

especially the intramolecular one, as weak C-H ··· O hydrogen bonds. It is interesting that the four interaction directions from O(5') are roughly tetrahedrally distributed.

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The Crystal Structures of NbAs₂ and NbSb₂

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The compounds NbAs₂ and NbSb₂ are isostructural. The monoclinic unit cells have the dimensions:

$$\begin{aligned} \text{NbAs}_2: a = 9.357, b = 3.3823, c = 7.792 \text{ \AA}; \beta = 119.46^\circ. \\ \text{NbSb}_2: a = 10.239, b = 3.6319, c = 8.333 \text{ \AA}; \beta = 120.07^\circ. \end{aligned}$$

The space group is $C2$ (C_2^3) and the unit cell contains 4 Nb and 2×4 As (Sb) in general positions 4(c). The parameters were found to be Nb: $x_1 = 0.3444$, $y_1 = \frac{1}{2}$, $z_1 = 0.3044$; As_I: $x_2 = 0.0948$, $y_2 = 0.488$, $z_2 = 0.3928$; As_{II}: $x_3 = 0.1399$, $y_3 = 0.067$, $z_3 = 0.0257$ for NbAs₂ and Nb: $x_1 = 0.343$, $y_1 = \frac{1}{2}$, $z_1 = 0.304$; Sb_I: $x_2 = 0.096$, $y_2 = 0.5$, $z_2 = 0.393$; Sb_{II}: $x_3 = 0.142$, $y_3 = 0.0$, $z_3 = 0.027$ for NbSb₂.

The relationships to the CuAl₂, PbCl₂, MoP₂ and marcasite types of structure are discussed in terms of the general (8-N) rule.

Introduction

In a recent study of niobium arsenides and antimonides (Furuseth & Kjekshus, 1964) the existence of phases with compositions NbAs₂ and NbSb₂ was established.* No extended ranges of homogeneity of these phases exist, and the compositions were unequivocally determined to be NbAs₂ and NbSb₂. According to Furuseth & Kjekshus (1964) the unit cells are monoclinic with the following dimensions:

$$\begin{aligned} \text{NbAs}_2: \\ a = 9.357, b = 3.3823, c = 7.792 \text{ \AA}; \beta = 119.46^\circ. \\ \text{NbSb}_2: \\ a = 10.239, b = 3.6319, c = 8.333 \text{ \AA}; \beta = 120.07^\circ. \end{aligned}$$

On the basis of the observed densities, 7.41 g.cm⁻³ (NbAs₂) and 8.22 g.cm⁻³ (NbSb₂), the unit cells contain 4 NbX₂-groups ($Z_c = 3.96$ for NbAs₂ and $Z_c = 3.98$ for NbSb₂).

* Note added in proof. — The paper by Saini, Calvert & Taylor (1964) which independently confirms the existence of NbAs₂ has come to hand since this article was accepted for publication. Their lattice dimensions and observed density are: $a = 9.354 \pm 0.002$, $b = 3.381 \pm 0.002$, $c = 7.799 \pm 0.002$ \AA; $\beta = 119.43 \pm 0.08^\circ$; $d_{\text{obs}} = 7.01$ g.cm⁻³.

All reflexions hkl with $h+k=2n+1$ are missing and the possible space groups are accordingly $C2$ (C_2^3), Cm (C_2^3) and $C2/m$ (C_2^3).

Needle-shaped single crystals of NbSb₂ grew from the vapour phase. Single crystals of NbAs₂ (with a similar shape, but of somewhat smaller dimensions) were obtained by means of a transport reaction using traces of iodine as a transport agent.

Interest in the nature of the chemical bonding in these compounds and their properties as possible semiconducting materials has prompted the investigation of their crystal structures.

Structure determination of NbAs₂

A single crystal with a parallelogram-formed (almost square) cross-section was investigated in an integrating Weissenberg camera with Cu K radiation. Intensity measurements of the $h0l$ and $h1l$ reflexions were carried out microphotometrically by the multiple-film technique. The intensities were corrected for the combined Lorentz and polarization factor and for absorption ($\mu R = 1.5$). For the calculation of F_c values the atomic scattering factors were taken from Forsyth

& Wells (1959) for the $h0l$ reflexions and from Vand, Eiland & Pepinsky (1957) for the $h1l$ reflexions. The agreement between F_o and F_c is expressed by the reliability index

$$R = \sum ||F_o| - |F_c|| / \sum |F_o|.$$

The short b axis in NbAs_2 excludes the space group Cm which would lead to interatomic distances $\leq 1.7 \text{ \AA}$. For the same reason the possible positions in the two remaining space groups are limited to $4(c)$ in $C2$ and $4(i)$ in $C2/m$. As these possibilities are indistinguishable in the (010) projection, it was decided to start with a Patterson projection on the basis of the corrected $F_o^2(h0l)$ values.

