phosphates. Second, it seems unlikely that the small bond angle at phosphorus is necessarily the most important factor for the increased hydrolysis rates in the five-membered cyclic phosphates, inasmuch as the small angle in triphenyl phosphate does not enhance this hydrolysis rate appreciably.

Our simple consideration of the π bonding does not seem to account for the orientation of the P-O-C planes to provide maximum d-p overlap between the oxygen and phosphorus orbitals. A more complete analysis, such as that of Collins (1966), may be able to extend this treatment.

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The Crystal Structure of La₂Sb

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Crystals of La₂Sb are tetragonal, a=4.626 (3), c=18.06 (2) Å, c/a=3.904; space group I4/mmm (D_{4h}^{17}), Z=4; 4 La(1) in 4(c), $0\frac{1}{2}0$; 4 La(2) in 4(e), 00z with z=0.3204 (2); 4 Sb in 4(e), 00z with z=0.1377 (2). The structure of La₂Sb corresponds to two C38 structure units joined together by reflexion across a mirror plane perpendicular to the c axis. Intensities for 298 h0l and h1l reflexions were obtained from multiple-film Weissenberg exposures by visual comparison with a film density scale. The parameters were refined using a structure-factor least-squares program.

Introduction

The lanthanum-antimony system was first studied by Vogel & Klose (1954) who reported the phases La₂Sb, La₃Sb₂, LaSb and LaSb₂. The rock-salt structure of LaSb had already been established by Iandelli & Botti (1937). Wang & Steinfink (1967) have determined the structure of LaSb₂, Gambino (1967) has assigned the Gd_4Bi_3 (anti-Th₃P₄) structure to La₄Sb₃, and Rieger & Parthé (1968) have recently assigned the Mn₅Si₃ structure to La₅Sb₃. The structure determination of La₂Sb was undertaken as part of a reinvestigation of the La–Sb system which is still underway (Mansey, Sato, Taylor & Calvert, to be published).

Experimental

La₂Sb was prepared as described by Sato, Taylor & Calvert (1967) (La > 99.8, Sb > 99.99%; total impurities in the alloy were found to be in the range 0.05-0.5% by semi-quantitative spectroscopic analysis). The single

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crystals studied came from a pellet of composition La₂Sb which was annealed for 2 days at 1100 °C *in vacuo* and slowly cooled. The powder data were from a sample of composition La₂Sb (annealed for 8 days at 750 °C, air-cooled). Precession photographs (Mo K α radiation, Zr filter) of nets *h*0*l*, *h*1*l*, 0*kl*, 1*kl*, *hk*0, *hk*1, *hk*2, *hk*4, *hk*5, *hhl* and two general *hkl* nets were recorded; some nets were recorded from two further specimens to check the space group and axial dimensions. Multiple-film zero-level Weissenberg photographs (Cu K α radiation, Ni filtered) of the *hhl* net of the best crystal were used to obtain intensity data for 35 *hhl* reflexions (45

reflexions accessible). The intensities were estimated visually and corrected for Lorentz and polarization effects. Later, when these data had been found to be unsatisfactory, three much smaller crystals were checked (precession photographs) and levels h0l and h1l were recorded by the multiple-film (interleaved brass foils) Weissenberg technique from a crystal $0.05 \times 0.12 \times 0.12$ mm in size using Zr-filtered and radiation; 144 out of 232 accessible h0l reflexions and 154 out of 215 accessible h1l reflexions were measured. Intensities were estimated visually, against a scale prepared from the same crystal, and corrected for the Lp effect and absorption

Table 1. Atomic parameters for La₂Sb

	Cu radiation	Mo ra	Mo radiation		
	$z(hhl)(\sigma)$	$z(h0l)(\sigma)$	$z(h1l)(\sigma)$	$z(\text{final})(\sigma)$	
La(1)	0	0	0	0	
La(2)	0.32024 (65)	0.32052 (33)	0.32039 (24)	0.32042 (19)	
Sb	0.13838 (70)	0.13736 (36)	0.13785 (31)	0.13771 (22)	
	$*B(hhl)(\sigma)$	$*B(h0l)(\sigma)$	$*B(h1l)(\sigma)$	* B(final) (σ)	
La(1)	0.72 (15)	0.670 (79)	0.788 (71)	0.73 (5)	
La(2)	0.67 (17)	0.477 (63)	0.352 (53)	0.42 (4)	
Sb	1.10 (20)	0.409 (76)	0.433 (64)	0.46 (5)	
	(hhl)	(<i>h</i> 0 <i>l</i>)	(<i>h</i> 1 <i>l</i>)	Reflexions	
	45	232	215	Accessible	
	35	144	154	Observed	
	27	133	142	Refined	
	0.078	0.134	0.131	R value	



Fig. 1. Structural relationships between LaSb, La₂Sb and C38 type structures. The figures beside the atoms are fractional heights. The small square marks the origin of the La₂Sb cell in each projection. (a) Projection along the [001] axis of LaSb (B1 type).
(b) Three LaSb cells stacked together; projection along [110] of LaSb (B1 type). (c) Projection along [100] in tetragonal La₂Sb. (d) Projection along [100] in tetragonal C38 type.

