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# Bis{(*E*)-2-[(2-chloro-3-pyridyl)iminomethyl]-6-methoxyphenolato-$\kappa^2N,O^1$}copper(II)

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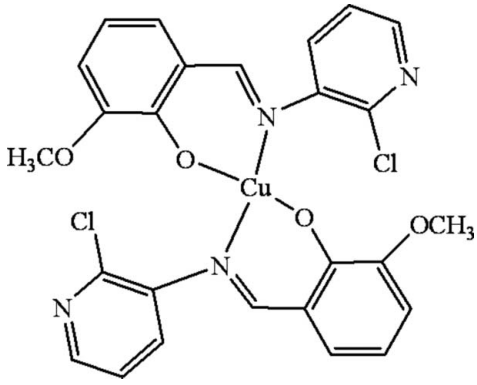
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.035; $wR$ factor = 0.075; data-to-parameter ratio = 13.3.

In the title mononuclear copper(II) complex, $[Cu(C_{13}H_{10}ClN_2O_2)_2]$, the $Cu^{II}$ ion, lying on an inversion center, is four-coordinated in a *trans*-$CuN_2O_2$ square-planar geometry by two phenolate O and two imino N atoms from two symmetry-related *N*,*O*-bidentate Schiff base ligands. The shortest Cu···Cu distance is 7.5743 (9) Å. However, there are weak intramolecular electrostatic interactions between the Cu atom and the Cl atom of the ligand, with a Cu···Cl distance of 3.3845 (9) Å.

## Related literature

For the synthesis and related crystal strcutures, see: Dong *et al.* (2009, 2010); Ding *et al.* (2009).




## Experimental

### Crystal data

$[Cu(C_{13}H_{10}ClN_2O_2)_2]$
$M_r$ = 586.90
Monoclinic, $C2/c$
$a$ = 21.242 (2) Å
$b$ = 7.5743 (9) Å
$c$ = 16.141 (2) Å
$\beta$ = 97.652 (1)°
$V$ = 2573.9 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.10 mm$^{-1}$
$T$ = 298 K
0.18 × 0.16 × 0.11 mm

### Data collection

Siemens SMART 1000 CCE diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.827, $T_{max}$ = 0.889
6295 measured reflections
2262 independent reflections
1651 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.075
$S$ = 1.01
2262 reflections
170 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Foundation of the Education Department of Gansu Province (0904–11), which is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2379).

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# supporting information

*Acta Cryst.* (2011). E**67**, m91 [https://doi.org/10.1107/S1600536810052414]

## Bis{(*E*)-2-[(2-chloro-3-pyridyl)iminomethyl]-6-methoxyphenolato-$\kappa^2N,O^1$}copper(II)

**Wen-Kui Dong, Yuan Wang, Jian-Chao Wu and Shou-Ting Zhang**

### S1. Comment

The centrosymmetric structure of the title complex is shown in Fig. 1. In the title complex all bond lengths are in normal ranges. The $Cu^{II}$ ion, lying on the inversion centre, is four-coordinated in a *trans*-$CuN_2O_2$ square-planar geometry, with two phenolate O and two imino N atoms from two N,*O*-bidentate Schiff-base ligand (HL) (Dong *et al.*, 2009; Ding *et al.*, 2009). The shortest Cu···Cu distance is 7.5743 (9) Å. However, there are weak intramolecular electrostatic interactions between the Cu and Cl of the ligand, with Cu1··· Cl1 distance of 3.3845 (9) Å.

### S2. Experimental

(*E*)-2-((2-chloropyridin-3-ylimino)methyl)-6-methoxyphenol (HL) was prepared according to previously reported procedure (Dong *et al.*, 2010; Ding *et al.*, 2009). To a warm pale-yellow ethanol solution (4 ml) of 3-methoxysalicylaldehyde (152.2 mg, 1.00 mmol), colorless ethanol solution (4 ml) of 3-amino-2-chloropyridine (128.6 mg, 1.00 mmol) was added dropwise, and the color of the mixture turned orange. The solution was maintained under reflux for 24 h, and a saffron yellow powder product was obtained. It was filtered off, washed with ethanol and ethanol-hexane (1:4, V/V), respectively, and then dried *in vacuo* yielding 245.3 mg powder. Yield, 93.38%. m.p. 397–398 K. Anal. Calcd. for $C_{13}H_{11}ClN_2O_2$ (%): C, 59.44; H, 4.22; N, 10.66. Found: C, 59.40; H, 4.18; N, 10.71.

