cules treated in the one configuration approximation. Likewise continuum orbitals could be invoked in situations where the optimum forms of the molecular orbitals of a molecular fragment change substantially during the process of molecule formation.

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CANADA

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The Crystal Structure of $Yb_{11}Sb_{10}$

Sir:

The compound previously designated as α-Yb_5Sb_4 is the low-temperature form of one of the intermediate phases occurring in the Yb–Sb system investigated by Bodnar and Steinfink.[1] The stoichiometry of the compound had not previously been established with certainty, although a single phase was observed on an X-ray powder diffraction pattern when the elements reacted in a 5:4 ratio. The lattice parameters and space group of this compound indicated that it was isostructural with one of the monogermanide phases reported by Tharp, Smith, and Johnson.[2] A later single-crystal analysis by Smith, Johnson, and Tharp[3] established the structure of this new rare earth germanide phase and showed that the composition corresponded to an 11:10 ratio of the elements.

TABLE II
INTERATOMIC DISTANCES IN $Yb_{11}Sb_{10}$[a]

Atom 1	Atom 2	Distance, Å	Esd, Å
Yb(1)	Sb(4)	3.125	0.003
	Sb(2)	3.159	0.006
	Sb(5)	3.413	0.007
	Sb(1)	3.420	0.005
	Sb(5)	3.527	0.007
	Yb(4)	3.701	0.004
	Yb(4)	3.819	0.004
	Yb(3)	3.920	0.005
	Yb(2)	3.910	0.009
	Yb(1)	4.223	0.004
Yb(2)	Sb(1)	2.933	0.010
	Sb(3)	3.464	0.018
	Sb(2)	3.556	0.010
	Sb(5)	3.672	0.011
	Yb(4)	4.319	0.009
	Yb(2)	3.963	0.013
Yb(3)	Sb(3)	3.491	0.016
	Sb(5)	3.465	0.008
	Yb(4)	4.119	0.005
Yb(4)	Sb(5)	3.148	0.007
	Sb(1)	3.165	0.005
	Sb(3)	3.393	0.016
	Sb(4)	3.176	0.003
	Yb(4)	3.881	0.004
Sb(1)	Sb(1)	3.572	0.006
Sb(3)	Sb(3)	2.998	0.022
	Sb(5)	3.280	0.017
Sb(5)	Sb(5)	2.936	0.009

[a] Esd's include only uncertainties in positional parameters.

TABLE I
FINAL ATOMIC PARAMETERS ($\times 10^4$) FOR $Yb_{11}Sb_{10}$[a]

Atom	Wycoff notation	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Yb(1)	16n	0	2518 (2)	1886 (1)	38 (1)	22 (1)	6 (0)	0	0	−1 (1)
Yb(2)	8h	1671 (5)	1671 (5)	0	71 (4)	71 (4)	14 (1)	40 (3)	0	0
Yb(3)	4e	0	0	3374 (2)	32 (4)	32 (4)	11 (1)	0	0	0
Yb(4)	16n	0	3364 (2)	3974 (1)	26 (1)	36 (1)	4 (0)	0	0	−1 (1)
Sb(1)	8i	3494 (4)	0	0	26 (3)	45 (3)	5 (1)	0	0	0
Sb(2)	4e	0	0	1283 (3)	23 (5)	23 (5)	8 (2)	0	0	0
Sb(3)	8h	3736 (9)	3736 (9)	0	104 (8)	104 (8)	19 (2)	−1 (5)	0	0
Sb(4)	4d	0	$^1/_2$	$^1/_4$	25 (4)	25 (4)	3 (1)	0	0	0
Sb(5)	16m	2062 (4)	2062 (4)	3245 (2)	35 (2)	35 (2)	8 (1)	6 (2)	−1 (2)	−1 (2)

[a] The esd's × 10^4 are given in parentheses. The form of the thermal ellipsoids is $\exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + 2B_{12}hk + 2B_{13}hl + 2B_{23}kl)]$.

Procedure.—The preparation of this compound has been described previously.[1] The material is spongy, and single crystals were difficult to find. The single crystal used in this investigation was an irregular fragment with encompassing dimensions of about 0.06 × 0.07 × 0.10 mm and with a shape which could be approximated by six planar faces.

The calculated density assuming 4 units of $Yb_{11}Sb_{10}$ per unit cell is 8.6 g/cm^3. Density measurements on the spongy material by loss of weight in acetone resulted in a suspiciously low value of 7.6 g/cm^3, probably because acetone failed to displace entrapped air. The density was redetermined by immersing the specimen in benzene and evacuating the system so that boiling occurred and benzene vapors could penetrate into the pores to displace the air. When the system was opened to the atmosphere, the vapors condensed to liquid in the pores and additional liquid was sucked in so that a true weight loss was determined. Several such measurements yielded values ranging from 8.11 to 8.24 g/cm^3, with an average value of 8.17 (7) g/cm^3, considerably closer to the calculated value for the stoichiometry $Yb_{11}Sb_{10}$.

Weissenberg and precession photographs, made with Cu Kα and Mo Kα radiation, respectively, showed that the diffraction symmetry was 4/mmm, that the crystal was mounted along an axis which was labeled b, and that hkl diffraction spectra were present only when $h + k + l = 2n$ with no other systematic absences being

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(1) R. E. Bodnar and H. Steinfink, *Inorg. Chem.*, **6**, 327 (1967).

