STRUCTURE REPORTS

for 1985

Volume 52A

METALS AND INORGANIC SECTIONS

General editor

G. Ferguson

Section editor

J. Trotter

Published for the

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

by

D. REIDEL PUBLISHING COMPANY

A MEMBER OF THE KLUWER ACADEMIC PUBLISHERS GROUP

DORDRECHT / BOSTON / LANCASTER / TOKYO

First published in 1986

ISSN 0166-6983

ISBN 90-277-2385-0

Printed in the Netherlands

INTRODUCTION

The present volume continues the aim of Structure Reports to present critical accounts of all crystallographic structure determinations. Details of the arrangement in the volumes, symbols used etc. are given in previous volumes (e.g. 41B or 42A, pages vi–viii).

University of Guelph,
Guelph, Ontario, Canada

G. FERGUSON

15 July 1986

TABLE OF CONTENTS

STRUCTURE REPORTS

SECTION I

METALS

Edited by

J. Trotter
(University of British Columbia)

ARRANGEMENT

As in previous volumes the arrangement in the Metals section is approximately, but not strictly, alphabetical, and to find particular substances the subject index or formula index should be used.

ALKALI-METAL RHENIUM SULPHIDES and SELENIDES
$M_4Re_6X_{12}$ or 13 (M = K, Rb, Cs; X = S, Se)

W. BRONGER, H.-J. MIESSEN, R. NEUGRÖSCHEL, D. SCHMITZ and M. SPANGENBERG, 1985. Z. anorg. Chem. **525**, 41-53.

Monoclinic, Z = 4. Ag radiation.

		a (Å)	b (Å)	c (Å)	β	R
$Cs_4Re_6Se_{13}$	C2/c	10,244	17,792	14,190	100,89	0,068
$Cs_4Re_6S_{9,45}Se_{3,55}$	C2/c	10,203	17,511	13,866	101,46	0,082
$Rb_4Re_6S_{13}$	C2/c	9,773	16,584	13,865	99,82	0,078
$Rb_2K_2Re_6S_{13}$	C2/c	9,896	16,543	13,611	100,76	0,066
$Rb_4Re_6Se_{12}$	C2/c	17,487	10,024	12,350	90,59	0,063
$K_4Re_6Se_{12}$	C2/c	17,167	10,029	12,293	91,37	0,047

The structures (Fig. 1) contain Re_6X_8 clusters linked by X and X_2 bridges. Re-Re = 2.60-2.66 A.

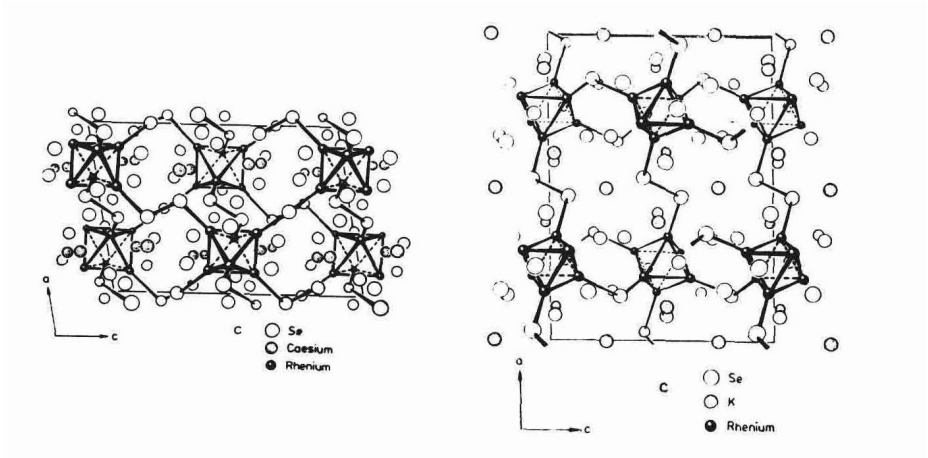


Fig. 1. Structures of $Cs_4Re_6Se_{13}$ (left) and $K_4Re_6Se_{12}$ (right).

ALUMINUM ARSENIC POTASSIUM
$K_3Al_2As_3$

G. CORDIER, H. OCHMANN and H. SCHÄFER, 1985. Rev. Chim. Minér., **22**, 58-63.

Monoclinic, $P2_1/m$, a = 10.494, b = 5.991, c = 7.534 A, β = 110.5°, Z = 2. R = 0.034 for 1407 reflexions.

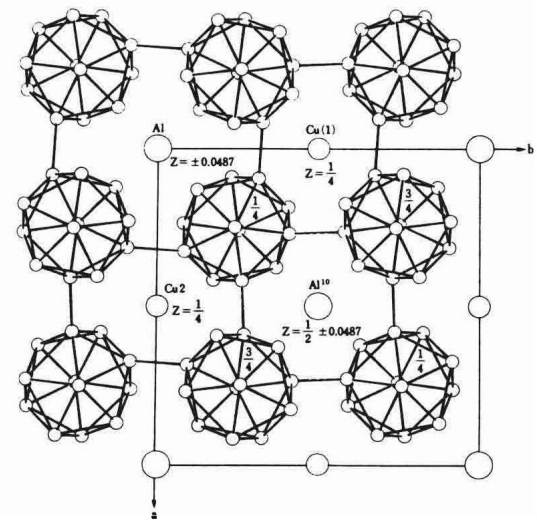
The structure contains $(Al_2As_3^{3-})_\infty$ chains of edge-sharing $AlAs_4$ tetrahedra, linked by K^+ ions.