Tentative atomic positions could be deduced from the Patterson map and a set of structure factors calculated on this basis gave $R=0.26$. A Fourier synthesis was evaluated, which clearly showed all atoms resolved. The atomic parameters were refined further by means of Fourier and difference synthesis. R decreased to 0.13 after the final difference synthesis. In order to determine the effect of individual B values (up to this stage $B=0.1$ had been used for all atoms) on the final parameters least-square refinements were carried out. The refinements gave $R=0.111$, only minor shifts in the atomic coordinates and B values: $B_{\text{Nb}} = -0.276$, $B_{\text{AsI}} = 0.099$ and $B_{\text{AsII}} = 0.118$. (The apparent negative B_{Nb} value most probably represents the slight incorrectness in the absorption correction resulting from the shape of the crystal.)

Table 1. Observed and calculated structure factors for NbAs_2

The three numbers in each column represent respectively l , F_o and F_c

$h=0, k=0,$	5 0 4	0 66 -57	-5 32 38
1 50 -27	6 0 3		-4 44 32
2 31 22			-3 83 76
3 27 234	$h=6, k=0,$	-8 62 74	-2 116 101
4 23 12	-9 29 -22	-7 80 76	-1 28 18
5 31 40	-8 151 -151	-6 149 161	0 86 77
6 40 36	-7 80 68	-5 0 13	1 154 159
7 73 80	-6 0 -6	-4 125 88	2 55 50
8 24 -15	-5 177 -173	-3 138 115	3 112 104
	-4 137 134	-2 155 133	4 98 114
	-3 0 1	-1 30 40	5 60 73
$h=2, k=0,$	-2 74 -60	0 61 61	
-9 76 86	-1 75 78	1 198 230	$h=7, k=1,$
-8 96 -111	0 67 56	2 174 157	-7 36 24
-7 102 -86	1 59 62	3 50 35	-6 117 128
-6 142 151	2 33 -26	4 155 137	-5 0 13
-5 122 112	3 105 131	5 133 135	-4 68 53
-4 135 139	4 70 75	6 0 14	-3 217 224
-3 137 155	5 53 -57	7 22 22	-2 34 38
-2 58 46			-1 27 27
-1 61 -80	$h=8, k=0,$	$h=3, k=1,$	0 164 174
0 46 -33	-9 115 121	-9 37 40	1 35 35
1 0 4	-8 23 -25	-8 52 40	2 34 38
2 0 13	-7 69 68	-7 0 4	3 58 56
3 167 -198	-6 100 65	-6 99 96	
4 24 25	-5 117 99	-5 124 118	$h=9, k=1,$
5 0 2	-4 0 16	-4 73 59	-9 101 116
6 172 -197	-3 62 54	-3 141 207	-8 109 102
7 21 28	-2 180 189	-2 101 152	-7 84 79
	-1 76 -68	-1 109 133	-6 130 118
$h=4, k=0,$	0 49 54	0 155 180	-5 88 67
-9 41 -42	1 131 145	1 0 12	-4 30 21
-8 54 40	2 75 -75	2 105 87	-3 21 22
-7 91 98	3 57 32	3 109 96	-2 54 41
-6 88 -75		4 116 118	-1 59 42
-5 92 88	$h=10, k=0,$	5 0 26	0 118 100
-4 0 3	-8 120 106	6 58 63	1 50 48
-3 159 -181	-7 0 2		
-2 145 -168	-6 119 -103	$h=5, k=1,$	$h=11, k=1,$
-1 98 111	-5 133 120	-9 116 176	-6 97 88
0 205 -241	-4 47 -50	-8 0 7	-5 96 85
1 103 -109	-3 106 -93	-7 0 20	-4 85 78
2 89 76	-2 40 35	-6 132 191	-3 155 136
3 113 -144	-1 40 -47		
4 50 39			

