$wR = 0.038$
$S = 1.7$
1268 reflections
48 parameters
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} < 0.005$
$\Delta\rho_{max} = 0.6$ e Å^{-3}
$\Delta\rho_{min} = -1.0$ e Å^{-3}

Extinction coefficient: 12.6×10^{-6}
Atomic scattering factors, including f' and f'', from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Li	0	0.2642 (5)	1/4	0.0184 (7)
Ga	0	0.90154 (2)	1/4	0.00461 (3)
Si	0.29673 (3)	0.09112 (3)	0.26088 (6)	0.00443 (5)
O(1)	0.11357 (8)	0.08377 (8)	0.1442 (1)	0.0054 (1)
O(2)	0.36547 (8)	0.26160 (9)	0.3232 (1)	0.0086 (1)
O(3)	0.35682 (7)	0.0001 (1)	0.0491 (2)	0.0096 (1)

Table 2. *Selected geometric parameters* (Å, °)

Si tetrahedron		Ga octahedron		
Si—O(1)	1.644 (1)	Ga—O(1)*A*1,*B*1		2.085 (1)
Si—O(2)	1.589 (1)	Ga—O(1)*A*2,*B*2		1.987 (1)
Si—O(3)*A*1	1.620 (1)	Ga—O(2)*C*1,*D*1		1.893 (1)
Si—O(3)*A*2	1.626 (1)	Mean of six		1.988
Mean of four	1.620			
		O(1)*A*1—O(1)*B*1		2.763 (1)
O(1)—O(2)	2.728 (1)	O(2)*C*1—O(2)*D*1		2.930 (1)
O(1)—O(3)*A*1	2.642 (1)	O(1)*A*1—O(2)*C*1	×2	2.769 (1)
O(1)—O(3)*A*2	2.654 (1)	O(1)*A*1—O(1)*A*2	×2	3.000 (1)
O(2)—O(3)*A*1	2.651 (1)	O(1)*A*2—O(2)*C*1	×2	2.863 (1)
O(2)—O(3)*A*2	2.554 (1)	O(1)*A*2—O(2)*D*1	×2	2.732 (1)
O(3)*A*1—O(3)*A*2	2.634 (1)	O(1)*A*1—O(1)*B*2	×2	2.608 (1)
Si—Si	3.0620 (4)	Ga—Ga		3.1280 (1)
O(1)—Si—O(2)	115.05 (4)	O(1)*A*1—Ga—O(1)*B*1		83.00 (3)
O(1)—Si—O(3)*A*1	108.04 (4)	O(1)*A*1—Ga—O(2)*C*1	×2	88.08 (3)
O(1)—Si—O(3)*A*2	108.49 (4)	O(1)*A*1—Ga—O(1)*A*2	×2	94.88 (3)
O(2)—Si—O(3)*A*1	111.39 (5)	O(1)*A*1—Ga—O(1)*B*2	×2	79.63 (3)
O(2)—Si—O(3)*A*2	105.19 (4)	O(1)*A*2—Ga—O(2)*C*1	×2	95.10 (3)
O(3)*A*1—Si—O(3)*A*2	108.46 (4)	O(1)*A*2—Ga—O(2)*D*1	×2	89.51 (3)
		O(2)*C*1—Ga—O(2)*D*1		101.40 (3)
Li antiprism				
Li—O(1)*A*1,*B*1	2.073 (3)	Si—O(3)—Si		141.21 (5)
Li—O(2)*C*2,*D*2	2.181 (1)	Ga—O(1)—Ga		100.37 (3)
Li—O(3)*C*1,*D*1	2.466 (3)	O(3)—O(3)—O(3)		180.00 (1)
Mean of six	2.240			

The calculations were initiated with the atomic parameters of $LiAlSi_2O_6$ given by Clark, Appleman & Papike (1969). All calculations were performed with the *SDP* program system (B. A. Frenz & Associates, Inc., 1982).

Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71629 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1040]

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Strontium Cobalt(II) Diarsenate

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Abstract

The novel compound, $SrCoAs_2O_7$, has been obtained from a hydrothermal reaction. $SrCoAs_2O_7$ adopts a tunnel structure and its framework consists of corner-sharing CoO_5 square pyramids and As_2O_7 groups. Sr atoms are located in the pentagonal-shaped tunnels, which are formed by the edges of two square pyramids and three arsenate tetrahedra.

Comment

Recently, a large number of new structures in the *A*–V–P–O system, where *A* includes alkali, alkaline-earth and transition-metal cations, have been synthesized under hydrothermal conditions (Kang, Lee, Wang & Lii, 1992; Lii, 1992; Lii, Wen, Su & Chueh, 1992). These phosphates show a variety of new structural types with tunnel or layer structures. However, little structural work on transition-metal arsenates has been reported. Recently, we noted that single crystals of $VO(H_2AsO_4)_2$ could be grown under hydrothermal conditions (Wang & Lee, 1991). Subsequent research revealed that many vanadium arsenates containing alkali or alkaline-earth metals can also be obtained by hydrothermal methods (Cheng & Wang, 1992; Wang & Cheng, 1993). The present study is an extention of our previous work on the cobalt arsenate system.

