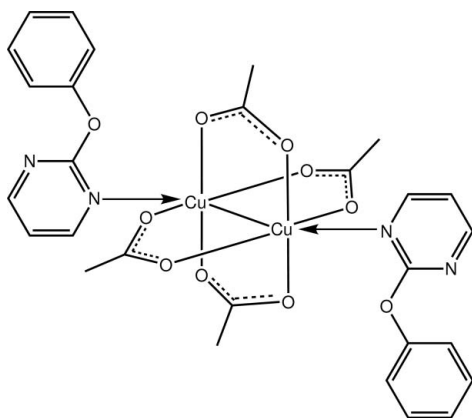
Received 24 October 2011; accepted 25 October 2011

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C—C}) = 0.008$  Å;  $R$  factor = 0.056;  $wR$  factor = 0.175; data-to-parameter ratio = 12.8.

The complete dinuclear molecule of the title complex,  $[\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{C}_{10}\text{H}_8\text{N}_2\text{O})_2]$ , is generated by a centre of inversion. The  $\text{Cu}^{\text{II}}$  atom is in a distorted octahedral coordination geometry defined by four O atoms derived from four bridging acetate ligands, a terminally connected pyrimidine N atom and a Cu atom.

### Related literature

For structures of related examples of tetrakisacetatobis[( $N$ -donor)copper] complexes, see: Fairuz *et al.* (2010*a,b*).



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### Experimental

#### Crystal data

$[\text{Cu}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{10}\text{H}_8\text{N}_2\text{O})_2]$   
 $M_r = 707.64$   
 Monoclinic,  $P2_1/n$   
 $a = 11.0738$  (9) Å  
 $b = 7.5002$  (6) Å  
 $c = 18.0539$  (14) Å  
 $\beta = 100.579$  (1)°

$V = 1474.0$  (2) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.51$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.25 \times 0.24 \times 0.04$  mm

#### Data collection

Bruker SMART APEX diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.637$ ,  $T_{\text{max}} = 0.746$

11124 measured reflections  
 2581 independent reflections  
 2249 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.175$   
 $S = 1.08$   
 2581 reflections

201 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.83$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.55$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Cu1—O3	1.954 (4)	Cu1—O2 <sup>i</sup>	1.979 (4)
Cu1—O1	1.966 (4)	Cu1—N1	2.207 (4)
Cu1—O4 <sup>i</sup>	1.977 (3)	Cu1—Cu1 <sup>i</sup>	2.6154 (10)

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

We thank the University of Malaya (grant No. RG027/09AFR) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5123).

### References

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**supplementary materials**

*Acta Cryst.* (2011). E67, m1637 [ doi:10.1107/S1600536811044345 ]

## Tetra- $\mu$ -acetato- $\kappa^8 O:O'$ -bis[(2-phenoxy pyrimidine- $\kappa N^1$ )copper(II)](*Cu-Cu*)

Z. A. Fairuz, Z. Abdullah, S. B. Nasir, S. W. Ng and E. R. T. Tiekink

### Comment

It was in connection with recent structural studies of tetrakisacetatobis[(*N*-donor)copper(II)] complexes (Fairuz *et al.*, 2010*a*; Fairuz *et al.*, 2010*b*), that the crystal structure of the title complex, (I), was investigated. The complex, Fig. 1, is centrosymmetric and features four symmetrically bridging acetate ligands and two terminally connected N atoms from the 2-phenoxy pyrimidine ligands, Table 1. The Cu—Cu distance is 2.6154 (10) Å. The resulting CuNO<sub>4</sub> donor set defines a distorted octahedral geometry. The 2-phenoxy pyrimidine ligand is twisted with the dihedral angle between the pyrimidyl and benzene rings being 63.3 (3)°.

### Experimental

2-Phenoxy pyrimidine (1.1 mmol) was dissolved in acetonitrile (15 ml), added to trimethyl orthoformate (10 ml) and the mixture then heated to 50°C. Copper acetate (0.5 mmol) dissolved in acetonitrile (15 ml) was added to the solution. The green precipitate that formed was collected and recrystallized from acetonitrile to give green crystals.