The observed and calculated $F(h0l)$ values are listed in Table 1, and the final Fourier map is shown in Fig. 1. The corresponding parameters are:

- 4 Nb in $x_1=0.3444, z_1=0.3044, etc.$
- 4 As_I in $x_2=0.0948, z_2=0.3928, etc.$
- 4 As_{II} in $x_3=0.1399, z_3=0.0257, etc.$

By considering the interatomic distances on the basis of the parameters in the (010) projection it appeared that only $y_2 - y_1 \approx 0$ and $y_3 - y_1 \approx \frac{1}{2}$ would lead to reasonable distances. As y_1 can be fixed arbitrarily, e.g. $y_1 = \frac{1}{2}$, the values exactly 0 and $\frac{1}{2}$ would suggest space group $C2/m$, whereas values slightly different from 0 and $\frac{1}{2}$ would lead to $C2$.

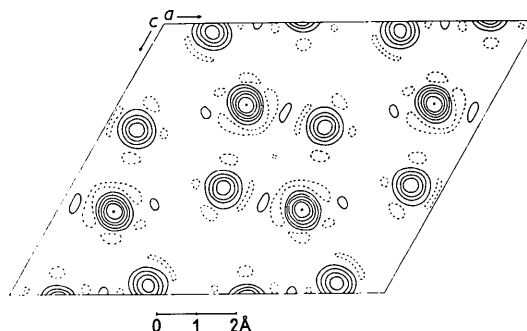


Fig. 1. Electron density projection of NbAs_2 on (010) . Contours are at intervals of 10 e.\AA^{-2} . The zero contours are broken.

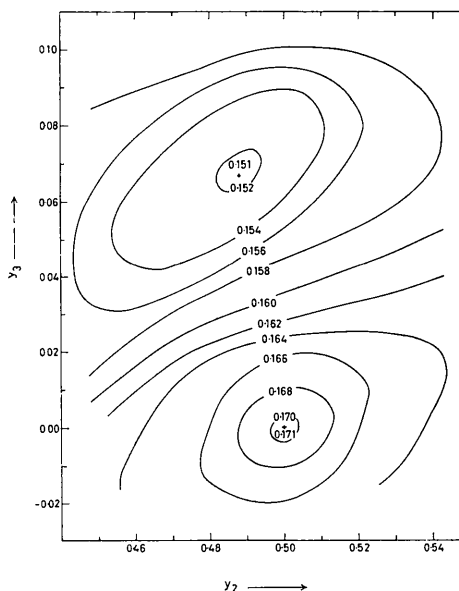


Fig. 2. Projection on the y_2, y_3 -plane of $R(y_2, y_3)$ for NbAs_2 . Contours are drawn at constant values of R .

The latter, having the lower symmetry of the two space groups, was chosen and y_2 and y_3 were refined by a trial-and-error method on the basis of the $h1l$ reflexions. (The six parameters x_1, z_1, \dots, z_3 were

assumed to be correct.) A set of F_c was prepared for different values of y_2 and y_3 and to check the agreement with F_o the R -test was applied. An $R(y_2, y_3)$ map is drawn on the basis of these values. As will be seen from Fig. 2 the map turned out to be fairly flat with a maximum at $\frac{1}{2}, 0$ and a minimum at 0.488, 0.067.

According to practice the final parameters are equal to the y_2, y_3 -values at the minimum in R . (The corresponding F_c and F_o values are listed in Table 1.) The deduced atomic arrangement (Fig. 3) is thus described in terms of the space group $C2 (C_2^3)$ as follows:

- $(0, 0, 0; \frac{1}{2}, \frac{1}{2}, 0) +$
 4 Nb in $(c) x, y, z; \bar{x}, y, \bar{z}$,
 with $x_1=0.3444, y_1=\frac{1}{2}, z_1=0.3044$.
 4 As_I in (c)
 with $x_2=0.0948, y_2=0.488, z_2=0.3928$.
 4 As_{II} in (c)
 with $x_3=0.1399, y_3=0.067, z_3=0.0257$.

Structure determination of NbSb₂

The obvious relationships between unit-cell dimensions, space group, intensities on Guinier photographs, etc. very strongly suggest that NbAs₂ and NbSb₂ are isostructural. As single crystals were available of NbSb₂ as well it seemed to be an easy task to refine the corresponding parameters in the NbSb₂ structure.

