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Bis{5-methyl-2-phenyl-4-[(3-tolylamino-κ*N*)-phenylmethylene]-1*H*-pyrazol-3(4*H*)-onato-κ*O*}-cobalt(II)

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The Co^{II} ion in the title compound, [Co($C_{24}H_{20}N_3O$)$_2$], is chelated by two deprotonated monoanions through their amido N and carbonyl O atoms in a distorted tetrahedral geometry.

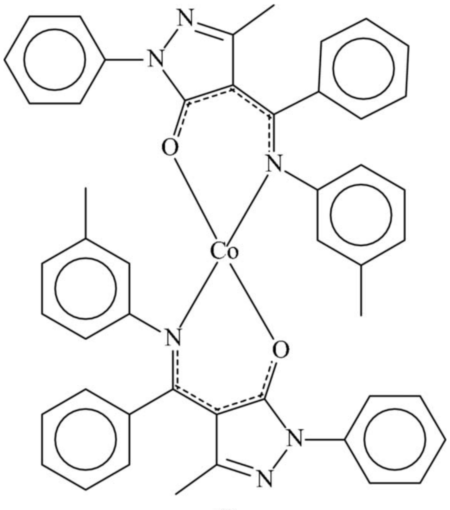
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.155
Data-to-parameter ratio = 21.0

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

Comment

A recent report described the structure of the cobalt(II) complex of 4-[(4-tolylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one, in which the metal atom exists in a tetrahedral environment (Ma *et al.*, 2005). The corresponding cobalt(II) complex of the 3-tolylamino isomer, (I), an organic chelating ligand that has recently been crystallographically authenticated (Qiao *et al.*, 2005), also has the metal atom in a distorted tetrahedral environment (Fig. 1). The bond dimensions involving the metal atom in the two compounds are not significantly different; however, in terms of packing, the 3-isomer is less dense, its density being 1.270 Mg m^{-3} whereas that of the 4-isomer is 1.298 Mg m^{-3} (Ma *et al.*, 2005).



(I)

Experimental

To a chloroform (5 ml) solution of 5-methyl-2-phenyl-4-[(3-tolylamino)phenylmethylene]-1*H*-pyrazol-3(4*H*)-one (Qiao *et al.*, 2005) (40 mg, 0.11 mmol) were added triethylamine (0.155 ml, 0.11 mmol) and cobalt(II) chloride (8 mg, 0.06 mmol) dissolved in ethanol (5 ml). The brown mixture was filtered and the solution set aside for several days to give red crystals in about 80% yield. Elemental analysis calculated for $C_{48}H_{40}CoN_6O_2$: C 72.81, H 5.09, N 10.61%; found: C 72.79, H 5.28, N 10.53%.

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Crystal data

[Co($C_{24}H_{20}N_2O$)$_2$]
M_r = 791.79
Triclinic, $P\overline{1}$
a = 10.0829 (5) Å
b = 12.2184 (7) Å
c = 17.857 (1) Å
α = 99.864 (1)°
β = 94.422 (1)°
γ = 105.554 (1)°
V = 2070.4 (2) Å^3
Z = 2
D_x = 1.270 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3856 reflections
θ = 2.3–20.4°
μ = 0.46 mm^{-1}
T = 295 (2) K
Block, red
0.30 × 0.20 × 0.12 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.874, T_{max} = 0.947
24322 measured reflections
9382 independent reflections
5098 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -15 \rightarrow 15$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.155
S = 0.88
9382 reflections
446 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.933 (2)	Co1—N3	1.969 (2)
Co1—O2	1.932 (2)	Co1—N6	1.982 (2)
O1—Co1—O2	119.3 (1)	O2—Co1—N3	113.3 (1)
O1—Co1—N3	97.1 (1)	O2—Co1—N6	96.8 (1)
O1—Co1—N6	111.1 (1)	N3—Co1—N6	120.8 (1)

The benzene rings were refined as rigid hexagons of 1.39 Å sides. All C atoms were restrained to vibrate in an approximately isotropic manner. H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [aromatic C—H = 0.93 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.

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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

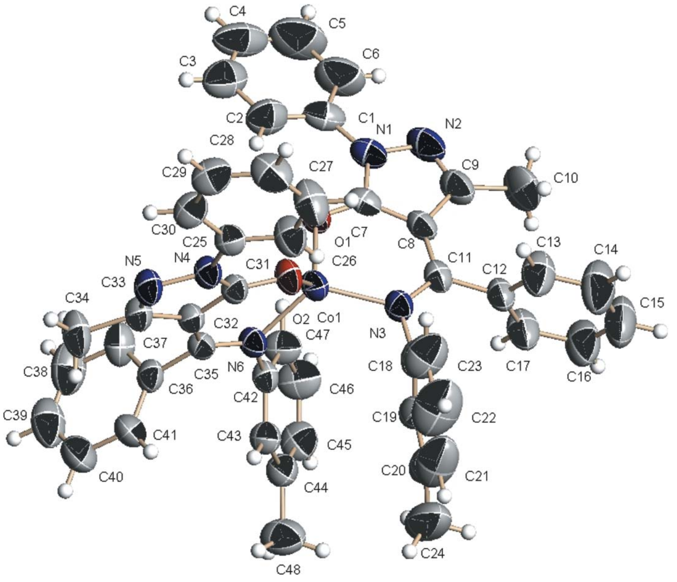

Figure 1
ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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