The title compound was obtained as violet crystals by heating a reaction mixture of $Co(OH)_2$ (0.4639 g), $Sr(OH)_2.8H_2O$ (1.3267 g) and 12 ml 13.3% aq. H_3AsO_4 in a 23 ml teflon-lined autoclave at 503 K for 4 d followed by slow cooling (5 K h^{-1}) to room temperature.

The crystal structure is isotypic with those of $SrCoP_2O_7$ (Riou & Raveau, 1991) and $CaCuP_2O_7$ (Riou & Goreaud, 1990). The Co atom in $SrCoAs_2O_7$ is close to the centre of the CoO_5 square pyramid, as in its phosphate analogue, unlike the Cu atom in $CaCuP_2O_7$ which is close to the square basal plane.

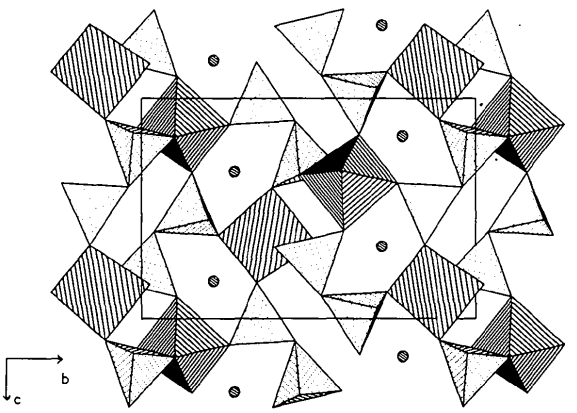

Fig. 1. Polyhedral representation of $SrCoAs_2O_7$ projected along the *a* axis. The corners of the square pyramids and tetrahedra are O atoms. The Co and As atoms are at the centre of each square pyramid and tetrahedron, respectively.

Experimental

Crystal data

$SrCoAs_2O_7$
M_r = 408.4
Monoclinic
$P2_1/n$
a = 5.520 (1) Å
b = 8.391 (2) Å
c = 13.083 (3) Å
β = 90.90 (2)°
V = 605.9 (3) Å^3
Z = 4
D_x = 4.477 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 20 reflections
θ = 6–13°
μ = 22.365 mm^{-1}
T = 297 K
Acicular
0.28 × 0.06 × 0.05 mm
Violet

Data collection

Nicolet *R3m/V* diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical, ψ scans
T_{min} = 0.699, T_{max} = 0.856
1890 measured reflections
1394 independent reflections
1048 observed reflections [$I \geq 3\sigma(I)$]

R_{int} = 0.017
θ_{max} = 27.5°
h = 0 → 7
k = 0 → 10
l = −17 → 17
3 standard reflections monitored every 50 reflections
intensity variation: 2.5%

Refinement

Refinement on F
R = 0.0268
wR = 0.0284
S = 0.92
1048 reflections
101 parameters
$w = 1/[\sigma^2(F) + 0.0008F^2]$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Extinction correction: $F^* = F[1 + (0.002 \times \chi F^2/\sin 2\theta)]^{-1/4}$
Extinction coefficient: χ = 0.00102 (11)

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Sr	0.2892 (1)	0.3300 (1)	0.2808 (1)	0.010 (1)
As(1)	0.7458 (1)	0.5246 (1)	0.1621 (1)	0.007 (1)
As(2)	0.3243 (1)	0.1955 (1)	0.9857 (1)	0.007 (1)
Co	0.8312 (2)	0.1413 (1)	0.1097 (1)	0.009 (1)
O(1)	0.6543 (8)	0.3367 (5)	0.1523 (4)	0.011 (1)
O(2)	0.6666 (9)	0.4016 (6)	0.3930 (3)	0.012 (1)
O(3)	0.9566 (8)	0.1190 (6)	0.2661 (3)	0.011 (1)
O(4)	0.7786 (9)	0.1020 (6)	0.4614 (3)	0.011 (1)
O(5)	0.4726 (8)	0.0474 (5)	0.2961 (4)	0.012 (1)
O(6)	0.1201 (8)	0.3442 (6)	0.4748 (4)	0.012 (1)
O(7)	0.1980 (8)	0.1736 (6)	0.0993 (3)	0.011 (1)

Table 2. *Selected lengths* (Å) *and angles* (°)