(2) A. G. Tharp, G. S. Smith, and Q. Johnson, *Acta Crystallogr.*, **20**, 583 (1966).

(3) G. S. Smith, Q. Johnson, and A. G. Tharp, *ibid.*, **23**, 640 (1967).

TABLE III

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $Yb_{11}Sb_{10}$[a]

K	L	FOBS	FCAL
*** H = 0 ***			
0	4	50	33*
0	8	232	245
0	10	1952	1946
0	12	1330	1314
0	14	899	-854
0	16	968	979
0	18	539	536
0	20	689	692
0	22	585	617
0	24	183	-244
*** H = 1 ***			
0	3	74	16
0	5	508	429
0	7	109	-110
0	9	189	164
0	11	68	25*
0	13	322	-312
0	15	636	632
0	17	132	73
0	19	371	-386
0	21	245	278
0	23	92	13*
1	4	38	19*
1	6	919	874
1	8	262	-224
1	10	416	-373
1	12	56	-65*
1	14	449	426
1	16	135	99
1	18	1	21*
1	20	400	-412
1	22	43	40*
1	24	204	231
*** H = 2 ***			
0	0	108	141
0	2	6	26*
0	4	342	-316
0	6	771	-725
0	8	653	620
0	10	200	-188
0	12	196	-192
0	14	75	35*
0	16	168	-174
0	18	123	-124
0	20	319	342
0	22	272	-282
0	24	121	11
1	1	61	-4*
1	3	78	-38
1	5	1288	-1233
1	7	150	-124
1	9	469	421
1	11	324	-302
1	13	203	-197
1	15	454	-430
1	17	128	-112
1	19	168	149
1	21	151	-154
1	23	40	-7*
2	0	288	-323
2	2	71	-28*
2	4	87	93
2	6	246	223
2	8	601	547
2	10	1222	-1151
2	12	456	433
2	14	307	285
2	16	193	-198
2	18	350	348
2	20	438	-451
2	22	231	-244
2	24	648	730
*** H = 3 ***			
0	1	283	-275
0	3	426	-388
0	5	1567	1559
0	7	91	117
0	9	892	-823
0	11	105	76
0	13	151	-144
0	15	828	791
0	17	400	410
0	19	850	-886
0	21	64	-30*
0	23	399	420
1	0	29	21*
1	2	104	-131
1	4	938	-908
1	6	156	-158
1	8	153	-151
1	10	56	-56*
1	12	315	-314
1	14	135	-111
1	16	345	-346
1	18	125	76
1	20	123	-74
1	22	121	-69
1	24	142	-131
2	1	225	-233
2	3	1310	1305
2	5	333	-309
2	7	450	419
2	9	744	703
2	11	625	-584
2	13	484	457
2	15	538	539
2	17	140	-79
2	19	143	140
2	21	115	-36
2	23	171	191
3	2	863	929
3	4	493	-438
3	6	807	807
3	8	741	697
3	10	1353	1309
3	12	759	731
3	14	170	-159
3	16	80	58*
3	18	857	888
3	20	462	471
3	22	353	375
3	24	21	-86*
*** H = 4 ***			
0	0	1291	1503
0	2	1317	-1495
0	4	768	-778
0	6	394	325
0	8	1067	-1028
0	10	158	118
0	12	117	-18
0	14	1014	-987
0	16	395	391
0	18	431	-436
0	20	75	-78*
0	22	75	73*
0	24	296	-335
1	1	339	387
1	3	559	-534
1	5	445	-418
1	7	445	-396
1	9	432	405
1	11	280	257
1	13	748	-712
1	15	58	-48*
1	17	96	-49*
1	19	159	-165
1	21	307	306
1	23	256	-280
2	0	230	-238
2	2	328	-334
2	4	244	231
2	6	124	108
2	8	137	118
2	10	731	-681
2	12	69	-84*
2	14	268	257
2	16	164	156
2	18	275	-281
2	20	174	-152
2	22	177	-203
2	24	263	291
3	1	138	127
3	3	371	-383
3	5	608	551
3	7	108	-89
3	9	128	-121
3	11	244	225
3	13	377	-364
3	15	398	394
3	17	220	226
3	19	432	-446
3	21	181	192
3	23	85	105*
4	0	922	1071
4	2	832	-870
4	4	353	356
4	6	1115	1060
4	8	725	-666
4	10	36	-48*
4	12	188	166
4	14	173	-179
4	16	814	791
4	18	465	-488
4	20	178	-206
4	22	172	146
4	24	2	21*
*** H = 5 ***			
0	1	165	179
0	3	832	869
0	5	507	496
0	7	226	238
0	9	726	713
0	11	60	-31*
0	13	122	59
0	15	937	945
0	17	69	27*
0	19	128	-122
0	21	381	411
0	23	41	-8*
1	0	148	-170
1	2	234	-244
1	4	236	-234
1	6	651	612
1	8	390	-369
1	10	448	-415
1	12	139	-96
1	14	211	212
1	16	40	8*
1	18	68	23*
1	20	432	-433
1	22	56	25*
1	24	145	190
2	1	151	170
2	3	261	-263
2	5	758	-705
2	7	62	-18*
2	9	165	144
2	11	82	-32*
2	13	173	-152
2	15	450	-448
2	17	89	103*
2	19	80	72*
2	21	180	-176
2	23	144	152
3	0	116	83
3	2	359	395
3	4	444	-405
3	6	160	-134
3	8	361	350
3	10	204	199
3	12	247	-230
3	14	219	222
3	16	252	-242
3	18	162	141
3	20	174	183
3	22	82	-50*
3	24	100	-87*
4	1	72	46*
4	3	399	-408
4	5	612	-582
4	7	504	-469
4	9	359	330
4	11	109	-36
4	13	671	-646
4	15	128	-19
4	17	202	-183
4	19	148	-149
4	21	250	257
4	23	302	-305
5	0	443	493
5	2	120	-92
5	4	42	-52*
5	6	1061	1021
5	8	292	-284