A pale-blue ethanol solution (3 ml) of $Cu^{II}$ acetate monohydrate (2.9 mg, 0.015 mmol) was added dropwise to a pale-yellow acetone solution (3 ml) of HL (7.0 mg, 0.027 mmol) at room temperature. The color of the mixing solution turned to yellow immediately, then turned to brown slowly and the filtrate was allowed to stand at room temperature for about three weeks. The solvent was partially evaporated and obtained green single crystals suit for X-ray crystallographic analysis. Anal. Calcd. for [Cu(*L*)$_2$] ($C_{26}H_{20}Cl_2CuN_4O_4$) (%): C, 53.21; H, 3.43; N, 9.55; Cu, 10.83. Found: C, 53.24; H, 3.46; N, 9.50, Cu, 10.79.

### S3. Refinement

H atoms were placed in calculated positions and non-H atoms were refined anisotropically. H atoms were treated as riding atoms with distances C—H = 0.96 Å ($CH_3$) and 0.93 Å (CH). The isotropic displacement parameters for all H atoms were set equal to 1.2 or 1.5 $U_{eq}$ of the carrier atom.

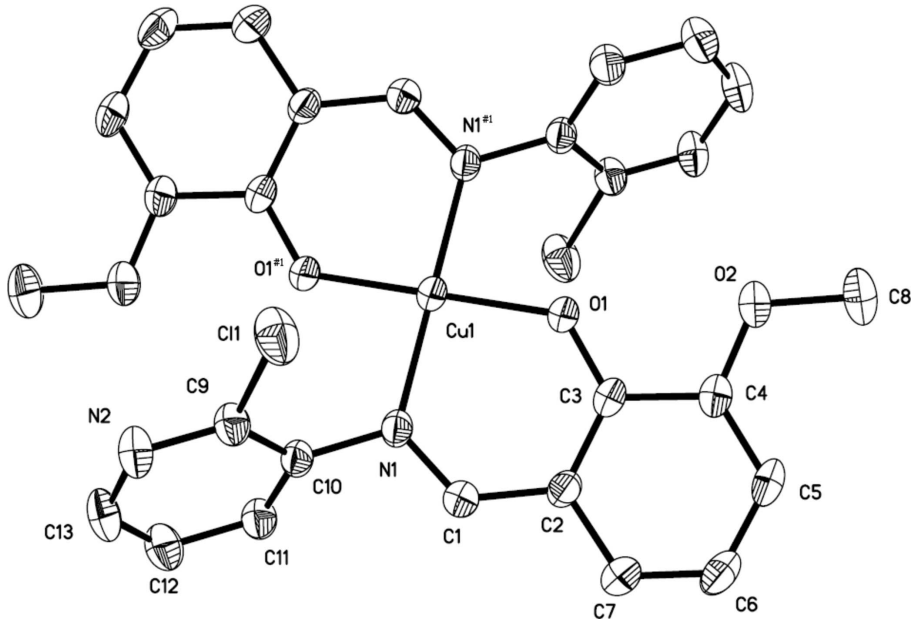


**Figure 1**

The molecular structure of the title complex with the atom numbering scheme [Symmetry code: #1 = -*x* + 1,-*y* + 1,-*z*]. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

**Bis{(*E*)-2-[(2-chloro-3-pyridyl)iminomethyl]-6-methoxyphenolato- $\kappa^2N,O^1$}copper(II)**

*Crystal data*

$[Cu(C_{13}H_{10}ClN_2O_2)_2]$
$M_r$ = 586.90
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
*a* = 21.242 (2) Å
*b* = 7.5743 (9) Å
*c* = 16.141 (2) Å
$\beta$ = 97.652 (1)°
*V* = 2573.9 (5) Å$^3$
*Z* = 4
*F*(000) = 1196
$D_x$ = 1.515 Mg m$^{-3}$
Mo *K*$\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1824 reflections
$\theta$ = 2.9–25.2°
$\mu$ = 1.10 mm$^{-1}$
*T* = 298 K
Block, brown
0.18 × 0.16 × 0.11 mm