assuming a sphere of radius 0.056 mm. The internal consistency of the F values was assessed by comparing the 17 available symmetry-related reflexions (10l and 011) for which $R_{\text{internal}} = \sum |\Delta F| / \sum \langle F \rangle$ was 0.15. The lattice parameters were measured on 30° precession photographs ($\lambda K \alpha_1 = 0.7092$ Å) of the crystal used for the intensity measurements. There is evidence from powder photographs of a very small variation in the lattice parameters. The powder pattern given in Table 4 is indexed on parameters $a = 4.636 (\sigma = 3)$ and c = 18.11 $(\sigma=2)$ Å, and was recorded in an 11.46 cm Debye-Scherrer camera using monochromatized Cu Ka radiation ($\lambda \alpha_1 = 1.5405$ Å); low angle cut off 14 Å; t = 25 °C. The Icalc values are peak intensities derived from integrated intensities by use of the curve of Swanson, Morris, Stinchfield & Evans (1962). The integrated intensities were calculated for the following parameters: La(1), $B=0.73 \text{ Å}^2$; La(2), $z = 0.32045 B=0.41 \text{ Å}^2$; Sb, z=0.13760, B=0.42 Å², using a program of Smith (1967) suitably revised for an IBM 360. Values of I_{obs} were obtained by visual comparison with a scale prepared in a powder camera.

Crystal data

La₂Sb, F.W.399·60, tetragonal, a=4.626 ($\sigma=3$) and c=18.06 ($\sigma=2$) Å at 25°C, c/a=3.904, Z=4, U=386.5 Å³, $D_x=6.87$ g.cm⁻³, μ_l for Mo K $\alpha=287$ cm⁻¹, μ_l for Cu K $\alpha=2170$ cm⁻¹. Space group *I4/mmm* ($D_{4h}^{(T)}$) No. 139 based on structure and diffraction symbol 4/*mmmI*...; 4 La(1) in 4(c), 0 $\frac{1}{2}$ 0 with B=0.73 ($\sigma=5$) Å²; 4 La(2) in 4(e), 0 0 z with z=0.32042 ($\sigma=19$) and B=0.42 ($\sigma=4$) Å², 4 Sb in 4(e), 0 0 z with z=0.13771 ($\sigma=22$) and B=0.46 ($\sigma=5$) Å².

The extreme values of the cell dimensions obtained by indexing the back-reflexion lines on powder patterns were a=4.636 ($\sigma=2$), c=18.11 ($\sigma=2$) Å, c/a=3.906 and a=4.630 ($\sigma=1$), c=18.062 ($\sigma=3$) Å c/a=3.901 at 25 °C (Cu $K\alpha_1=1.5405$ Å); these patterns are detectably different in the back-reflexion region when compared visually.

Trial structure and refinement

The trial structure was derived from that of LaSb (NaCl, B1 type) by noting first that a is equal to half the face-diagonal for LaSb (4.63 Å×2 \simeq 6.5 Å×1/2) [Fig. 1(a)] and secondly that c is slightly less than three times the a dimension for LaSb (18 Å \simeq 3×6.5=19.5 Å, [Fig. 1(b), (c)]. The composition La₂Sb is obtained by changing one out of every 3 layers from La+Sb to La+La and a reduction in the c dimension is then achieved by shifting the La layers by a/2 parallel to a. If the mixed atom planes are buckled, reasonable calculated structure factors are obtained.

At first the copper radiation data *hhl* could not be refined because the 11*l* reflexions calculated much too large for the models tried. Extinction was thought to be a possible cause of these discrepancies, although it had not been considered to be important in the first instance because the crystal had a noticeable mosaic structure. By eliminating the low order 11*l* reflexions the trial structure was readily refined, using a block-diagonal structure-factor least-squares program which minimized $\sum w(|F_o| - |F_c|)^2$ (Ahmed, 1966); the σ values were also calculated by this program.

The reflexions reduced appreciably by extinction were removed by using a test on $|\Delta F| = |F_o| - |F_c|$. This test removed from the least-squares calculations all reflexions having an $|\Delta F|/F_o$ value greater than some predetermined number T. This quantity was taken to be

Table 2. Observed and calculated structure factors $(\times 10)$ for La₂Sb

The F_c values for h0l and hll were calculated separately from the parameters given in columns 3 and 4 of Table 1. The effects of anomalous dispersion are included in the values of $|F_c|$, but the phase angles were restored to 0 or π during print-out.

