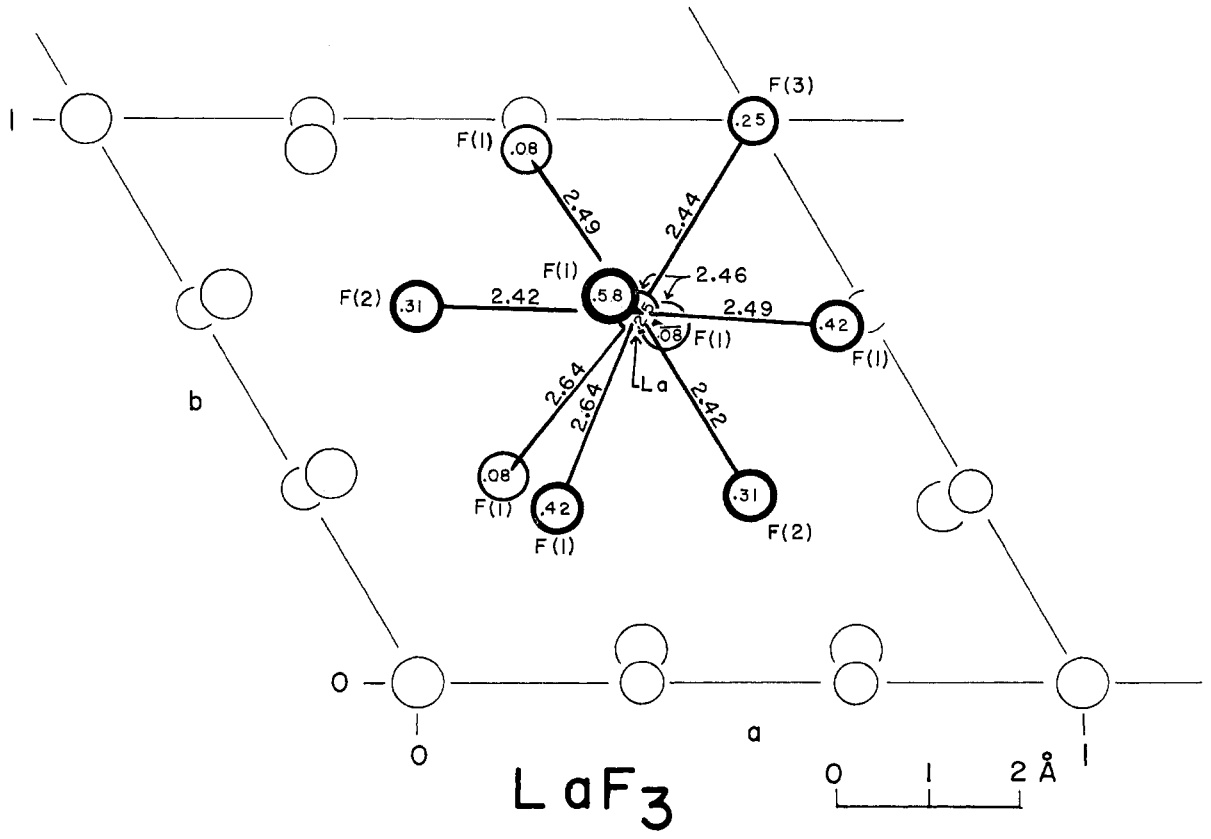

Figure 1.—The ninefold coordination of lanthanum in lanthanum trifluoride as viewed down the *c* axis.

TABLE IV
INTERATOMIC DISTANCES OF LESS THAN 3 A IN LANTHANUM TRIFLUORIDE

Atoms	Distance, A	Atoms	Distance, A
La-2F(2)	2.416 ± 0.003	F(1)-1F(2)	2.69 ± 0.02
La-1F(3)	2.443 ± 0.004	F(1)-2F(1)	2.74 ± 0.02
La-2F(1)	2.46 ± 0.02	F(1)-1F(3)	2.76 ± 0.01
La-2F(1)	2.49 ± 0.01	F(1)-1F(2)	2.79 ± 0.01
La-2F(1)	2.64 ± 0.01	F(1)-1F(2)	2.87 ± 0.02
La-2F(1)	3.01 ± 0.01	F(2)-3La	2.416 ± 0.003
F(1)-1La	2.46 ± 0.02	F(2)-3F(1)	2.69 ± 0.02
F(1)-1La	2.49 ± 0.01	F(2)-3F(1)	2.79 ± 0.01
F(1)-1La	2.64 ± 0.01	F(2)-3F(1)	2.87 ± 0.02
F(1)-1La	3.01 ± 0.01	F(3)-3La	2.443 ± 0.004
F(1)-1F(1)	2.57 ± 0.03	F(3)-6F(1)	2.76 ± 0.01
F(1)-1F(1)	2.68 ± 0.03		

than the calculated standard deviations when just high-angle data were used or when the extinction correction was introduced. Our estimates of the standard deviations bracket these fluctuations more realistically, and, because of the highly nonrandom nature of the errors here, the authors believe that an educated guess is preferable to a mathematical fiction. The thermal parameters (other than B_{13} and B_{23}) are systematically lower than the true values, because of neglect of absorption, by an unknown amount which is estimated to be about 0.6 A[2]. This effect is not included in the estimated standard deviations. Table IV shows a list of interatomic distances.