5	10	139	-122
5	12	297	281
5	14	132	133
5	16	203	194
5	18	246	253
5	20	393	-417
5	22	185	186
*** H = 6 ***			
0	0	1538	1848
0	2	528	554
0	4	216	-193
0	6	149	80
0	8	981	947
0	10	841	808
0	12	641	634
0	14	258	-241
0	16	119	72
0	18	514	545
0	20	604	638
0	22	121	93
0	24	67	24*
1	1	125	-106
1	3	713	706
1	5	171	-165
1	7	340	335
1	9	368	354
1	11	369	-357
1	13	338	318
1	15	292	282
1	17	84	55*
1	19	115	46
1	21	148	-119
1	23	224	252
2	0	200	-233
2	2	289	290
2	4	372	-353
2	6	667	-647
2	8	872	843
2	10	603	-594
2	12	152	117
2	14	141	85
2	16	503	-511
2	18	333	333
2	20	84	43*
2	22	297	-339
2	24	291	353
3	1	705	-780
3	3	553	539
3	5	220	174
3	7	210	201
3	9	344	-331
3	11	813	-783
3	13	368	346
3	15	508	488
3	17	54	-27*
3	19	348	-369
3	21	333	-362
3	23	329	379
4	0	375	412
4	2	277	-300
4	4	364	-350
4	6	187	-175
4	8	177	108
4	10	227	-213
4	12	70	44*
4	14	289	-258
4	16	106	-75*
4	18	75	-31*
4	20	91	38*
4	22	153	-147
5	1	42	-67*
5	3	663	707
5	5	111	-69
5	7	355	347
5	9	357	353
5	11	317	-309
5	13	359	346
5	15	328	331
5	17	46	73*
5	19	90	56*
5	21	109	-85*
5	23	235	259
6	0	710	785
6	2	728	805
6	4	217	-217
6	6	378	-376
6	8	1271	1251
6	10	250	246
6	12	533	511
6	14	95	45*
6	16	354	-360
6	18	689	706
6	20	458	498
6	22	128	-118
*** H = 7 ***			
0	1	211	224
0	3	554	-621
0	5	668	642
0	7	64	-56*
0	9	337	-326
0	11	397	381
0	13	382	-377
0	15	205	215
0	17	333	351
0	19	456	-484
0	21	119	115
0	23	144	188
1	0	330	-326
1	2	1	-27*
1	4	45	16*
1	6	470	456
1	8	174	-159
1	10	359	-347
1	12	192	-191
1	14	394	387
1	16	67	32*
1	18	68	-88*
1	20	291	-315
1	22	112	-16
1	24	126	152
2	1	167	-179
2	3	407	389
2	5	1192	-1161
2	7	170	-166
2	9	682	660
2	11	527	-516
2	13	151	-134
2	15	170	-158
2	17	338	-345
2	19	221	226
2	21	110	-25
2	23	184	-206
3	0	384	431
3	2	314	-340
3	4	723	-727
3	6	292	269
3	8	420	-420
3	10	74	-31*
3	12	100	-15
3	14	350	-340
3	16	164	-168
3	18	161	150
3	20	271	-266
3	22	94	57*
4	1	299	320
4	3	689	-721
4	5	224	-230
4	7	364	-351
4	9	120	61
4	11	344	326
4	13	677	-674
4	15	222	-202
4	17	83	63*
4	19	190	-232
4	21	190	192
4	23	158	-180
5	0	582	-662
5	2	60	17*
5	4	74	-76*
5	6	48	40*
5	8	83	-37*
5	10	410	-390
5	12	422	-405
5	14	429	432
5	16	118	-107
5	18	192	-182
5	20	189	-176
5	22	149	-122
6	1	137	-89
6	3	371	393
6	5	149	-141
6	7	190	199
6	9	208	198
6	11	282	-265
6	13	190	178
6	15	187	166
6	17	82	35*
6	19	74	-7*
6	21	136	-115
7	0	159	142
7	2	237	-275
7	4	68	-96*
7	6	712	718
7	8	429	-439
7	10	258	-267
7	12	94	80*
7	14	88	56*
7	16	179	139
7	18	79	25*
7	20	459	-473
7	22	134	113
*** H = 8 ***			
0	0	1056	1135
0	2	320	-301
0	4	74	-47
0	6	239	209
0	8	89	-53
0	10	498	486
0	12	113	41
0	14	292	-273
0	16	434	425
0	18	229	-253
0	20	338	362
0	22	159	77
0	24	170	-233
1	1	197	204
1	3	559	-560
1	5	222	-209
1	7	351	-328
1	9	118	114
1	11	222	225
1	13	583	-575
1	15	84	-58*
1	17	49	21*
1	19	214	-205
1	21	194	226
1	23	154	-145
2	0	388	435
2	2	306	-315
2	4	147	145
2	6	514	503
2	8	64	-33*
2	10	338	-331
2	12	256	261
2	14	68	18*
2	16	280	286
2	18	69	-24*
2	20	189	-192
2	22	53	-8*
2	24	248	291
3	1	178	201
3	3	330	337
3	5	568	550
3	7	161	163
3	9	326	321
3	11	165	141
3	13	67	-34*
3	15	663	671
3	17	147	148
3	19	191	-207
3	21	290	309
3	23	96	82*
4	0	394	433
4	2	697	-743
4	4	99	53
4	6	404	399
4	8	556	-526
4	10	171	-151
4	12	125	-107
4	14	205	-177
4	16	474	482
4	18	497	-491
4	20	134	-102
4	22	64	24*
5	1	311	357
5	3	430	-469
5	5	82	61
5	7	148	-135
5	9	126	81
5	11	385	368
5	13	412	-418
5	15	84	-26*
5	17	181	168
5	19	151	-174
5	21	209	201
5	23	75	-29*
6	0	403	462
6	2	107	-97
6	4	204	-199
6	6	105	-98
6	8	225	214
6	10	68	-13*
6	12	118	95
6	14	164	-162
6	16	69	14*
6	18	62	39*
6	20	135	139
6	22	2	-77*
7	1	109	119
