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Refinement of the crystal structure of stibnite, Sb_2S_3 [1]

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Auszug

Für Antimonit, Sb_2S_3, wurde ein verfeinerter Satz von Atomkoordinaten und Temperaturparametern erhalten. Diese Struktur enthält parallele $(Sb_4S_6)_n$-Ketten, welche miteinander verbunden sind und gewellte Netze bilden (zwei pro Einheitszelle). Das fünfwertige Sb weist eine Fünferkoordination in Form einer quadratischen Pyramide mit Sb leicht aus dem Basiszentrum verschoben auf. Das dreiwertige Sb hat eine Dreierkoordination in Form einer trigonalen Pyramide mit Sb als Spitze. Zwei dreiwertige S-Atome besitzen eine Dreierkoordination in Form einer trigonalen Pyramide mit S als Spitze. Das andere zweiwertige S-Atom hat eine Zweierkoordination. Die physikalischen Eigenschaften stehen mit der Kristallstruktur in Beziehung.

Abstract

A refined set of atomic coordinates and temperature parameters have been obtained for stibnite, Sb_2S_3. This structure contains parallel $(Sb_4S_6)_n$ chains, which are linked to form crumpled sheets (two per unit cell). The quinvalent Sb has fivefold coordination in a square pyramid, where the Sb is slightly displaced out of the base center. The trivalent Sb has threefold coordination in a trigonal pyramid, where the Sb occupies the vertex. Two trivalent S have threefold coordination in a trigonal pyramid, where the S occupies the vertex. The other divalent S has twofold coordination. The physical properties are related to the crystal structure.

Introduction

The crystal structure of stibnite (Sb_2S_3) was initially solved with a trial and error method by HOFMANN (1933). Later ŠĆAVNIČAR (1960) redetermined the structure with a Fourier from two-dimensional Weissenberg-film data. The crystallochemical relations between Sb and

[1] Contribution No. 222, Part 64 on sulfides and sulfosalts.

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S appear in the stibnite structure without any interference from other elements. Therefore it is worthwhile to refine such an important structure in the sulfosalt-mineral class with three-dimensional counter data to obtain more accurate interatomic distances and bond angles, because of their deviation from the expected more ideal structure.

Experimental

Stibnite crystals donated by Mr. S. LIECHTI (Number 212, Mineralogisch-Petrographisches Institut, Universität Bern) were examined. Since the mineral is both too soft (hardness 2) and easily cleavable along perfect cleavage (100) to grind a cylinder without crystal distorsion, a needle with dimensions $23 \times 296 \times 29\ \mu$m was used to measure the lattice constants and intensities.

The lattice constants were determined from two back-reflection Weissenberg photographs of $h0l$ and $0kl$, which were calibrated for film shrinkage by the diffraction pattern of silicon ($a = 5.43054$ Å). A least-squares best fit of the lattice constants was calculated by the program written by N. D. JONES (unpublished). The results are

	Present study	ŠĆAVNIČAR (1960)	HOFMANN (1933)
a	11.3107 (9) Å	11.33 (2) Å	11.28 kX
b	3.8363 (4)	3.84 (1)	3.83
c	11.2285 (5)	11.25 (2)	11.20

The observed density given by DANA (1941) is 4.63 (2) g cm^{-3}, and that calculated for 4 Sb_2S_3 on the basis of the new lattice constants is 4.62 g cm^{-3}. The space group $Pnma$ was chosen as assigned by both ŠĆAVNIČAR (1960) and HOFMANN (1933) after reorientation to the standard setting with systematic absences of $0kl$ with $k + l = 2n + 1$ and $hk0$ with $h = 2n + 1$. Three-dimensional data was collected by a Weissenberg counter autodiffractometer (Supper-Pace type) with Cu$K\alpha$ radiation (1.54178 Å). The intensities were corrected for both background and Lorentz and polarization factors. Corrections for absorption were calculated by a local version of the ACAC program written by WUENSCH and PREWITT (1965), because the linear absorption coefficient is high ($\mu = 1011$ cm^{-1} for Cu$K\alpha$).