ALUMINUM BORON COPPER
$AlCu_{0.79}B_{25}$

I. HIGASHI and Y. TAKAHASHI, 1985. J. Less-Common Metals, **108**, 177-188.

Tetragonal, $P\bar{4}n2$, a = 9.002, c = 5.069 A, Z = 2. Mo radiation, R = 0.053 for 874 reflexions.

The boron framework is essentially as in tetragonal α-B (1), with Al in a large hole surrounded tetrahedrally by four B_{12} icosahedra, but distributed in two sites separated by 0.5 A (Fig. 1). Cu atoms are in two holes, with 76.0 and 2.8% occupancies. B-B = 1.68-2.03, Al-B = 2.23-2.78, Cu-B = 1.91-2.69 A.



		x	y	z
B(1)	8i	0.3259	0.0832	0.4050
B(2)	8i	0.2369	0.0809	0.0850
B(3)	8i	0.1304	0.1232	0.3803
B(4)	8i	0.0901	0.2303	0.0856
B(5)	8i	0.0937	0.3140	0.4128
B(6)	8i	0.2485	0.2404	0.5848
B(7)	2b	0	0	1/2
Al	4e	0	0	0.0487
Cu(1)	2c	0	1/2	1/4
Cu(2)	2d	1/2	0	1/4

Fig. 1. Structure of $AlCu_{0.79}B_{25}$ (Al occupancy = 0.5).

1. Structure Reports, **15**, 137; **22**, 211.

ALUMINUM EUROPIUM
AlEu

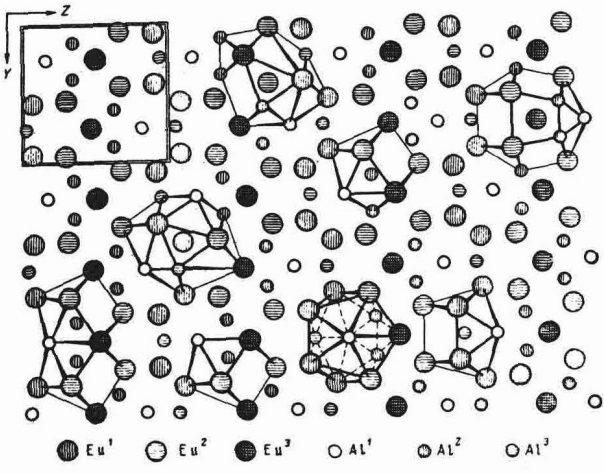
N.B. MANJAKO, I.V. ROŽDESTVENSKAJA, O.S. ZAREČNJUK and T.I. JANSON, 1985. Kristallografija, **30**, 484-487 [Soviet Physics - Crystallography, **30**, 280-282].

Orthorhombic, Pmmn, a = 5.806, b = 9.652, c = 10.088 A, Z = 10. Mo radiation, R = 0.055 for 559 reflexions.

Atomic positions

		x	y	z
Eu(1)	in 4(e)	1/4	0.5683	0.8151
Eu(2)	4(e)	1/4	0.4482	0.6889
Eu(3)	2(b)	1/4	3/4	0.4956
Al(1)	4(f)	0.490	3/4	0.817
Al(2)	4(e)	1/4	0.387	0.370
Al(3)	2(a)	1/4	1/4	0.957

New structure type (Fig. 1), closely related to those of AlCe (1) and AlDy (2).



Interatomic Distances (Å)

Eu1	-1Al3	3.333(7)	Al1	-1Al3	2.737(18)
	-1Al2	3.365(13)		-2Al2	2.754(15)
	-2Al3	3.419(2)		-1Al1	2.790(18)
	-1Eu1	3.507(3)		-1Al1	3.018(18)
	-2Al1	3.516(10)		-2Eu2	3.478(7)
	-2Al1	3.564(7)		-2Eu1	3.516(10)
	-2Eu1	3.623(2)		-1Eu3	3.527(12)
	-2Eu2	3.695(2)		-2Eu1	3.564(7)
	-1Eu2	4.162(3)			
	-1Eu3	4.297(3)	Al2	-1Al2	2.654(20)
				-2Al1	2.754(15)
Eu2	-1Al2	3.270(12)		-1Eu2	3.270(12)
	-1Al3	3.314(13)		-2Eu2	3.363(7)
	-2Al2	3.363(7)		-1Eu1	3.365(13)
	-2Al1	3.478(7)		-2Eu3	3.468(7)
	-1Eu3	3.506(3)		-1Eu3	3.723(14)
	-2Eu1	3.695(2)			
	-1Eu2	3.826(3)	Al3	-2Al1	2.737(18)
	-2Eu3	3.944(3)		-2Eu2	3.314(13)
	-1Eu1	4.162(3)		-2Eu1	3.333(7)
	-1Al2	4.564(13)		-4Eu1	3.419(2)
Eu3	-4Al2	3.468(7)			
	-2Eu2	3.506(3)			
	-2Al1	3.527(12)			
	-2Al2	3.723(14)			
	-1Eu2	3.944(3)			
	-2Eu1	4.297(3)			

Fig. 1. Structure of AlEu.

