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Strontium dihydrogenphosphite

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(P–O) = 0.006 Å
H-atom completeness 0%
R factor = 0.068
wR factor = 0.182
Data-to-parameter ratio = 13.2

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

The crystal structure of strontium dihydrogenphosphite, $Sr(H_2PO_3)_2$, contains eightfold-coordinated Sr ions connected by dihydrogenphosphite anions so that a layer structure is formed.

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Comment

Crystal structure analyses of alkaline-earth phosphites have been undertaken for several decades. The first one was $MgHPO_3{\cdot}6H_2O$ (Corbridge, 1956); this structure was later reinvestigated by neutron and X-ray diffraction (Powell *et al.*, 1994). $Ca(H_2PO_3)_2{\cdot}H_2O$ was reported by Larbot *et al.* (1984).

We present here the crystal structure of $Sr(H_2PO_3)_2$ (Fig. 1). The framework of the title compound can be described as layers perpendicular to the crystallographic *c* axis (Fig. 2). Sr is coordinated by eight O atoms, with bond distances ranging from 2.489 (5) to 2.753 (6) Å. There are three different types of O atoms: O13 is bonded only to P; O11 and O21 are bonded to P and one Sr atom; O12, O22 and O23 are bonded to P and two different Sr atoms. The average P—O distance of 1.54 (5) Å is similar to those reported in other dihydrogenophosphites: 1.523 Å in $Ca(H_2PO_3)_2{\cdot}H_2O$ or 1.513 Å in $Zn(H_2PO_3)_3{\cdot}0.333H_2O$ (Durand *et al.*, 1992).

Experimental

25 ml of $SrCl_2{\cdot}6H_2O$ (0.1 *M*) was added to a 25 ml aliquot of 1 *M* H_3PO_3 in water. The resulting solution was stirred for 8 h, at 333 K, before being left at room temperature. After a few days, large colourless block-shaped crystals were deposited. These were filtered off and washed with a solution of ethanol (80%).

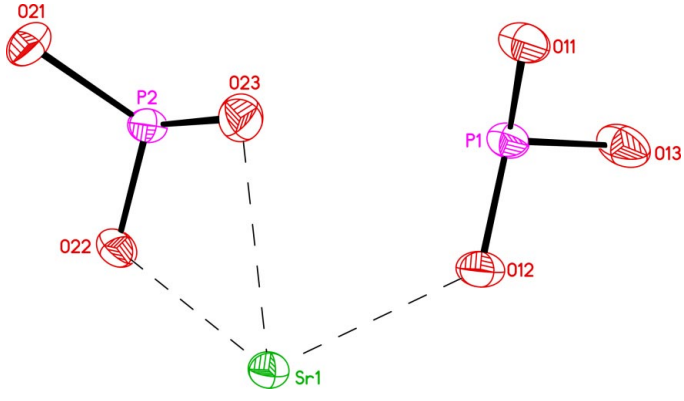

Figure 1
The asymmetric unit of the title compound with atom labelling and displacement ellipsoids drawn at the 50% probability level.

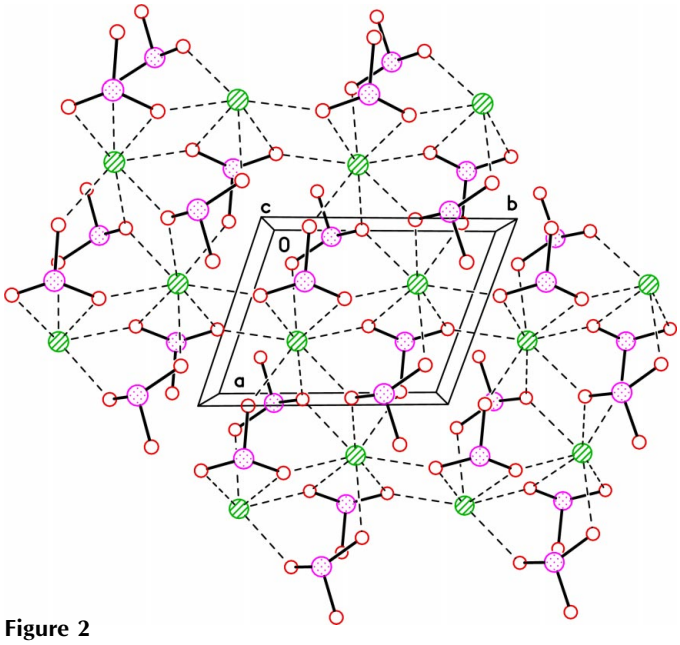

Figure 2
The crystal structure of $Sr(H_2PO_3)_2$, viewed perpendicular to the *c* axis. Key: Sr green, P violet and O red.

Crystal data

$Sr(H_2PO_3)_2$
M_r = 249.59
Triclinic, $P\overline{1}$
a = 5.797 (1) Å
b = 7.206 (1) Å
c = 8.068 (1) Å
α = 97.87 (1)°
β = 104.51 (1)°
γ = 106.55 (1)°
V = 304.78 (8) Å^3
Z = 2
D_x = 2.720 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 688 reflections
θ = 3.6–28.2°
μ = 9.33 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multiscan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.121, T_{max} = 0.394
1079 measured reflections
1079 independent reflections
1045 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
$h = -6 \rightarrow 6$
$k = -8 \rightarrow 8$
$l = 0 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.182
S = 1.09
1079 reflections
82 parameters
H atoms not located
$w = 1/[\sigma^2(F_o^2) + (0.1484P)^2 + 0.2956P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −3.05 e Å^{-3}

Table 1
Selected interatomic distances (Å).

Sr1—O23^{i}	2.489 (5)	Sr1—O21^{iv}	2.753 (6)
Sr1—O22^{ii}	2.513 (5)	P1—O12	1.504 (5)
Sr1—O12^{iii}	2.537 (5)	P1—O11	1.502 (5)
Sr1—O12	2.593 (5)	P1—O13	1.591 (6)
Sr1—O11^{i}	2.682 (5)	P2—O22	1.495 (5)
Sr1—O23	2.687 (5)	P2—O23	1.515 (5)
Sr1—O22	2.723 (5)	P2—O21	1.608 (5)

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 2-y, 1-z$; (iii) $-x, 1-y, 1-z$; (iv) $x-1, y, z$.

The H atoms could not be located and were therefore not included in the refinement process.

Data collection: *X-Area* (Stoe & Cie, 2001); cell refinement: *X-Area*; data reduction: *X-Area*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

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