Data were therefore collected and calculations carried out as described for NbAs₂. Although both the Patterson and the electron-density projections showed the expected relationships to those of NbAs₂ the proposed structure would not refine below $R=0.25$.

A difficulty which we were aware of, but had not expected to be so important as it turned out to be, was the different shape of the NbSb₂ crystal compared with that of NbAs₂. Owing to a pronounced parallelogram form of the cross-section of the NbSb₂ crystal the absorption was much larger in some directions than in others.

Instead of trying a new, more complicated correction for absorption it was decided to attempt to allow for anisotropic thermal motion of the atoms. Although this is not quite the same, it was thought that this would give improved results for the parameters. The least-square refinement calculations carried out ($R=0.20$) did not give a satisfactory answer as some reflexions still showed too large discrepancies between F_c and F_o .

As a check of the correctness of the parameters from the least-square refinement a comparison between F_c and F_o from photometer recordings of Guinier photographs was tried. The NbAs₂ type atomic arrangement with the following parameters

- Nb: $x_1=0.343, y_1=\frac{1}{2}, z_1=0.304$
 Sb_I: $x_2=0.096, y_2=0.5, z_2=0.393$
 Sb_{II}: $x_3=0.142, y_3=0.0, z_3=0.027$

gave $R=0.13$ for the $h0l$ reflexions and $R=0.21$ for the $h1l$ and $h2l$ reflexions included in this calculation ($\theta \leq 30^\circ$, Table 2). Whereas the x and z parameters seem to be reasonably correct the higher R value for the $h1l$ and $h2l$ reflexions indicates that y_2 and y_3 differ from $\frac{1}{2}$ and 0. Further refinement of y_2 and y_3 has in the present circumstances not been attempted as experiments to make better crystals for a detailed refinement are in progress.

Table 2. Observed (from Guinier photographs) and calculated structure factors for NbSb₂

hkl	F_o	$ F_c $	hkl	F_o	$ F_c $
001	—	12	11 $\bar{4}$	163	197
002	125	90	11 $\bar{3}$	105	117
20 $\bar{5}$	100	118	11 $\bar{2}$	297	215
20 $\bar{4}$	119	132	11 $\bar{1}$	78	48
20 $\bar{3}$	226	212	110	107	42
20 $\bar{2}$	—	1	111	330	330
20 $\bar{1}$	88	62	112	242	178
200	32	30	31 $\bar{4}$	62	70
201	122	72	31 $\bar{3}$	311	289
203	193	214	31 $\bar{1}$	250	237
40 $\bar{5}$	109	136	311	—	22
40 $\bar{4}$	—	22	312	175	187
40 $\bar{3}$	200	216	51 $\bar{3}$	48	87
40 $\bar{2}$	265	268	51 $\bar{2}$	82	115
40 $\bar{1}$	129	110	51 $\bar{1}$	54	84
400	284	304	510	85	121
401	98	118	020	304	391
60 $\bar{1}$	92	102	021	—	8
			22 $\bar{1}$	58	43

Overlapping reflexions:

- $hkl, |F_c|$: (003, 270; 31 $\bar{2}$, 158), (202, 39; 310, 222),
 (60 $\bar{4}$, 158; 605, 180)

Discussion of the structures

The coordination around the niobium and arsenic (antimony) atoms can be seen from Fig. 3. The interatomic distances between nearest neighbours are listed in Table 3.