1. Structure Reports, **43A**, 8.
2. Ibid., **32A**, 8.

ALUMINUM TERNARY ALLOYS
$Ca_4Cd_5Al_3$, $CaAg_4Al_7$, $MM'_{6.5}Al_{6.5}$

G. CORDIER, E. CZECH and H. SCHÄFER, 1985. J. Less-Common Metals, **108**, 225-239.

$Ca_4Cd_5Al_3$, orthorhombic, Imma, a = 7.536, b = 4.816, c = 8.339 A, Z = 1. Mo radiation, R = 0.044 for 262 reflexions. 4 Ca in 4(e): 0,1/4,0.7069; 5 Cd + 3 Al in 8(i): 0.2019,1/4,0.0857. KHg_2-type (1).

$CaAg_4Al_7$, cubic, Pm3m, a = 8.685 A, Z = 3. Mo radiation, R = 0.090 for 239 reflexions. $BaHg_{11}$-type (2).

Atomic positions

			x	y	z
Ca	in	3(d)	1/2	0	0
Ag(1)		1(b)	1/2	1/2	1/2
M(2)		12(j)	1/2	0.2654	0.2654
M(3)		12(i)	0	0.3427	0.3427
M(4)		8(j)	0.1660	0.1660	0.1660

M(2) = 4.3 Ag + 7.7 Al
M(3) = 4.5 Ag + 7.5 Al
M(4) = 2.3 Ag + 5.7 Al

$CaCu_{6.5}Al_{6.5}$, $LaCu_{6.5}Al_{6.5}$, $CeCu_{6.5}Al_{6.5}$, $SrAg_{6.5}Al_{6.5}$, cubic, Fm3c, a = 11.935, 11.949, 11.822, 12.543 A, Z = 8. Mo radiation, R = 0.077, 0.070, 0.057, 0.042 for 124, 123, 123, 143 reflexions. $NaZn_{13}$-type (3).

Atomic positions (for $CaCu_{6.5}Al_{6.5}$, similar values for others)

		x	y	z
Ca	in 8(a)	1/4	1/4	1/4 [not 0]
Cu(1)	8(b)	0	0	0
M(2)	96(i)	0	0.1780	0.1163

M(2) = 44 Cu + 52 Al

1. Structure Reports, **19**, 231.
2. Ibid., **16**, 25.
3. Strukturbericht, **6**, 8, 157; Structure Reports, **16**, 139.

ANTIMONY BARIUM
Ba_2Sb_3

B. EISENMANN, H. JORDAN and H. SCHÄFER, 1985. Z. Naturforsch., **40B**, 1603-1606.

Monoclinic, $P2_1/c$, a = 6.934, b = 13.453, c = 15.817 A, β = 90.25°, Z = 8. Mo radiation, R = 0.100 for 620 reflexions.

Atomic positions

	x	y	z
Ba(1)	0.7522	0.1227	0.9921
Ba(2)	0.2509	0.3737	0.9924
Ba(3)	0.0241	0.2728	0.2387
Ba(4)	0.5267	0.0246	0.7553
Sb(1)	0.7402	0.3664	0.0708
Sb(2)	0.4929	0.2291	0.1590
Sb(3)	0.5900	0.2950	0.8352
Sb(4)	0.8982	0.0481	0.3423
Sb(5)	0.0025	0.4785	0.6679
Sb(6)	0.2416	0.1161	0.9202

Isostructural with Sr_2Sb_3 (**1**), with discrete Sb_6^{8-} chain anions, Sb-Sb = 2.865-3.006 A, Sb-Sb-Sb = 103.5-113.7°. Ba-Sb = 3.461-3.759, Ba-Ba = 4.262-4.654 A.

1. Structure Reports, **45A**, 19.

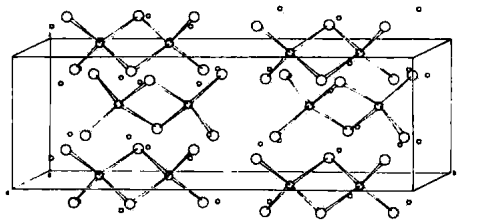
ANTIMONY BARIUM GALLIUM
ARSENIC CALCIUM GALLIUM
CALCIUM INDIUM PHOSPHORUS
Ba_3GaSb_3, Ca_3GaAs_3, Ca_3InP_3

G. CORDIER, H. SCHÄFER and M. STELTER, 1985. Z. Naturforsch., **40B**, 1100-1104.

Ba_3GaSb_3, orthorhombic, Pnma, a = 14.117, b = 21.167, c = 7.128 A, Z = 8. Mo radiation, R = 0.082 for 1429 reflexions.