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н≠.	С, к.	o	37	662	604	23	3714	-166	13	. 777	585	7	598	605	13	241•	294
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1	85*	-99	43	332	299	29	350	350	19	234.	117	13	399	423	19	231 *	56
8	1240	1372	47	1534	13	33	848	-841	23	3454	-132	17	851	-774	21	224+	197
10	1059	1033				35	335	224	25	248*	105	19	250	82	25	204+	51
14	1045	994	- 14 8	2. K	. 0	39	553	-557	27	342	294	21	247	271	27	1914	-233
16	2132	2338	0	4154	5055	41	2090	11	31	332	384	25	236.	76		1/6-	,
20	197.	81	- 4	3514	386	43	183•	278	33	709	-711	27	2464	-320	HÞ	10, K	= 0
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24	218*	257	10	1481	1172		3540	1400	39	444	-475	33	507	-562	2	237*	10
28	1651	1617	12	1619	1326	ž	385	240	••	1784	-,	37	380	360		236*	-102
30	507	475	14	1124	894	4	175*	-90	He	6, K	= 0		<u> </u>		8	232*	220
34	765	609	18	338	207	8	1053	840	o	2235	2378	н-	8. K	- 0	10	2290	157
36	256	318	20	205*	65	10	892	657	2	216*	130	0	1441	1596	14	220+	199
40	231*	118	24	225*	2337	14	942	684		1791	1800	2	247*	-107	16	477	575
42	215*	-31	26	301	-284	16	1751	1701	-						10	207-	-17
**	170+	715	25	403	1530	18	217*	147	8	679	565	6	1217	1208	20	196*	-13
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1	485	305	38	533	550	28	1202	1306	18	2424	83	16	353	317	26	276	575
3	614	439	40	225*	111	30	354	379	20	246*	5	18	229.	33	H×	11. K	= 0
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9	1534	1327				36	236*	260	26	312	-227	24	235.	69	ż	205*	61
13	2730 -	938	He	3. 6	. 0	38	205*	4 81	28	82C	1025	26	226*	-191	5	203*	-356
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17	1689 -	1574	3	473	326	44	472	614	34	313	354				11	467	-553
zí	636	504	í	1591	1200	H=	5, K	• 0	38	187+	383		41.4	- 0	15	1770	331
23	304 .	-188		1357	1054		10/ *	146				1	240*	74	17	335	-371
27	787	-559	13	1061	781	3	277	728	нч	/, K	• 0	5	527	-534	Ha	12. 8	
29	540	385	15	1438	1224	5	1347 -	-1129	1	234*	103	ĩ	231+	418	10-		- 0
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33 35 L H 13 35 7 91 13 15 7 91 13 15 7 91 13 15 7 91 33 35 7 91 33 35 7 91 14 15 7 91 13 15 7 91 14 15 7 91 14 19 19 19 19 19 19 19 19 19 19 19 19 19	925 390 0, K= 549 1755 - 1236 1233 - 1236 1457 - 350 645 233 - 1057 500 645 235 231 500 255 500 255 255	FC 1 301 434 122129 1576 122129 12704 1007 11291 2704 1007 1515 1860 -956 3089 -956 3089 -956 3089 -056 3089 -056 3089 -056 -059 -056 -059 -056 -059 -056 -0	19 21 L 24 26 28 30 32 36 38 36 38 40 42 44 46 48 1 1 3 5 7 9 11 1157 157 19	F0 1174 - 1409 - 578 664 932 250= 459 253= 459 253= 459 253= 459 253= 459 253= 459 253= 459 253= 1405 1405 1505 10	FC -1258 FC -1258 -1538 -1538 -393 -166 -393 -393 -316 -393 -13808 1361 -13808 1364 -13808 1364 -12808 -13164 -1298 -13164 -1298 -13164	4 11 L 0 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	887 1835 - 1594 2760 - 1594 1962 - 1962 - 1924 1962 - 1924 1925 1925 1925 1925 1925 1925 1925 1925	767 -1661 -1661 -1661 -1651 -1627 -1653 -1550 -1551 -1235 -627 -1350 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -1357 -15	5 L 333 35 37 37 41 43 H × 0 2 4 4 6 8 10 0 2 2 4 4 14 16 18 8 20 22 24 2 22 4 30 32 32	F0 669 252* 180* 5, K 1109 1830 5, K 1109 1830 1284 1204* 1285 1284 1204 237* 1284 1204 237* 1284 1204 237* 1286 1204 5, 570 5, 700 5, 7000 5, 700 5, 7000 5, 7000 5, 7000 5, 7000 5, 70	-784 FC -811 262 262 262 267 = 1 10703 -1007 -1084 -608 -1064 -692 -1145 -878 -1136 -878 -1136 -878 -440 -461 -612	11 1 15 15 15 17 19 21 23 25 27 29 9 1 33 33 33 33 33 4 4 4 6 8 10 10 10 10 10 10 10 10 10 10	FQ 994 888 267* 262* 262* 262* 262* 262* 262* 262*	-620 FC 787 -964 176 305 -176 142 -247 358 218 429 -497 -497 -1276 377 -1276 3771 -1276 377 -1276 377 -1276 377 -1276 377 -1276 -127	2 L 7 9 11 13 15 17 19 21 23 22 7 23 1 33 3 H- 0 2 4 6 8 0 12 14 16 12	1570 640 524 641 545 545 2479 255a 2479 2552 2479 2479 2552 2479 2479 2552 2479 2552 2479 2552 2479 2552 2479 2552 2479 2552 2479 2552	-14 FC 497 469 398 -712 272 272 272 272 274 281 -284 -284 -283 -284 -112 194 281 -523 -745 -8307 -451 -243 113 -245 -451 -243 -245 -245 -245 -245 -245 -245 -245 -245