The structure was refined from the coordinates of ŠĆAVNIČAR (1960) with a local version of the block-diagonal least-squares program

Table 1. *Observed and calculated structure factors for stibnite*

h	k	l	$\|F_o\|$	$\|F_c\|$
2	0	0	124.8	114.8
4			23.1	21.4
6			160.4	154.6
8			38.0	36.8
10			107.6	111.2
12			71.1	71.2
1	0	1	34.3	31.2
2			124.5	123.7
3			180.5	181.6
4			7.2	4.9
5			6.9	3.9
6			87.4	82.8
7			54.3	52.2
8			83.8	82.8
9			75.8	75.9
10			83.8	88.7
11			34.3	34.1
12			39.5	39.3
13			73.8	74.9
0	0	2	58.6	59.6
1			27.9	28.7
2			101.7	105.5
3			129.1	134.9
4			200.7	223.3
5			157.2	164.0
6			58.4	57.8
7			78.5	78.2
8			57.5	56.2
9			74.0	74.6
10			75.4	77.0
11			69.3	71.2
12			38.4	38.9
13			29.3	29.2
1	0	3	157.7	183.6
2			95.0	101.3
3			41.4	40.6
4			81.2	79.5
5			58.7	56.1
6			123.3	126.9
7			140.8	142.3
8			47.1	46.1
9			53.4	52.3
10			6.5	3.7
11			45.5	45.5
12			57.0	57.7
13			17.0	15.9
0	0	4	6.2	2.8
1			49.7	48.4
2			105.0	114.1
3			101.7	104.9
4			114.5	114.3
5			7.0	10.3
6			46.2	44.8
7			130.7	132.8
8			39.6	37.4
9			133.7	136.2
10			22.3	18.9
11			17.6	17.9
12			30.3	29.8
13			46.0	46.2
1	0	5	67.2	68.9
2			115.9	126.0
3			166.1	178.7
4			99.3	99.2
5			33.7	29.8
6			142.1	144.0
7			18.6	17.7
8			25.7	26.9
9			28.9	26.1
10			36.2	35.8
11			5.3	4.3
12			89.5	91.3
0	0	6	138.0	149.1
1			106.4	113.2
2			85.6	90.5
3			7.0	8.2
4			91.5	91.7
5			80.7	80.2
6			61.6	58.7
7			42.2	41.6
8			6.7	1.6
9			26.5	24.1
10			21.4	19.5
11			64.3	62.3
12			32.3	31.8
1	0	7	15.6	10.6
2			168.3	187.4
3			22.0	13.9
4			7.7	11.9
5			50.8	49.4
6			59.2	56.9
7			20.5	12.6
8			140.0	142.8
9			6.3	3.1
10			79.4	78.3
11			20.9	19.9
0	0	8	132.0	137.3
1			59.1	61.0
2			22.3	20.7
3			7.2	2.1
4	0	8	23.2	17.8
5			127.6	128.3
6			55.4	54.4
7			27.8	26.7
8			30.8	29.5
9			16.8	13.2
10			4.8	3.1
11			75.8	77.5
1	0	9	95.2	100.7
2			29.7	29.6
3			104.9	106.8
4			59.4	57.6
5			23.9	24.5
6			99.4	98.2
7			6.4	1.3
8			33.4	33.3
9			13.4	12.3
10			30.4	29.6
0	0	10	51.4	50.7
1			56.3	56.6
2			7.1	5.7
3			64.7	64.3