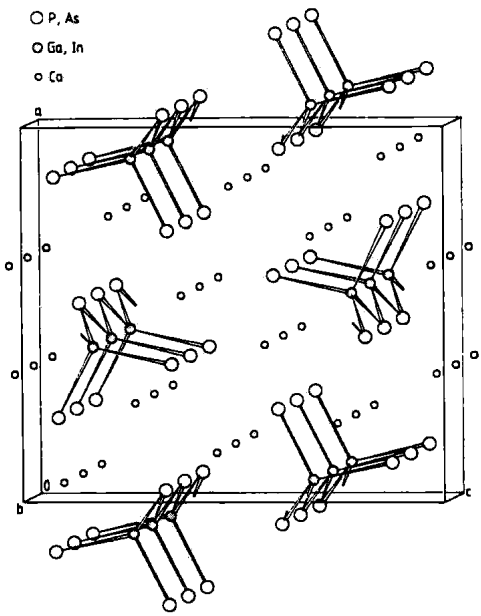
Ca_3GaAs_3, Ca_3InP_3, orthorhombic, Pnma, a = 12.171, 12.019, b = 4.197, 4.138, c = 13.414, 13.460 A, Z = 4. Mo radiation, R = 0.074, 0.042 for 1117, 1103 reflexions.

The three structures (Fig. 1) contain $GaSb_4$, $GaAs_4$, and InP_4 tetrahedra, which share edges in the first compound to form isolated Ga_2Sb_6 groups, and corners in the other two compounds to form chains. Ba ions have 6 Sb neighbours, and Ca ions have 5 or 6 As or P neighbours.



Ba_3GaSb_3

		x	y	z
8 Ba1	8d:	0,0095	0,4235	0,7716
8 Ba2	8d:	0,7371	0,4236	0,1943
4 Ba3	4c:	0,7346	0,25	0,8022
4 Ba4	4c:	0,0168	0,25	0,1754
8 Ga1	8d:	0,8739	0,1632	0,4848
4 Sb1	4c:	0,7678	0,25	0,2904
4 Sb2	4c:	0,9810	0,25	0,6806
8 Sb3	8d:	0,5135	0,9097	0,7691
8 Sb4	8d:	0,2587	0,0895	0,8012



Ca_3GaAs_3

		x	y	z
4 Ca1	4c:	0,2721	0,25	0,2844
4 Ca2	4c:	0,5623	0,25	0,3920
4 Ca3	4c:	0,3510	0,25	0,9978
4 Ga1	4c:	0,5628	0,25	0,7978
4 As1	4c:	0,6075	0,25	0,6135
4 As2	4c:	0,7499	0,25	0,8774
4 As3	4c:	0,0413	0,25	0,3509

Ca_3InP_3

		x	y	z
4 Ca1	4c:	0,2688	0,25	0,2889
4 Ca2	4c:	0,5651	0,25	0,3975
4 Ca3	4c:	0,3454	0,25	0,0037
4 In1	4c:	0,5521	0,25	0,8003
4 P1	4c:	0,6048	0,25	0,6137
4 P2	4c:	0,7538	0,25	0,8716
4 P3	4c:	0,0496	0,25	0,3662

Fig. 1. Structures of Ba_3GaSb_3, Ca_3GaAs_3, and Ca_3InP_3.

ANTIMONY CALCIUM GALLIUM
ANTIMONY CALCIUM INDIUM
ANTIMONY INDIUM STRONTIUM
$Ca_5Ga_2Sb_6$, $Ca_5In_2Sb_6$, $Sr_5In_2Sb_6$

G. CORDIER, H. SCHÄFER and M. STELTER, 1985. Z. Naturforsch., 40B, 5-8.

Orthorhombic, Pbam, a = 14.021, 14.256, 14.749, b = 12.106, 12.133, 12.696, c = 4.452, 4.572, 4.660 A, Z = 2. Mo radiation, R = 0.087, 0.052, 0.065 for 763, 1294, 1413 reflexions.

Atomic positions (for $Ca_5Ga_2Sb_6$; similar values for others)

		x	y	z
Sb(1)	in 4(g)	0.4073	0.8444	0
Sb(2)	4(h)	0.1786	0.6610	1/2
Sb(3)	4(g)	0.4007	0.4761	0
Ca(1)	4(h)	0.4848	0.6746	1/2
Ca(2)	4(h)	0.2476	0.4089	1/2
Ca(3)	2(d)	0	1/2	1/2
Ga(1)	4(g)	0.2880	0.6707	0

The structures (Fig. 1) contain M_2Sb_6 sheets (M = Ga, In), linked by alkaline-earth cations. Ga-Sb = 2.69-2.84, In-Sb = 2.81-3.03 A.

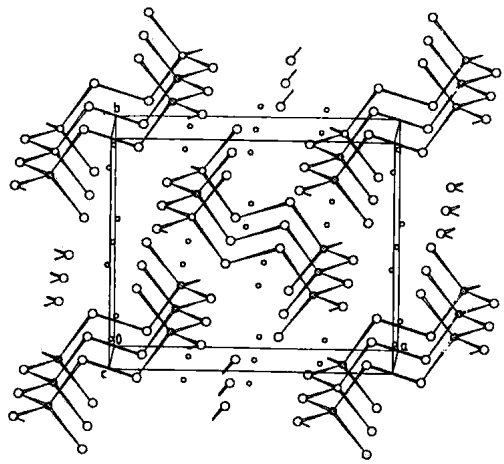


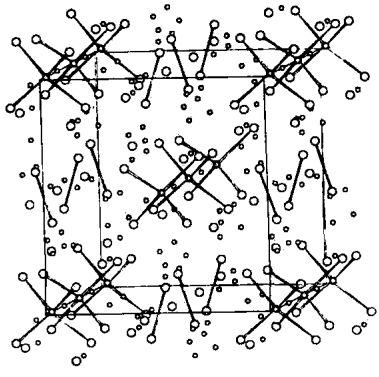
Fig. 1. Structure of $Ca_5In_2Sb_6$.