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3 3 5 1 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 5 7 9 1 5 7 9 1 3 5 7 9 1 5 7 1 7 7 7 7 1 7 7 7 7 7 7 7 7 7 7 7 7 7	F0 0, k= 456 549 1755 - 549 1755 - 1755 - 549 1755 - 1755	FC 1 301 434 434 2129 1576 2129 1576 2129 1576 2129 1576 511 1207 1415 511 1207 1415 3004 -345 3004 -345 300 -345 300 -345 -340 300 -345 -3	191 21 24 26 28 28 30 32 44 44 44 48 H= 13 57 79 13 13 13 13 25 57 79 21 22 57 27 27 27 13 33 33 41 34 34 41 34 41 34 41 34 41 34 41 34 41 34 34 41 34 41 34 41 34 34 34 34 34 34 34 34 34 34 34 34 34	F0 1174 - 1 1409 - 578 578 664 932 2008 348 2, Ki 4194 22008 348 2, Ki 4194 22008 348 2, Ki 4194 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 348 22008 2578 2008	-1518 +444 -1258 -15258 -1525 -1056 -1525 -106 -1536 -1536 -1304 -304 -304 -31808 13618 -31808 -21808	911 L 022468 10211466 10211466 102222268 30222268 3023346444 H= 13357 911131179 113117791 113117791 113117791	887 1835 - 1835 - 1835 - 1835 - 1835 - 1992 - 1992 - 1992 - 1992 - 1992 - 1992 - 1992 - 1992 - 1993 - 1992 - 1993 - 1993 - 1993 - 1993 - 1993 - 1993 - 1994 - 1995 - 1	767 767 766 1324 22481 22481 22481 1530 -1551 -2754 497 -1350 -1551 -562 -1453 783 -1455 -	5 L 333 35 37 37 41 4 4 4 6 6 8 10 22 22 22 24 30 32 34 6 38 8 42 24 5 37 30 32 34 5 37 14 14 14 14 14 14 14 14 14 14 14 14 14	FO 669 252- 480 501 180- 5, K 1189 1245 470 1044 1255 771 1044 1044 1045 772 1044 1045 772 1044 1045 772 1045 772 1045 773 1045 773 230 45 772 230 45 772 230 45 772 230 45 772 230 45 772 230 45 772 230 45 772 230 45 772 230 45 772 230 45 775 785 785 785 785 785 785 78	-784 FC -811 2622 515 -593 80 267 -1003 -1703 80 267 -1003 -1003 -1003 -1003 -1004 -1091 -1084 -1091 -1105 -461 -1105 -461 -1105 -291 -295 -295 -295 -295 -295 -297 -297 -297 -297 -297 -297 -297 -297	11 15 17 17 21 22 27 29 29 31 33 35 37 39 H. 02 24 46 68 10 21 14 18 20 22 24 46 80 10 22 24 24 24 24 24 24 25 27 29 29 21 33 35 55 37 39 H. 10 10 10 10 10 10 10 10 10 10	771 F0 994 878 878 2602 257*	-620 FC 787 -964 176 305 -0176 142 247 -176 142 247 -176 142 249 -1276 358 -673 358 -673 218 429 -775 -725 -725 -725 -630 385 550 -643 3-75 -630 385 -633 -633 -633 -633 -633 -633 -635 -635	2 L 7 9 1 1 3 3 1 7 7 9 2 1 3 3 3 3 H= 0 2 4 4 8 10 2 2 2 2 9 1 3 3 3 H= 1 2 2 4 4 6 8 10 2 2 2 2 6 7 7 9 1 3 3 3 H= 1 1 2 2 5 7 7 9 1 3 3 3 1 7 7 1 2 2 5 5 7 2 9 1 3 3 3 1 7 7 1 1 3 5 7 7 9 1 3 3 3 1 7 7 1 2 2 5 5 7 2 9 1 3 3 3 1 7 7 1 2 2 5 5 7 2 9 1 3 3 3 1 7 7 1 2 2 5 5 7 7 2 9 1 3 3 3 1 7 7 1 2 2 5 5 7 2 9 1 3 3 3 1 7 7 1 2 2 5 5 7 7 2 9 1 3 3 3 1 2 2 5 5 7 7 2 9 1 3 3 3 1 2 2 5 5 7 2 9 1 3 3 3 1 2 2 5 5 7 2 9 1 3 3 3 1 2 2 5 5 7 2 9 1 3 3 3 1 2 2 5 5 7 7 2 9 1 3 3 3 1 2 2 5 5 7 7 2 9 1 3 3 7 2 1 1 2 5 5 7 2 2 9 1 3 3 3 1 2 2 5 5 7 2 2 5 5 7 2 2 9 1 3 3 3 1 2 2 5 5 7 2 2 1 2 2 5 5 7 2 2 2 5 5 7 2 2 1 1 2 2 5 5 7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	F0 640 524 772 772 645 747 2479 2479 2479 2479 2479 2479 2479	-14 FC 407 469 -712 1023 398 -712 202 202 202 202 202 202 202 2
3 3 5 H= 13 5 7 9 113 15 7 9 113 15 7 9 113 15 7 9 13 3 5 7 9 13 3 5 7 9 13 3 5 7 9 13 3 5 7 9 13 3 5 7 9 13 5 5 7 9 13 5 5 7 9 11 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 1 1 3 5 7 9 1 1 3 5 7 9 1 3 5 7 9 1 5 7 9 1 3 5 7 9 1 1 5 7 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	F0 0, K= 540 5430 1364 1365 1364 1236 1236 1236 1236 1357 1362 1357 1365 1357 13	FC 1 301 434 1269 12	19 21 L 246 288 368 322 324 446 48 H= 13 57 9 113 117 17 121 2257 229 133 3357 341 45	F0 1174 - 1409 - 578 664 2300 2532 2302 2332 2432 2432 2432 2444 - 1353 2144 - 1357 2352 2412 558 2412 558 2412 558 2412 558 2412 558 2412 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2597 2325 2412 2412 2597 2412 207 207 207 207 207 207 207 20	-1511 -1258 -1258 -1258 -1575 -0355 -1055 -1	911 L 0244689122468022464 11224146802224644 H 1357791131577131213257	887 1835 - FG 1598 2760 - 1598 2760 - 1982 - 1983 - 1982 - 1982 - 1983 - 1982 - 1983 - 1982 - 1983 - 1982 - 1982 - 1982 - 1982 - 1983 - 1982 - 1982 - 1982 - 1983 - 1983 - 1982 - 1983 - 1982 - 1983 - 1985 - 1	767 1061 FC 1324 4409 1530 1551 -1557 -1557	5 L 33 357 379 413. H= 02 244 800 122 244 259 324 366 327 324 402 244 135 377 9 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 41 357 279 279 274 274 274 274 274 274 274 274	F0 669 252+ 480 501 204+ 180+ 5, K 2151 470 2151 1205 2151 1205 470 237+ 1205 237+ 237+ 237+ 237+ 237+ 237+ 237+ 237- 237- 237- 210- 217- 2	-784 FC -811 2622 515 -593 267 -1003 267 -1003 -1703 -008 -1703 -008 -1703 -008 -1703 -008 -1703 -008 -1703 -008 -00	11 15 17 17 17 17 21 27 27 27 27 27 27 27 27 27 27	771 FQ 994 888 257 2602 262 262 262 262 262 262 262 262 262 262 262 262 262 262 262 262 262 261 261	-820 FC 787 -964 112 305 -176 112 2497 -176 -176 -176 -176 -218 -218 -218 -218 -218 -218 -219 -218 -219 -219 -219 -219 -219 -219 -219 -219	2 L 7 911 1351 1792 2333 H 024 68 1022246 H 13577 1	157* F0 640 524 172 5455 249* 2319 2249* 2319 2243* 2243* 2243* 2243* 2243* 2243* 2243* 2250* 3094 2250* 3094 2250* 3094 2250* 2250* 3094 2250* 2250* 3094 2250* 2250* 3094 3094 2250* 3094 3094 2250* 3094 3094 2250* 3094 3094 2250* 3094	-14 FC 407 469 1023 398 -712 2023 1030