7	3	194	-197
7	5	278	-284
7	7	272	-255
7	9	279	294
7	11	106	69
7	13	443	-426
7	15	74	60*
7	17	138	-89
7	19	132	-94
7	21	215	240
8	0	775	861
8	2	312	-373
8	4	241	229
8	6	711	710
8	8	247	-266
8	10	184	152
8	12	253	241
8	14	80	-114*
8	16	580	576
8	18	165	-170
8	20	83	-19*
*** H = 9 ***			
0	1	606	-621
0	3	160	144
0	5	368	371
0	7	136	-128
0	9	268	-270
0	11	518	-499
0	13	114	-92
0	15	665	671
0	17	113	-106
0	19	498	-531
0	21	54	-12*
0	23	52	61*
1	0	231	243
1	2	16	9*
1	4	438	-432
1	6	157	142
1	8	76	-47
1	10	109	37
1	12	85	-47
1	14	48	-49*
1	16	148	-166
1	18	170	159
1	20	75	-90*
1	22	103	11*
2	1	1	20*
2	3	314	318
2	5	71	24*
2	7	275	271
2	9	118	116
2	11	129	-140
2	13	229	215
2	15	151	139
2	17	167	155
2	19	55	-26*
2	21	164	-134
2	23	251	286
3	0	726	790
3	2	547	573
3	4	390	-393
3	6	107	-40
3	8	562	554
3	10	677	666
3	12	125	121
3	14	71	30*
3	16	193	-191
3	18	413	434
3	20	395	429
3	22	133	84
4	1	108	97
4	3	146	129
4	5	262	248
4	7	61	34*
4	9	230	206
4	11	73	34*
4	13	121	-121
4	15	430	404
4	17	72	58*
4	19	180	-184
4	21	194	182
4	23	55	6*
5	0	330	340
5	2	98	-84
5	4	461	-474
5	6	205	192
5	8	170	-165
5	10	68	40*
5	12	65	28*
5	14	176	-165
5	16	144	-140
5	18	202	197
5	20	158	-135
5	22	47	50*
6	1	470	-524
6	3	346	387
6	5	93	77
6	7	127	133
6	9	214	-197
6	11	578	-578
6	13	244	248
6	15	344	357
6	17	62	-36*
6	19	257	-258
6	21	235	-271
7	0	59	-63*
7	2	98	90
7	4	281	-286
7	6	127	-81
7	8	106	73
7	10	52	-8*
7	12	181	-168
7	14	124	88
7	16	178	-189
7	18	81	32*
7	20	2	16*
8	1	118	98
8	3	97	-61
8	5	338	347
8	7	48	45*
8	9	68	-4*
8	11	134	126
8	13	115	-107
8	15	292	298
8	17	160	159
8	19	207	-228
8	21	137	122
9	0	687	734
9	2	271	295
9	4	305	-321
9	6	174	150
9	8	251	257
9	10	490	472
9	12	209	207
9	14	125	-119
9	16	128	-100
9	18	345	386
9	20	143	208
*** H = 10 ***			
0	0	580	591
0	2	387	-379
0	4	360	-355
0	6	131	114
0	8	113	-104
0	10	174	-177
0	12	228	224
0	14	386	-397
0	16	54	-20*
0	18	108	85
0	20	147	-129
0	22	48	-50*
1	1	132	-85
1	3	114	108
1	5	906	-870
1	7	134	-123
1	9	366	375
1	11	323	-325
1	13	161	-139
1	15	261	-263
1	17	197	-199
1	19	154	151
1	21	91	-94*
1	23	116	-107
2	0	795	-829
2	2	197	193
2	4	142	134
2	6	423	-398
2	8	599	576
2	10	813	-815
2	12	145	-127
2	14	459	478
2	16	271	-282
2	18	51	-24*
2	20	133	-118
2	22	307	-351
3	1	47	-29*
3	3	163	165
3	5	93	-29
3	7	196	197
3	9	17	24*
3	11	145	-135
3	13	142	142
3	15	77	46*
3	17	140	138
3	19	49	-54*
3	21	157	-170
3	23	235	254
4	0	49	39*
4	2	322	-328
4	4	93	84*
4	6	281	271
4	8	110	-110
4	10	480	-473
4	12	98	87
4	14	79	33*
4	16	149	145
4	18	137	-127
4	20	267	-270
4	22	83	-79*
5	1	120	-97
5	3	352	372
5	5	799	-799
5	7	83	-52
5	9	543	510
5	11	387	-377
5	13	67	-26*
5	15	137	-77
5	17	249	-247
5	19	221	220
5	21	75	-14*
6	0	145	-141
6	2	100	101
6	4	233	-231
6	6	357	-356
6	8	435	440
6	10	424	-421
6	12	82	73*
6	14	87	19*
6	16	332	-338
6	18	189	201
6	20	22	-25*
6	22	209	-237
7	1	59	29*
7	3	269	-278
7	5	529	-540
7	7	127	-121
7	9	76	48*
7	11	112	-67
7	13	210	-219
7	15	399	-389
7	17	35	-14*
7	19	25	24*
7	21	90	-145*
8	0	169	-169
8	2	149	-144
8	4	108	78
8	6	73	-26*
8	8	99	72
8	10	369	-352
8	12	123	-86
8	14	143	137
8	16	84	62*
8	18	147	-175
8	20	99	-75*
9	1	123	-136
9	3	369	369
9	5	232	-235
9	7	130	101
9	9	246	226
9	11	311	-307
9	13	159	138
9	15	163	142
9	17	74	-79*
9	19	57	67*
10	0	175	-183
10	2	179	-53
10	4	41	51*
10	6	20	65*
10	8	135	144
10	10	545	-522
10	12	154	145
10	14	98	131*
10	16	92	-80*
10	18	117	99
*** H = 11 ***			
0	1	223	198
0	3	77	91
0	5	579	544
0	7	160	144
0	9	113	96
0	11	207	210
0	13	66	-45*
0	15	453	471
0	17	218	224
0	19	215	-234
0	21	192	211
0	23	144	150
1	0	1	-57*
1	2	139	-41
1	4	107	-68
1	6	348	347
1	8	130	-126