ANTIMONY CALCIUM INDIUM
$Ca_{11}InSb_9$

G. CORDIER, H. SCHÄFER and M. STELTER, 1985. Z. Naturforsch., 40B, 868-871.

Orthorhombic, Iba2, a = 11.894, b = 12.594, c = 16.730 A, Z = 4. Mo radiation, R = 0.068 for 3636 reflexions.

The structure (Fig. 1) contains isolated Sb^{3-} anions, Sb_2^{4-} dumbells, and isolated $InSb_4^{9-}$ tetrahedra, linked by 6- and 7-, and 8-coordinate Ca^{2+} ions.



	x	y	z
8 Ca(1) auf 8c	0.4266	0.2219	0.6534
8 Ca(2) auf 8c	0.6835	0.0543	0.6259
8 Ca(3) auf 8c	0.4118	0.2255	0.3366
8 Ca(4) auf 8c	0.6854	0.0592	0.3657
8 Ca(5) auf 8c	0.8366	0.1761	0.9957
4 Ca(6) auf 4a	0.0	0.0	0.6686
4 In(1) auf 4a	0.0	0.0	0.3877
8 Sb(1) auf 8c	0.8646	0.1180	0.5
4 Sb(2) auf 4b	0.0	0.5	0.2470
8 Sb(3) auf 8c	0.1750	0.1759	0.6787
8 Sb(4) auf 8c	0.4653	0.1080	0.4930
8 Sb(5) auf 8c	0.1499	0.1426	0.3053

Sb(1)–In(1)	288.6	
–Ca(1,2,3,4,5,6)	311.8–362.9	8
Sb(2)–Ca(1,2,3,4)	305.5–337.8	8
Sb(3)–Ca(1,2,3,5,6)	304.5–351.3	7
Sb(4)–Sb(4)	284.3	
–Ca(1,2,3,4,5)	307.3–359.9	8
Sb(5)–In(1)	288.1	
–Ca(1,3,5,6)	319.5–341.1	7
Ca(1)–Sb(1,2,3,4,5)	307.7–334.6	6
Ca(2)–Sb(1,2,3,4)	305.5–351.3	6
Ca(3)–Sb(1,2,3,4,5)	307.3–341.7	6
Ca(4)–Sb(1,2,3,4,5)	305.9–383.4	
–In(1)	383.4	7
Ca(5)–In(1)	345.8	
–Sb(1,3,4,5)	306.5–371.9	8
Ca(6)–Sb(1,3,5)	304.5–357.2	6
In(1) –Sb(5)	288.1 2×	4
–Sb(1)	288.6 2×	
Sb(5)–In(1)–Sb(5)	122.8°	
Sb(5)–In(1)–Sb(1)	109.6° 2×	
Sb(5)–In(1)–Sb(1)	106.7° 2×	
Sb(1)–In(1)–Sb(1)	98.8°	

Fig. 1. Structure of $Ca_{11}InSb_9$, with interatomic distances (A x 10^2) and coordination numbers.

ANTIMONY-COPPER TYPE STRUCTURES
Cu_2Sb

W.B. PEARSON, 1985. Z. Kristallogr., **171**, 23-39.

Previous confusion regarding occupancy of the two independent 2(c) sites is clarified for all Cu_2Sb-type structures (**1**) whose z parameters have been determined.

1. Strukturbericht, **2**, 742; **3**, 33, 288.

ANTIMONY COPPER SULPHUR
(TETRAHEDRITE (ARGENTIAN))
$(Cu,Ag,Fe)_{12}(Sb,As)_4S_{13}$

M.L. JOHNSON and C.W. BURNHAM, 1985. Amer. Min., **70**, 165-170.

Cubic, $I\bar{4}3m$, a = 10.530 A, Z = 2. Mo radiation, R = 0.046 for 169 reflexions.

Atomic positions

		x	y	z
Cu(1)	in 12(d)	1/4	1/2	0
Cu(2)	12(e)	0.2160	0	0
Sb	8(c)	0.2683	0.2683	0.2683
S(1)	24(g)	0.1238	0.1238	0.3661
S(2)	2(a)	0	0	0

Cu(1) = 0.63 Cu + 0.24 Fe
Cu(2) = 0.65 Cu + 0.35 Ag
Sb = 0.68 Sb + 0.32 As

Tetrahedrite structure (**1**), with substitution of Ag for Cu and As for Sb resulting in smaller and more-regular Cu(1) tetrahedra and Sb pyramids.