* Unobserved, Fo is value of local threshold.

 $\blacktriangle |\triangle F|/F_o > 0.40.$

 $[\]circledast$ Unknown F_o , back-stop interfered; F_o is value of local threshold.

approximately three times R_{internal} , the internal consistency in the F_o data. On the assumption that the errors in F_o have a normal distribution and that $R_{\text{internal}} \simeq \sigma(F_o)$, a valid F_o will be rejected by this test less than 1% of the time, provided that the model for F_c is correct. In the present case, use of this test gave a rapid convergence using F_o data which had previously not been successfully refined. Use of such a test obviously requires caution, but is satisfactory when the parameters are adequately determined and there is good reason to believe in the model.



Fig. 2. Atomic coordinations in La₂Sb. Solid lines for nearest neighbours, broken lines for next-nearest neighbours. (a) Sb atom at 0, 0, 0.138 (0 0 z), (b) La (1) atom at 0, $\frac{1}{2}$, 0, (c) La (2) atom at $\frac{1}{2}$, $\frac{1}{2}$, 0.180 ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, z).

Rather than attempt corrections for extinction and to continue the refinement, it appeared better to collect a more extensive set of data from a different crystal with Mo radiation. A preliminary analysis of this data revealed some extinction and absorption effects, both considerably reduced, however, as well as discrepancies tentatively attributed to multiple-reflexion (*e.g.* 204 with a possible contribution from $\overline{400}$).

Following this preliminary analysis, the two sets of reflexions h0l and h1l were refined separately using the structure-factor least-squares program described above with T=0.40. Isotropic temperature factors were used, all observed planes were given unit weight and scattering factors (TFD, *International Tables for X-ray Crystallography*, 1962) were corrected for dispersion ($\delta f'$ and $\delta f''$). The refinements were considered complete when the final shifts were less than 10% of the σ values. The results are given in Tables 1,2 and 3.

Comparison of the results obtained from the separate refinements of h0l and h1l gave a check on the accuracy of the overall procedure. It was possible that the results might have been affected by the experimental errors but unlikely that these would have equal effect in both zones. The results are subject to the criticism that the parameters are a function of the unit weighting scheme used. To test this, the hol data were refined, using weights $\sqrt{w} = 1/\{1 + [(|F_o| - P_2)/P_1]^2\}^{1/2}$ with $P_1 = 13$ and $P_2 = 45$ which gave nearly constant, but not unit values for $\sum w |\Delta F|^2 / N$, where N is the number of reflexions in small ranges of $\sin^2 \theta$ and F_o . No test on $|\Delta F|$ was applied and hence all observed reflexions were included in the refinement. The results obtained for the positional parameters [La(2), z=0.32043 ($\sigma=13$); Sb, z=0.13740 ($\sigma = 15$)] are substantially identical, with σ values smaller than before by about 50% (see Table 1); the thermal parameters have increased while the corresponding σ values have decreased [La(1), B=0.96 $(\sigma=3)$ Å²; La(2), B=0.73 $(\sigma=3)$ Å²; Sb, B=0.72 $(\sigma=3)$ Å²]. Thus the positional parameters of Table 1 are adequately determined but the temperature parameters are less accurate, although of the right order. Lower σ values could undoubtedly be obtained by a combined refinement of the hol and h1l data with appropriate weights, but this was not essential for the pres-

Table 3. Interatomic distances in La

(σ includes uncertainty in unit-cell dimensions)