The structure we find has lanthanum in almost exactly the positions reported by Oftedal. The fluorine atoms have been shifted so that of the six second-nearest neighbors of each lanthanum, four have moved closer and two have moved away; thus, lanthanum has a normal coordination number of nine. We have failed to find any simple description for the geometry of these neighbors. Each fluorine has three lanthanum neighbors. A sketch showing the ninefold coordination of lanthanum as viewed down the *c* axis is shown in Figure 1.[10]

(10) NOTE ADDED IN PROOF.—M. Mansmann, *Z. Krist.*, **122**, 375 (1965), has recently reported atomic coordinates for this structure which correspond to our results within 0.06 A in the worst case and with complete agreement concerning the symmetry.

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The Structure of $YbSb_2$, a $ZrSi_2$ Isotype[1]

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In the recent study of the ytterbium–antimony phase diagram,[2] $YbSb_2$ was found to exist as one of the most stable phases in this system. It crystallizes in a pro-

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(2) R. E. Bodnar and H. Steinfink, Fifth Rare Earth Research Conference Preprints, Iowa State University, Ames, Iowa, 1965.

nounced layered structure and is stable to atmospheric exposure. $YbSb_2$ is the first rare earth intermetallic compound found to be isostructural with $ZrSi_2$, whose structure was determined by Naray-Szabo.[3] Since the cell constants of $YbSb_2$ are significantly larger than those of $ZrSi_2$, a complete structure determination was carried out to evaluate interatomic distances more accurately.

Single crystals of $YbSb_2$ were grown from a liquid–liquid reaction of the elements in sealed tantalum tubes at 1000°. A flat single crystal with dimensions $0.038 \times 0.053 \times 0.008$ mm was selected. Molybdenum Kα radiation was used to record the $hk0$ reflections in a Weissenberg camera and $0kl$ and $h0l$ reflections in a precession camera. The intensities were measured visually; the linear absorption coefficient is 467.5 cm^{-1} but no absorption corrections were applied to the data.

The systematic extinctions observed on upper-level Weissenberg and on precession diagrams were: hkl, $h + k = 2n + 1$; $h0l$, $l = 2n + 1$, which are consistent with the space group Cmcm. Cell dimensions obtained from a least-squares treatment of powder data are $a = 4.536 \pm 0.002$, $b = 16.63 \pm 0.01$, $c = 4.271 \pm 0.002$ A, and there are four formula weights per unit cell.

The three crystallographically independent atoms are located at 0, y, $^1/_4$, position 4(c) of the space group. Table I shows the positional parameters and isotropic temperature factors obtained from a full-matrix, least-squares refinement of the $hk0$, $h0l$, and $0kl$ reflections using unit weights. The parameters for $ZrSi_2$[4] are also included in Table I for comparison.

TABLE I

PARAMETERS FOR $YbSb_2$

Atom	y	$\sigma(y)$	B, A²	$\sigma(B)$	y ($ZrSi_2$)
Yb	0.1039	0.0003	1.55	0.16	0.104
Sb(I)	0.4382	0.0005	1.60	0.18	0.439
Sb(II)	0.7451	0.0005	1.55	0.19	0.750

Table II lists the calculated and observed structure factors. The discrepancy coefficient for these reflections is 0.118.

Table III lists the interatomic distances observed in this structure between nearest neighbors and Figure 1 shows the coordination around the ytterbium atoms.

The structure of $YbSb_2$ contains two slightly puckered layers of Sb(II) atoms at the approximate y positions $^1/_4$ and $^3/_4$, respectively. The puckering is described by a variation in the y positions of the Sb(II) atoms of 0.163 A, considerably larger than the maximum standard deviation of 0.016 A. Each ytterbium atom is located 0.70 A above a plane formed by four Sb(I) atoms. These four Sb(I) atoms form a rectangle defined by the a and c unit cell parameters. The Yb–Sb(I) separation is 3.193 A. Located 2.43 A above this ytterbium atom is a distorted and tilted square of four Sb(II) atoms rotated approximately 45° with respect to the rectangle of Sb(I) atoms. The orthorhombic

(3) St. v. Naray-Szabo, *Z. Krist.*, **A97**, 223 (1937).

(4) H. Schachner, H. Nowotny, and H. Kudielka, *Monatsh. Chem.*, **85**, 1147 (1954).