1. Structure Reports, **29**, 15; **37A**, 4; **45A**, 14.

ANTIMONY EUROPIUM PALLADIUM
$EuPd_2Sb_2$

ARSENIC PALLADIUM STRONTIUM
$SrPd_2As_2$

W.K. HOFMANN and W. JEITSCHKO, 1985. Mh. Chem., **116**, 569-580.

$EuPd_2Sb_2$, tetragonal, P4/nmm, a = 4.629, c = 10.568 A, Z = 2. Mo radiation, R = 0.039 for 366 reflexions. Eu, Pd(2), Sb(2) in 2(c): 1/4,1/4,z, z = 0.2424, 0.6284, 0.8745; Pd(1) in 2(a): 3/4,1/4,0; Sb(1) in 2(b): 3/4,1/4,1/2. $CaBe_2Ge_2$-type (**1**).

$SrPd_2As_2$, tetragonal, I4/mmm, a = 4.380, c = 10.169, Z = 2. Mo radiation, R = 0.020 for 182 reflexions. Sr in 2(a): 0,0,0; Pd in 4(d): 0,1/2,1/4; As in 4(e): 0,0,0.3768. $ThCr_2Si_2$-structure type (**2**).

Other related arsenides have the Th Cr_2Si_2-structure type, and antimonides and bismuthides the $CaBe_2Ge_2$-type.

1. Structure Reports, **43A**, 28.
2. Ibid., **43A**, 99.

ANTIMONY LANTHANUM COMPOUNDS
$LaMSb_2$, M = $Zn_{0.52}$, $Co_{0.68}$, $Mn_{0.65}$, $Mn_{0.76}$, $Cu_{0.82}$, $Cu_{0.87}$

G. CORDIER, H. SCHÄFER and P. WOLL, 1985. Z. Naturforsch., **40B**, 1097-1099.

Tetragonal, P4/nmm, a = 4.380, 4.394, 4.387, 4.372, 4.402, 4.373, c = 10.488, 9.954, 10.780, 10.933, 10.154, 10.400 A, Z = 2. Mo radiation, R = 0.053-0.074 for 208-268 reflexions. La in 2(c): 1/4,1/4,z, z = 0.2578, 0.2418, 0.2675, 0.2701, 0.2465, 0.2498; M in 2(a): 3/4,1/4,0; Sb(1) in 2(b): 3/4,1/4,1/2; Sb(2) in 2(c): z = 0.8468, 0.8764, 0.8450, 0.8421, 0.8562, 0.8525.

$CaMnBi_2$-type structures (**1**). La-8Sb = 3.27-3.40, M-4Sb = 2.52-2.79 A.

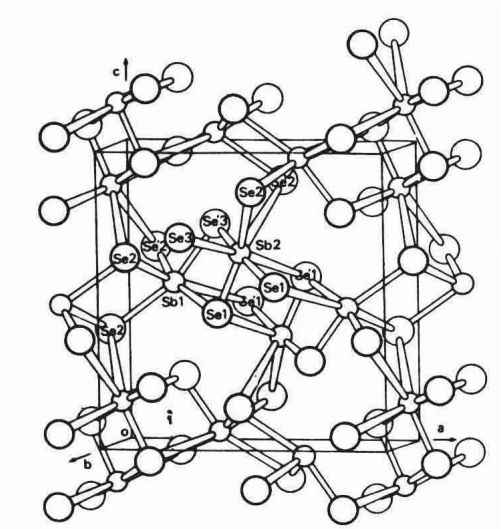
1. Structure Reports, **46A**, 32.

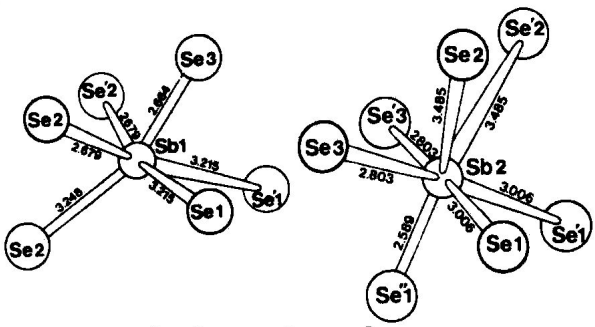
ANTIMONY SELENIUM
Sb_2Se_3

G.P. VOUTSAS, A.G. PAPAZOGLOU, P.J. RENTZEPERIS and D. SIAPKAS, 1985. Z. Kristallogr., **171**, 261-268.

Orthorhombic, Pnma, a = 11.794, b = 3.986, c = 11.648 A, Z = 4. Mo radiation, R = 0.052 for 610 reflexions.

Structure (Fig. 1) as previously described (**1**), with 6- and 7-coordinate Sb.





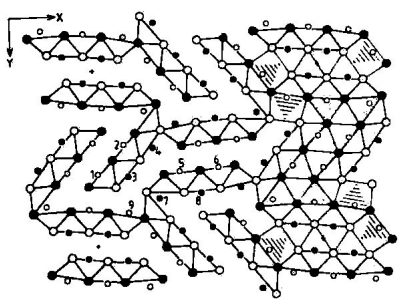
	x	y	z
Sb(1)	0.03036	¼	0.32789
Sb(2)	0.14745	¾	0.03965
Se(1)	0.0536	¼	0.8713
Se(2)	0.1289	¾	0.4447
Se(3)	0.2141	¼	0.19486

Fig. 1. Structure of Sb_2Se_3.

