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A redetermination of the crystal structure of livingstonite, $HgSb_4S_8$*

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Auszug

Die Kristallstruktur von Livingstonit wurde neu bestimmt, um die neue chemische Formel $HgSb_4S_8$ (statt $HgSb_4S_7$) zu bestätigen und um die Koordination von Hg und die (S—S)-Bindung in der von Niizeki und Buerger (1957) veröffentlichten Struktur zu studieren. Livingstonit kristallisiert monoklin mit den Gitterkonstanten $a = 30{,}567 \pm 0{,}006$, $b = 4{,}015 \pm 0{,}001$, $c = 21{,}465 \pm 0{,}003$ Å und $\beta = 103{,}39 \pm 0{,}01\,°$, in der Raumgruppe C^6_{2h}—$A\,2/a$ mit 8 Formeleinheiten pro Zelle. Die Struktur wurde mittels Block-Diagonal-Least-Squares-Methoden bis zu einem R-Wert von 7,3% für 596 beobachtete (10,2% für alle 1099) Reflexe verfeinert.

Die Strukturbestimmung bestätigt die neue chemische Formel. Es kommt eine S_2-Gruppe mit S—S = 2,06 Å, die das zusätzliche achte S-Atom in der neuen Formel liefert, vor. In der Struktur sind zwei Schichtarten $\parallel c$ vorhanden. Die (S—S)-Bindung verknüpft zwei Sb_2S_4-Doppelketten, wodurch zwischen ihnen eine S_2-Gruppe entsteht. Die anderen Sb_2S_4-Doppelketten werden durch Hg-Atome untereinander verbunden. Die Bindungen zwischen diesen Doppelketten sind eher schwach und erklären die perfekte Spaltbarkeit $\parallel$ (001).

Die Koordination der Hg-Atome ist oktaedrisch; zwei der S-Atome sind stark und linear gebunden, ähnlich wie in Zinnober. In der Struktur sind vier unabhängige Sb-Atome vorhanden. Zwei davon weisen eine Viererkoordination durch S-Atome auf, in Form einer deformierten trigonalen Pyramide plus ein zusätzliches S-Atom. Die beiden anderen Sb-Atome haben eine quadratisch-pyramidale bzw. die normale trigonal-pyramidale Koordination. Die Strukturformel von Livingstonit kann als $[(Sb_2S_4)_2\,|\,Hg^{II+IV}]$ geschrieben werden [Typ IV.a_1 der Klassifikation von Nowacki (1969)].

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* Contribution No. 243b; part 72 on sulfides and sulfosalts (Preliminary note: Srikrishnan and Nowacki, 1973).

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Abstract

The crystal structure of livingstonite has been redetermined with a view to confirm the new chemical formula, $HgSb_4S_8$ (not $HgSb_4S_7$) as well as to study the coordination of mercury and the S—S bond in the structure, reported by NIIZEKI and BUERGER (1957). Crystals of livingstonite are monoclinic, having the cell dimensions $a = 30.567 \pm 0.006$, $b = 4.015 \pm 0.001$, $c = 21.465 \pm 0.003$ Å and $\beta = 103.39 \pm 0.01°$. The space-group symmetry is C_{2h}^6—$A\,2/a$ and there are eight formula units in the unit cell. The structure was refined by block-diagonal least-squares method to a final R value of 7.3% for the 596 observed reflections (10.2% for all 1099 reflections).

The structure confirms the new chemical formula. There is an S_2 group with an S—S distance of 2.06 Å, which gives raise to the additional sulfur atom in the new chemical formula. There are two kinds of layers running parallel to the c axis in the structure. The S—S bond joins two Sb_2S_4 double chains. The other Sb_2S_4 double chains are joined together by the Hg atoms. The bonds between these two double chains are rather weak and hence explain the presence of a perfect cleavage || (001).

The coordination of the Hg atoms is octahedral; two of the S atoms are strongly and linearly bonded, as in cinnabar. There are four independent Sb atoms in the structure. Two of them have a coordination of four sulfur atoms which could be described as distorted trigonal pyramid plus one additional sulfur atom. The other two Sb atoms have a square pyramidal coordination and the familiar trigonal pyramidal coordination, respectively. The structural formula of livingstonite could be described as $[(Sb_2S_4)_2 \mid Hg^{II+IV}]$ [type IV.a_1 in the classification of the sulfosalts by NOWACKI (1969)].

Introduction

Livingstonite is a mercury antimony sulfide and derives its name after its discoverer, DAVID LIVINGSTONE. It is quite often found to occur along with cinnabar, which is regarded as its pseudomorph. It occurs in association with stibnite, sulfur, cinnabar and valentinite in a matrix of calcite and gypsum, at Huitzuco, Guerrero, Mexico and also at Guadalcázar, San Luis Potozi, with gypsum and sulfur (DANA, 1944). For a long time, its chemical composition was taken to be $HgSb_4S_7$, until NIIZEKI and BUERGER (in 1957) gave the correct chemical composition as $HgSb_4S_8$.

Livingstonite was first investigated by RICHMOND (1936), who described it as monoclinic, belonging to the space group $P\,2_1/c$. Later GORMAN (1954) reported it as triclinic. The cell dimensions reported by them are given in Table 1. NIIZEKI and BUERGER (1957) investigated its structure and found it to be monoclinic. They also found an anomaly in the chemical composition and concluded that the correct composition is $HgSb_4S_8$ instead of $HgSb_4S_7$. Their analysis, although based on three-dimensional diffractometer data, was not very accurate, probably due to the limitations of the quality of the data and to the limitations on computing and least-squares refinement techniques in 1957.

Quite recently, another mercury-containing sulfosalt, vrbaite, $Hg_3Tl_4As_8Sb_2S_{20}$ has been investigated in this laboratory (Ohmasa and Nowacki, 1971). We have undertaken the redetermination of livingstonite to resolve the anomaly in its chemical composition with more accurate data and also to study the coordination of mercury and compare it with that of vrbaite.

Experimental

The crystal used for the present study was prepared from a sample of livingstonite from the type locality in Mexico. It was a thin and fibrous needle, having the dimensions 0.152 × 0.081 × 0.046 mm, with approximately cylindrical cross-section.

The lattice constants were determined with the help of back-reflection Weissenberg photographs, on which the diffraction pattern of standard silicon had been superimposed to calibrate the film shrinkage. The precise cell constants determined from a least-squares

Table 1. *Crystallographic data of livingstonite*

	Richmond (1936)	Gorman (1954)	Niizeki and Buerger (1957)	Present study
Space group	$P2_1/c$	$P1$ or $P\bar{1}$	$A2/a$	$A2/a$
a	15.14 Å	7.67 Å	30.25 Å	30.567 ± 0.006 Å
b	3.98	4.00	4.00	4.015 ± 0.001
c	21.60	10.84	21.49	21.465 ± 0.003
α	—	99° 12′	—	—
β	104° 00′	102° 1′	104° 12′	103.39 ± 0.02
γ	—	73° 48′	—	—
V				2562 Å^3
Cell content	4 $HgSb_4S_7$	$HgSb_4S_7$	8 $HgSb_4S_8$	8 $HgSb_4S_8$
Computed density			5.06	4.89 g cm^{-3}
Measured density			5.00 (Frondel)	
$F(000)$				3296 electrons
R for observed reflections			0.19	0.073

best fit of 20 ($h0l$) and 14 ($0kl$) reflections are given in Table 1, together with the values of NIIZEKI and BUERGER (1957), GORMAN (1945) and RICHMOND (1936). The calculations were made with the help of a program written by N. D. JONES (unpublished).