4			59.3	57.6
5			26.1	26.6
6			40.9	40.2
7			49.2	48.1
8			34.7	34.3
9			98.9	100.5
1	0	11	94.9	97.9
2			6.7	3.9
3			29.3	29.1
4			69.9	69.9
5			30.2	28.4
6			38.9	38.4
7			55.3	56.1
8			18.8	18.0
0	0	12	24.7	22.5
1			44.9	44.1
2			62.0	61.0
3			13.3	11.1
4			73.0	74.6
5			58.8	58.7
6			7.2	9.4
1	0	13	47.9	47.6
2			21.8	21.0
3			57.9	57.9
4			43.2	43.6
2	1	0	106.1	93.1
4			196.2	186.0
6			268.9	281.1
8			6.9	2.2
10			65.4	64.6
12			103.9	103.9
0	1	1	104.0	107.2
1			82.8	84.3
2			91.0	81.0
3			48.6	41.6
4			154.4	145.1
5			93.9	86.5
6			37.5	33.1
7			82.0	79.1
8			7.0	6.1
9			99.3	99.9
10			33.2	32.2
11			40.3	41.3
12			38.5	38.5
13			22.7	21.4
1	1	2	159.6	187.9
2			189.0	218.1
3			110.9	109.0
4			45.5	42.0
5			62.5	60.4
6			7.0	3.1
7			60.3	58.3
8			122.0	123.5
9			73.5	73.9
10			70.4	69.5
11			48.8	48.6
12			25.9	26.0
13			9.8	8.1
0	1	3	183.6	214.8
1			97.9	102.8
2			5.9	1.8
3			54.4	52.8
4			74.0	71.2
5			155.5	157.2
6			60.0	58.7
7			50.3	48.7
8			20.5	19.6
9			45.0	44.0
10			61.0	60.0
11			95.1	94.7
12			26.9	25.6
13			70.1	69.7
1	1	4	83.0	85.2
2			113.8	119.3
3			192.8	207.3
4			22.0	20.6
5			17.6	15.4
6			7.3	13.2
7	1	4	6.8	3.9
8			101.1	98.6
9			34.8	32.2
10			30.5	29.2
11			5.3	5.2
12			27.9	28.2
0	1	5	207.5	238.0
1			45.6	45.5
2			30.8	28.2
3			116.9	115.6
4			49.8	52.0
5			24.0	22.7
6			113.2	114.6
7			74.2	73.5
8			63.5	62.4
9			109.0	108.9
10			58.8	58.9
11			5.0	2.4
12			17.0	17.4
1	1	6	46.2	45.4
2			47.6	47.9
3			62.8	62.5
4			68.4	64.7
5			7.1	7.4
6			97.1	95.2
7			108.0	106.1
8			55.4	53.1
9			48.9	48.2
10			76.1	74.8
11			18.6	17.1
12			54.5	54.5
0	1	7	40.1	39.0
1			31.1	30.9
2			124.3	129.5
3			7.3	5.3
4			177.5	182.4
5			17.2	14.1
6			35.1	34.1
7			10.9	12.0
8			51.4	48.9
9			16.7	16.9
10			42.6	42.8
11			36.3	36.2
1	1	8	110.8	117.1
2			21.6	21.3
3			36.5	35.2
4			24.0	19.1
5			40.7	39.6
6			92.0	89.0
7			79.5	80.4
8			5.8	9.2
9			32.5	31.2
10			41.3	40.0
0	1	9	137.4	146.0
1			31.4	32.1
2			7.2	3.3
3			53.8	52.8
4			7.2	10.1
5			58.5	55.8
6			56.6	56.1