TABLE II

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $YbSb_2$

h	k	l	F_o	F_c	h	k	l	F_o	F_c
0	0	2	433	−483	0	16	0	84	83
0	0	4	311	273	0	16	1	116	122
0	0	6	145	−135	0	16	2	60	−71
0	2	0	33	15	0	16	3	81	−92
0	2	1	145	−124	0	16	4	52	45
0	2	2		−12	0	18	0	57	59
0	2	3	76	81	0	18	1	63	74
0	2	4		7	0	18	2	45	−51
0	2	5	57	−45	0	18	3	50	−56
0	4	0	63	−35	0	20	0	106	118
0	4	1	79	66	0	20	1	40	43
0	4	2	38	30	0	20	2	89	−103
0	4	3	33	−38	0	20	3	35	−33
0	4	4	38	−20	0	22	0	65	−77
0	4	5	35	18	0	22	1	54	−57
0	6	0	456	−425	0	22	2	66	68
0	6	1	283	226	2	0	2	460	−397
0	6	2	323	331	2	0	4	244	238
0	6	3	172	−149	4	0	2	260	−251
0	6	4	204	−195	4	0	4	158	164
0	6	5	97	81	6	0	2	133	−136
0	8	0	115	93	2	0	0	539	499
0	8	1	228	200	4	0	0	260	295
0	8	2	76	−76	6	0	0	138	155
0	8	3	152	−137	1	3	0	112	−142
0	8	4	60	47	1	5	0	154	−187
0	10	0	33	−34	1	7	0	97	129
0	10	1	153	−153	1	9	0	227	245
0	10	2	35	26	1	11	0	145	179
0	10	3	107	106	1	13	0	124	−148
0	10	4		−13	1	15	0	119	−145
0	10	5	75	−59	2	6	0	366	−340
0	12	0	92	95	2	8	0	80	78
0	12	1	229	−209	3	3	0	69	−93
0	12	2	97	−79	3	5	0	148	−129
0	12	3	126	150	3	7	0	100	88
0	12	4	54	50	3	9	0	196	177
0	12	5	103	−86	3	11	0	153	132
0	14	0	177	−148	3	13	0	106	−111
0	14	1	132	−134	3	15	0	128	−111
0	14	2	139	126	4	6	0	224	−210
0	14	3	88	98	5	9	0	113	104
0	14	4	94	−83	6	6	0	138	−112

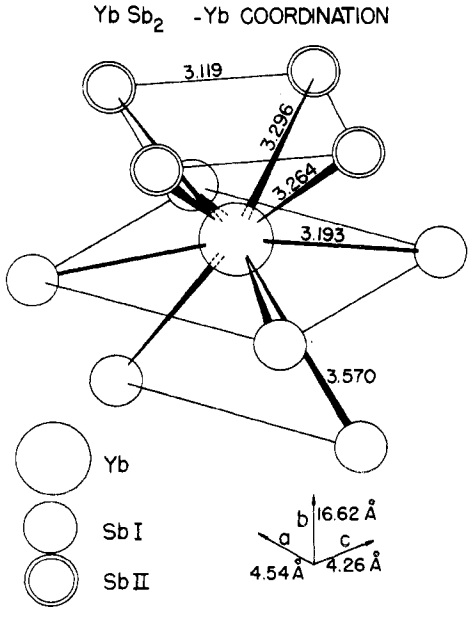

Figure 1.—Coordination of Sb around Yb.

TABLE III

INTERATOMIC DISTANCES (A) AND THEIR STANDARD DEVIATIONS IN $YbSb_2$

Yb–2Yb	4.062 ± 0.007	Sb(I)–4Yb	3.193 ± 0.010	Sb(II)–2Yb	3.264 ± 0.010
Yb–4Sb(I)	3.193 ± 0.010	Sb(I)–2Yb	3.570 ± 0.010	Sb(II)–2Yb	3.296 ± 0.010
Yb–2Sb(I)	3.570 ± 0.010	Sb(I)–2Sb(I)	2.966 ± 0.012	Sb(II)–2Sb(I)	3.721 ± 0.012
Yb–2Sb(II)	3.264 ± 0.010	Sb(I)–2Sb(II)	3.721 ± 0.012	Sb(II)–2Sb(I)	3.930 ± 0.012
Yb–2Sb(II)	3.296 ± 0.010	Sb(I)–2Sb(II)	3.930 ± 0.012	Sb(II)–4Sb(II)	3.119 ± 0.012

symmetry is due to the distortion and the tilt due to the puckering of the Sb(II) atoms. Two of these Sb(II) atoms are at a distance of 3.264 A from the ytterbium atom while the other two are located at a distance of 3.296 A. Two additional Sb(I) atoms are located 3.570 A from the ytterbium, and they are below the rectangle formed by four Sb(I) atoms. Thus, each ytterbium atom is coordinated by ten antimony atoms.

The shortest Yb–Sb(I) distance is 3.193 A and the shortest Sb(I)–Sb(I) distance is 2.966 A. Assuming contact, the Sb(I) radius is 1.483 A and the Yb radius is 1.710 A. The shortest Sb(I)–Sb(II) separation is 3.119 A giving an Sb(II) radius of 1.559 A. These radii indicate metallic bonding in the structure, and this is verified by high electrical conductivity measurements on polycrystalline samples of $YbSb_2$.