The crystal belongs to the monoclinic system. The systematic absences, as observed from Weissenberg photographs are

$$hkl\colon\ k + l = 2n + 1$$

$$h0l\colon\ l = 2n + 1 \qquad (h \neq 4n)$$

$$0k0\colon\ k = 2n + 1.$$

The possible space groups are $A\,2/a$ or Aa. But the former space group has been assumed, because an analysis of the distribution of the normalized structure amplitudes suggested the centric rather than the acentric space group (see Table 2). The systematic absences in $h0l$ reflections are rather unusual. In addition to the space group extinctions of $h = 2n + 1$ and $l = 2n + 1$, there is an additional absence of $h \neq 4n$. This could be only interpreted as due to the structural arrangement. There are eight formula units in the unit cell and one in the asymmetric octant. In all this we follow and confirm the 1957 analysis by NIIZEKI and BUERGER.

Table 2. *Distribution of normalized structure factors*

	Experimental	Theoretical	
		centric	acentric
$< \|E\| >$	0.657	0.798	0.886
$< \|E^2\| >$	1.029	1.000	1.000
$< \|E^2 - 1\| >$	1.312	0.968	0.736
$\|E\| > 3.0$	2.3%	0.3%	0.01%
$\|E\| > 2.0$	6.9%	5.0%	1.8%
$\|E\| > 1.0$	24.4%	32.0%	36.8%

Three-dimensional intensity data were collected by a Supper-Pace automated diffractometer having Weissenberg geometry and using Cu$K\alpha$ radiation. The intensities were corrected for Lorentz and polarization factors. Correction for absorption was made with the help of an ICR-10 program (JOHNSON, 1963), because of the high linear absorption coefficient of the material ($\mu = 1068$ cm^{-1} for Cu$K\alpha$ radiation).

Structure determination and refinement

The coordinates of the Hg atoms were determined from an analysis of the Patterson synthesis. There were two big peaks in the three-

