

Bis[4-methyl-*N*-[(*Z*)-(3-methyl-5-oxo-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-ylidene)(phenyl)-methyl]anilinato- κ^2 *N,O*]cobalt(II)**Rong-Ming Ma,^a Shao-Fa Sun^a
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Key indicators

Single-crystal X-ray study

 $T = 292$ KMean $\sigma(\text{C}-\text{C}) = 0.005$ Å R factor = 0.064 wR factor = 0.182

Data-to-parameter ratio = 17.5

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

The Co atom in the molecule of the title compound, $[\text{Co}(\text{C}_{24}\text{H}_{20}\text{N}_3\text{O})_2]$, is chelated by two deprotonated 4-[(4-tolylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one ligands through the amido N and carbonyl O atoms in a distorted tetrahedral geometry.

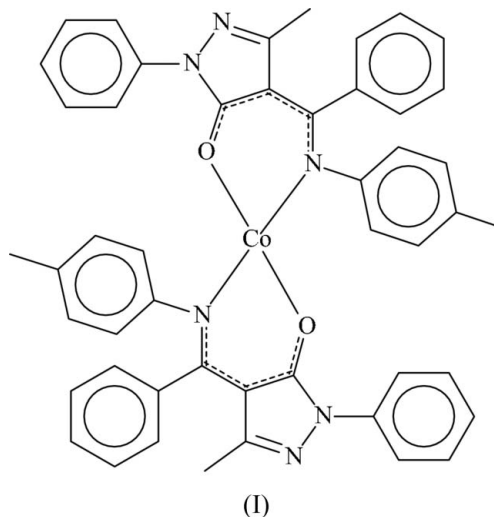
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Comment

The ligand 4-[(benzylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one, whose crystal structure has previously been determined (Jiang *et al.*, 2004), forms a bis-chelated copper complex with a distorted square-planar coordination environment (Bao *et al.*, 2005). In contrast, the title cobalt(II) complex, (I), of the similar organic ligand, 4-[(4-tolylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one (Ma, 2005), features the Co atom in a distorted tetrahedral coordination environment (Fig. 1). The two six-membered chelate rings are oriented essentially perpendicular to each other.

**Experimental**

To a dichloromethane (5 ml) solution of 4-[(4-tolylamino)phenylmethylene]-5-methyl-2-phenylpyrazol-3-one (Ma, 2005) (40 mg, 0.11 mmol) and triethylamine (15 μl , 0.11 mmol) was added cobalt(II) chloride hexahydrate (13 mg, 0.055 mmol) dissolved in ethanol (5 ml). The mixture was filtered and the solution set aside for several days to give dark-red crystals of (I) in about 50% yield. CHN analysis, calculated for $\text{C}_{48}\text{H}_{40}\text{N}_6\text{O}_2\text{Co}$: C 72.81, H 5.09, N 10.66%; found: C 73.09, H 5.34, N 10.39%.

Crystal data

[Co(C₂₄H₂₀N₃O)₂]
M_r = 791.79
 Triclinic, *P* $\bar{1}$
a = 10.6785 (6) Å
b = 13.3996 (8) Å
c = 16.1443 (9) Å
 α = 106.334 (1)°
 β = 96.640 (1)°
 γ = 109.950 (1)°
V = 2025.6 (2) Å³

Z = 2
D_x = 1.298 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3763 reflections
 θ = 2.2–22.5°
 μ = 0.47 mm⁻¹
T = 292 (2) K
 Prism, red
 0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART area-detector diffractometer
 ω and φ scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.786, *T_{max}* = 0.954
 18522 measured reflections

9047 independent reflections
 6469 reflections with *I* > 2σ(*I*)
R_{int} = 0.034
 θ_{max} = 27.5°
h = -13 → 13
k = -17 → 17
l = -20 → 20

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.064
wR(*F*²) = 0.182
S = 1.03
 9047 reflections
 518 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0948P)^2 + 0.5831P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 $\Delta\rho_{max}$ = 0.39 e Å⁻³
 $\Delta\rho_{min}$ = -0.40 e Å⁻³

Table 1 Selected geometric parameters (Å, °).

| | | | |
|-----------|-------------|-----------|-------------|
| Co1—O1 | 1.927 (2) | Co1—N3 | 1.993 (2) |
| Co1—O2 | 1.939 (2) | Co1—N6 | 1.998 (3) |
| O1—Co1—O2 | 116.53 (9) | O1—Co1—N6 | 114.10 (10) |
| O1—Co1—N3 | 96.46 (9) | O2—Co1—N6 | 94.90 (10) |
| O2—Co1—N3 | 121.30 (10) | N3—Co1—N6 | 114.91 (10) |

When refined without any distance restraints, the structure gave short C_{ar}—C_{ar} (ar = aromatic) distances that averaged 1.37 Å. Consequently, all C_{ar}—C_{ar} distances were restrained to 1.395 (5) Å. The aromatic C atoms show somewhat larger than usual displacement ellipsoids, but attempts to model the benzene rings as disordered did not lead to meaningful results. H atoms were positioned geometrically and were included in the refinement in the riding-model approximation, with C—H_{phenyl} = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C), and C—H_{methyl} = 0.96 Å and *U*_{iso}(H) = 1.5*U*_{eq}(C). The methyl groups were rotated to fit the electron density.

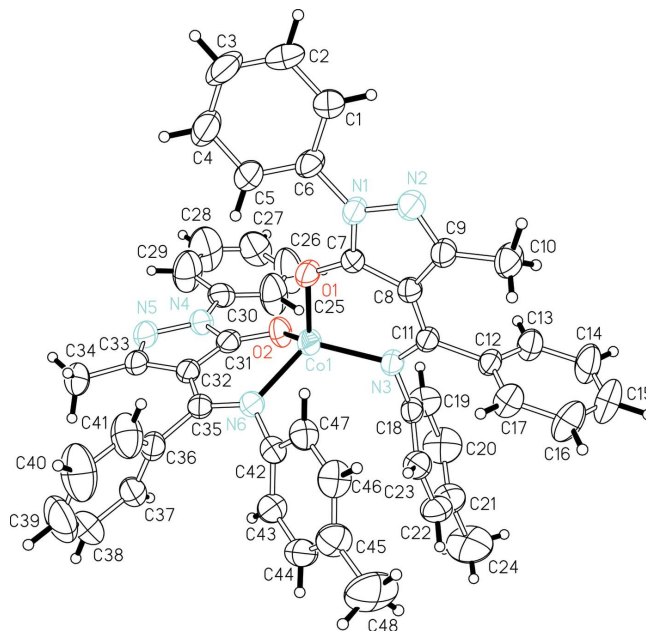


Figure 1 A plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

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.

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References

Bao, F., Feng, J. & Ng, S. W. (2005). *Acta Cryst.* E61, m2393–m2395.
 Bruker (2003). SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.
 Jiang, J.-J., Lü, X.-Q., Bao, F., Kang, B.-S. & Ng, S. W. (2004). *Acta Cryst.* E60, o1149–o1150.
 Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 Ma, R.-M. (2005). *Acta Cryst.* E61, o3264–o3265.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.