1	10	153	-156
1	12	94	-69
1	14	187	196
1	16	38	47*
1	18	123	15
1	20	197	-205
1	22	31	40*
2	1	59	31
2	3	144	148
2	5	505	-473
2	7	35	8*
2	9	321	315
2	11	150	-147
2	13	54	-33*
2	15	114	-87
2	17	2	-61*
2	19	138	114
2	21	60	-12*
2	23	118	13
3	0	387	395
3	2	118	101
3	4	304	-299
3	6	167	165
3	8	52	40*
3	10	211	220
3	12	63	29*
3	14	55	-50*
3	16	87	-58*
3	18	190	187
3	20	12	31*
3	22	132	80
4	1	182	198
4	3	316	-298
4	5	100	-91
4	7	185	-168
4	9	137	148
4	11	186	195
4	13	391	-368
4	15	67	6*
4	17	57	52*
4	19	141	-125
4	21	179	201
5	0	144	78
5	2	135	119
5	4	82	50
5	6	384	391
5	8	64	48*
5	10	71	-23*
5	12	114	14*
5	14	284	266
5	16	143	94
5	18	98	90*
5	20	129	-104
5	20	1	-97*
5	22	51	67*
6	1	64	-36*
6	3	372	386
6	5	72	45*
6	7	222	215
6	9	195	177
6	11	154	-163
6	13	218	210
6	15	254	256
6	17	109	70
6	19	92	-44
6	21	42	-36*
7	0	97	-61
7	2	143	-119
7	4	125	-100
7	6	278	278
7	8	222	-196
7	10	191	-166
7	12	104	-81
7	14	125	99
7	16	87	40*
7	18	95	-24*
7	20	238	-228
8	1	180	157
8	3	142	-180
8	5	113	-15
8	7	117	-98
8	9	158	128
8	11	162	151
8	13	231	-252
8	15	104	64
8	17	74	42*
8	19	94	-102*
9	0	128	156
9	2	131	62
9	4	269	-244
9	6	81	23*
9	8	50	46*
9	10	80	91*
9	12	47	-50*
9	14	71	-9*
9	16	130	-98
9	18	117	112
10	1	66	77*
10	3	117	85
10	5	297	-292
10	7	76	28*
10	9	223	228
10	11	105	-50
10	13	95	-25*
10	15	105	-75
10	17	54	-1*
11	0	151	152
11	2	118	68
11	4	64	32*
11	6	362	318
11	8	1	7*
11	10	130	39
11	12	55	58*
11	14	158	143
11	16	150	109
*** H = 12 ***			
0	0	1015	966
0	2	80	-16*
0	4	163	-164
0	6	142	-80
0	8	231	214
0	10	624	606
0	12	52	57*
0	14	245	-265
0	16	164	195
0	18	76	-64*
0	20	448	513
0	22	103	56*
1	1	152	142
1	3	116	-122
1	5	351	316
1	7	54	9*
1	9	37	15*
1	11	182	167
1	13	163	-181
1	15	260	259
1	17	146	143
1	19	207	-237
1	21	131	145
1	23	57	53*
2	0	556	538
2	2	304	-301
2	4	242	-229
2	6	160	144
2	8	102	-99
2	10	89	-65
2	12	192	176
2	14	309	-312
2	16	103	70
2	18	52	35*
2	20	103	-70
2	22	87	-11*
3	1	367	-369
3	3	116	82
3	5	310	316
3	7	133	-96
3	9	193	-175
3	11	315	-304
3	13	121	-101
3	15	504	526
3	17	139	-65
3	19	387	-421
3	21	85	38*
4	0	531	534
4	2	317	-334
4	4	135	-93
4	6	127	105
4	8	140	-176
4	10	142	141
4	12	92	-45*
4	14	210	-231
4	16	257	242
4	18	224	-253
4	20	129	116
4	22	63	7*
5	1	130	150
5	3	249	-268
5	5	354	378
5	7	92	11
5	9	170	-139
5	11	222	229
5	13	187	-180
5	15	156	166
5	17	218	219
5	19	254	-273
5	21	82	86*
6	0	674	721
6	2	134	131
6	4	168	-173
6	6	72	-62*
6	8	335	348
6	10	333	331
6	12	208	207
6	14	203	-192
6	16	86	13*
6	18	181	187
6	20	272	314
7	1	109	-7
7	3	134	99
7	5	57	62*
7	7	57	-50*
7	9	200	180
7	11	75	-56*
7	13	119	-138
7	15	321	300
7	17	123	-47
7	19	116	-134
8	0	596	649
8	2	378	-381
8	4	182	-169
8	6	196	219
8	8	268	-267
8	10	139	148
8	12	115	87
8	14	357	-350
8	16	218	234
8	18	131	-121
8	20	103	25*
9	1	136	-147
9	3	132	-127
9	5	392	378
9	7	86	-20*
9	9	294	-277
9	11	71	-54*
9	13	77	-88*
9	15	279	280
9	17	147	102
9	17	83	103*
9	19	353	-369
10	0	86	17*
10	2	71	-51*
10	4	132	-88
10	6	192	-181
10	8	159	132
10	10	78	-102*
10	12	88	-79*
10	14	57	-14*
10	16	120	-45
10	18	97	-96*
11	1	79	37*
11	3	73	5*
11	5	175	185
11	7	44	13*
11	9	105	30
11	11	82	42*
11	13	82	-71*
11	15	213	221
11	17	54	60*
12	0	798	764
12	2	159	-146
12	4	177	-166
12	6	230	193
12	8	50	-64*
12	10	333	332
12	12	223	192
12	14	335	-326
*** H = 13 ***			
0	1	111	78
0	3	82	-83*
0	5	253	232
0	7	85	20*
0	9	2	-16*
0	11	90	76*
0	13	169	-118
0	15	191	188
1	0	300	-253
1	2	82	-72*
1	4	94	-67*
1	6	201	187
1	8	143	-132
1	10	294	-277
1	12	185	-148
1	14	200	200
1	16	2	-33*
2	1	48	-20*
2	3	131	125
2	5	599	-568
2	7	45	-54*
2	9	326	316
2	11	211	-210
2	13	117	-79*
2	15	168	-141
3	0	186	169
