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Key indicators

Single-crystal X-ray study
 T = 273 K
 Mean $\sigma(C-C)$ = 0.002 Å
 R factor = 0.026
 wR factor = 0.076
 Data-to-parameter ratio = 15.6

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

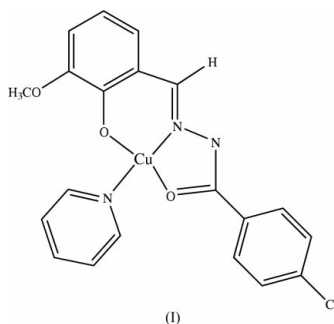
{4-Chloro-2'-[(3-methoxy-2-oxidophenyl)-methylidene]benzohydrazido}(pyridine)-copper(II)

In the title compound, $[Cu(C_{15}H_{11}ClN_2O_3)(C_5H_5N)]$, the hydrazide ligand chelates to the central Cu atom in an *O,N,O'*-tridentate manner and the pyridine molecule coordinates through the N atom, forming a distorted square-planar geometry. The compound has a *trans* configuration with *cis* angles about the Cu atom between 81.1 (2) and 95.7 (2)°. The molecule is discrete, with no significant intermolecular interactions.

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Comment

It is known that tetracoordinate Schiff base metal complexes may adopt *trans* or *cis* planar or tetrahedral geometry. $[Cu(C_{20}H_{12}Br_2N_2O_2)]$ (Elmali *et al.*, 2000) and $[Cu(C_{15}H_{22}NO)_2]$ (Zhang *et al.*, 2001) are examples of *cis*- and *trans*- CuN_2O_2 coordination geometry, respectively.



The present compound, $[Cu(C_{20}H_{16}ClN_3O_3)]$, (I), shows a *trans*- CuN_2O_2 configuration in a distorted square-planar environment (Fig. 1), as in the compound above. However, the ligand is chelated to the Cu atom in an *O,N,O'*-tridentate manner and the pyridine molecule coordinates through the N atom. The *cis* angles lie between 81.1 (2) and 95.7 (2)° and show more variation than in $[Cu(C_{15}H_{22}NO)_2]$, which is centrosymmetric with *cis* N1–Cu1–O1 and O1'–Cu1–N1

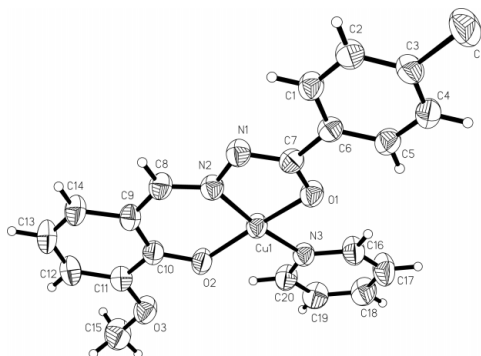


Figure 1
 The molecular structure of the title compound, (I), shown with 50% probability displacement ellipsoids.

angles of 88.91 (13) and 91.09 (13)°. The whole molecule is not planar, with a maximum deviation at C15 of 0.483 (2) Å from the mean plane. The maximum deviation among the atoms Cu1, O1, O2, N2 and N3 is for atom O2 of 0.265 (1) Å, in such a way that the Cu1–O1 bond length [1.93 (11) Å] is slightly longer than the Cu1–O2 bond length [1.88 (11) Å], although in agreement with other square-planar complexes, such as [Cu(C₂₀H₁₂Br₂N₂O₂)] [Cu–O = 1.88 (4) and 1.88 (3) Å; Cu–N = 1.93 (4) and 1.94 (4) Å; Elmali *et al.*, 2000] and centrosymmetric [Cu(C₁₅H₂₂O)₂] [Cu–O = 1.88 (3) and Cu–N = 2.00 (3) Å; Zhang *et al.*, 2001]. The structural dimensions of the ligand are normal (Allen *et al.*, 1987; Orpen *et al.*, 1989). No significant intermolecular interactions are observed in the crystal structure.

Experimental

The title complex was synthesized by the template condensation of 2-hydroxy-3-methoxybenzaldehyde (0.30 g, 1.0 mmol) and 4-chlorobenzhydrazide (0.34 g, 1.0 mmol) with copper acetate dihydrate (0.34 g, 0.5 mmol) by refluxing and stirring in ethanol for 5 h. The dark-blue solid was filtered off and recrystallized from pyridine.

Crystal data

[Cu(C ₁₅ H ₁₁ ClN ₂ O ₃)(C ₅ H ₅ N)]	<i>Z</i> = 2
<i>M_r</i> = 445.35	<i>D_x</i> = 1.607 Mg m ^{−3}
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 7.6672 (6) Å	Cell parameters from 7701 reflections
<i>b</i> = 8.3085 (7) Å	<i>θ</i> = 2.4–27.0°
<i>c</i> = 14.6960 (12) Å	<i>μ</i> = 1.36 mm ^{−1}
<i>α</i> = 97.960 (2)°	<i>T</i> = 273 (2) K
<i>β</i> = 93.595 (2)°	Block, dark blue
<i>γ</i> = 95.405 (1)°	0.41 × 0.36 × 0.24 mm
<i>V</i> = 920.31 (13) Å ³	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3984 independent reflections
<i>ω</i> scans	3772 reflections with <i>I</i> > 2 <i>s</i> (<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> _{int} = 0.017
<i>T</i> _{min} = 0.592, <i>T</i> _{max} = 0.721	<i>θ</i> _{max} = 27.0°
10319 measured reflections	<i>h</i> = −9 → 9
	<i>k</i> = −10 → 10
	<i>l</i> = −18 → 18

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.1871P]$
$R[F^2 > 2\sigma(F^2)] = 0.026$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.076$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.06	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
3984 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
255 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.0119 (18)

After their location in a difference map, all H atoms were positioned geometrically and allowed to ride on the parent C atoms, with C–H = 0.93–0.96 Å and *U*_{iso}(H) = 1.2 or 1.5*U*_{eq}(C).

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Elmali, A., Elerman, Y. & Svoboda, I. (2000). *Acta Cryst.* **C56**, 423–424.
- Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1–3.
- Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Zhang, L. Z., Bu, P.-Y., Wang, L.-J. & Cheng, P. (2001). *Acta Cryst.* **C57**, 1166–1167.