Table 3. *Observed and calculated structure factors for livingstonite*

h	F_o	F_c
h	**0 0**	
8	661	667
12	496	-490
16	422	373
h	**0 2**	
4	528	-487
-4	162	159
8	674	694
-8	1098	1028
12	698	686
-12	649	664
-16	464	413
h	**0 4**	
-4	630	568
8	521	536
-12	850	785
-20	894	876
h	**0 6**	
0	308	-297
4	839	894
-4	1371	1476
-8	833	755
-12	991	948
h	**0 8**	
0	348	-375
4	1217	1276
8	384	414
-8	430	-433
-12	1003	1001
-16	420	421
-20	590	586
-24	125	129
h	**0 10**	
0	789	788
4	474	432
8	342	-338
-8	822	916
-12	163	-179
-16	219	206
-24	324	350
h	**0 12**	
0	258	238
8	716	750
-8	578	630
-16	661	725
-24	121	142
h	**0 14**	
0	858	824
-16	252	267
-20	367	381
-24	376	366
-28	105	122
h	**0 16**	
0	84	-53
4	95	-88
-4	410	386
8	309	323
-8	574	633
-12	414	448
-16	89	89
-24	116	-114
-28	103	113
h	**0 18**	
0	151	153
4	416	410
-4	178	168
-8	333	-323
-12	200	208
-20	445	479
-28	180	194
h	**0 20**	
0	137	-124
-4	521	531
-12	375	365
-28	208	227
h	**0 22**	
-4	111	97
-8	134	-137
-12	225	210
-16	238	251
-20	158	150
h	**0 24**	
0	134	158
-4	143	135
-8	133	125
-16	87	84
-20	69	-59
h	**0 26**	
-8	202	179
h	**1 1**	
6	1097	-1140
-6	345	-365
7	161	160
-7	88	77
9	110	-120
-9	106	-111
10	770	-744
-10	405	352
-11	200	210
-12	119	-121
13	95	109
-13	241	235
-14	795	-734
-15	155	-161
-17	109	94
18	74	-66
-18	262	-251
h	**1 3**	
-2	278	-262
4	134	172
-4	89	-59
5	277	310
-5	327	304
6	693	690
-6	1999	-1717
7	224	-260
-7	449	-382
-8	139	144
-9	236	-211
10	521	-531
-11	106	105
-14	203	-206
15	100	-103
-19	157	163
-22	314	-344
h	**1 5**	
2	222	-246
-3	267	295
-5	122	94
6	387	-399
-6	1127	-969
9	235	-274
10	1013	-1025
-10	461	-418
-13	207	198
-14	970	-872
-15	171	-167
-18	223	-201
h	**1 7**	
2	725	-729
3	149	163
-5	117	-114
6	341	-366
-9	117	-137
10	359	-361
-10	215	-197
-13	163	-154
-14	314	269
-15	203	177
-16	95	104
-17	107	104
-18	492	-494
-22	88	-72
27	52	51
h	**1 9**	
1	279	267
-1	85	57
2	459	477
-2	531	-557
3	241	-240
6	354	-382
-7	94	79
-9	265	281
-10	965	-982
-11	243	-271
-14	485	-459
-18	431	-420
-21	166	-161
-22	341	308
-23	125	125
h	**1 11**	
-1	104	110
2	410	-393
-2	1027	-1024
-3	182	-183
-4	88	-103
5	153	-142
-5	208	-237
6	658	-661
7	196	196
-10	215	-212
-17	124	131
-18	506	-529
19	63	-69
-22	180	-175
23	53	41
h	**1 13**	
1	125	124
-2	379	-382
-5	117	120
-6	484	-539
-10	125	-139
-11	77	-87
-14	185	-195
-17	113	-125
-18	136	140
-19	94	95
-22	150	-144
24	46	31
26	35	-31
-26	152	-157
-29	52	61
h	**1 15**	
1	101	-108
2	355	-340
-2	79	74
-3	105	107
6	154	-160
-6	189	-197
-10	80	-73
-11	96	109
-13	157	167
-15	130	-129
-22	400	-416
-23	96	-90
-25	91	-89
-26	111	111
-27	54	60
h	**1 17**	
2	518	-537
5	101	107
6	84	101
-6	577	-577
-9	92	-85
-11	75	41
-14	78	-69
-18	215	263
-19	97	103
-22	144	-148
-26	183	-199
h	**1 19**	
-1	89	-95
2	105	-110
-2	158	160
6	63	-64
-10	268	-277
12	62	80
-13	83	77
-14	358	-374
-18	109	-87
h	**1 21**	
2	201	-207
-2	294	-258
-3	72	-80
-10	182	-188
-13	99	-68
-14	133	126
-15	99	85
-17	62	55
-18	291	-291
-19	59	-28
-22	55	-43
-26	158	-156
-27	52	-55
h	**1 23**	
2	92	119
-2	137	-145
-10	281	-260
-12	66	65
-14	48	51
-18	84	-82
-21	61	-62
-22	75	76
-23	58	51
h	**1 25**	
-2	52	-53
-5	51	-52
-10	54	-58
-14	40	43
-15	45	21
h	**2 0**	
8	350	394
11	271	-289
14	128	132
16	259	255
h	**2 2**	
-1	97	-124
-5	162	-170
6	109	-88
8	265	320
-8	391	407
12	341	355
-12	238	243
-14	79	83
15	183	194
-16	245	233
-17	82	57
21	101	86
h	**2 4**	
-3	69	64
4	279	312
-4	363	378
5	191	-200
-5	72	93
-6	109	-122
-7	297	296
8	244	250
-8	127	148
9	94	-107
-9	236	-244
-10	113	-90
11	143	-160
12	85	81
-12	551	548
13	70	47
-19	216	-212
-20	460	420
-21	177	189
-22	72	69
-24	70	91
29	47	27
h	**2 6**	
0	71	-55
-1	246	-271
4	618	639
-4	587	616
-5	289	297
7	179	-203
-8	352	367
9	246	241
11	159	161
12	355	399
-12	503	473
-13	268	269
-15	318	314
-16	211	-182
-17	203	-198
-20	87	80
-21	32	34
h	**2 8**	
1	293	280
-1	90	-80
3	341	366
-3	74	97
4	655	590
-5	79	-76
-7	166	174
8	190	195
-9	265	-270
11	84	68
-11	200	-216
-12	559	571
-16	154	153
-17	82	81
-19	71	-97
-20	284	286
-21	125	112
-24	102	105
27	37	40
28	44	47
h	**2 10**	
0	362	388
3	84	-82
-3	116	-142
4	376	338
-4	258	272
7	209	-211
8	98	-85
-8	460	490
9	141	138
-9	177	181
-11	186	201
-16	240	250
-20	95	92
-21	120	-115
-23	105	-113
-24	154	154
h	**2 12**	
0	217	237
-3	169	179
4	96	110
-5	259	-262
-6	73	70
7	246	213
-7	169	-179
8	421	390
9	122	-121
-9	104	108
-15	162	-175
-16	280	303
-17	212	231
18	62	-60
-18	74	-65
-19	127	116
-27	56	58
h	**2 14**	
0	335	344
1	269	-235
-1	212	225
-2	81	84
-3	91	90
8	228	213
-8	341	371
9	68	-88
-13	162	-199
14	59	-73
-14	81	-82
-16	172	189
17	46	-56
-20	248	252
21	69	57
-23	92	-90
-24	164	165
-25	97	99
h	**2 16**	
-1	97	-113
3	119	-102
-4	277	293
5	126	121
-6	70	81
7	69	89
-7	160	-150
-8	302	328
-9	111	111
-12	184	195
-13	138	134
-14	64	48
16	55	72
18	78	-89
19	34	-3
-23	85	83
-25	75	-80
h	**2 18**	
0	95	73
3	133	133
4	210	185
-4	111	111
-7	169	168
-9	145	-150
-10	83	-84
-12	152	157
-17	56	-52
-19	131	-134
-20	205	210
-21	137	134
-22	47	-42
h	**2 20**	
1	55	70
-1	111	-92
4	62	75
-4	278	268
-6	58	49
-12	211	205
-15	109	96
-16	100	100
-17	81	-80
-20	52	60
h	**2 22**	
0	82	82
2	71	-50
3	46	63
-4	121	109
-7	63	61
-9	79	-77
-11	80	-74
-12	125	117
-15	52	-60
-16	119	124
-17	68	61
-20	77	69
h	**3 1**	
7	71	83
-9	64	-79
11	102	100
-12	91	-65
-13	208	207
14	114	-113
-14	100	-113
-18	58	-53
22	49	-35
27	35	-34
h	**3 3**	
4	120	110
5	213	239
-5	225	223
-6	382	-415
-7	336	-330
-8	93	70
-9	235	-209
10	279	-294
15	85	-93
-16	83	101
-18	218	-204
-19	132	148
-20	63	-60
-21	84	87
-22	81	-97
h	**3 5**	
0	65	69
-1	151	-177
-4	86	75
-5	141	151
-6	441	-440
9	204	-220
-9	59	75
10	207	-206
-10	111	-121
11	188	197
12	61	-40
-12	69	-80
13	84	91
-13	153	138
-14	214	-199
-15	150	-127
-16	81	-58
-22	58	-68
h	**3 7**	
-1	77	95
2	138	-128
-2	109	-114
3	112	106
-5	140	-134
-8	68	66
-9	68	-82
10	275	-281
-10	199	-209
-14	71	-70
-16	83	77
-17	138	124
-18	170	-161
h	**3 9**	
-1	118	97
-2	221	-232
4	72	46
6	187	-176
-7	120	118
-8	99	-73
-9	232	226
-11	223	-219
-14	220	-244
-18	188	-185
-20	81	95
-21	164	-149
-23	106	113
-24	50	-45
-25	43	40
h	**3 11**	
-1	109	117
-2	377	-372
-3	200	-204
4	65	-67
-4	81	-62
-5	205	-218
6	110	-93
7	192	185
-7	112	125
-8	64	79
9	105	94
-10	163	-161
-14	106	-95
-15	102	98
-16	62	-73
-17	105	107
18	40	-18
-18	114	-134
-19	69	-82
-23	52	-33
-24	52	31
h	**3 13**	
-1	88	72
-2	138	-117
-5	72	76
-6	78	-91
-8	57	-65
-13	66	-54
-14	103	-92
-16	49	72
-17	98	-93
-18	70	-61
-22	99	-94
h	**3 15**	
0	60	70
1	144	-118
-2	121	-120
-4	70	73
-6	168	-154
-10	156	-142
11	36	52
12	34	24
-12	77	-69
-13	181	163
-15	104	-116
-16	53	-65
-21	46	31
-22	141	-145
-23	102	-99
h	**3 17**	
2	213	-187
-4	86	66
5	80	97
-5	141	119
7	79	-69
-9	123	-85
-14	94	-77
-17	79	-71
h	**3 19**	
-1	96	-88
2	50	-66
-7	59	51
-9	65	42
-10	114	-100
-13	64	59
-14	100	-101
-15	94	-69
h	**4 0**	
9	85	-99
10	59	-41
11	70	-53
h	**4 2**	
6	67	-35
7	77	99
-7	65	-89
h	**4 4**	
0	54	74
-7	56	50
-8	233	214
-11	87	-81
-12	210	196
16	49	66
h	**4 6**	
-2	48	33
4	266	242
-5	60	71
8	90	87
9	65	64
-13	125	125
-14	74	-68
-17	61	-61
-18	53	-51
h	**4 8**	
2	66	58
4	59	53
-4	47	13
5	74	-77
8	54	52
-9	74	-89
-11	90	-105
h	**4 10**	
0	73	71
1	74	-51
-6	43	50
7	61	-64
8	36	34
-8	97	103
-9	69	67
-11	58	66
-14	36	-14
h	**4 12**	
-1	60	37
-2	40	-69
4	96	75
-11	37	39

dimensional Patterson synthesis, corresponding to the Hg—Hg interactions. There are two kinds of Hg atoms in the structure. Hg(1) is located at the centre of symmetry and Hg(2) is placed on the twofold axis. A three-dimensional Fourier synthesis was computed with the Hg atoms and the antimony atoms could be located from this Fourier map. A structure-factor calculation with the mercury and antimony atomic coordinates and with the overall B of 4.6 Å^2, as indicated from the Wilson plot, yielded an R value of 45.6$^0/_0$ for all 1099 reflections. A three-dimensional Fourier synthesis computed with these atoms, showed up all the sulfur atoms. The additional sulfur atom, found by the same procedure as by NIIZEKI and BUERGER, also showed up, with almost the same strength as the other sulfur atoms.