Atom							
and symmetry	Neighbours	(h0l)	(σ)	(<i>h</i> 1 <i>l</i>)	(σ)	weighted mean	(σ)
La(1)	4 La (1)	3.271	(3)	3.271	(3)	3.271	(2)
mmm	4 La(2)	3.982	(6)	3.984	(5)	3.983	(4)
	4 Sb	3.392	(6)	3.398	(5)	3.395	(4)
La(2)	4 La(1)	3.982	(6)	3.984	(5)	3.983	(4)
4mm	4 La(2)	4.146	(6)	4.143	(5)	4.144	(4)
	1 Sb	3.358	(4)	3.357	(4)	3.357	(3)
	4 Sb	3.308	(9)	3.297	(7)	3.302	(6)
Sb	4 La(1)	3.392	(6)	3.398	(5)	3.395	(4)
4mm	1 La(2)	3.358	(4)	3.357	(4)	3.357	(3)
· · · · •	4 La(2)	3.308	Ì	3.297	(7)	3.302	(6)

ent purpose. The mean interatomic distances (Table 3) are all within 1.0σ of the independent values from the h0l and hll data, indicating that the estimates for σ are of the right order.

An overall check of the correctness of this structure was now made by calculating the powder pattern (Table 4). The observed powder intensities could be expected to be substantially free from extinction, the absorption could be adequately corrected because the specimen was cylindrical and multiple reflexion should affect the results much less because of the random orientation of the powder particles. The good overall agreement is indicative of an adequately refined structure (Smith, 1968). Table 2 includes 23 weak reflexions excluded from the least-squares refinement by the test on $|\Delta F|$. These are about equally divided between lowangle reflexions with $|F_o| > |F_c|$ and high-angle reflexions with $|F_o| < |F_c|$. The error analysis results (Ahmed & Barnes, 1963) were of the form usually observed with the photographic method. The larger discrepancies are observed at the lower and higher angles and also with the smaller and larger $|F_o|$ values. The analysis of the $|\Delta F|$ values for the unobserved planes, which were not used in the least-squares refinement, shows a normal distribution with about 1 % having a $|\Delta F|$ greater than $2F_{\text{threshold}}$ ($F_{\text{threshold}}$ calculated from I_{obs} (minimum) $\times 0.6$).

The final values listed in column five of Table 1 and column five of Table 3 are weighted means ($w_i = 1/\sigma_i$). Further refinement with anisotropic temperature factors was not undertaken in view of the approximate absorption correction.

Alternative structures

Lanthanum and antimony have very similar scattering powers and it is possible to formulate other arrangements of the atoms in the same sets of positions. The arrangements listed in Table 5 were refined by the leastsquares method described above but in this case including all observed reflexions in the calculation in order to keep the total number of reflexions constant. The significance of the changes in R (based on observed planes only) was examined by Hamilton's (1965) R test. The refinement included 6 parameters (K, B_{La}, B_{La}) B_{Sb}, z_1, z_2) so that there were 138 and 148 degrees of freedom for h0l and h1l respectively. The results are listed in Table 6. Structures (II) and (III) can be safely rejected at the 0.005 level with both sets of data. Hence structure (I) was accepted as having the correct arrangement of atoms.

Table 4.	Powder	X-ray	diffractio	n pattern	of La ₂ Sb
		(se	e text)		

d _{obs}	dcalc	h	k	£	I _{obs}	^I calc	dobs	dcalc	h	k, t	lobs	I _{calc}
3.23	3.28	1	1	024	<22 66	13 100	1.040 1.034	1.043	2	1 15 0 17	<22 66	16 (7]] 3
2.81	2.85	1	0	54	42 82	39 110	1.029	11.037 11.035 J1.032	4 3 4	0 13 0 8	<22	13
2.29	2.32 12.26 2.26	2 0 1	0	0 8 ·7	82 22	95 24 20	1.015	11.031 11.017 11.015	4 2 2	1 7 0 16 2 14	26	26 23
1.85	1.86	2	0	28	26	23	1.011 .978	1.013	34	2 11	42 66	43 68 J 8
1.78	1.84 1.80	2	0	9 6 5	82 34	93 111 40	968	1,980 .970 .962	43	2 6 1 14 1 18	26 26	16
1.63	1.64	22	20	067	42	54 20 [27	.945	.948 .931	22	1 17 2 16	34 22	26
1.575	1.585	2	21	2 10	26	29 21	.918	.919	45	0 12 1 0	<22 <22	2000
1.539 1.456 1.435	1.551 1.466 [1.447	1 3 3	0 1 1	11 0 2	42 <22 82	41 9 [62	.903 .897	.905 .900 .898	5 4 5	1 2 2 10 0 5	42 42	38 30 4
1.413	1.444	2 2 2	1 2 0	9 6	20	128 14 52	.891	l.898 .891 880	4 5 3	3 5	66	51 51
1.366	1.421 1.395	3	0	54	66	17 (13 77	.876 .8715	.877 .8728	35	0 17 0 7	<22	14
1.318	$\begin{cases} 1.3/1\\ 1.327\\ 1.326 \end{cases}$	23	20	8	<22	12 { 5 7	.8537	1 .8728 .8728 .8545	24	3 7 1 20 2 12	26 <22	38211 [21 13
1.283	[1.294 [1.289 1.265	0 2 2	010	14 11 12	66 <22	59 {58 6	.6429 .8414	.8437 .6421	55	1809	26 26	19 15√15
1.224	1.231	322	1 2 2	18	22 22	20 22	.6375 .8348	.8376	5	2 5	22 22	20
1.198	1.203	ĭ	100	4 15	<22 <22	10 10	.8225	{ .8232 .8228	104	0 22 1 15	52	37 22
1.146	1.156	23	1 2	13 7	<22 <22	36{28 11	.8195	8203 8195 .8169	3 4 5	2 17 4 0 2 7	62 42 *	65 {33 13
1.136 1.123	1.139 [1.130 [1.127	323	1 0 0	10 14 11	22 26	22 26 23	.8123 .8095 .8074	.8125 .8098 [.8079	5 4 4	1 10 0 16 3 11	42 34 128	25 30
1.079	1.085 1.083	334	320	296	42	60	.7918	1 .8079	55	0 11 3 2	-52	92 (31 54
1.070 1.058 1.050	1.074 1.062 1.052	433	ĭ 3 1	5 4 12	22 26 <22	16 24 10	.7831 .7788 .7756	.7831 .7788 .7757	552	3 4 1 12 0 22	102 22 102	79 16 103

