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Bis{[(*Z*)-4-(5-methyl-3-oxo-2-phenylpyrazol-4-yl)-phenylmethylene]benzylamido-κ^2N,O}cobalt(II)

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Key indicators

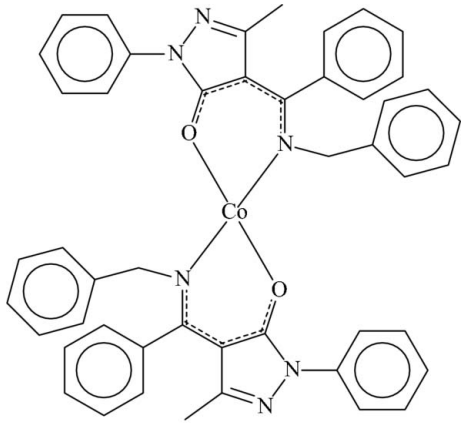
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.155
Data-to-parameter ratio = 17.9

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

The Co^{II} atom in the title compound, $[Co(C_{24}H_{20}N_3O)_2]$, 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 tetrahedral geometry.

Comment

4-[(Benzylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one (Jiang *et al.*, 2004) in the monoprotonated form chelates to copper(II) through its amido N and carbonyl O atoms, to render a square-planar geometry to the metal (Bao *et al.*, 2005). The geometry is distorted towards tetrahedral, the distortion being limited by the general preference of d^9 Cu for square-planar coordination.



(I)

In the title d^7 Co analogue, (I), the geometry is the preferred tetrahedral (Fig. 1). The exocyclic carbonyl C═O bonds [1.285 (3) and 1.287 (2) Å for C31═O2 and C7═O1, respectively] are lengthened relative to that in the free ligand [1.247 (2) Å; Jiang *et al.*, 2004]. The bond dimensions involving the metal are similar to those found in tetrahedral bis{[(5-methyl-2-phenylpyrazolyl-3-one)phenylmethylene]-4-tolylamido}cobalt(II) (Ma *et al.*, 2005).

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 cobalt(II) chloride (6.5 mg, 0.05 mmol) dissolved in ethanol (5 ml). The mixture was filtered and the solution set aside for several days to give red crystals in about 70% yield. CHN analysis, calculated for $C_{48}H_{40}N_6O_2Co$: C 72.81, H 5.09, N 10.61%; found: C 72.68, H 5.26, N 10.58%.

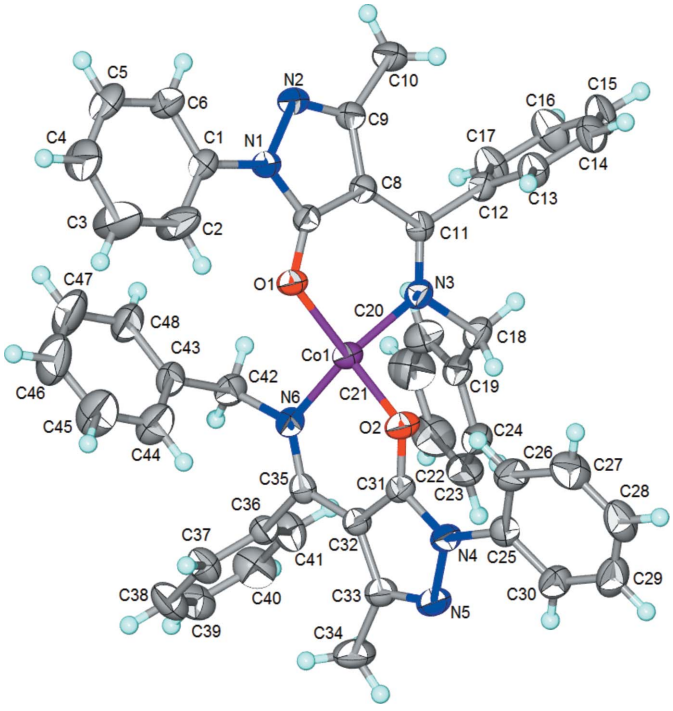


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Crystal data

$[Co(C_{24}H_{20}N_3O)_2]$
M_r = 791.79
Monoclinic, $P2_1/c$
a = 19.736 (1) Å
b = 17.389 (1) Å
c = 12.002 (1) Å
β = 102.234 (1)°
V = 4025.4 (4) Å^3
Z = 4
D_x = 1.307 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 293 (2) K
Block, red
0.36 × 0.30 × 0.20 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.848, T_{max} = 0.911
46193 measured reflections
9243 independent reflections
6652 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
S = 1.00
9243 reflections
516 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0922P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.925 (2)	Co1—N3	1.993 (2)
Co1—O2	1.931 (2)	Co1—N6	1.996 (2)
O1—Co1—O2	128.2 (1)	O2—Co1—N3	103.8 (1)
O1—Co1—N3	96.8 (1)	O2—Co1—N6	95.7 (1)
O1—Co1—N6	111.9 (1)	N3—Co1—N6	122.7 (1)

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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