3	2	82	-18*
3	4	314	-301
3	6	113	92*
3	8	69	-58*
3	10	75	9*
3	12	2	-27*
3	14	77	-58*
3	16	127	-122
4	1	142	74
4	3	335	-337
4	5	313	-291
4	7	255	-227
4	9	64	85*
4	11	53	49*
4	13	407	-375
4	15	155	-142
5	0	253	-268
5	2	103	-13*
5	4	101	-45*
5	6	93	121*
5	8	70	-60*
5	10	220	-223
5	12	181	-162
5	14	211	222
5	16	2	-40*
6	1	92	-77*
6	3	198	201
6	5	152	-113
6	7	54	100*
6	9	108	96*
6	11	204	-189
6	13	76	100*
6	15	95	79*
7	0	70	-110*
7	2	83	-88*
7	4	76	-46*
7	6	253	270
7	8	176	-164
7	10	228	-214
7	12	78	-51*
7	14	149	123
8	1	146	125
8	3	57	-71*
8	5	142	-138
8	7	91	-81*
8	9	223	209
8	11	60	75*
8	13	221	-199
8	15	2	29*
9	0	69	-60*
9	2	118	12
9	4	212	-210
9	6	78	-16*
9	8	53	-6*
9	10	2	-24*
9	12	129	-89
9	14	53	8*
10	1	1	-14*
10	3	163	-93
10	5	414	-386
10	7	118	-73
10	9	76	91*
10	11	128	-102
10	13	165	-114
10	15	58	-215*
11	0	98	-99*
11	2	117	-33
11	4	81	-50*
11	6	126	124
11	8	110	-70
11	10	88	-123*
11	12	113	-75
11	14	96	106*
12	1	58	-2*
12	3	1	-1*
12	5	53	41*
12	7	101	-28*
12	9	73	50*
12	11	62	-20*
12	13	120	-90
*** H = 14 ***			
0	0	564	486
0	2	50	-68*
0	4	196	-155
0	6	116	72
0	8	155	125
0	10	86	31*
0	12	245	209
0	14	213	-180
1	1	108	20*
1	3	217	198
1	5	420	-377
1	7	2	49*
1	9	311	286
1	11	184	-144
1	13	77	40*
2	0	315	-302
2	2	265	235
2	4	159	137
2	6	189	-151
2	8	535	485
2	10	397	-377
2	12	99	39*
2	14	337	336
3	1	45	-11*
3	3	262	254
3	5	91	96*
3	7	230	213
3	9	50	59*
3	11	38	-89*
3	13	214	202
4	0	82	97*
4	2	141	-131
4	4	57	46*
4	6	164	156
4	8	73	21*
4	10	259	-232
4	12	169	95*
4	14	74	24*
5	1	89	-48*
5	3	241	266
5	5	425	-398
5	7	2	29*
5	9	342	308
5	11	207	-218
5	13	105	57*
6	0	74	37*
6	2	171	174
6	4	175	-112
6	6	218	-217
6	8	411	407
6	10	158	-149
6	12	66	108*
6	14	2	41*
7	1	156	109
7	3	2	18*
7	5	183	-193
7	7	2	61*
7	9	129	137
7	11	98	24*
7	13	2	-6*
8	0	108	88*
8	2	112	43*
8	4	139	124
8	6	129	89
8	8	202	184
8	10	102	-94*
8	12	132	73
9	1	94	-79*
9	3	323	313
9	5	35	-62*
9	7	170	131
9	9	182	154
9	11	198	-194
9	13	177	169
10	0	94	-111*
10	2	61	-12*
10	4	81	-66
10	6	74	8*
10	8	184	138
10	10	330	-311
10	12	117	78
11	1	71	17*
11	3	94	45*
11	5	159	-162
11	7	49	23*
11	9	128	104
11	11	75	-53*
12	0	86	97*
12	2	73	19*
12	4	72	-52*
12	6	146	-103
12	8	181	149
12	10	52	-9*
*** H = 15 ***			
0	1	312	-259
0	3	86	85*
0	5	247	216
0	7	61	-54*
0	9	86	-119*
0	11	241	-232
1	0	167	140
1	2	139	-45
1	4	264	-221
1	6	89	111*
1	8	63	-89*
1	10	2	17*
1	12	134	-32
2	1	51	9*
2	3	43	40*
2	5	2	4*
2	7	98	82*
2	9	84	-6*
2	11	83	-47*
3	0	358	342
3	2	226	209
3	4	274	-250
3	6	61	-61*
3	8	208	206
3	10	334	319
3	12	2	-10*
4	1	124	25*
4	3	89	-22*
4	5	101	82*
4	7	59	-37*
4	9	164	66
4	11	84	17*
5	0	213	224
5	2	83	-80*
5	4	272	-239
5	6	191	166
5	8	172	-131
5	10	2	28*
6	1	264	-248
6	3	174	187
6	5	107	67*
6	7	83	52*
6	9	138	-104
6	11	291	-282
7	0	8	-31*
7	2	89	16*
7	4	188	-150
7	6	2	-27*
7	8	2	-11*
7	10	2	-1*
8	1	114	63
8	3	124	-167
8	5	172	182
8	7	74	6*
8	9	74	-40*
8	11	45	90*
9	0	408	369
9	2	113	101*
9	4	170	-213
9	6	83	65*
9	8	2	78*
9	10	243	235
10	1	79	-68*
10	3	183	165
10	5	171	-138
10	7	2	25*
10	9	165	127
11	0	113	107
11	2	67	2*
11	4	170	-141
11	6	2	47*
11	8	2	-23*
12	1	87	-80*
12	3	145	-108
12	5	219	210
12	7	119	-18
*** H = 16 ***			
0	0	484	402
0	2	295	-226
0	4	53	-60*
0	6	77	69*
0	8	132	-119
2	0	2	62*
2	2	268	-212
2	4	2	33*
2	6	167	140
2	8	104	-109*
4	2	349	-299
4	4	115	69*
4	6	211	209
4	8	254	-225
5	1	171	146
5	3	244	-190
5	5	58	-35*
5	7	106	-88*
6	0	244	196
6	2	94	-113*
6	4	121	-99
6	6	118	-17*
6	8	41	12*
8	0	218	188
8	2	251	-251
8	4	67	32*
8	6	199	185
10	0	2	-17*
10	2	118	-86*
10	4	87	72*
10	6	113	74*
12	0	274	242
12	2	194	-176
*** H = 17 ***			
5	0	96	-94*
5	2	197	130

