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Tris(*N*-ethyl-*N*-phenyldithiocarbamato-*S*,*S*′)cobalt(III)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.013 Å
R factor = 0.058
wR factor = 0.185
Data-to-parameter ratio = 16.1

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

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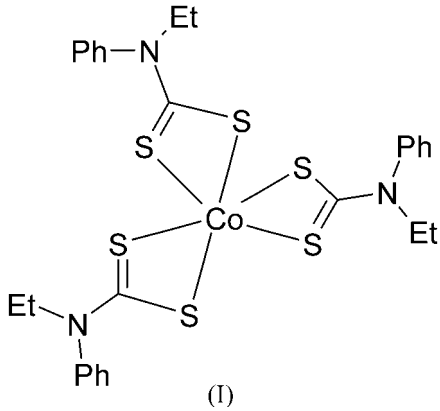
The crystal and molecular structure of the title mononuclear Co^{III} complex, $[Co(EtPhdtc)_3]$ (EtPhdtc is *N*-ethyl-*N*-phenyldithiocarbamate, $C_9H_{10}NS_2$), has been studied by single-crystal X-ray diffraction methods at 293 (2) K.

Comment

The title compound, (I), was prepared in an exchange reaction between a chloroform solution of commercially manufactured vulcanization ultra-accelerator $[Zn(EtPhdtc)_3]$ (commercial designation Vulkacit P Extra; EtPhdtc is *N*-ethyl-*N*-phenyldithiocarbamate) (Debnath & Basu, 1995) and an aqueous solution of cobalt(II) sulfate. The bond lengths in (I) are consistent with average values quoted in the usual sources (*International Tables for Crystallography*, 1992, Vol. C, Table 9.5.1.1).



(I)

Experimental

$[Co(EtPhdtc)_3]$ was prepared by the reaction of a chloroform solution of $[Zn(EtPhdtc)_2]$ and an aqueous solution of cobalt(II) sulfate at room temperature. The dark-brown product was recrystallized from chloroform.

Crystal data

$[Co(C_9H_{10}NS_2)_3]$
M_r = 647.83
Triclinic, $P\overline{1}$
a = 10.193 (2) Å
b = 11.159 (2) Å
c = 14.253 (3) Å
α = 105.14 (3)°
β = 103.09 (3)°
γ = 92.30 (3)°
V = 1515.7 (5) Å^3
Z = 2
D_x = 1.419 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 3.8–9.1°
μ = 1.00 mm^{-1}
T = 293 (2) K
Prism, dark brown
0.6 × 0.3 × 0.3 mm

Data collection

Syntex $P2_1$ diffractometer
θ–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.544, T_{max} = 0.741
6616 measured reflections
6560 independent reflections
2593 reflections with $I > 2\sigma(I)$

R_{int} = 0.082
θ_{max} = 27.5°
$h = -9 \rightarrow 1$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 18$
3 standard reflections
every 100 reflections
intensity decay: 15%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.185
S = 0.86
5379 reflections
334 parameters

H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1151P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—S2	2.256 (2)	Co1—S6	2.263 (2)
Co1—S4	2.255 (2)	Co1—S3	2.267 (2)
Co1—S5	2.259 (2)	Co1—S1	2.279 (2)
S2—Co1—S4	93.33 (8)	S5—Co1—S3	164.15 (7)
S2—Co1—S5	94.74 (7)	S6—Co1—S3	93.84 (7)
S4—Co1—S5	92.41 (8)	S2—Co1—S1	76.13 (7)
S2—Co1—S6	166.96 (7)	S4—Co1—S1	166.80 (7)
S4—Co1—S6	96.57 (8)	S5—Co1—S1	96.32 (8)
S5—Co1—S6	76.43 (7)	S6—Co1—S1	95.09 (8)
S2—Co1—S3	96.76 (7)	S3—Co1—S1	97.00 (8)
S4—Co1—S3	76.09 (7)		

Since the crystal diffracted very weakly, the completeness of the data is just 81.1% to 25° in θ.

Data collection: $P2_1$ *Diffractometer Control Software* (Syntex, 1973); cell refinement: $P2_1$ *Diffractometer Control Software*; data reduction: *XP*21 (Pavelčík, 1993); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1965); software used to prepare material for publication: *SHELXL*97.

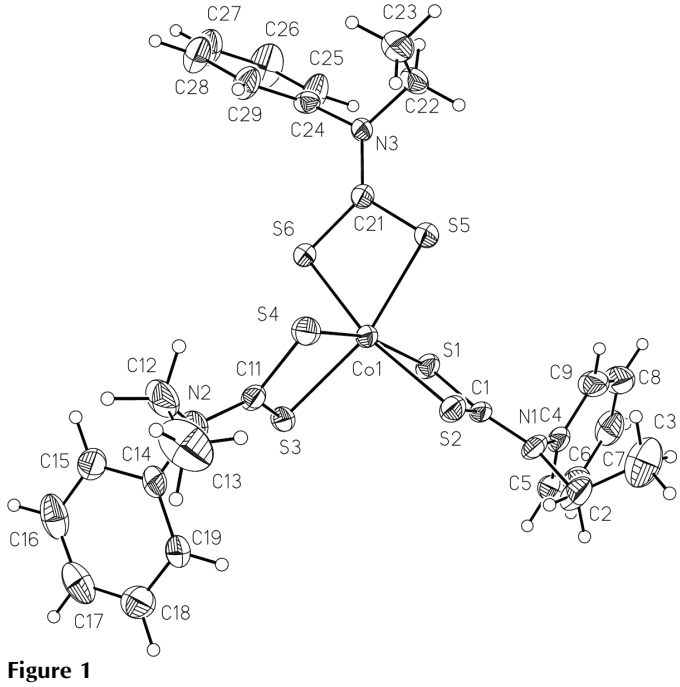


Figure 1
The structure of tris(*N*-ethyl-*N*-phenyldithiocarbamato-*S*,*S*′)cobalt(III) with displacement ellipsoids drawn at the 30% probability level.

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