7			100.8	99.9
8			8.9	3.8
9			68.4	67.2
10			48.5	49.0
1	1	10	12.1	12.2
2			72.0	72.4
3			124.8	125.1
4			45.0	43.8
5			47.2	46.3
6			21.1	19.7
7			18.0	16.4
8			17.7	17.9
9			16.2	16.0
0	1	11	62.4	63.1
1			35.7	36.1
2			51.2	50.5
3			47.1	46.1
4			9.4	12.1
5			93.4	93.6
6			34.7	35.4
7			31.8	32.3
1	1	12	61.2	59.6
2			58.6	56.3
3			5.3	7.8
4			4.9	4.7
5			16.0	15.1
6			4.0	4.1
0	1	13	78.4	77.2
1			23.7	23.3
2			62.4	63.4
3			21.6	22.1
2	2	0	94.6	85.0
4			19.2	12.9
6			125.5	122.3
8			30.7	29.9
10			85.9	93.6
12			60.5	62.2
1	2	1	19.5	18.1
2			93.1	84.7
3			144.2	136.5
4	2	1	14.0	11.1
5			6.8	4.8
6			69.7	66.7
7			41.4	39.9
8			66.6	68.4
9			61.5	63.3
10			73.3	76.2
11			28.0	28.0
12			34.8	34.9
0	2	2	40.2	39.5
1			21.3	19.4
2			82.1	81.8
3			95.5	94.8
4			162.3	167.3
5			126.2	129.2
6			44.8	44.6
7			66.5	65.4
8			46.9	46.6
9			65.4	64.4
10			62.6	63.7
11			58.6	61.1
12			32.8	33.4
1	2	3	133.7	142.5
2			72.4	73.9
3			33.6	32.0
4			63.1	61.4
5			48.9	46.4
6			102.0	102.1
7			115.3	115.8
8			37.0	36.8
9			45.0	43.3
10			5.0	3.5
11			37.5	38.4
12			30.8	32.3
0	2	4	8.7	3.1
1			43.9	42.5
2			83.2	85.2
3			84.2	81.5
4			92.8	90.0
5			6.4	11.4
6			35.7	35.6
7			110.7	110.8
8			33.8	31.3
9			115.7	114.9
10			15.6	14.7
11			15.0	13.7
1	2	5	55.7	55.6
2			95.0	96.7
3			140.7	141.7
4			82.7	79.5
5			26.9	25.2
6			119.4	118.6
7			16.4	14.3
8			22.2	20.7
9			24.1	22.9
10			31.6	30.8
11			3.9	4.5
0	2	6	115.6	119.5
1			86.1	88.2
2			73.6	74.5
3			6.6	6.3
4			79.2	76.7
5			66.1	62.8
6			51.5	49.0
7			36.4	34.9
8			6.2	1.7
9			20.1	19.2
10			17.6	16.9
1	2	7	6.8	9.3
2			144.6	152.4
3			14.5	11.9
4			6.7	12.2
5			45.3	41.7
6			52.2	49.7
7			6.2	10.6
8			121.5	121.4
9			4.6	2.7
10			67.6	68.7
0	2	8	109.5	114.0
1			48.1	48.8
2			19.6	17.2
3			6.9	0.9
4			16.4	14.8
5			109.3	107.2
6			46.7	46.3
7			23.9	23.6
8			26.1	26.1
9			10.2	10.0
1	2	9	83.3	86.6
2			23.9	23.1
3			91.1	90.3
4			49.2	48.8
5			22.3	21.1
6			83.7	83.2
7			4.6	0.4
8			26.9	27.2
0	2	10	41.9	42.7
1			47.9	47.5
2			5.8	5.0
3			54.7	54.6