### Refinement

Hydrogen atoms were placed at calculated positions (C—H 0.95–0.98 Å) and were treated as riding on their parent carbon atoms, with  $U(H)$  set to 1.2–1.5 times  $U_{eq}(C)$ . The maximum and minimum residual electron density peaks of 1.83 and 0.55 e Å<sup>-3</sup>, respectively, were located 1.42 Å and 0.44 Å from the H6 and Cu atoms, respectively.

### Figures

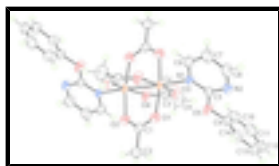


Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The complex is centrosymmetric. The unlabelled atoms are related by the symmetry operation  $1 - x, 1 - y, 1 - z$ .

## Tetra- $\mu$ -acetato- $\kappa^8 O:O'$ -bis[(2- phenoxy pyrimidine- $\kappa N^1$ )copper(II)](*Cu—Cu*)

### Crystal data

[Cu<sub>2</sub>(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>4</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O)<sub>2</sub>]

$M_r = 707.64$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 11.0738$  (9) Å

$F(000) = 724$

$D_x = 1.594$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3884 reflections

$\theta = 2.3$ – $27.1^\circ$

# supplementary materials

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$b = 7.5002 (6) \text{ \AA}$	$\mu = 1.51 \text{ mm}^{-1}$
$c = 18.0539 (14) \text{ \AA}$	$T = 100 \text{ K}$
$\beta = 100.579 (1)^\circ$	Plate, green
$V = 1474.0 (2) \text{ \AA}^3$	$0.25 \times 0.24 \times 0.04 \text{ mm}$
$Z = 2$	

## Data collection

Bruker SMART APEX diffractometer	2581 independent reflections
Radiation source: fine-focus sealed tube graphite	2249 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.037$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 2.0^\circ$
$T_{\text{min}} = 0.637$ , $T_{\text{max}} = 0.746$	$h = -13 \rightarrow 13$
11124 measured reflections	$k = -8 \rightarrow 8$
	$l = -21 \rightarrow 21$

## Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.175$	H-atom parameters constrained
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.1094P)^2 + 3.359P]$
2581 reflections	where $P = (F_o^2 + 2F_c^2)/3$
201 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 1.83 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.55 \text{ e \AA}^{-3}$

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.41133 (5)	0.58752 (7)	0.52267 (3)	0.0279 (3)
O1	0.3059 (3)	0.4099 (4)	0.4621 (2)	0.0415 (9)
O2	0.4556 (3)	0.2595 (5)	0.4231 (2)	0.0463 (9)
O3	0.4384 (4)	0.4244 (5)	0.6085 (2)	0.0479 (10)
O4	0.5873 (3)	0.2712 (5)	0.5697 (2)	0.0421 (9)
O5	0.1716 (4)	0.5271 (5)	0.5969 (3)	0.0520 (11)

