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Key indicators

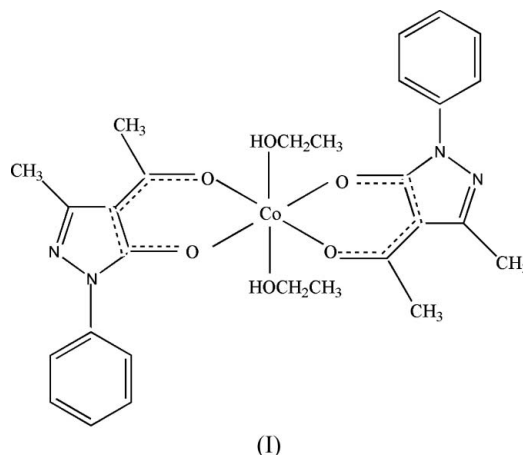
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.038
 wR factor = 0.098
Data-to-parameter ratio = 14.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***trans*-Bis[4-acetyl-3-methyl-1-phenyl-1*H*-pyrazol-
5(4*H*)-onato- $\kappa^2\text{O},\text{O}'$]diethanolcobalt(II)**

In the mononuclear title complex, $[\text{Co}(\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_2)_2(\text{C}_2\text{H}_6\text{O})_2]$, the six-coordinate Co^{II} atom lies on an inversion centre and is coordinated by six O atoms, two from the ethanol molecules and the remaining four from two chelating 4-acetyl-3-methyl-1-phenyl-5-pyrazolonate monovalent anions. $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds involving the ethanol $\text{O}-\text{H}$ and the pyrazolonate N atoms stabilize the structure.

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Comment

Derivatives of pyrazolone play an important role in chelate complexes (Uzoukwu *et al.*, 1996). Interest in understanding the relationship between the coordination modes in such ligands led us to synthesize the title Co^{II} complex, (I), and we report its structure here (Fig. 1).



The Co^{II} atom, located on an inversion centre, assumes a distorted octahedral CoO_6 coordination geometry (Table 1). The two ethanol molecules are mutually *trans*, while the two bidentate 1-phenyl-3-methyl-4-aceto-5-pyrazolone ligands adopt a deprotonated enol form in chelating to the Co^{II} centre *via* their O atoms.

$\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 2) involving the ethanol $\text{O}-\text{H}$ and the pyrazolonate N atoms link adjacent molecules to form chains in approximately orthogonal directions with respect to the central Co^{II} atom.

Experimental

1-Phenyl-3-methyl-4-aceto-5-pyrazolone (0.0932 g, 0.431 mmol) in ethanol (15 ml) was added to $\text{Co}(\text{ClO}_4)_2\cdot 6\text{H}_2\text{O}$ (0.0812 g, 0.222 mmol) in ethanol (15 ml), and the solution was stirred for a few minutes. Orange crystals of (I) were obtained after allowing the solution to stand at room temperature for three weeks.

Crystal data

[Co(C₁₂H₁₁N₂O₂)₂(C₂H₆O)₂]
M_r = 581.52
 Monoclinic, *P*2₁/*n*
a = 9.5694 (13) Å
b = 14.3386 (19) Å
c = 10.7533 (15) Å
 β = 109.070 (2)°
V = 1394.5 (3) Å³
Z = 2

D_x = 1.385 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 5383 reflections
 θ = 2.5–27.8°
 μ = 0.66 mm⁻¹
T = 298 (2) K
 Prism, orange
 0.50 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.733, *T*_{max} = 0.879
 7335 measured reflections

2589 independent reflections
 2380 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.040
 θ _{max} = 25.5°
h = -8 → 11
k = -14 → 17
l = -13 → 11

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.038
wR (*F*²) = 0.098
S = 1.08
 2589 reflections
 181 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 5.209P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.32 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co1—O2	2.0412 (13)	Co1—O3	2.1100 (15)
Co1—O1	2.0746 (14)		
O2—Co1—O1	89.80 (6)	O1—Co1—O3	86.17 (6)
O2—Co1—O3	89.36 (7)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O3—H16...N2 ¹	0.89	1.92	2.810 (2)	174

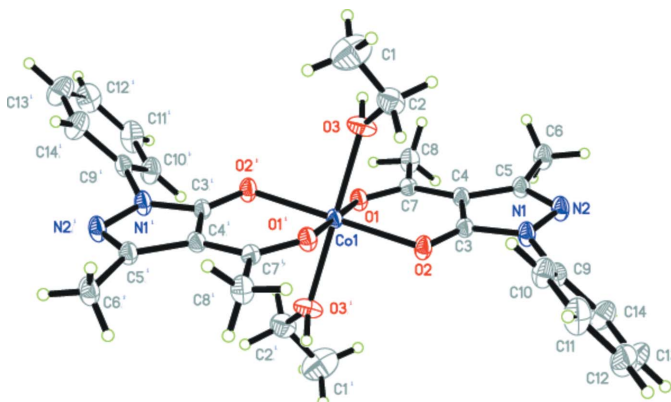
Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$.

Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, -y + 1, -z + 1$].

The hydroxyl H atom was located in a difference Fourier map and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.5_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions, with C—H = 0.93 for phenyl, 0.96 for methyl and 0.97 Å for methylene H atoms, and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2_{\text{eq}}(\text{C})$ for phenyl and methylene H, and 1.5_{eq}(C) for methyl H.

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

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