* α_2 overlap major contribution.

Table 5. R values for different atomic arrangements in La₂Sb

		I4/mmm	R value		
Structure	$4(c) \\ 0\frac{1}{2}0$	$4(e) \\ 00z_1$	$4(e) \\ 00z_2$	(h0l)	(h1l)
I II III IV	La(1) La(1) Sb La(1) (0.95)	La(2) Sb La(2) La(2)	Sb La(2) La(1) Sb	0·149 0·163 0·157 0·147	0·140 0·163 0·151 0·139

Table 6. Comparison of different atomic arrangements in La₂Sb

Structures	(h0l)	(<i>h</i> 1 <i>l</i>)
II vs. I	$R_{\rm II}/R_{\rm I} = 1.094$	$R_{\rm II}/R_{\rm I} = 1.164$
	$\mathcal{R}_{1, 138, 0.005} < 1.034$	$\mathcal{R}_{1, 148, 0.005} < 1.034$
III vs. I	$R_{\rm III}/R_{\rm I} = 1.054$	$R_{\rm III}/R_{\rm I} = 1.079$
	$\mathcal{R}_{1,\ 138,\ 0.005} < 1.034$	$\mathcal{R}_{1, 148, 0.005} < 1.034$
I vs. IV	$R_{\rm I}/R_{\rm IV} = 1.014$	$R_{\rm I}/R_{\rm IV} = 1.007$
	$\mathcal{R}_{1, 137, 0.10} < 1.011$	$\Re_{1, 147, 0.25} < 1.006$

In structure (I) the La(1) atoms lie in densely packed planes. This type of plane in the related structure of NdTe_{1.80} (Wang, Steinfink & Bradley, 1966) has been shown to have vacancies. In addition the unit-cell parameters for La₂Sb as derived from different X-ray powder diffraction patterns have slightly different values. Hence the occupancy factor for the La(1) atom was refined. Starting with a value of 0.5, the final occupancy factor was found to be 0.95. For this refinement [structure (IV)] the R values for the (h0l) and (h1l) data are given in Table 5. The change in R [with respect to structure (I)] was examined by Hamilton's R test. The results shown in Table 6 do not compel the rejection of structure (I), since the probability of error in rejection would be 10 to 25%. The occupancy factor for La(1) was therefore taken as unity.

Description of the La₂Sb structure

A projection of the La₂Sb structure along the *a* axis is shown in Fig. 1(*c*), while the arrangement of nearest neighbours and next-nearest neighbours for each atom is illustrated in Fig.2.

The eight nearest neighbours of the La(1) atom lie at the corners of a cube, slightly distorted by extension along the La₂Sb [001] direction [Fig. 2(*b*)]. The La–Sb distances of 3.39 Å are quite normal, but the La(1)– La(1) distances of 3.27 Å are noticeably shorter than the free-metal contact distances (3.73 and 3.77 Å). There are also next-nearest neighbours, four La(2) at 3.98 Å, making a total coordination of 12.

The nearest neighbours of the La(2) atoms [Fig. 2(c)] are Sb atoms arranged at the corners of a square pyramid, which is a distinctive feature of the La₂Sb and related (C 38) structures and will be discussed briefly below. The distances are 3.36 Å to the atom at the vertex of the pyramid and 3.30 Å to the four Sb atoms at the corners of the square base. There are also eight nextnearest neighbours, four La(1) atoms at 3.98 Å and four La(2) atoms at 4.15 Å, making a total coordination of 13.

The Sb atom [Fig. 2(*a*)] has nine nearest neighbours forming a mono-capped square antiprism with distances ranging from 3.30 to 3.40 Å. An alternative description for this arrangement is as a trigonal prism with; 1 La(1) + 2 La(2) forming each end face with three extra atoms, 2 La(1) + 1 La(2), opposite the prism faces. This coordination occurs widely for the *B* group atoms, in their transition metal compounds, *e.g.* Co₂P and Ta₂P.

The La₂Sb structure belongs to a fairly diverse group of structures of the metal-rich compounds between transition metals and chalcogenides or pnictides. These structures are characterized by metal-metal bonds and nearest neighbour coordinations of less than 12, in this case 8, 5 and 9 as compared with total coordination numbers of 12, 13 and 9.