A structure-factor calculation with all these atoms, yielded an R value of 38.5$^0/_0$ for all reflections (the final atomic coordinates, as reported by NIIZEKI and BUERGER, with an overall B of 4.6 Å^2 gave an R value of 19$^0/_0$ for observed reflections and 27.7$^0/_0$ for all 1099 reflections). Three-dimensional block-diagonal least-squares refinements were started with the initial R value of 38.5$^0/_0$. After a series of isotropic block-diagonal least-squares refinements, the R value fell to 13.5$^0/_0$ for all 1099 reflections. The refinements were continued with anisotropic thermal parameters for all the atoms and the final R value was 7.3$^0/_0$ for the observed 596 reflections (10.2$^0/_0$ for all 1099 reflections). The effect of anomalous dispersion was taken into account but no significant difference was found between the two enantiomorphs. Reflections with $I < 2.233\sigma(I)$ were assigned as unobserved reflections. Neutral atom scattering factors as given by THOMAS, UMEDA were used for the Hg and Sb atoms and those given by DAWSON were used for the S atoms (*International tables*, 1962).

A block-diagonal least-squares refinement programm written by ENGEL (1972) for IBM 370/155 was used in the structure refinement.

In the beginning stages of the refinement, unit weights were assigned to all the reflections, but in the final stages weights were calculated using the weighting function (ENGEL, 1972)

$$W = \frac{1}{(G_1 + F_{\text{obs}} + G_2 \cdot F^2_{\text{obs}})} ,$$

where $G_1 = 8$ and $G_2 = 0$.

A list of the final observed and calculated structure amplitudes is given in Table 3.

Description of the structure

The final atomic coordinates are given in Table 4*a* and the anisotropic thermal parameters in Table 4*b*. The root-mean-squared displacements of the atoms along the principal axes of the vibration ellipsoid

Table 4a. *The final atomic coordinates of livingstonite, their standards deviations* (in parentheses) *and occupancy factors.* In brackets: coordinates given by NIIZEKI and BUERGER (1957)

Atom	x		y		z		Occupancy factor
Hg(1)	0	[0]	0.5	[0.5]	0	[0]	0.5
Hg(2)	0.25	[0.25]	0.0089(11)	[0.001]	0	[0]	0.5
Sb(1)	0.0395(2)	[0.042]	0.0628(12)	[0.095]	0.2115(2)	[0.214]	1.0
Sb(2)	0.1244(1)	[0.120]	0.0563(12)	[0.063]	0.0779(2)	[0.075]	
Sb(3)	0.1355(2)	[0.131]	0.0586(12)	[0.064]	0.4281(2)	[0.425]	
Sb(4)	0.2057(2)	[0.208]	0.1091(12)	[0.078]	0.2847(2)	[0.287]	
S(1)	0.0148(6)	[0.022]	0.005(3)	[0.021]	0.3169(7)	[0.318]	
S(2)	0.0642(5)	[0.062]	0.517(3)	[0.493]	0.0979(5)	[0.092]	
S(3)	0.0757(6)	[0.078]	0.516(3)	[0.507]	0.4625(6)	[0.460]	
S(4)	0.1077(6)	[0.102]	0.501(4)	[0.483]	0.2881(6)	[0.277]	
S(5)	0.1527(6)	[0.149]	0.511(3)	[0.521]	0.2300(5)	[0.222]	
S(6)	0.1698(9)	[0.172]	0.520(5)	[0.506]	0.0352(13)	[0.039]	
S(7)	0.2060(9)	[0.189]	0.512(3)	[0.494]	0.4216(9)	[0.407]	
S(8)	0.2177(7)	[0.229]	0.024(4)	[0.028]	0.1795(9)	[0.180]	

Table 4b. *The final anisotropic temperature factor coefficents*
The values are the coefficients in the expression
$\exp [- (h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + hk\beta_{12} + hl\beta_{13} + kl\beta_{23}$

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Hg(1)	0.00188(11)	0.086(3)	0.00303(12)	0.0004(8)	0.0013(2)	−0.0015(9)
Hg(2)	177(10)	81(3)	266(10)	—	12(2)	—
Sb(1)	140(10)	86(4)	229(11)	− 18(8)	14(2)	3(10)
Sb(2)	134(10)	83(4)	200(10)	− 52(7)	11(2)	− 41(8)
Sb(3)	125(9)	80(3)	217(11)	− 41(7)	10(2)	− 29(8)
Sb(4)	185(11)	78(3)	228(11)	56(8)	17(2)	26(10)
S(1)	0.0010(3)	0.039(7)	0.0023(4)	0.006(2)	0.0026(6)	0.007(3)
S(2)	3(2)	37(6)	10(2)	− 3(2)	− 3(3)	− 2(2)
S(3)	15(3)	39(7)	11(3)	− 7(2)	15(5)	− 5(2)
S(4)	5(2)	70(10)	10(2)	− 1(2)	2(4)	4(2)
S(5)	13(2)	26(6)	5(2)	2(2)	− 13(3)	− 2(2)
S(6)	15(5)	64(12)	49(8)	− 10(3)	25(10)	− 4(5)
S(7)	35(5)	2(6)	36(5)	− 4(2)	52(9)	− 3(3)
S(8)	4(2)	73(11)	24(4)	− 1(2)	12(5)	− 5(3)

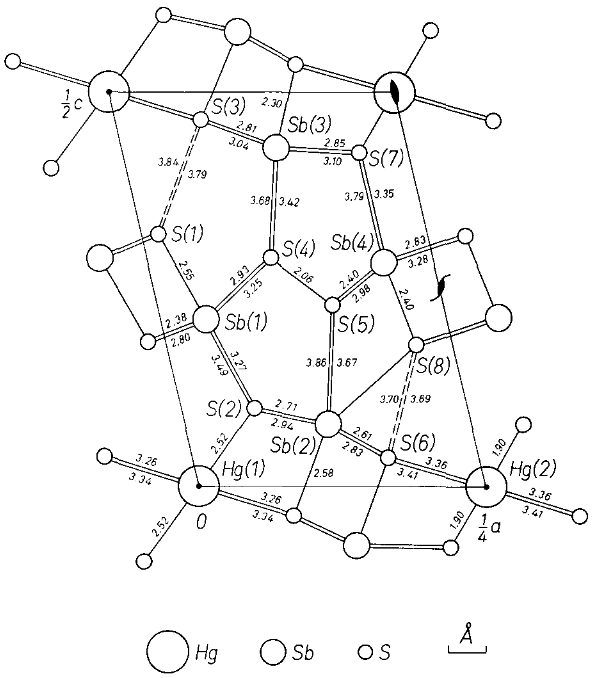

Fig. 1. The structure of livingstonite projected down [010]