Table 1. *(Continued)*

h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$	h	k	l	$\|F_o\|$	$\|F_c\|$
4	2	10	49.3	48.6	5	3	2	42.5	42.3	8	3	5	44.8	46.0	4	4	0	5.4	3.2
5			20.5	21.6	6			5.9	0.3	9			77.2	80.6	6			63.0	72.1
6			33.4	34.1	7			39.3	38.3	1	3	6	29.1	28.4	1	4	1	4.6	6.1
7			41.3	42.6	8			83.1	86.1	2			36.1	34.7	2			51.9	47.8
1	2	11	84.1	83.8	9			51.7	53.8	3			41.8	39.7	3			74.9	74.0
2			5.1	1.8	10			49.1	52.3	4			47.4	46.0	4			5.2	8.2
3			26.9	26.5	0	3	3	123.6	127.2	5			5.3	6.3	5			4.8	2.6
4			59.8	60.1	1			59.0	58.6	6			68.0	67.9	6			39.3	41.5
5			25.0	25.5	2			5.6	0.5	7			75.2	74.2	0	4	2	17.7	18.1
0	2	12	19.1	17.8	3			40.1	35.5	8			41.1	41.5	1			7.9	7.4
1			37.6	37.4	4			47.3	45.6	0	3	7	33.5	32.6	2			50.6	47.7
2			52.8	53.3	5			102.8	104.1	1			23.0	22.3	3			59.3	58.1
3			10.0	9.7	6			39.4	38.6	2			91.1	92.2	4			94.7	97.7
2	3	0	62.9	53.1	7			35.6	35.5	3			5.5	4.1	5			75.3	78.4
4			129.1	120.1	8			14.6	13.8	4			129.7	128.7	6			22.3	23.9
6			180.4	190.7	9			34.6	35.2	5			11.8	11.2	1	4	3	79.2	81.8
8			7.5	4.0	1	3	4	58.6	59.5	6			22.3	22.0	2			43.5	40.9
10			46.0	48.4	2			75.2	76.0	7			10.0	9.1	3			26.3	23.8
0	3	1	66.5	66.5	3			135.8	134.5	1	3	8	80.7	82.2	4			35.5	36.5
1			51.9	52.7	4			18.4	16.4	2			18.3	15.9	5			28.7	30.6
2			61.8	57.0	5			14.8	11.4	3			22.2	21.5	0	4	4	5.2	3.3
3			30.7	26.7	6			15.0	12.4	4			15.2	15.9	1			21.3	22.0
4			98.6	93.6	7			5.2	0.8	5			29.5	29.6	2			55.4	51.6
5			55.6	52.6	8			69.4	70.4	6			65.3	66.0	3			51.7	47.5
6			25.5	24.1	9			21.8	23.2	0	3	9	102.7	103.6	4			53.4	53.5
7			53.1	55.1	0	3	5	144.9	155.5	1			23.3	22.2	5			13.1	12.8
8			4.9	3.7	1			28.7	30.2	2			4.9	4.5	1	4	5	35.6	36.9
9			66.2	69.8	2			22.5	21.0	3			38.9	38.9	2			58.9	56.1
10			22.5	22.6	3			82.1	78.5	4			4.3	5.1	3			88.6	86.7
1	3	2	110.4	115.9	4			36.1	33.2	5			42.6	44.2	4			46.9	47.6
2			128.0	129.8	5			19.1	18.9	1	3	10	12.5	11.1	0	4	6	69.4	73.3
3			74.4	70.3	6			79.8	79.3	2			51.8	52.3	1			51.2	50.0
4			25.2	23.7	7			53.8	53.9	2	4	0	62.1	54.1	2			48.6	48.5

written by D. VAN DER HELM. The neutral-atom form scattering factors corrected for the real dispersion correction for S and Sb were taken from the *International tables* (1962). The final discrepancy index R is 0.044 for all 532 reflections. Both observed and calculated structure amplitudes are shown in Table 1. No secondary-extinction correction has been made, although it has had an effect as shown by the results in Table 1.

Discussion of the structure

The atomic coordinates and temperature parameters, which are given in Table 2, are similar to both HOFMANN (1933) and ŠĆAVNIČAR (1960). The interatomic distances and bond angles are tabulated in Table 3. A projection of the structure on the (010) plane is shown in Fig. 1.

The structure is formed of infinite Sb_4S_6 chains parallel to the b axis (needle axis) with interatomic distances between 2.455 and 2.854 Å. These chains are linked to form crumpled sheets perpendicular to the a axis with interatomic distances of 3.167 Å. These sheets (two per unit cell) are held together with interatomic distances between 3.373 and 3.642 Å, whereas the sum of van der Waals radii for Sb and S is 4.05 Å. The Sb to S bonds are mainly covalent.