N1	0.2668 (3)	0.7572 (5)	0.5552 (2)	0.0304 (8)
N2	0.0888 (4)	0.8062 (6)	0.6078 (3)	0.0436 (11)
C1	0.5176 (4)	0.3045 (6)	0.6154 (3)	0.0326 (10)
C2	0.5298 (7)	0.1861 (9)	0.6841 (3)	0.0597 (17)
H2A	0.6101	0.2059	0.7163	0.090*
H2B	0.5228	0.0609	0.6683	0.090*
H2C	0.4646	0.2146	0.7122	0.090*
C3	0.3455 (5)	0.2911 (6)	0.4241 (3)	0.0331 (10)
C4	0.2508 (5)	0.1755 (8)	0.3750 (3)	0.0484 (14)
H4A	0.2681	0.0497	0.3872	0.073*
H4B	0.2545	0.1964	0.3218	0.073*
H4C	0.1687	0.2056	0.3841	0.073*
C5	0.1732 (4)	0.7050 (6)	0.5869 (3)	0.0316 (10)
C6	0.2763 (5)	0.9324 (7)	0.5446 (3)	0.0413 (13)
H6	0.3425	0.9762	0.5231	0.050*
C7	0.1930 (6)	1.0506 (8)	0.5640 (4)	0.0546 (16)
H7	0.1998	1.1753	0.5565	0.065*
C8	0.0997 (6)	0.9796 (8)	0.5947 (4)	0.0565 (16)
H8	0.0394	1.0582	0.6075	0.068*
C9	0.0924 (5)	0.4472 (6)	0.6393 (3)	0.0374 (12)
C10	0.1489 (5)	0.3652 (9)	0.7058 (3)	0.0515 (14)
H10	0.2348	0.3764	0.7234	0.062*
C11	0.0762 (6)	0.2666 (9)	0.7457 (3)	0.0567 (16)
H11	0.1127	0.2093	0.7913	0.068*
C12	-0.0480 (6)	0.2509 (8)	0.7200 (3)	0.0487 (14)
H12	-0.0970	0.1818	0.7473	0.058*
C13	-0.1003 (5)	0.3352 (8)	0.6553 (3)	0.0461 (13)
H13	-0.1864	0.3255	0.6383	0.055*
C14	-0.0313 (5)	0.4344 (7)	0.6136 (3)	0.0405 (12)
H14	-0.0690	0.4921	0.5684	0.049*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0235 (4)	0.0277 (4)	0.0343 (4)	0.0048 (2)	0.0105 (2)	0.0017 (2)
O1	0.0300 (19)	0.040 (2)	0.054 (2)	0.0005 (14)	0.0077 (17)	-0.0082 (16)
O2	0.0293 (18)	0.048 (2)	0.062 (2)	-0.0022 (16)	0.0099 (16)	-0.0188 (19)
O3	0.052 (2)	0.052 (2)	0.044 (2)	0.0165 (18)	0.0223 (19)	0.0130 (17)
O4	0.043 (2)	0.0395 (19)	0.049 (2)	0.0127 (16)	0.0212 (17)	0.0127 (16)
O5	0.046 (2)	0.0279 (18)	0.094 (3)	0.0067 (16)	0.045 (2)	0.0048 (19)
N1	0.0276 (19)	0.0273 (19)	0.039 (2)	0.0041 (15)	0.0134 (16)	0.0005 (17)
N2	0.039 (2)	0.033 (2)	0.064 (3)	0.0047 (18)	0.025 (2)	-0.006 (2)
C1	0.032 (2)	0.031 (2)	0.035 (2)	-0.005 (2)	0.005 (2)	0.0059 (19)
C2	0.067 (4)	0.064 (4)	0.049 (3)	0.010 (3)	0.013 (3)	0.026 (3)
C3	0.035 (3)	0.033 (2)	0.031 (2)	-0.002 (2)	0.005 (2)	0.0073 (19)
C4	0.040 (3)	0.048 (3)	0.055 (3)	-0.008 (2)	0.002 (3)	-0.006 (3)
C5	0.025 (2)	0.029 (2)	0.042 (3)	0.0016 (18)	0.0096 (19)	-0.0058 (19)
C6	0.038 (3)	0.035 (3)	0.055 (3)	0.002 (2)	0.020 (3)	0.001 (2)

## supplementary materials

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C7	0.068 (4)	0.031 (3)	0.072 (4)	0.007 (3)	0.033 (3)	0.001 (3)
C8	0.059 (4)	0.032 (3)	0.089 (5)	0.013 (3)	0.041 (3)	-0.007 (3)
C9	0.035 (3)	0.028 (2)	0.054 (3)	0.002 (2)	0.023 (2)	-0.004 (2)
C10	0.036 (3)	0.058 (3)	0.055 (4)	0.002 (3)	-0.006 (3)	-0.007 (3)
C11	0.074 (4)	0.058 (4)	0.037 (3)	0.006 (3)	0.007 (3)	0.004 (3)
C12	0.055 (3)	0.044 (3)	0.055 (3)	0.001 (3)	0.032 (3)	0.001 (3)
C13	0.028 (3)	0.047 (3)	0.067 (4)	0.004 (2)	0.019 (2)	-0.003 (3)
C14	0.035 (3)	0.040 (3)	0.045 (3)	0.007 (2)	0.004 (2)	0.003 (2)