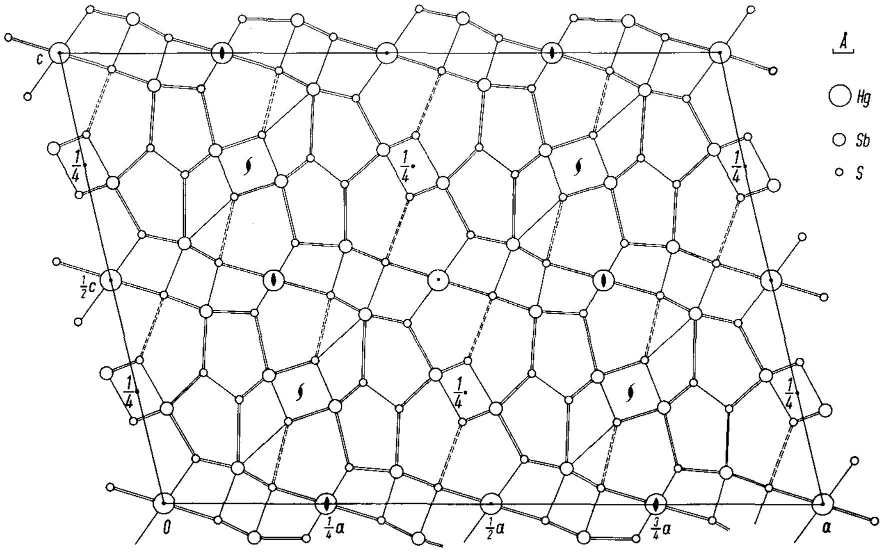

Fig. 2. A schematic representation of the structure of livingstonite, in the whole unit cell, projected down the *b* axis

are given in Table 5. The arrangement of atoms projected down the *b* axis is given in Fig. 1. In Fig. 2, the structural scheme is illustrated for the unit cell.

The structure proposed by NIIZEKI and BUERGER is essentially correct. For purposes of comparison, the final atomic coordinates of NIIZEKI and BUERGER are also given in Table 4*a*, in brackets, along with those of this investigation. The average shift in the coordinates of the Sb atoms from the model of NIIZEKI and BUERGER is 0.077 Å, while those in the S atoms is 0.128 Å. The largest shift in a Sb-atom coordinate is 0.086 Å and that in a sulfur atom is 0.302 Å.

The interatomic distances and angles are given in Tables 6*a* and 6*b* respectively. There are two kinds of Hg atoms in the structure. One of them is located at the centre of symmetry and the other on the twofold axis. Both these Hg atoms are included in the structure-factor calculation, with an occupancy factor of 0.5, so as to be consistent with the unit cell content of 8 Hg atoms. The coordination of the two Hg atoms by the S atoms are octahedral; two of the S atoms are nearer than the other four and linked to Hg in a diagonal linear bond. The octahedron around Hg(1) is formed by S(2), S(2)′, S(3)′, S(3)″, S(3)‴ and S(3)⁗. Out of these, S(2) and S(2)′ are linearely bonded to Hg at a distance of 2.52 Å [S(2)—Hg(1)—S(2)′ = 180.0°]. Such diagonal linear covalent linkage is characteristic of the structural chemistry of the Hg atom (GRDENIĆ, 1965) and is also found in the structure of cinnabar, HgS (Hg—S = 2.36 Å, S—Hg—S = 172°; AURIVILLIUS, 1950) and also in vrbaite (Hg—S = 2.38 Å, S—Hg—S = 166.0°; OHMASA and NOWACKI, 1971). The octahedral arrangement around Hg(1) is almost regular and runs almost parallel to the *c* axis. The average Hg—S distance is 3.04 Å and the average standard deviation in them is 0.013 Å. Hg(2) also has an octahedral arrangement with S(7)′, S(7)″, S(6), S(6)′, S(6)″ and S(6)‴. The atoms S(7)′ and S(7)″ are almost linearely bonded to mercury. The angle S(7)′—Hg(2)—S(7)″ = 179.1°, but the covalent distance between the Hg and S atoms is 1.90 Å, shorter than the sum of the covalent radii of the atoms (2.36 Å). The standard deviation in these bonds is 0.02 Å and it is rather difficult to assert that this bond is really short. Similar short bonds, those less than, or equal to, the sum of the covalent radii, have been reported in some mercury-bearing compounds: in dimethyl thio-mercury (BRADLEY and KUNCHUR, 1964), the Hg—S distance is 2.36 Å; in KI · $Hg(CN)_2$, the Hg—C diagonal bond is 2.08 Å (KRUSE, 1963), which is less than the sum of the covalent radii 2.3 Å

Table 5. *The root-mean-squared displacements of the atoms along the principal axes of the vibration ellipsoids and direction cosines of these axes with respect to the crystallographic axes*

Atom	B_{isotr}	Axes	B	$\sqrt{\overline{u^2}}$	$\cos\alpha_1$	$\cos\alpha_2$	$\cos\alpha_3$
Hg(1)	5.78	1	6.66	0.290	0.954	0.058	0.294
		2	5.69	0.268	0.092	0.877	−0.472
		3	5.00	0.252	−0.285	0.477	0.831
Hg(2)	5.35	1	6.27	0.282	0.977	0.000	0.215
		2	5.21	0.257	0.000	1.000	0.000
		3	4.56	0.240	−0.215	0.000	0.977
Sb(1)	4.72	1	4.96	0.251	0.664	0.490	0.565
		2	5.77	0.270	−0.477	0.859	−0.184
		3	3.43	0.209	−0.575	−0.147	0.805
Sb(2)	4.47	1	3.79	0.219	0.811	0.584	0.021
		2	6.39	0.284	−0.555	0.782	−0.284
		3	3.23	0.202	−0.182	0.218	0.959
Sb(3)	4.41	1	3.78	0.219	0.666	0.583	0.465
		2	5.90	0.273	−0.511	0.811	−0.285
		3	3.53	0.212	−0.543	−0.048	0.838
Sb(4)	5.03	1	7.42	0.307	0.801	0.487	0.348
		2	4.28	0.233	−0.386	0.865	−0.322
		3	3.40	0.207	−0.457	0.124	0.881
S(1)	2.92	1	0.56	0.084	0.832	−0.158	−0.531
		2	1.82	0.152	−0.098	0.901	−0.422
		3	6.38	0.284	0.545	0.404	0.735
S(2)	1.84	1	0.50	0.079	0.738	0.357	0.573
		2	2.64	0.183	−0.356	0.927	−0.119
		3	2.39	0.174	−0.573	−0.116	0.811
S(3)	3.03	1	6.14	0.279	0.831	−0.421	0.363
		2	1.79	0.151	0.506	0.843	−0.181
		3	1.16	0.121	−0.230	0.334	0.914
S(4)	2.71	1	1.88	0.154	0.989	0.145	0.019
		2	4.75	0.245	−0.145	0.963	0.228
		3	1.50	0.138	0.015	−0.228	0.973
S(5)	2.72	1	6.34	0.283	0.940	0.134	−0.315
		2	1.62	0.143	−0.162	0.985	−0.065
		3	0.19	0.049	0.301	0.112	0.947

Table 5. *(Continued)*

Atom	B_{isotr}	Axes	B	$\sqrt{\bar{u}^2}$	$\cos\alpha_1$	$\cos\alpha_2$	$\cos\alpha_3$
S(6)	5.69	1	5.80	0.271	0.635	−0.648	−0.422
		2	2.13	0.164	0.696	0.716	−0.051
		3	9.12	0.340	0.335	−0.261	0.905
S(7)	5.51	1	13.74	0.417	0.817	−0.067	0.572
		2	0.07	0.031	0.051	0.998	0.044
		3	2.72	0.186	−0.574	−0.007	0.819
S(8)	3.35	1	1.01	0.113	0.985	0.000	−0.174
		2	5.43	0.262	−0.111	0.769	−0.630
		3	3.62	0.214	0.133	0.640	0.757