[a] Starred entries were statistically unacceptable reflections and were not used in the refinement.

observed. Thus the data are consistent with one of the space groups I4/mmm, I422, I4mm, I$\bar{4}$2m, and I$\bar{4}$m2. Lattice constants obtained from a least-squares analysis of data from Weissenberg photographs taken at room temperature with Cu Kα radiation (λ 1.54178 Å) are $a = 11.86$ (1) Å and $c = 17.10$ (1) Å, slightly different from those reported previously.

Approximately 4500 integrated intensities were collected for hkl and $hk\bar{l}$ to a limit of $\Upsilon = 63°$ with a Philips automatic single-crystal diffractometer, PAILRED, using crystal monochromatized Mo Kα radiation (λ 0.71069 Å) and an ω scan. Reflections from levels $h0l$-$h3l$ were scanned over a 2° interval, those from levels $h4l$-$h5l$ were scanned over a 2.4° interval, and reflections from levels $h6l$-$h12l$ were scanned over a 2.4° interval with $\Upsilon > 30°$ and over a 4° interval with $\Upsilon \leq 30°$. The scanning rate was 1°/min, and background was counted on each side of the peaks for 1 min.

The intensity data were processed and Lorentz and polarization factors applied by means of a program written in this laboratory. Absorption corrections were made using the program GNABS written by Burnham[4] and using a linear absorption coefficient of $\mu = 514$ cm^{-1}, obtained by using the measured density of 8.2 g/cm^3 and assuming a stoichiometry of $Yb_{11}Sb_{10}$. The caclulated transmission factors varied between 0.10 and 0.77. Intensities were accepted as being statistically nonzero on the basis that $\Delta I/I \leq 0.50$.[5] The amplitudes of the equivalent reflections were averaged using their $\sigma(F)$'s as weights, where $\sigma(F)$ is given by