1. Structure Reports, **21**, 34.

ANTIMONY SELENIUM TIN
$SnSb_2Se_4$

P.P.K. SMITH and J.B. PARISE, 1985. Acta Cryst., B**41**, 84-87.



	x	y	z
M(1)*	86	5903	0
M(2)	1265	4256	0
M(3)	1434	6057	½
M(4)	2549	4485	½
M(5)	3702	5852	0
M(6)	5432	5678	0
M(7)	2785	7359	½
M(8)	4647	7105	½
M(9)	1406	8134	0
Se(1)	9671	6579	½
Se(2)	769	5119	½
Se(3)	1787	3612	½
Se(4)	872	6655	0
Se(5)	1969	5138	0
Se(6)	2913	3477	0
Se(7)	3021	5977	½
Se(8)	4610	5834	½
Se(9)	6158	5607	½
Se(10)	2206	6961	0
Se(11)	3865	7065	0
Se(12)	5488	6904	0

* (Sn,Sb) distributed randomly over the nine available metal (*M*) sites.

M(1)-Se(4)	2·624 (3) Å	M(6)-Se(12)	2·587 (3)
-Se(1) ×2	2·708 (2)	-Se(9) ×2	2·800 (2)
-Se(2) ×2	3·181 (2)	-Se(8) ×2	2·996 (2)
-Se(2) ×2	3·728 (3)	-Se(8) ×2	3·774 (2)
M(2)-Se(5)	2·638 (3)	M(7)-Se(10) ×2	2·676 (3)
-Se(3) ×2	2·803 (2)	-Se(7)	2·978 (2)
-Se(2) ×2	3·022 (2)	-Se(6)	2·999 (2)
-Se(1) ×2	3·658 (3)	-Se(3) ×2	3·514 (2)
		-Se(11) ×2	3·568 (2)
M(3)-Se(2)	2·653 (3)		
-Se(4) ×2	2·812 (2)	M(8)-Se(8)	2·677 (3)
-Se(5) ×2	3·140 (2)	-Se(11) ×2	2·902 (2)
-Se(10) ×2	3·454 (2)	-Se(12) ×2	3·045 (2)
		-Se(1) ×2	3·433 (2)
M(4)-Se(3)	2·737 (3)		
-Se(5) ×2	2·891 (2)	M(9)-Se(9)	2·733 (3)
-Se(6) ×2	3·087 (2)	-Se(6) ×2	2·809 (2)
-Se(7)	3·385 (2)	-Se(12) ×2	3·172 (2)
-Se(9)	3·446 (2)	-Se(10)	3·262 (3)
		-Se(4)	3·424 (3)
M(5)-Se(11)	2·592 (3)		
-Se(7) ×2	2·727 (2)		
-Se(8) ×2	3·150 (2)		
-Se(9) ×2	3·697 (2)		

Fig. 1. Structure of $SnSb_2Se_4$, with atomic positional parameters (decimal fractions, x 10^4).

Orthorhombic, Pnnm, a = 26.610, b = 21.066, c = 4.0423 A, Z = 12. Mo radiation, R = 0.045 for 1687 reflexions, and electron microscopy. $SnSb_2S_4$ is isostructural.

The structure (Fig. 1) contains ribbons along c of edge-sharing MSe_3 trigonal pyramids, linked by sharing Se atoms to give 7- and 8-coordinations for M atoms.

ANTIMONY SULPHUR
$Sb_{10}S_{15}$

J.S. SWINNEA, A.J. TENORIO and H. STEINFINK, 1985. Amer. Min., **70**, 1056-1058.

Monoclinic, C2/c, a = 13.393, b = 11.7170, c = 16.737 A, β = 93.763°, Z = 4. Mo radiation, R = 0.062 for 2893 reflexions.

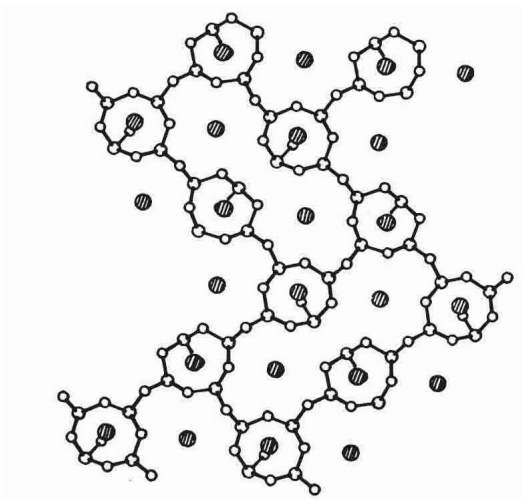
Atomic positions (x 10^4)

	x	y	z
Sb(1)	3754.9	1450.4	4952.2
Sb(2)	4090.8	1810.9	1535.9
6.82 Sb(3)	883.7	522.6	4149.7
Sb(4)	1414.6	2495.5	636.6
6.18 Sb(5)	3026.6	4444.6	3409.5
2.33 Sb(6)	0	3977.1	¼
S(1)	3520	442	2510
S(2)	0	8109	¼
S(3)	2640	264	364
S(4)	1912	2464	3950
S(5)	4656	3640	4619
S(6)	284	4136	878
S(7)	732	1295	1677
S(8)	2739	3207	1618

Isostructural with fuloppite, $Pb_3Sb_8S_{15}$ (1), with partial occupancy of some Sb sites. Sb-S = 2.43-2.77 A. Reinvestigation of the fuloppite structure (1) indicates that Pb(1) = Pb, Pb(2) = 0.825Pb + 0.175Sb, Sb(3) = 0.145Pb + 0.865Sb.