Table 6a. *Interatomic distances in livingstonite*

Hg(1)—S(2)	2.52 ± 0.01 Å	[2×]
S(3)‴	3.34 ± 0.01	[2×]
S(3)′	3.26 ± 0.01	[2×]
Mean	3.04	
Hg(2)—S(7)′	1.90 ± 0.02	[2×]
S(6)	3.41 ± 0.02	[2×]
S(6)′	3.36 ± 0.02	[2×]
Mean	2.89	
Sb(1)—S(1)	2.55 ± 0.02	
S(1)′	2.38 ± 0.01	
S(1)″	2.80 ± 0.01	
S(4)	2.93 ± 0.02	
Mean	2.67	
Sb(2)—S(6)	2.61 ± 0.02	
S(6)′	2.83 ± 0.02	
S(2)	2.71 ± 0.01	
S(2)′	2.94 ± 0.01	
S(3)′	2.58 ± 0.01	
Mean	2.73	
Sb(3)—S(6)′	2.30 ± 0.03	
S(3)	2.81 ± 0.01	
S(7)	2.85 ± 0.02	
Mean	2.65	
Sb(4)—S(8)	2.40 ± 0.02 Å	
S(5)	2.40 ± 0.01	
S(8)′	2.83 ± 0.02	
S(5)′	2.98 ± 0.01	
Mean	2.65	
S(1)—S(1)′	3.42 ± 0.02	
S(1)″	3.47 ± 0.02	
S(4)	3.64 ± 0.02	
S(4)′	3.66 ± 0.02	
S(3)	3.84 ± 0.02	
S(3)′	3.79 ± 0.02	
S(4)″	3.90 ± 0.02	
Sb(3)	3.91 ± 0.02	
S(2)—Sb(1)	3.27 ± 0.01	
Sb(1)′	3.35 ± 0.02	
S(5)	3.44 ± 0.02	
Sb(1)′	3.49 ± 0.01	
S(3)′	3.61 ± 0.02	
S(3)″	3.62 ± 0.02	
S(6)	3.77 ± 0.03	
S(4)	3.99 ± 0.02	
S(3)—S(6)′	3.55 ± 0.03	
S(6)″	3.57 ± 0.03	

Table 6a. *(Continued)*

S(4)—S(5)		2.06 ± 0.02 Å
	Sb(1)′	3.25 ± 0.02
	Sb(3)	3.42 ± 0.01
	S(7)	3.64 ± 0.02
	Sb(3)′	3.69 ± 0.01
	Sb(4)′	3.88 ± 0.02
	Sb(4)	3.40 ± 0.02
S(5)—S(8)		3.15 ± 0.02
	S(8)′	3.22 ± 0.02
	Sb(2)	3.67 ± 0.01
	Sb(1)	3.84 ± 0.02
	Sb(2)′	3.86 ± 0.01
	S(8)′	3.99 ± 0.02
S(6)—S(7)′		3.51 ± 0.03
S(6)—S(7)″		3.55 ± 0.03 Å
	S(8)	3.69 ± 0.03
	S(8)′	3.70 ± 0.03
S(7)—Sb(3)′		3.10 ± 0.02
	Sb(4)	3.35 ± 0.02
	S(8)′	3.53 ± 0.03
	Sb(4)′	3.79 ± 0.02
	S(7)′	3.79 ± 0.03
S(8)—Sb(2)		3,17 ± 0.02
	Sb(4)″	3.28 ± 0.02
	S(8)′	3.79 ± 0.02
	S(8)″	3.79 ± 0.02
	S(9)′	3.99 ± 0.02

Table 6b. *Bond angles in livingstonite*

S(2)′—Hg(1)—	S(2)	180.0°
	S(3)′	76.2(3)
	S(3)″	103.8(3)
	S(3)‴	74.7(3)
	S(3)⁗	105.4(3) (2×]
S(3)′—Hg(1)—	S(3)″	180.0(3) [2×]
	S(3)‴	74.9(3) [2×]
	S(3)⁗	105.1(3) [2×]
S(7)′—Hg(2)—	S(7)″	179.1(7)°
	S(6)′	78.5(7) [2×]
	S(6)″	102.1(7) [2×]
	S(6)‴	78.1(7) [2×]
	S(6)	101.3(7) [2×]
S(6)′—Hg(2)—	S(6)″	108.6(5)
	S(6)‴	72.7(5) [2×]
	S(6)	178.7(5) [2×]
S(6)‴—Hg(2)—	S(6)	106.0(5)
S(1)′—Sb(1)—	S(1)	87.8(5)°
	S(1)″	101.2(5)
	S(4)	94.0(5)
	S(4)′	164.5(1.7)
	S(2)	70.8(5)
S(1)—Sb(1)—	S(1)″	80.7(4)
	S(4)	82.8(4)
	S(4)′	77.0(4)
	S(2)	151.3(7)
S(1)″—Sb(1)—	S(4)	157.0(3)
	S(4)′	79.8(4)
	S(2)	121.2(5)
S(4)—Sb(1)—	S(4)′	81.0(4)
	S(2)	80.0(3)
S(4)′—Sb(1)—	S(2)	122.1(5)
S(3)′—Sb(2)—	S(6)	86.8(7)
	S(2)	86.2(4)
	S(6)′	81.9(6)
	S(2)′	81.5(4)
	S(8)	152.3(6)

Table 6b. *(Continued)*

S(6)—Sb(2)—	S(2)	90.3(5)°
	S(6)′	95.1(6)
	S(2)′	168.2(5)
	S(8)	78.7(5)
S(2)—Sb(2)—	S(6)′	166.6(6)
	S(2)′	90.5(4)
	S(8)	117.0(4)
S(6)′—Sb(2)—	S(2)′	81.8(5)
	S(8)	76.1(6)
S(2)′—Sb(2)—	S(8)	111.3(4)
S(6)′—Sb(3)—	S(3)	87.4(6)
	S(7)	85.2(6)
	S(3)′	82.6(6)
	S(7)′	80.6(6)
	S(4)	151.0(1.4)
S(3)—Sb(3)—	S(7)	98.1(5)
	S(3)′	86.6(4)
	S(7)′	167.5(8)
	S(4)	81.2(4)
S(7)—Sb(3)—	S(3)′	166.7(1.5)
	S(7)′	84.7(5)
	S(4)	70.3(5)
S(3)′—Sb(3)—	S(7)′	88.1(4)
	S(4)	122.9(5)
S(7)′—Sb(3)—	S(4)	111.1(5)
S(8)—Sb(4)—	S(5)	82.4(5)
	S(8)′	92.5(6)
	S(5)′	72.6(5)
	S(8)″	82.1(5)
	S(7)	157.7(1.0)
S(5)—Sb(4)—	S(8)′	99.2(5)
	S(5)′	96.0(4)
	S(8)″	164.5(9)
	S(7)	88.2(4)
S(8)′—Sb(4)—	S(5)′	157.1(5)°
	S(8)″	81.8(4)
	S(7)	69.1(5)
S(5)′—Sb(4)—	S(8)″	79.0(4)
	S(7)	128.7(4)
S(8)″—Sb(4)—	S(7)	106.5(4)
Sb(1)′—S(1)—	Sb(1)	92.1(5)
	Sb(1)″	101.2(5)
	S(2)′	67.1(4)
	S(1)′	48.1(6)
	S(1)″	100.7(5)
Sb(1)—S(1)—	Sb(1)″	99.3(4)
	S(2)′	152.0(5)
	S(1)′	44.0(6)
	S(1)″	52.8(6)
Sb(1)′—S(1)—	S(2)′	68.5(4)
	S(1)′	104.9(5)
	S(1)″	46.5(3)
S(2)′—S(1)—	S(1)′	112.9(5)
	S(1)″	110.7(5)
S(1)′—S(1)—	S(1)″	71.2(6)
Hg(1)—S(2)—	Sb(2)	106.0(4)
	Sb(2)′	106.9(3)
	Sb(1)	109.7(4)
	Sb(1)′	86.2(4)
	S(5)	178.0(4)
Sb(2)—S(2)—	Sb(2)′	90.5(4)
	Sb(1)	91.2(3)
	Sb(1)′	132.1(4)
	S(5)	72.2(4)
Sb(2)′—S(2)—	Sb(1)	141.3(6)
	S(1)′	130.8(5)
	S(5)	74.1(3)
Sb(1)—S(2)—	S(1)′	42.1(5)
	S(5)	69.8(4)

