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Sodium tris(acetylacetonato-κ^2O,O')cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.119
Data-to-parameter ratio = 14.8

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

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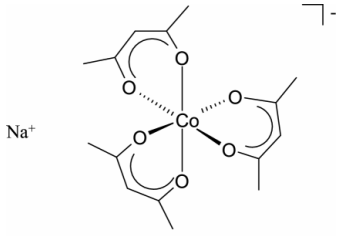
The title compound, Na[Co(acac)$_3$], where acac is acetylacetonate ($C_5H_7O_2$), crystallizes in the rhombohedral space group $R\bar{3}c$. The sodium ion is found to sit on a 32 crystallographic site. The cobalt complex is located on a site of $\bar{3}$ symmetry.

Comment

Metal carboxylate complexes have been the subject of interest for many years (Oldham, 1968; Doedens, 1976). Although a great deal of work has been reported on the synthesis and characterization of various cobalt(III) complexes of the acetylacetonate ligand, only a few cobalt(II) complexes have been reported (Cotton & Elder, 1965, 1966). As part of a general method for the preparation of stable cobalt(II) complexes, we prepared Na[Co(acac)$_3$], (I), and its crystal structure is presented here.



(I)

Experimental

A solution of Co(acac)$_3$ dissolved in methanol was added to a methanol solution of $NaBH_4$. After stirring the reaction mixture for 2 h, the solution was concentrated by removing the solvent *in vacuo*. Light-brown needle-shaped crystals were formed by vapor diffusion of diethyl ether.

Crystal data

Na[Co($C_5H_7O_2$)$_3$]
M_r = 379.24
Rhombohedral, $R\bar{3}c$
a = 16.1201 (19) Å
c = 11.715 (3) Å
V = 2636.3 (7) Å^3
Z = 6
D_x = 1.433 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2493 reflections
θ = 2.5–25.9°
μ = 1.03 mm^{-1}
T = 100 (2) K
Needle, light brown
0.50 × 0.10 × 0.07 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.624, T_{max} = 0.931
6796 measured reflections
548 independent reflections
404 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.0°
h = −19 → 19
k = −19 → 19
l = −14 → 14

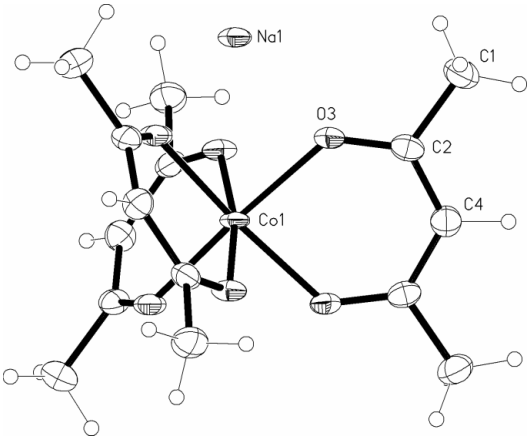


Figure 1
Drawing of $Na[Co(acac)_3]$, with 50% probability displacement ellipsoids.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 10P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.119$	$\Delta\rho_{max} = 0.70$ e Å^{-3}
$S = 1.25$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
548 reflections	
37 parameters	
H-atom parameters constrained	

H-atom positions were refined using a riding model and H-atom displacement parameters were set at 1.2 (1.5 for methyl H atoms) times the U_{eq} vlaue of the bonded atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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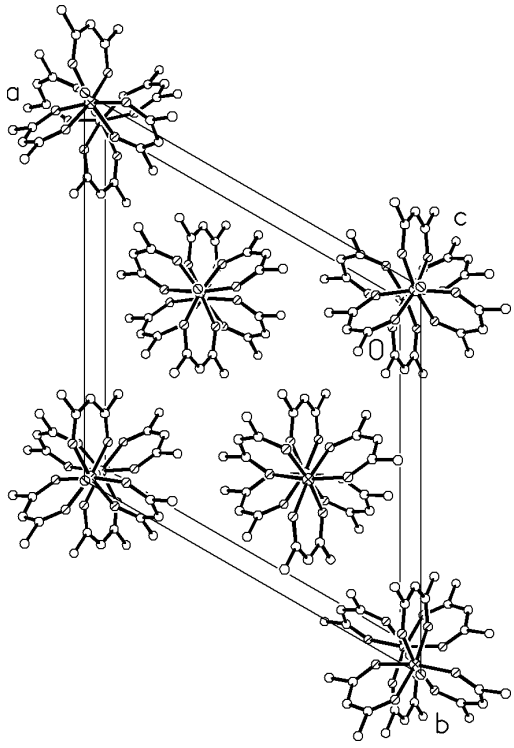

Figure 2
Packing diagram viewed down the *c* axis. The sodium ion is located at a distance of 2.321 (2) Å from the nearest O atom of the acac ligand and 2.9287 (6) Å from the cobalt center.

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