*Data collection*

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.827, $T_{max}$ = 0.889
6295 measured reflections
2262 independent reflections
1651 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
*h* = −20→25
*k* = −8→8
*l* = −19→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.075
*S* = 1.01
2262 reflections
170 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.5000 | 0.5000 | 0.0000 | 0.04162 (16) |
| Cl1 | 0.41342 (4) | 0.44977 (10) | 0.15993 (6) | 0.0749 (3) |
| N1 | 0.53184 (10) | 0.3389 (3) | 0.09230 (13) | 0.0415 (5) |
| N2 | 0.40093 (12) | 0.1120 (3) | 0.17745 (16) | 0.0590 (7) |
| O1 | 0.56672 (8) | 0.6625 (2) | 0.03158 (12) | 0.0494 (5) |
| O2 | 0.65231 (10) | 0.9115 (3) | 0.03223 (14) | 0.0662 (6) |
| C1 | 0.58981 (13) | 0.3453 (4) | 0.13165 (17) | 0.0452 (7) |
| H1 | 0.6021 | 0.2534 | 0.1685 | 0.054* |
| C2 | 0.63603 (12) | 0.4787 (4) | 0.12382 (16) | 0.0442 (7) |
| C3 | 0.62132 (12) | 0.6322 (4) | 0.07655 (16) | 0.0426 (7) |
| C4 | 0.67016 (13) | 0.7650 (4) | 0.07845 (18) | 0.0495 (7) |
| C5 | 0.72880 (14) | 0.7374 (4) | 0.12438 (19) | 0.0586 (8) |
| H5 | 0.7603 | 0.8228 | 0.1244 | 0.070* |
| C6 | 0.74167 (15) | 0.5833 (4) | 0.1708 (2) | 0.0642 (9) |
| H6 | 0.7815 | 0.5668 | 0.2015 | 0.077* |
| C7 | 0.69649 (14) | 0.4579 (4) | 0.17153 (18) | 0.0572 (8) |
| H7 | 0.7052 | 0.3568 | 0.2037 | 0.069* |
| C8 | 0.69847 (17) | 1.0482 (4) | 0.0302 (2) | 0.0785 (11) |
| H8A | 0.7120 | 1.0891 | 0.0860 | 0.118* |
| H8B | 0.6801 | 1.1444 | −0.0034 | 0.118* |
| H8C | 0.7344 | 1.0028 | 0.0066 | 0.118* |
| C9 | 0.43771 (13) | 0.2320 (4) | 0.14983 (17) | 0.0476 (7) |
| C10 | 0.49353 (13) | 0.1971 (3) | 0.11672 (16) | 0.0427 (7) |
| C11 | 0.50962 (14) | 0.0223 (4) | 0.10883 (17) | 0.0516 (7) |
| H11 | 0.5457 | −0.0086 | 0.0853 | 0.062* |
| C12 | 0.47121 (16) | −0.1066 (4) | 0.13646 (19) | 0.0637 (9) |
| H12 | 0.4813 | −0.2255 | 0.1321 | 0.076* |
| C13 | 0.41833 (17) | −0.0569 (4) | 0.1702 (2) | 0.0647 (9) |
| H13 | 0.3931 | −0.1446 | 0.1891 | 0.078* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0330 (3) | 0.0411 (3) | 0.0496 (3) | −0.0060 (2) | 0.0010 (2) | 0.0007 (2) |
| Cl1 | 0.0740 (6) | 0.0506 (5) | 0.1082 (7) | −0.0009 (4) | 0.0415 (5) | −0.0033 (4) |
| N1 | 0.0370 (13) | 0.0402 (13) | 0.0472 (13) | −0.0072 (10) | 0.0046 (11) | −0.0018 (10) |
| N2 | 0.0575 (16) | 0.0524 (17) | 0.0704 (18) | −0.0181 (14) | 0.0207 (14) | −0.0051 (14) |
| O1 | 0.0380 (11) | 0.0423 (11) | 0.0642 (12) | −0.0088 (9) | −0.0065 (10) | 0.0060 (9) |
| O2 | 0.0574 (14) | 0.0533 (13) | 0.0852 (16) | −0.0221 (11) | −0.0004 (12) | 0.0056 (12) |
| C1 | 0.0438 (17) | 0.0451 (17) | 0.0461 (17) | −0.0024 (14) | 0.0034 (14) | 0.0014 (13) |
| C2 | 0.0347 (15) | 0.0508 (18) | 0.0458 (15) | −0.0041 (14) | 0.0009 (12) | −0.0008 (14) |
| C3 | 0.0342 (15) | 0.0491 (17) | 0.0437 (17) | −0.0069 (13) | 0.0028 (14) | −0.0073 (14) |
| C4 | 0.0444 (18) | 0.0483 (19) | 0.0557 (19) | −0.0108 (14) | 0.0059 (15) | −0.0065 (15) |
| C5 | 0.0393 (18) | 0.065 (2) | 0.070 (2) | −0.0177 (15) | 0.0003 (16) | −0.0121 (17) |
| C6 | 0.0391 (19) | 0.077 (2) | 0.072 (2) | −0.0053 (17) | −0.0096 (16) | −0.0098 (19) |
| C7 | 0.0467 (19) | 0.063 (2) | 0.0586 (19) | −0.0025 (15) | −0.0063 (15) | 0.0012 (15) |
| C8 | 0.082 (3) | 0.060 (2) | 0.095 (3) | −0.0335 (19) | 0.016 (2) | −0.0060 (19) |
| C9 | 0.0486 (18) | 0.0405 (17) | 0.0553 (18) | −0.0050 (14) | 0.0125 (15) | −0.0034 (14) |
| C10 | 0.0403 (17) | 0.0442 (17) | 0.0425 (16) | −0.0093 (13) | 0.0016 (13) | 0.0005 (13) |
| C11 | 0.0503 (18) | 0.0469 (18) | 0.0583 (18) | −0.0059 (15) | 0.0096 (14) | −0.0011 (15) |
| C12 | 0.073 (2) | 0.0439 (19) | 0.075 (2) | −0.0104 (17) | 0.0156 (19) | −0.0005 (17) |
| C13 | 0.075 (2) | 0.047 (2) | 0.076 (2) | −0.0255 (17) | 0.022 (2) | −0.0016 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1$^{i}$ | 1.8951 (17) | C4—C5 | 1.378 (4) |
| Cu1—O1 | 1.8951 (17) | C5—C6 | 1.395 (4) |
| Cu1—N1 | 1.974 (2) | C5—H5 | 0.9300 |
| Cu1—N1$^{i}$ | 1.974 (2) | C6—C7 | 1.351 (4) |
| Cl1—C9 | 1.743 (3) | C6—H6 | 0.9300 |
| N1—C1 | 1.309 (3) | C7—H7 | 0.9300 |
| N1—C10 | 1.434 (3) | C8—H8A | 0.9600 |
| N2—C9 | 1.314 (3) | C8—H8B | 0.9600 |
| N2—C13 | 1.341 (4) | C8—H8C | 0.9600 |
| O1—C3 | 1.304 (3) | C9—C10 | 1.389 (4) |
| O2—C4 | 1.363 (3) | C10—C11 | 1.378 (4) |
| O2—C8 | 1.429 (3) | C11—C12 | 1.384 (4) |
| C1—C2 | 1.426 (3) | C11—H11 | 0.9300 |
| C1—H1 | 0.9300 | C12—C13 | 1.365 (4) |
| C2—C3 | 1.403 (4) | C12—H12 | 0.9300 |
| C2—C7 | 1.416 (4) | C13—H13 | 0.9300 |
| C3—C4 | 1.443 (4) | | |
| | | | |
| O1$^{i}$—Cu1—O1 | 180.00 (14) | C7—C6—C5 | 120.3 (3) |
| O1$^{i}$—Cu1—N1 | 88.30 (8) | C7—C6—H6 | 119.9 |
| O1—Cu1—N1 | 91.70 (8) | C5—C6—H6 | 119.9 |
| O1$^{i}$—Cu1—N1$^{i}$ | 91.70 (8) | C6—C7—C2 | 120.8 (3) |
| O1—Cu1—N1$^{i}$ | 88.30 (8) | C6—C7—H7 | 119.6 |