Each trivalent Sb_I at the vertex of a trigonal pyramid is bonded to three S atoms (two divalent and one trivalent), which occupy the corners of the basal plane. This trigonal pyramid is slightly distorted as shown by the interatomic distances of S_{III} at 2.521 Å and two S_{II}

at 2.539 Å, and also the bond angles S_{II}—Sb_I—S_{III} of 87.49° and S_{II}—Sb_I—S_{II} of 98.13°. In addition another four S atoms (two S_I at 3.111 Å, S_{II} at 3.167 Å and S_{III} at 3.642 Å) lie near Sb_I. Each quinvalent Sb_{II}, which lies just below the center (0.17 Å) of the basal plane of a distorted square pyramid, is bonded to five trivalent S atoms, which occupy the corners of the square pyramid. This square pyramid is distorted as

Table 2. *Atomic coordinates and temperature parameters of stibnite*

		HOFMANN (1933)	ŠĆAVNIČAR (1960)	Present study	
Sb_I	x	0.031	0.030 (3)	0.0293 (1)	β_{11} 0.0030 (2)
	y	1/4	1/4	1/4	β_{22} 0.0144 (15)
	z	0.328	0.326 (4)	0.3261 (1)	β_{33} 0.0025 (2)
					β_{13} 0.0006 (1)
Sb_{II}	x	0.149	0.149 (4)	0.1495 (1)	β_{11} 0.0027 (2)
	y	3/4	3/4	3/4	β_{22} 0.0230 (15)
	z	0.039	0.036 (4)	0.0360 (1)	β_{33} 0.0036 (2)
					β_{13} 0.0013 (1)
S_I	x	0.047	0.055 (15)	0.0497 (3)	β_{11} 0.0032 (2)
	y	1/4	1/4	1/4	β_{22} 0.0180 (25)
	z	0.883	0.880 (15)	0.8769 (3)	β_{33} 0.0027 (3)
					β_{13} 0.0004 (3)
S_{II}	x	0.125	0.131 (14)	0.1251 (3)	β_{11} 0.0035 (3)
	y	3/4	3/4	3/4	β_{22} 0.0177 (25)
	z	0.439	0.441 (14)	0.4386 (3)	β_{33} 0.0024 (3)
					β_{13} 0.0008 (3)
S_{III}	x	0.208	0.214 (14)	0.2079 (3)	β_{11} 0.0031 (3)
	y	1/4	1/4	1/4	β_{22} 0.0267 (26)
	z	0.194	0.189 (13)	0.1917 (3)	β_{33} 0.0023 (3)
					β_{13} 0.0002 (3)

shown by the interatomic distances of S_I at 2.455 Å, two S_{III} at 2.678 Å and two S_I at 2.854 Å, and also the bond angles given in Table 3. In addition another two S atoms (two S_{II} at 3.373 Å) lie near Sb_{II}. Both Sb_I (three S bonded and four S nearby) and Sb_{II} (five S bonded and two nearby) are surrounded by seven S atoms, which have a similar orientation as shown by their bond angles in Table 3. Both the trigonal pyramid (trivalent Sb_I) and square pyramid

Table 3. *Interatomic distances and bond angles of stibnite*

Sb_I —S_{III}	2.521 (3) Å	S_{II}—Sb_I—S_{III}(2)	87.49 (8) °	S_I —Sb_{II}—S_{III}(2)	88.08 (8)°	Sb_{II}—S_I —Sb_{II}	84.46 (8)°
—S_{II}(2)	2.539 (2)	S_I — —S_{III}(2)	77.95 (8)	S_I — —S_I(2)	83.47 (8)	Sb_{II}— —Sb_{II}(2)	96.53 (9)
—S_I(2)	3.111 (3)	S_I — —S_I	76.14 (5)	S_I — —S_I	84.46 (6)		
—S_{II}	3.167 (3)	S_I — —S_{II}(2)	91.22 (7)	S_I — —S_{III} (2)	91.42 (6)	Sb_I —S_{II} —Sb_I(2)	98.13 (11)
—S_{III}	3.642 (3)	S_{II}— —S_{II}	98.13 (8)	S_{III}— —S_{III}	91.50 (7)		
		S_{II}— —S_{II}(2)	79.65 (8)	S_I — —S_{II} (2)	73.37 (7)	Sb_I —S_{III}—Sb_{II}(2)	101.14 (8)
Sb_{II}—S_I	2.455 (3)	S_I — —S_{III}(2)	70.90 (7)	S_{II}— —S_{III} (2)	67.54 (8)	Sb_{II}— —Sb_{II}	91.50 (9)
—S_{III}(2)	2.678 (2)	S_{II}— —S_{III}	59.69 (7)	S_{II}— —S_{II}	69.31 (4)		
—S_I(2)	2.854 (2)						
—S_{II}(2)	3.373 (2)						

(quinvalent Sb_{II}) are joined together with their basal planes parallel to the b axis through common S atoms to form infinite chains.