### Geometric parameters (Å, °)

Cu1—O3	1.954 (4)	C2—H2C	0.9800
Cu1—O1	1.966 (4)	C3—C4	1.515 (7)
Cu1—O4 <sup>i</sup>	1.977 (3)	C4—H4A	0.9800
Cu1—O2 <sup>i</sup>	1.979 (4)	C4—H4B	0.9800
Cu1—N1	2.207 (4)	C4—H4C	0.9800
Cu1—Cu1 <sup>i</sup>	2.6154 (10)	C6—C7	1.371 (8)
O1—C3	1.252 (6)	C6—H6	0.9500
O2—C3	1.246 (6)	C7—C8	1.367 (9)
O2—Cu1 <sup>i</sup>	1.979 (4)	C7—H7	0.9500
O3—C1	1.246 (6)	C8—H8	0.9500
O4—C1	1.254 (6)	C9—C14	1.367 (8)
O4—Cu1 <sup>i</sup>	1.977 (3)	C9—C10	1.391 (8)
O5—C5	1.347 (6)	C10—C11	1.389 (9)
O5—C9	1.400 (6)	C10—H10	0.9500
N1—C5	1.331 (6)	C11—C12	1.373 (9)
N1—C6	1.335 (6)	C11—H11	0.9500
N2—C5	1.312 (6)	C12—C13	1.361 (8)
N2—C8	1.331 (8)	C12—H12	0.9500
C1—C2	1.511 (7)	C13—C14	1.383 (8)
C2—H2A	0.9800	C13—H13	0.9500
C2—H2B	0.9800	C14—H14	0.9500
O3—Cu1—O1	90.30 (18)	C3—C4—H4A	109.5
O3—Cu1—O4 <sup>i</sup>	168.58 (15)	C3—C4—H4B	109.5
O1—Cu1—O4 <sup>i</sup>	89.46 (16)	H4A—C4—H4B	109.5
O3—Cu1—O2 <sup>i</sup>	88.77 (18)	C3—C4—H4C	109.5
O1—Cu1—O2 <sup>i</sup>	168.63 (15)	H4A—C4—H4C	109.5
O4 <sup>i</sup> —Cu1—O2 <sup>i</sup>	89.22 (17)	H4B—C4—H4C	109.5
O3—Cu1—N1	99.39 (15)	N2—C5—N1	127.3 (4)
O1—Cu1—N1	98.78 (15)	N2—C5—O5	120.4 (4)
O4 <sup>i</sup> —Cu1—N1	91.93 (14)	N1—C5—O5	112.3 (4)
O2 <sup>i</sup> —Cu1—N1	92.55 (14)	N1—C6—C7	121.7 (5)
O3—Cu1—Cu1 <sup>i</sup>	85.37 (11)	N1—C6—H6	119.1
O1—Cu1—Cu1 <sup>i</sup>	83.66 (11)	C7—C6—H6	119.1
O4 <sup>i</sup> —Cu1—Cu1 <sup>i</sup>	83.26 (10)	C8—C7—C6	116.5 (5)
O2 <sup>i</sup> —Cu1—Cu1 <sup>i</sup>	84.97 (11)	C8—C7—H7	121.8

