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The rhombohedral polymorph of scandium formate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(O–C) = 0.001 Å
R factor = 0.027
wR factor = 0.078
Data-to-parameter ratio = 23.2

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

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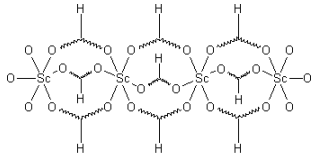
The structure of the rhombohedral polymorph of scandium formate, $[Sc(HCO_3)_2]$, consists of infinite chains. The Sc atom has a nearly ideal octahedral environment, with an Sc—O distance of 2.0794 (9) Å.

Comment

Owing to the ability of carboxylic acids to coordinate metals in different modes, even the simplest metal carboxylates exhibit polymorphism. The monoclinic modification of scandium formate was first described in 1968 (Gusejnova *et al.*, 1968) and confirmed in 1990 (Hasek *et al.*, 1990).



(I)

Here we report the crystal structure of the rhombohedral modification of scandium formate, (I), which is less dense than the monoclinic form (D_x = 1.95 and 2.00 Mg m^{-3} for the rhombohedral and monoclinic modifications, respectively). The Sc atom in (I) has a nearly ideal octahedral environment, with an Sc—O distance of 2.0794 (1) Å (Table 1). ScO_6 octahedra are linked into three-dimensional polymeric chains, similar to those of scandium acetate (Fuchs & Strahle, 1984).

Experimental

The compound studied is an analytical-grade commercial reagent (Novosibirsk Rare Metal Plant).

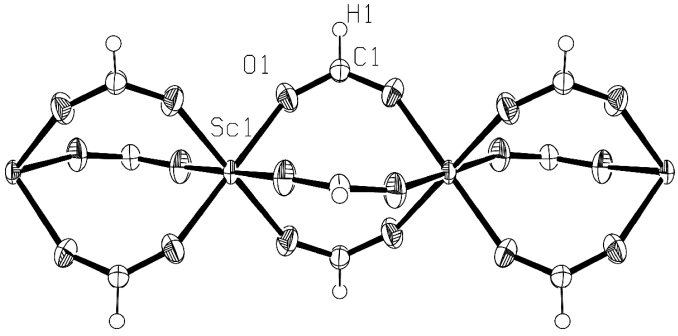


Figure 1
ORTEP perspective view of the $\{Sc(HCOO)_3\}_n$ infinite chain, with displacement ellipsoids drawn at the 50% probability level.

Crystal data

$[Sc(HCO_3)_2]$	Mo $K\alpha$ radiation
M_r = 180.01	Cell parameters from 24 reflections
Hexagonal, $R\bar{3}c$	θ = 14.9–16.7°
a = 10.7252 (9) Å	μ = 1.20 mm^{-1}
c = 8.9854 (8) Å	T = 293.0 (3) K
V = 895.11 (13) Å^3	Needle, colourless
Z = 6	0.16 × 0.08 × 0.08 mm
D_x = 2.004 Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.056
$\omega/2\theta$ scans	θ_{max} = 34.9°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -17 \rightarrow 17$
T_{min} = 0.798, T_{max} = 0.908	$k = -17 \rightarrow 17$
4738 measured reflections	$l = -14 \rightarrow 14$
440 independent reflections	3 standard reflections
388 reflections with $I > 2\sigma(I)$	frequency: 120 min
	intensity decay: 2%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.078	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
440 reflections	
19 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

Sc1—O1	2.0794 (9)	C1—H1	0.95 (3)
O1—C1	1.2414 (11)		
O1^{i}—Sc1—O1^{ii}	92.56 (4)	O1—Sc1—O1^{ii}	87.44 (4)

Symmetry codes: (i) $-x, -y, -z$; (ii) $y, -x+y, -z$.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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