

## Cobalt(II) formate hydroxide

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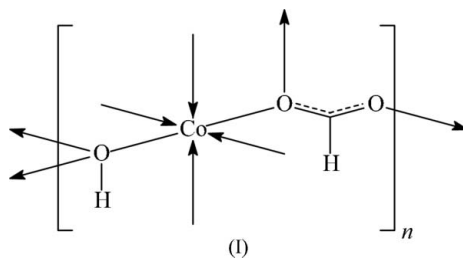
## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{O}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.031  
 $wR$  factor = 0.077  
Data-to-parameter ratio = 12.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title compound, poly[ $\mu_3$ -formato- $\mu_3$ -hydroxo-cobalt(II)],  $[\text{Co}(\text{CHO}_2)(\text{OH})]_n$ , adopts a polymeric three-dimensional network structure arising from the  $\mu_3$ -bridging mode of both the formate and the hydroxide. The Co atom lies in a *fac* octahedron of six O atoms, three of which belong to three different formates and the other three to different hydroxides.

## Comment

The structure of cobalt(II) diformate has been reported recently; the compound was synthesized hydrothermally from cobaltous nitrate and formic acid in dimethylformamide (DMF). It crystallizes with DMF (Fu *et al.*, 2005). With citric acid in place of formic acid, a similar synthesis affords cobalt(II) formate hydroxide, (I) (Fig. 1), the source of formic acid probably resulting from the decomposition of the citric acid. The compound adopts a three-dimensional network structure in which both the formate and hydroxide function in a  $\mu_3$ -bridging mode; the  $\text{Co}^{\text{II}}$  exists in a *fac*-octahedral arrangement; three of the O atoms belong to different formates and the other three to different hydroxides. The formate displays delocalized C—O bonds; one C—O bond is somewhat longer than the other. The O atom involved in the longer bond interacts with two Co atoms whereas the O atom involved in the shorter bond interacts with only one Co atom.



## Experimental

A mixture of cobaltous nitrate hexahydrate (0.23 g, 0.5 mmol), citric acid (0.22 g, 1 mmol) and DMF (8 ml) was heated in a 15 ml Teflon-lined steel bomb at 400 K for 50 d. Red block-shaped crystals were obtained in about 40% yield (based on Co).

## Crystal data

[ $\text{Co}(\text{CHO}_2)(\text{OH})$ ]  
 $M_r = 120.96$   
Trigonal,  $R\bar{3}$   
 $a = 11.698$  (1) Å  
 $c = 11.661$  (1) Å  
 $V = 1381.9$  (2) Å<sup>3</sup>  
 $Z = 18$   
 $D_x = 2.616$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation  
Cell parameters from 1480  
reflections  
 $\theta = 2.7$ – $28.0^\circ$   
 $\mu = 5.37$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
Block, red  
 $0.16 \times 0.11 \times 0.09$  mm

Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.501$ ,  $T_{\max} = 0.644$   
 2498 measured reflections

698 independent reflections  
 667 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -15 \rightarrow 7$   
 $k = -15 \rightarrow 14$   
 $l = -13 \rightarrow 14$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.077$   
 $S = 1.07$   
 698 reflections  
 54 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 11.747P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.62 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.50 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.122 (2)	Co1—O3	2.047 (2)
Co1—O1 <sup>i</sup>	2.156 (2)	Co1—O3 <sup>ii</sup>	2.042 (2)
Co1—O2 <sup>i</sup>	2.149 (2)	Co1—O3 <sup>iii</sup>	2.114 (2)
O1—Co1—O1	79.5 (1)	O1—Co1—O3 <sup>iii</sup>	93.3 (1)
O1—Co1—O2 <sup>i</sup>	84.2 (1)	O2 <sup>i</sup> —Co1—O3	170.8 (1)
O1—Co1—O3	92.9 (1)	O2 <sup>i</sup> —Co1—O3 <sup>ii</sup>	88.4 (1)
O1—Co1—O3 <sup>ii</sup>	102.6 (1)	O2 <sup>i</sup> —Co1—O3 <sup>iii</sup>	97.0 (1)
O1—Co1—O3 <sup>iii</sup>	172.5 (1)	O3—Co1—O3 <sup>ii</sup>	100.8 (1)
O1—Co1—O2 <sup>i</sup>	83.9 (1)	O3—Co1—O3 <sup>iii</sup>	84.8 (1)
O1—Co1—O3	86.9 (1)	O3 <sup>ii</sup> —Co1—O3 <sup>iii</sup>	84.9 (1)
O1—Co1—O3 <sup>ii</sup>	171.8 (1)		

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

H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (1) Å and C—H = 0.95 (1) Å; their displacement parameters were freely refined.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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.

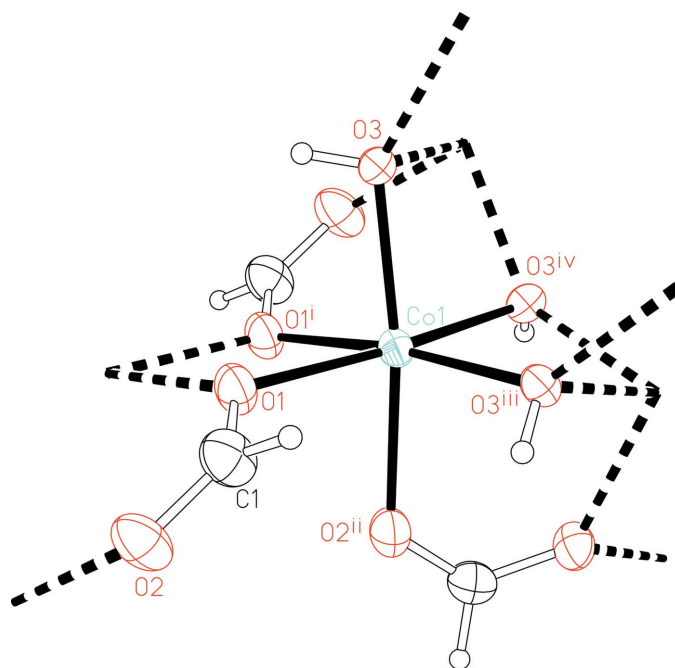


Figure 1

ORTEPII (Johnson, 1976) plot, illustrating the coordination geometry of Co and the  $\mu_3$ -bridging modes of the  $-\text{HCO}_2$  and  $-\text{OH}$  groups. Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as spheres of arbitrary radii. The symmetry codes are as given in Table 1.

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