Table 6b. *(Continued)*

S(1)′—S(2)—S(5)	94.5(4)°
Sb(2)′—S(3)—Sb(3)	91.6(5)
Sb(3)′	86.7(4)
Hg(1)′	90.6(4)
Hg(1)″	94.9(4)
S(6)′	52.0(6)
Sb(3)—S(3)—Sb(3)′	86.6(4)
Hg(1)′	175.3(1.5)
Hg(1)″	100.8(4)
S(6)′	40.4(5)
Sb(3)′—S(3)—Hg(1)′	97.7(4)
Hg(1)″	172.4(1.8)
S(6)′	92.1(5)
Hg(1)′—S(3)—Hg(1)″	74.9(3)
S(6)′	140.8(6)
Hg(1)″—S(3)—S(6)′	94.7(4)
S(5)—S(4)—Sb(1)	99.3(6)
Sb(1)′	96.9(6)
Sb(4)	44.1(5)
Sb(3)	118.5(7)
S(1)	140.5(6)
Sb(1)—S(4)—Sb(1)′	81.0(4)
Sb(4)	103.1(4)
Sb(3)	100.5(4)
S(1)	44.2(3)
Sb(1)′—S(4)—Sb(4)	140.9(3)
Sb(3)	143.5(7)
S(1)	91.8(4)
Sb(4)—S(4)—Sb(3)	74.8(3)
S(1)	118.5(5)
Sb(3)—S(4)—S(1)	67.2(4)
S(4)—S(5)—Sb(4)	99.2(6)
Sb(4)′	99.0(5)
S(8)	139.2(7)
S(8)′	140.2(7)
S(2)	89.6(6)
Sb(4)—S(5)—Sb(4)′	96.0(5)°
S(8)	48.8(5)
S(8)′	101.3(6)
S(2)	136.3(7)
Sb(4)′—S(5)—S(8)	107.8(6)
S(8)′	45.2(4)
S(2)	124.9(4)
S(8)—S(5)—S(8)′	78.1(5)
S(2)	99.0(5)
S(8)′—S(5)—S(2)	98.5(4)
Sb(3)′S(6)—Sb(2)	104.0(7)
Sb(2)′	97.4(7)
Hg(2)′	85.6(7)
Hg(2)	90.2(7)
S(7)′	54.0(1.0)
Sb(2)—S(6)—Sb(2)′	95.1(7)
Hg(2)′	165.9(2.1)
Hg(2)	96.6(5)
S(7)′	157.4(2.5)
Sb(2)′—S(6)—Hg(2)′	93.9(5)
Hg(2)	164.1(1.4)
S(7)′	93.1(6)
Hg(2)′ —S(6)—Hg(2)	72.7(5)
S(7)′	31.9(8)
Hg(2)—S(6)—S(7)′	80.0(6)
Hg(2)′—S(7)—Sb(3)	109.9(6)
Sb(3)′	108.8(6)
Sb(4)	129.2(1.0)
S(6)′	69.6(8)
S(8)′	96.4(8)
Sb(3)—S(7)—Sb(3)′	84.7(6)
Sb(4)	83.5(4)
S(6)′	40.8(7)
S(8)′	130.8(8)

Table 6b. *(Continued)*

Sb(3)′—S(7)—	Sb(4)	121.4(5)°
	S(6)′	91.8(6)
	S(8)′	125.7(4)
Sb(4)—S(7)—	S(6)′	113.6(5)
	S(8)′	48.5(5)
S(6)′—S(7)—	S(8)′	142.4(1.1)
Sb(4)—S(8)—	Sb(4)′	97.2(6)
	S(5)	48.8(6)
	Sb(2)	109.6(6)
	S(5)′	62.1(5)
	Sb(4)″	86.2(5)
Sb(4)′—S(8)—	S(5)	145.0(3)°
	Sb(2)	140.1(9)
	S(5)′	93.9(5)
	Sb(4)″	81.8(4)
S(5)—S(8)—	Sb(2)	70.9(4)
	S(5)′	78.1(5)
	Sb(4)″	87.0(5)
Sb(2)—S(8)—	S(5)′	74.4(4)
	Sb(4)″	127.8(4)
S(5)′—S(8)—	Sb(4)″	147.4(2)

and in the addition compound of mercuric chloride with coumarin (Kitaigorodskii, Khotsyanova and Struchkov, 1953), the Hg—0 distance is 2.38 Å. The average Hg(2)—S distance is 2.89 Å and the mean standard deviation is 0.02 Å.

There are four independent Sb atoms in the structure. Atom Sb(1) has a coordination of four sulfur atoms, which could be described as a distorted trigonal pyramid plus an additional sulfur atom. The Sb(1)—S distances are in the range 2.38 to 2.93 Å and have a mean standard deviation of 0.015 Å. Atom Sb(2) has a coordination of five sulfur atoms which form a distorted square-pyramidal configuration, similar to that found in stibnite, Sb_2S_3 (Bayliss and Nowacki, 1972). The Sb atom is almost at the centre of the basal plane of the square pyramid, which runs almost parallel to the *c* axis; the apex S is at a distance of 2.58 Å from the Sb. The other Sb(2)—S distances are in the range 2.61 to 2.94 Å with a mean standard deviation of 0.02 Å. Sb(3) has the familiar trigonal-pyramidal coordination, with three sulfur atoms in the range 2.3 to 2.85 Å. Similar coordination for antimony have been observed in many of the sulfosalts (Nowacki, 1969, 1970). The average Sb(3)—S distance is 2.65 Å with a mean standard deviation of 0.02 Å. Sb(4), similar to Sb(1), has a distorted trigonal-pyramidal coordination plus an additional sulfur atom, thus having four sulfur atoms in the range 2.40 to 2.98 Å, with a mean standard deviation of 0.02 Å. The average of all the Sb—S distances is 2.68 Å.