| | | | |
|---|---|---|---|
| N1—Cu1—N1$^{i}$ | 180.00 (16) | C2—C7—H7 | 119.6 |
| C1—N1—C10 | 115.2 (2) | O2—C8—H8A | 109.5 |
| C1—N1—Cu1 | 123.28 (18) | O2—C8—H8B | 109.5 |
| C10—N1—Cu1 | 121.36 (17) | H8A—C8—H8B | 109.5 |
| C9—N2—C13 | 116.5 (3) | O2—C8—H8C | 109.5 |
| C3—O1—Cu1 | 127.80 (17) | H8A—C8—H8C | 109.5 |
| C4—O2—C8 | 117.4 (2) | H8B—C8—H8C | 109.5 |
| N1—C1—C2 | 126.7 (3) | N2—C9—C10 | 125.1 (3) |
| N1—C1—H1 | 116.7 | N2—C9—Cl1 | 115.2 (2) |
| C2—C1—H1 | 116.7 | C10—C9—Cl1 | 119.6 (2) |
| C3—C2—C7 | 120.6 (3) | C11—C10—C9 | 117.0 (2) |
| C3—C2—C1 | 121.9 (2) | C11—C10—N1 | 122.5 (2) |
| C7—C2—C1 | 117.3 (3) | C9—C10—N1 | 120.5 (2) |
| O1—C3—C2 | 124.5 (2) | C10—C11—C12 | 119.0 (3) |
| O1—C3—C4 | 118.2 (3) | C10—C11—H11 | 120.5 |
| C2—C3—C4 | 117.3 (2) | C12—C11—H11 | 120.5 |
| O2—C4—C5 | 125.7 (3) | C13—C12—C11 | 119.1 (3) |
| O2—C4—C3 | 114.2 (2) | C13—C12—H12 | 120.5 |
| C5—C4—C3 | 120.1 (3) | C11—C12—H12 | 120.5 |
| C4—C5—C6 | 121.0 (3) | N2—C13—C12 | 123.3 (3) |
| C4—C5—H5 | 119.5 | N2—C13—H13 | 118.3 |
| C6—C5—H5 | 119.5 | C12—C13—H13 | 118.3 |