Finally it may be noted that the structure of Ti_2Bi (Auer-Welsbach, Nowotny & Kohl, 1958) is in fact analogous to that derived here for La₂Sb. The structure assigned to Ti₂Bi places 2 Ti in 2(*a*), 0 0 0; 2 Ti in 2(*b*), $\frac{1}{2}$ $\frac{1}{2}$ 0; 4 Ti in 4(*i*), 0 $\frac{1}{2}$ 0·133, 4Bi in 4(*i*), 0 $\frac{1}{2}$ 0·353, in the space group $P4_2/mmc$ (D_{4h}^9) No. 131. By first adding $\frac{1}{2}$ to all *y* coordinates (*i.e.* shifting the origin to -b/2) and then combining the Ti atoms in 2(*a*) with those in 2(*b*) we get the position 4(*c*) in *I*4/*mmm*. Similarly the positions 4(*i*) convert to 4(*e*) of *I*4/*mmm*. Thus the correct space group for the Ti₂Bi structure is *I*4/*mmm*.

Comparison of La₂Sb with C38 and $E0_1$ structures

The close-packed plane of La(1) atoms in La₂Sb prompted a geometrical study of the A_2B (C38) type structures. The occurrence of such layers in the similar structures of NdTe₂ (C38) and NdTe₃ has been discussed in terms of their electrical properties (Wang, Steinfink & Bradley, 1966; Norling & Steinfink, 1966).

The C38 structure is formally and geometrically equivalent to the $E0_1$ structure [Pearson (1965) gives data for these structure types]. This may be seen by tabulating *a*, *c* and *c/a* values and by calculating the interatomic distances and coordinations. It is convenient here to use the C38 structure as the reference. The reported structure for Cu₂Sb, commonly quoted as representative of the C38 type, is atypical in that the buckling of the mixed atom planes is reversed, with Cu atoms moving out of the mixed atom plane towards the all-Cu plane.

The most typical feature of the C38 structure is found to be the square pyramidal coordination of five generally larger B atoms around the A atom [Fig. 2(c)]. Both the a and c axial lengths are largely determined by the A-B distance in this pyramid in which the vertical and sloping distances are approximately equal. It may be noted that those A_2B (C38) compounds that involve metals of the first long period have small c/a ratios (<1.80), while those that involve metals of the second (and higher) long periods have large c/a ratios (>2.00). The radius ratios r_A/r_B (12 C.N.) in the A_2B compounds are (generally) 0.85 ± 5 and as a direct consequence the layer composed solely of A atoms [Fig. 2(b)] is usually not close-packed. Where the ratio is significantly greater than 1.0 the A atoms in this layer come into contact and the extreme example occurs with La₂Sb for which $r_A/r_B = 1.15$. It appears that the five La–Sb contacts in the square pyramid provide enough energy to compress the La(1) atoms by about 12%.

Thus the La₂Sb structure is comparable to the C38 type in that the La–Sb contacts in the pyramid largely determine the *a* and *c* axes. The large r_A/r_B ratio of 1.15 for La₂Sb, implying a pronounced compression of the La(1) atoms is, however, not characteristic of most C38 structures.

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The Crystal Structure of Anhydrous UO₂F₂*

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A neutron powder-diffraction study of UO_2F_2 has been carried out. The structure is trigonal with a unit-layer unit cell with $a=b=4\cdot192\pm0\cdot001$ and $c/3=5\cdot220\pm0\cdot003$ Å and bonding distances of $U-O=1\cdot74\pm0\cdot02$ and $U-F=2\cdot429\pm0\cdot002$ Å, confirming essentially a previous X-ray study but with considerably higher accuracy. The powder sample consisted of approximately equal cumulative volumes of four different types of ordered coherent domains, containing individually the layer sequences, $A^+B^+C^+$, $A^-B^-C^-$, $A^+B^+A^+B^+C^+B^+C^+A^+C^+$ and $A^-B^-A^-B^-C^-A^-C^-$, where (+) and (-) refer respectively to the right-side-up and upside-down unit-layer configurations. In each layer sequence, a backward stacking with the opposite-sign unit layer is equally possible in powder diffractometry. All structures belong to the centric trigonal space group $R\overline{3}m$ (D_{3d}^2) . The polymorphic, multidomain structure is not necessarily unique, although an exhaustive search for other probable models was fruitless.

Introduction

Zachariasen (1954) made a pioneering contribution to the structure chemistry of the 5*f* series of elements by solving the crystal structures of a number of actinide compounds using the X-ray diffraction method. His study included anhydrous uranyl fluoride, UO_2F_2 , which was found to exhibit growth layer-stacking faults almost inherently (Zachariasen, 1948). Based on the X-ray powder data, Zachariasen assigned a rhombohedral structure with a cubic close-packing layer sequence to the *ideally* ordered UO_2F_2 and interpreted the stacking faults by introducing a hexagonal close-packing sequence with a random-walk probability. The stacking ordering increases with heat treatment, but the *ideally* ordered structure is hardly achievable in practice. Since neutron diffraction is more sensitive to the structure parameters of UO_2F_2 , we have re-examined the subject using this technique. In this paper the rhombohedral crystal structure is conveniently described with reference to hexagonal axes unless otherwise stated.

Experimental

The anhydrous UO_2F_2 used in this work was prepared by treating UO_3 with gaseous anhydrous HF at temperatures between 350 and 500 °C in a nickel reactor (Hoekstra, 1963). Chemical analysis of the samples confirmed the stoichiometry, as indicated by a satisfactory agreement between the observed and calculated weight percentages (the latter values in parentheses), uranium 77.1 ± 0.1 (77.28), oxygen 10.3 ± 0.1 (10.39)

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