Each trivalent S_I at the vertex of a trigonal pyramid is bonded to three quinvalent Sb_{II} (Sb_{II} at 2.455 Å and two Sb_{II} at 2.854 Å), which occupy the corners of the basal plane. Two additional Sb_I at 3.111 Å also lie near S_I. Each divalent S_{II} is bonded to two trivalent Sb_I at 2.539 Å with an angle of 98.13°. Three additional Sb atoms (Sb_I at 3.167 Å and two Sb_{II} at 3.373 Å) also lie near S_{II}. Each trivalent S_{III} at

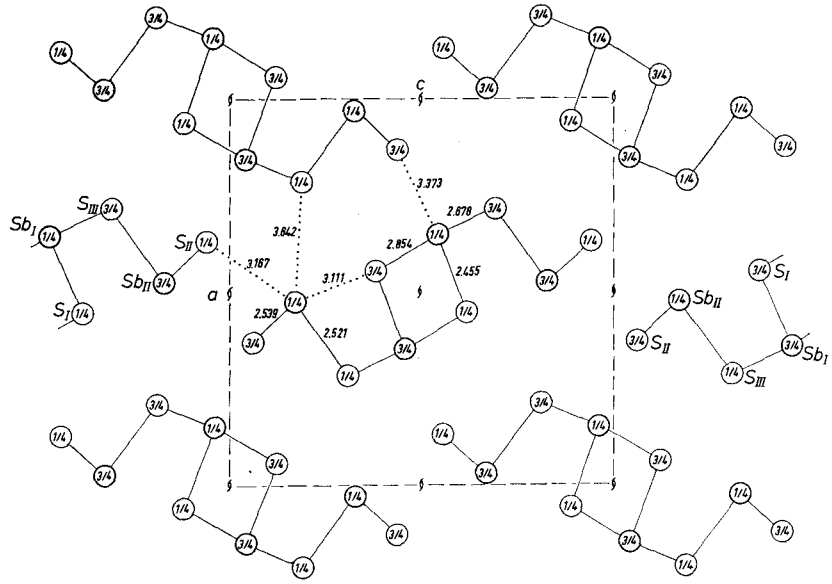

Fig. 1. Projection on b axis to show atomic arrangement and interatomic distances in stibnite. Thick circles —Sb atom with heights $\frac{1}{4}$ and $\frac{3}{4}$, thin circles —S atom with heights $\frac{1}{4}$ and $\frac{3}{4}$

the vertex of a trigonal pyramid is bonded to three Sb atoms (trivalent Sb_I at 2.521 Å and two quinvalent Sb_{II} at 2.678 Å), which occupy the corners of the basal plane. An additional Sb_I (3.642 Å) also lies near S_{III}.

The physical properties of stibnite described by DANA (1941) such as (1) habitual long slender prismatic crystals, (2) perfect cleavage (100) and imperfect cleavages (001) and (101), (3) translational gliding parallel to (100) in the [010] direction, (4) flexibility about [001], and (5) hardness 2 may be related to its crystal structure.

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References

J. D. DANA and E. S. DANA (1941), *The system of mineralogy*, Vol. 1. J. Wiley and Sons, New York.

W. HOFMANN (1933), Die Struktur der Minerale der Antimonitgruppe. Z. Kristallogr. **86**, 225—245.

International tables for x-ray crystallography (1962), Vol. III. Kynoch Press, Birmingham.

S. ŠĆAVNIČAR (1960), The crystal structure of stibnite. A redetermination of atomic positions. Z. Kristallogr. **114**, 85—97.

B. J. WUENSCH and C. T. PREWITT (1965), Corrections for x-ray absorption by a crystal of arbitary shape. Z. Kristallogr. **122**, 24—59.