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Bis{*N*-[(*Z*)-(3-Methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-ylidene)(phenyl)methyl]benzylamido-κ^2N,O}copper(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.111
Data-to-parameter ratio = 17.3

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

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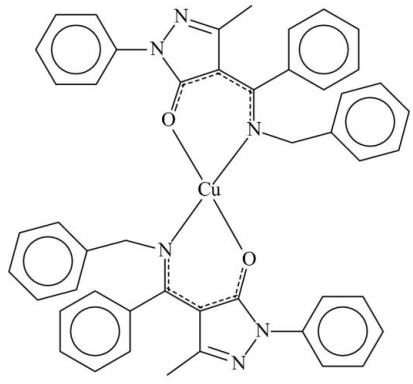
The Cu atom in the title compound, $[Cu(C_{24}H_{20}N_3O)_2]$, is chelated by two deprotonated 4-[(benzylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one ligands through their amide N and carbonyl O atoms in a distorted square-planar geometry.

Comment

4-[(Benzylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one (Jiang *et al.*, 2004) is an example of a class of potential bidentate chelating ligands that is synthesized from the condensation of commercially available 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone with the primary amine, benzylamine. In the copper(II) derivative, two deprotonated ligands chelate to the metal through their amido N and carbonyl O atoms (Fig. 1). For both six-membered chelate rings, the five C, N and O atoms are coplanar; however, the Cu atom lies out of the plane. The metal atom lies 0.352 (2) Å out of the O1/C7/C8/C11/N3 plane, and 0.714 (2) Å out of the O2/C31/C32/C35/N6 plane, in the opposite direction. As the two planes are twisted by 36.2 (1)°, the four-coordinate geometry of copper is better regarded as a distorted square planar. The carbonyl C═O bond distances [1.283 (2) and 1.287 (2) Å] are lengthened relative to that [1.247 (2) Å] in the free ligand (Jiang *et al.*, 2004); similarly, the exocyclic C═O double bond is also lengthened, so that the negative charge formally residing on the amide N is better regarded as being delocalized over the five-atom unit.



(I)

The structure of a similar organic compound, 4-[(1-naphthylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one, has been authenticated (Wang *et al.*, 2003). In addition, a structure of this compound as a 2:1 complex with silver hexafluorophosphate is known. In this salt, the Ag is coordinated by the two ligands through the N-atom sites of the pyrazolyl rings (Lü *et al.*, 2004).

Experimental

To a chloroform (5 ml) solution of 4-[(benzylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one (Jiang *et al.*, 2004) (37 mg, 0.1 mmol) and triethylamine (14 µl, 0.1 mmol) was added copper(II) chloride (9 mg, 0.05 mmol) dissolved in ethanol (5 ml). The brown mixture was filtered and the solution set aside for several days to give black crystals in about 65% yield. Analysis calculated for $C_{48}H_{40}CuN_6O_2$: C 72.39, H 5.06, N 10.55%; found: C 72.62, H 5.34, N 10.89%.

Crystal data

$[Cu(C_{24}H_{20}N_3O)_2]$
M_r = 796.40
Monoclinic, $P2_1/c$
a = 14.718 (2) Å
b = 18.686 (2) Å
c = 15.320 (2) Å
β = 104.337 (2)°
V = 4082.2 (9) Å^3
Z = 4
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 975 reflections
θ = 2.6–26.6°
μ = 0.58 mm^{-1}
T = 295 (2) K
Irregular block, black
0.49 × 0.48 × 0.27 mm

Data collection

Bruker SMART area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.730, T_{max} = 0.859
24434 measured reflections
8912 independent reflections
6429 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.1°
$h = -18 \rightarrow 18$
$k = -23 \rightarrow 14$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.111
S = 0.99
8912 reflections
516 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 1.4386P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.916 (1)	Cu1—N3	1.973 (2)
Cu1—O2	1.922 (1)	Cu1—N6	1.984 (2)
O1—Cu1—O2	152.25 (7)	O2—Cu1—N3	91.70 (7)
O1—Cu1—N3	94.45 (6)	O2—Cu1—N6	92.50 (6)
O1—Cu1—N6	93.39 (6)	N3—Cu1—N6	154.63 (7)

H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [phenyl C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C); methylene C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C); methyl C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C)]; the methyl groups were rotated to fit the electron density.

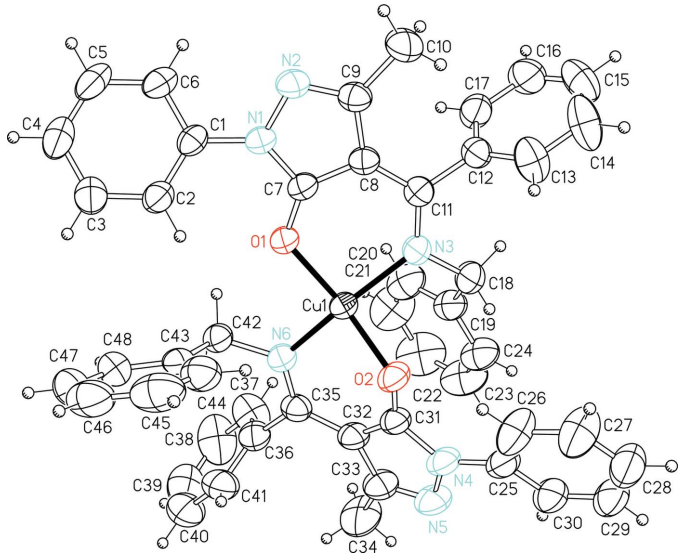


Figure 1
ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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