Co—O(1)	1.992 (5)	Co—O(6^{ii})	2.103 (5)
Co—O(2^i)	2.012 (5)	Co—O(7^{iii})	2.049 (5)
Co—O(3)	2.157 (5)		
As(1)—O(1)	1.660 (5)	As(2)—O(2^{iv})	1.691 (5)
As(1)—O(3^{vii})	1.671 (5)	As(2)—O(4^{iv})	1.746 (5)
As(1)—O(4^{vii})	1.744 (4)	As(2)—O(7^v)	1.662 (5)
As(1)—O(5^{vii})	1.651 (4)	As(2)—O(6^{vi})	1.675 (5)
Sr—O(1)	2.645 (5)	Sr—O(5)	2.586 (5)
Sr—O(2)	2.599 (5)	Sr—O(6)	2.720 (5)
Sr—O(3^{ix})	2.556 (5)	Sr—O(5^{viii})	2.526 (5)
Sr—O(3^{vii})	2.872 (5)	Sr—O(7)	2.753 (5)
O(1)—Co—O(3)	87.6 (2)	O(1)—Co—O(2^i)	146.2 (2)
O(3)—Co—O(2^i)	85.9 (2)	O(1)—Co—O(6^{ii})	85.4 (2)
O(3)—Co—O(6^{ii})	165.0 (2)	O(2^i)—Co—O(6^{ii})	92.7 (2)
O(1)—Co—O(7^{iii})	113.5 (2)	O(3)—Co—O(7^{iii})	76.8 (2)
O(2^i)—Co—O(7^{iii})	97.2 (2)	O(6^{ii})—Co—O(7^{iii})	118.1 (2)
O(1)—As(1)—O(3^{vii})	106.7 (2)	O(2^{iv})—As(2)—O(4^{iv})	105.5 (2)
O(3^{vii})—As(1)—O(4^{vii})	107.6 (2)	O(4^{iv})—As(2)—O(6^{vi})	108.5 (2)
O(3^{vii})—As(1)—O(5^{vii})	113.2 (2)	O(4^{iv})—As(2)—O(7^v)	102.1 (2)
O(1)—As(1)—O(4^{vii})	105.3 (2)	O(2^{iv})—As(2)—O(6^{vi})	109.5 (2)
O(1)—As(1)—O(5^{vii})	114.8 (2)	O(2^{iv})—As(2)—O(7^v)	111.7 (2)
O(4^{vii})—As(1)—O(5^{vii})	108.8 (2)	O(6^{vi})—As(2)—O(7^v)	118.5 (2)
As(1)—O(4)—As(2)	122.7 (3)		
O(1)—Sr—O(2)	75.1 (1)	O(1)—Sr—O(5)	76.5 (1)
O(2)—Sr—O(5)	81.9 (1)	O(1)—Sr—O(6)	150.2 (1)
O(2)—Sr—O(6)	75.4 (1)	O(5)—Sr—O(6)	96.2 (1)
O(1)—Sr—O(7)	66.0 (1)	O(2)—Sr—O(7)	137.0 (1)
O(5)—Sr—O(7)	72.2 (1)	O(6)—Sr—O(7)	139.9 (1)
O(1)—Sr—O(3^{ix})	121.3 (1)	O(2)—Sr—O(3^{ix})	140.4 (1)
O(5)—Sr—O(3^{ix})	69.5 (1)	O(6)—Sr—O(3^{ix})	81.0 (1)
O(7)—Sr—O(3^{ix})	58.9 (1)	O(1)—Sr—O(3^{vii})	57.8 (1)
O(2)—Sr—O(3^{vii})	62.4 (1)	O(5)—Sr—O(3^{vii})	126.8 (1)
O(6)—Sr—O(3^{vii})	109.8 (1)	O(7)—Sr—O(3^{vii})	107.5 (1)
O(3^{ix})—Sr—O(3^{vii})	157.1 (1)	O(1)—Sr—O(5^{viii})	99.7 (1)
O(2)—Sr—O(5^{viii})	120.4 (1)	O(5)—Sr—O(5^{viii})	156.1 (1)
O(6)—Sr—O(5^{viii})	97.9 (1)	O(7)—Sr—O(5^{viii})	84.5 (1)
O(3^{ix})—Sr—O(5^{viii})	93.7 (1)	O(3^{vii})—Sr—O(5^{viii})	65.4 (1)
O(1)—Sr—O(7^{viii})	105.9 (1)	O(2)—Sr—O(7^{viii})	61.1 (1)
I(5)—Sr—O(7^{viii})	139.8 (1)	O(6)—Sr—O(7^{viii})	61.4 (1)
O(7)—Sr—O(7^{viii})	146.4 (1)	O(3^{ix})—Sr—O(7^{viii})	130.9 (1)
O(3^{vii})—Sr—O(7^{viii})	49.7 (1)	O(5^{viii})—Sr—O(7^{viii})	64.2 (1)

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

Data collection: Nicolet *R3m/V* diffractometer control program. Cell refinement: *P3/PC Diffractometer Program* (Siemens, 1989). Data reduction: *XDISK* (Siemens, 1991). Programs used to solve and refine structure: *SHELXTL-Plus* (Sheldrick, 1991). Software used to generate structural plots and prepare material for publication: *SHELXTL-Plus*.

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Lists of structure factors, anisotropic displacement parameters, complete geometry and equivalent atoms bonded to unique atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71633 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: BR1042]

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