1. Structure Reports, **40A**, 11; **41A**, 14; **42A**, 19.

ARSENIC CAESIUM SULPHUR
$Cs_2As_8S_{13}$



	x	y	z
Cs1	0.2970	0.0464	0.1211
Cs2	0.3036	−0.4517	0.3674
As1	0.0781	0.1570	0.0318
As2	0.0821	0.2241	0.1743
As3	0.0684	−0.0839	0.1915
As4	0.0902	−0.1280	0.0377
As5	0.0603	−0.2993	0.3027
As6	0.0262	−0.3750	0.4386
As7	0.0822	−0.6495	0.4404
As8	0.0881	−0.5961	0.2893
S1	0.1518	0.2534	0.0959
S2	0.1346	0.0706	0.2156
S3	0.1417	−0.1689	0.1250
S4	0.1629	0.0174	0.0109
S5	0.1030	−0.2520	0.3897
S6	0.1180	−0.4851	0.4793
S7	0.1591	−0.6632	0.3622
S8	0.1426	−0.4292	0.2704
S11	0.0025	0.0700	0.0901
S21	0.1694	0.3257	0.2241
S31	0.1373	−0.1658	0.2633
S41	0.1705	−0.2544	−0.0059
S61	−0.0101	−0.4837	0.3688

Fig. 1. Structure of $Cs_2As_8S_{13}$.

W.S. SHELDRICK and J. KAUB, 1985. Z. Naturforsch., **40B**, 571-573.

Orthorhombic, Pbcn, a = 17.738, b = 11.950, c = 23.367 A, Z = 8. Mo radiation, R = 0.040 for 2855 reflexions.

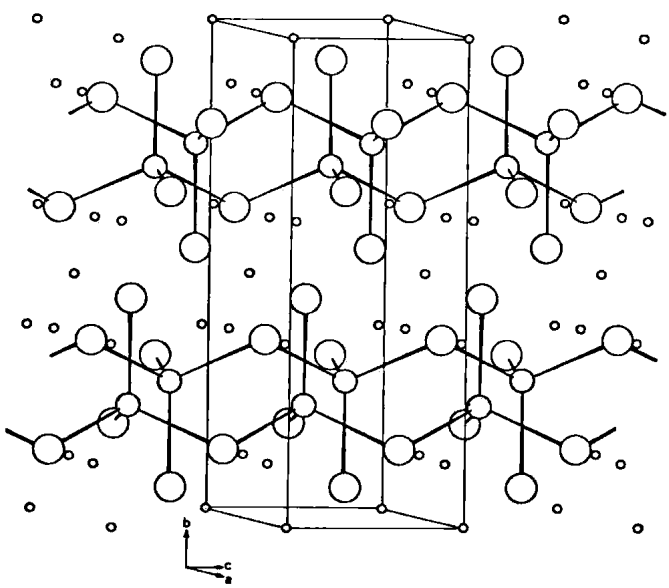
The structure (Fig. 1) contains an infinite anion layer of As_4S_4 rings connected by S bridges, with layers linked by 11-coordinate Cs cations. As-S = 2.18-2.31 A, S-As-S = 84-105, As-S-As = 95-110°, Cs-S = 3.45-4.32 A.

ARSENIC CALCIUM TIN
$Ca_5Sn_2As_6$

B. EISENMANN, H. JORDAN and H. SCHÄFER, 1985. Z. anorg. Chem., **530**, 74-78.

Orthorhombic, Pbam, a = 13.643, b = 11.830, c = 4.121 A, Z = 2. Mo radiation, R = 0.067 for 1098 reflexions.

The structure (Fig. 1) contains chains of corner-sharing $SnAs_4$ tetrahedra, linked by 6- and 7-coordinate Ca. Sn-As = 2.57-2.64, Ca-As = 2.96-3.29 A.



		x	y	z
Ca1	4g	0,2609	0,3774	0
Ca2	2a	0	0	0
Ca3	4g	0,4329	0,1282	0
Sn1	4h	0,1067	0,2152	0,5
As1	4h	0,9200	0,1696	0,5
As2	4h	0,1128	0,4325	0,5
As3	4g	0,2003	0,1271	0

Fig. 1. Structure of $Ca_5Sn_2As_6$.

ARSENIC RHODIUM
$Rh_{12}As_7$

ARSENIC HOLMIUM RHODIUM
$Ho_2Rh_{12}As_7$

I. J.Y. PIVAN, R. GUÉRIN and M. SERGENT, 1985. J. Less-Common Metals, **107**, 249-258.

II. B. LAMBERT-ANDRON, E. DHAHRI, P. CHAUDOÜET and R. MADAR, 1985. Ibid., **108**, 353-358.