N1—Cu1—Cu1 <sup>i</sup>	174.60 (11)	C6—C7—H7	121.8
C3—O1—Cu1	123.7 (3)	N2—C8—C7	123.5 (5)
C3—O2—Cu1 <sup>i</sup>	121.6 (3)	N2—C8—H8	118.2
C1—O3—Cu1	122.2 (3)	C7—C8—H8	118.2
C1—O4—Cu1 <sup>i</sup>	123.3 (3)	C14—C9—C10	121.7 (5)
C5—O5—C9	121.5 (4)	C14—C9—O5	122.3 (5)
C5—N1—C6	116.0 (4)	C10—C9—O5	115.7 (5)
C5—N1—Cu1	127.2 (3)	C11—C10—C9	118.1 (5)
C6—N1—Cu1	116.7 (3)	C11—C10—H10	120.9
C5—N2—C8	114.9 (5)	C9—C10—H10	120.9
O3—C1—O4	125.8 (4)	C12—C11—C10	120.7 (5)
O3—C1—C2	117.5 (5)	C12—C11—H11	119.6
O4—C1—C2	116.7 (5)	C10—C11—H11	119.6
C1—C2—H2A	109.5	C13—C12—C11	119.5 (5)
C1—C2—H2B	109.5	C13—C12—H12	120.3
H2A—C2—H2B	109.5	C11—C12—H12	120.3
C1—C2—H2C	109.5	C12—C13—C14	121.8 (5)
H2A—C2—H2C	109.5	C12—C13—H13	119.1
H2B—C2—H2C	109.5	C14—C13—H13	119.1
O2—C3—O1	125.9 (5)	C9—C14—C13	118.2 (5)
O2—C3—C4	117.1 (5)	C9—C14—H14	120.9
O1—C3—C4	117.0 (5)	C13—C14—H14	120.9
O3—Cu1—O1—C3	-87.8 (4)	Cu1—O1—C3—C4	-174.5 (4)
O4 <sup>i</sup> —Cu1—O1—C3	80.8 (4)	C8—N2—C5—N1	0.3 (8)
O2 <sup>i</sup> —Cu1—O1—C3	-2.6 (11)	C8—N2—C5—O5	-179.7 (6)
N1—Cu1—O1—C3	172.6 (4)	C6—N1—C5—N2	1.1 (8)
Cu1 <sup>i</sup> —Cu1—O1—C3	-2.5 (4)	Cu1—N1—C5—N2	178.4 (4)
O1—Cu1—O3—C1	83.2 (4)	C6—N1—C5—O5	-178.8 (5)
O4 <sup>i</sup> —Cu1—O3—C1	-5.6 (11)	Cu1—N1—C5—O5	-1.5 (6)
O2 <sup>i</sup> —Cu1—O3—C1	-85.5 (4)	C9—O5—C5—N2	-9.6 (8)
N1—Cu1—O3—C1	-177.9 (4)	C9—O5—C5—N1	170.4 (5)
Cu1 <sup>i</sup> —Cu1—O3—C1	-0.5 (4)	C5—N1—C6—C7	-1.2 (8)
O3—Cu1—N1—C5	-39.5 (4)	Cu1—N1—C6—C7	-178.8 (5)
O1—Cu1—N1—C5	52.2 (4)	N1—C6—C7—C8	0.0 (10)
O4 <sup>i</sup> —Cu1—N1—C5	142.0 (4)	C5—N2—C8—C7	-1.8 (10)
O2 <sup>i</sup> —Cu1—N1—C5	-128.7 (4)	C6—C7—C8—N2	1.7 (11)
O3—Cu1—N1—C6	137.7 (4)	C5—O5—C9—C14	72.4 (7)
O1—Cu1—N1—C6	-130.5 (4)	C5—O5—C9—C10	-114.0 (6)
O4 <sup>i</sup> —Cu1—N1—C6	-40.8 (4)	C14—C9—C10—C11	0.9 (9)
O2 <sup>i</sup> —Cu1—N1—C6	48.5 (4)	O5—C9—C10—C11	-172.8 (5)
Cu1—O3—C1—O4	-1.0 (8)	C9—C10—C11—C12	-0.1 (9)
Cu1—O3—C1—C2	-179.8 (4)	C10—C11—C12—C13	-0.9 (9)
Cu1 <sup>i</sup> —O4—C1—O3	2.4 (7)	C11—C12—C13—C14	1.1 (9)
Cu1 <sup>i</sup> —O4—C1—C2	-178.7 (4)	C10—C9—C14—C13	-0.7 (8)
Cu1 <sup>i</sup> —O2—C3—O1	-5.4 (7)	O5—C9—C14—C13	172.5 (5)

## supplementary materials

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Cu1 <sup>i</sup> —O2—C3—C4	174.6 (4)	C12—C13—C14—C9	-0.3 (8)
Cu1—O1—C3—O2	5.5 (7)		

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



Fig. 1