$$\sigma(F_o) = \left\{\frac{F_o^2}{4(T-B)^2}[T + B + 0.0009(T-B)^2]\right\}^{1/2}$$

where T is the total count and B is the computed total background count. The additive term involving $(T - B)$ makes allowance for errors proportional to the net count, such as variation in the beam intensity and absorption errors. An average $\sigma(F)$, $\bar{\sigma}(F)$, was calculated for each averaged F from the individual $\sigma(F)$'s in the equivalent set, using the individual F's as weighting factors. In the case where not all of the

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(4) C. W. Burnham, "An IBM 709/7090 Computer Program for Computing Transmission Factors for Crystals of Essentially Arbitrary Shape," Geophysical Laboratory, Carnegie Institute of Washington, Washington, D. C., 1963.

(5) M. Mack, *Norelco Rep.*, **12**, 40 (1965).

equivalents for an independent reflection were statistically acceptable, only the acceptable ones were used in calculating the average quantities. In the other cases all equivalents were used. The averaged reflections were combined with single reflections for which no equivalents were available in the data set to obtain a final set of 1370 independent reflections, of which 997 were statistically nonzero.

Determination of the Structure.—In the refinements discussed below, R is the conventional discrepancy coefficient, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. The function minimized was $\Sigma[w(|F_o| - |F_c|)^2]$, where w is $[\bar{\sigma}(F_o)]^{-2}$. The computer program used in the refinements was XFLS, a modified version of ORFLS.[6] Dispersion-corrected scattering factors incorporating the real and imaginary terms for Yb and Sb as given in ref 7 for Mo Kα were used throughout.

Beginning with a trial model consisting of the $Ho_{11}Ge_{10}$ parameters, eight cycles of full-matrix least-squares refinement of the scale factor, positional parameters, and isotropic thermal parameters resulted in an R value of 0.13. The thermal parameters after this refinement all fell within the range of 0.3–1.0 Å^2 with the exception of Sb(3), for which the thermal parameter was 3.9 Å^2. Five cycles of anisotropic refinement then resulted in $R = 0.080$, with the thermal parameters for Sb(3) remaining quite high relative to those for the other atoms in the structure.

The high thermal parameter for Sb(3) and the large value of the calculated density for $Yb_{11}Sb_{10}$ might be an indication that the Sb(3) site is partially occupied. A stoichiometry of $Yb_{11}Sb_9$ is obtained on the assumption that the occupant is $^1/_2$Sb. The calculated density for this formula is 8.3 g/cm^3. A full-matrix refinement on this basis reduced the temperature factors of Sb(3) to values comparable with those of the other atoms, as expected, but R increased to 0.084. The formula $Yb_{11}Sb_{10}$ was retained for all further calculations but the possibility that a deviation from the 11:10 composition exists cannot be ruled out.

The final parameters for $Yb_{11}Sb_{10}$ are shown in Table I, the interatomic distances are shown in Table II, and the final observed amplitudes and calculated structure factors are presented in Table III. The standard deviation of an observation of unit weight is 2.67. A difference Fourier synthesis was calculated and contained no peaks representing more than about 0.4 e$^-$/Å^3.

Discussion of the Structure.—The spatial parameters of "α-Yb_5Sb_4" show that it is isostructural with $Ho_{11}Ge_{10}$. A detailed discussion of this structure has been given by Smith, *et al.*[3] All of the bond distances in Table II fall within an acceptable range for the atoms involved. The same type of bonding is expected in this compound as in $Ho_{11}Ge_{10}$, because valence numbers of 3 and 4 for Ho and Ge, respectively, would provide the same number of electrons for bonding as valence numbers of 2 and 5 for Yb and Sb, respectively. Magnetic susceptibility data indicate that nearly all of the Yb is divalent in this phase.[8]

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(6) W. R. Busing, K. O. Martin, and H. A. Levy, USAEC Report ORNL-TM 305, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1962.

(7) "International Tables for X-Ray Crystallography," Vol. III, Kynoch Press, Birmingham, England, 1968.

(8) R. E. Bodnar, H. Steinfink, and K. S. V. L. Narasimhan, *J. Appl. Phys.*, **39**, 1485 (1968).

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