The coordination around the Hg and Sb atoms are schematically shown in Fig. 3*a* and those around the sulfur atoms are shown in

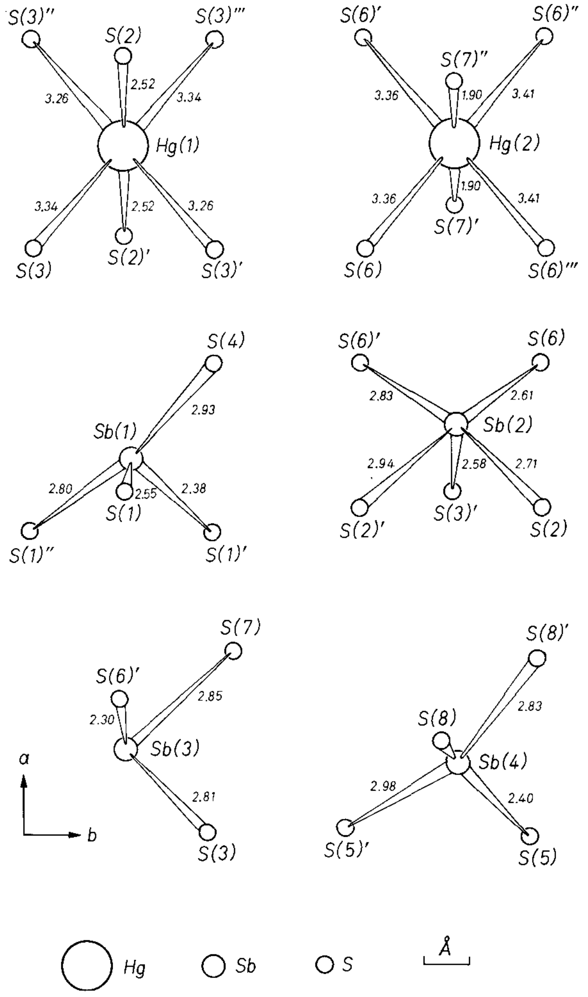

Fig. 3*a*. Coordination of the Hg and Sb atoms in livingstonite, projected down [001]

Fig. 3*b*, as projected down the *c* axis. The sulfur atoms S(2), S(3), S(5), S(6) and S(7) have five metal atoms surrounding them, while S(1) and S(8) have four metal atoms and S(4) has six metal atoms around them.

The structure of livingstonite can be described as essentially a double-layered structure. These double layers, formed by Sb atoms, run parallel to the *c* axis. If we consider the nearest three S atoms around each Sb atom, it could be represented as a SbS_3 unit. These SbS_3 units are connected as chains of composition SbS_2. In the

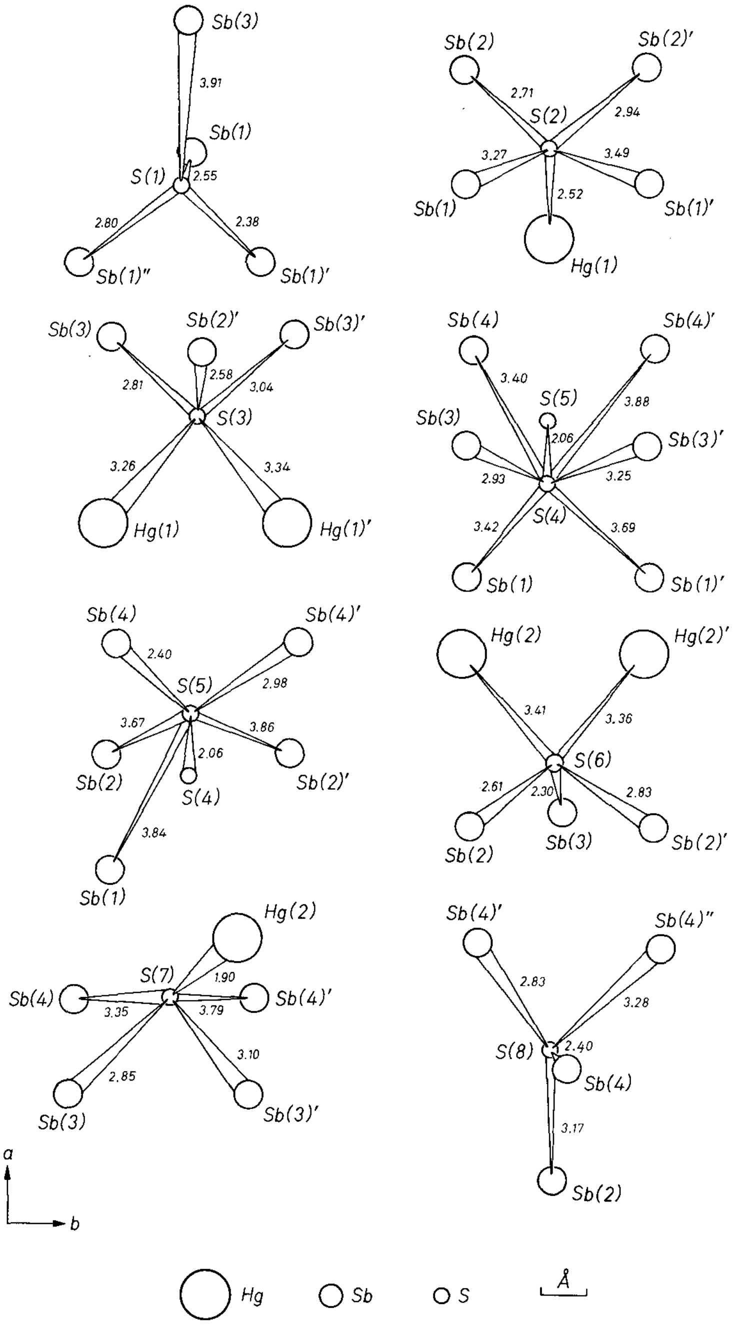

Fig. 3b. Coordination of the sulfur atoms in livingstonite, projected down [001]

structure there are three such groups of two SbS_2 chains. One group is related by a centre of symmetry, the second by a twofold axis and the third by no symmetry element. These SbS_2 chains are combined into Sb_2S_4 double chains, very similar to that in berthierite (BUERGER and HAHN, 1955). These two double chains of Sb_2S_4 differ in the way they are joined together. In one of them, they are connected as a layer, by a mutual S_2 group, S(4)—S(5) = 2.06 Å. This is probably the only example of an S_2 group in the structure of sulfosalts, although many examples are found in literature in simple sulfides. The S—S distance of 2.06 Å agrees very well with those found in CuS (S—S = 2.05 Å; OFTEDAL, 1932), in pyrite, FeS_2 (S—S = 2.10 Å; BRAGG, 1913) and in marcasite, FeS_2 (S—S = 2.25 Å, BUERGER, 1931). This S_2 group in livingstonite is so disposed that its midpoint is at a pseudocentre of symmetry in the structure. It is this S_2 group that necessitated the new chemical formula, $HgSb_4S_8$. The other two double chains of Sb_2S_4 are joined by the Hg atoms in the structure.

In livingstonite, the factor φ, expressing the ratio of the number of sulfur to the metal atoms is 2 and hence it falls under Type IV of the classification of the sulfosalts by NOWACKI (1969), for which $\varphi = 2$. The chemical formula of livingstonite can be expressed as $[(Sb_2S_4)_2\,Hg^{II+IV}]$. The structure could be described as SbS_3 pyramids interconnected so as to form double chains of composition Sb_2S_4 running along [001]. Hence it comes under Type IV.a_1, the other examples of this type being trechmannite, $AgAsS_2$ (MATSUMOTO and NOWACKI, 1969) and smithite, $AgAsS_2$ (HELLNER and BURZLAFF, 1964).

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