| | | | |
|---|---|---|---|
| O1$^{i}$—Cu1—N1—C1 | 161.5 (2) | O2—C4—C5—C6 | 178.8 (3) |
| O1—Cu1—N1—C1 | −18.5 (2) | C3—C4—C5—C6 | −1.2 (4) |
| O1$^{i}$—Cu1—N1—C10 | −13.9 (2) | C4—C5—C6—C7 | 0.0 (5) |
| O1—Cu1—N1—C10 | 166.1 (2) | C5—C6—C7—C2 | 1.5 (5) |
| N1—Cu1—O1—C3 | 21.0 (2) | C3—C2—C7—C6 | −1.7 (4) |
| N1$^{i}$—Cu1—O1—C3 | −159.0 (2) | C1—C2—C7—C6 | −176.5 (3) |
| C10—N1—C1—C2 | −175.3 (2) | C13—N2—C9—C10 | −2.2 (5) |
| Cu1—N1—C1—C2 | 9.1 (4) | C13—N2—C9—Cl1 | 179.7 (2) |
| N1—C1—C2—C3 | 6.3 (4) | N2—C9—C10—C11 | 3.2 (4) |
| N1—C1—C2—C7 | −179.0 (3) | Cl1—C9—C10—C11 | −178.8 (2) |
| Cu1—O1—C3—C2 | −13.0 (4) | N2—C9—C10—N1 | −176.8 (3) |
| Cu1—O1—C3—C4 | 167.22 (18) | Cl1—C9—C10—N1 | 1.2 (4) |
| C7—C2—C3—O1 | −179.3 (2) | C1—N1—C10—C11 | −60.3 (3) |
| C1—C2—C3—O1 | −4.8 (4) | Cu1—N1—C10—C11 | 115.4 (3) |
| C7—C2—C3—C4 | 0.4 (4) | C1—N1—C10—C9 | 119.7 (3) |
| C1—C2—C3—C4 | 175.0 (2) | Cu1—N1—C10—C9 | −64.6 (3) |
| C8—O2—C4—C5 | 0.7 (4) | C9—C10—C11—C12 | −2.2 (4) |
| C8—O2—C4—C3 | −179.2 (2) | N1—C10—C11—C12 | 177.8 (2) |
| O1—C3—C4—O2 | 0.7 (4) | C10—C11—C12—C13 | 0.4 (5) |
| C2—C3—C4—O2 | −179.0 (2) | C9—N2—C13—C12 | 0.2 (5) |
| O1—C3—C4—C5 | −179.2 (2) | C11—C12—C13—N2 | 0.6 (5) |
| C2—C3—C4—C5 | 1.0 (4) | | |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.