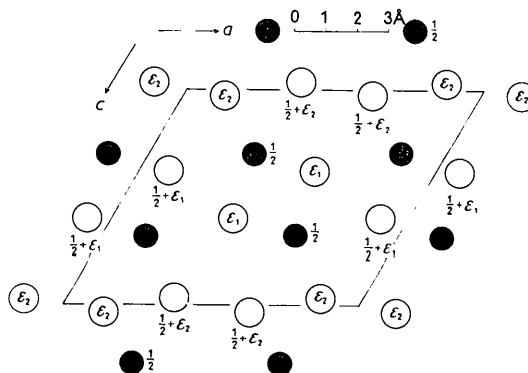
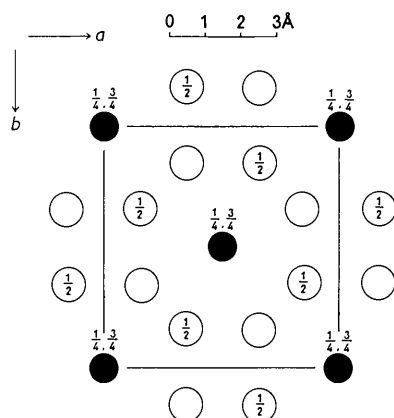
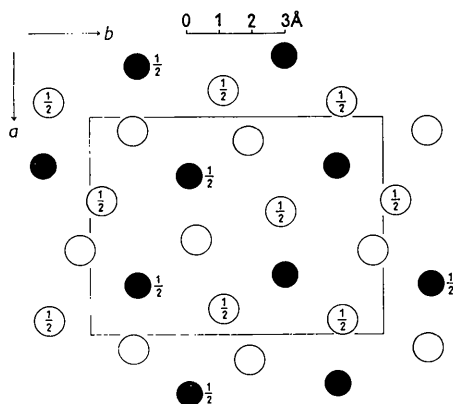
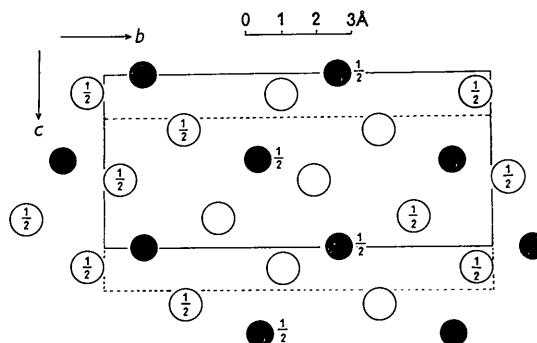
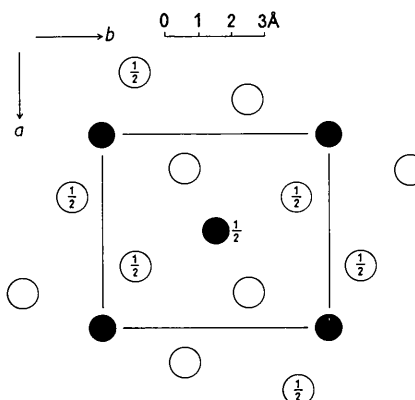


Fig. 3. The structure of NbAs₂ projected along [010]. In this and the following diagrams filled circles represent metal atoms and open circles represent metalloid atoms. The numbers indicate fractions of the projection axes.

(The y parameters of the metalloid atoms indicated on this diagram are related to those given in the text by: $\epsilon_1=y_2-\frac{1}{2}$ and $\epsilon_2=y_2$. For NbAs₂: $\epsilon_1=-0.012, \epsilon_2=0.067$; for NbSb₂: $\epsilon_1=\epsilon_2=0.0$.)

Fig. 4. The CuAl_2 type structure of TiSb_2 projected along $[001]$.Fig. 5. The PbCl_2 type structure of HfAs_2 projected along $[001]$. The origin has been shifted to $0, 0, \frac{1}{4}$ in this diagram.Fig. 6. The structure of MoP_2 projected along $[100]$. The broken unit cell has origin at $0, 0, \frac{1}{4}$.Fig. 7. The marcasite type structure of CrSb_2 projected along $[001]$.

Each niobium atom is surrounded by six arsenic (antimony) atoms at the corners of a triangular prism and by two other arsenic (antimony) atoms and one niobium atom outside the rectangular faces of the prism. Two more distant niobium atoms lie outside

Table 3. *Interatomic distances*Interatomic distances in NbAs_2 (Å)

Nb-3 Nb:	3.00 ₇ ; 3.382 ₃ (2)
-5 As _I :	2.66 ₅ ; 2.70 ₁ ; 2.71 ₆ ; 2.73 ₉ ; 2.75 ₁
-3 As _{II} :	2.53 ₇ ; 2.65 ₇ ; 2.82 ₃
As _I -5 Nb:	2.66 ₅ ; 2.70 ₁ ; 2.71 ₆ ; 2.73 ₉ ; 2.75 ₁
-5 As _I :	2.97 ₆ ; 3.05 ₂ (2); 3.382 ₃ (2)
-6 As _{II} :	3.23 ₉ ; 3.25 ₈ ; 3.45 ₂ ; 3.46 ₈ ; 3.79 ₄ ; 3.96 ₂
As _{II} -3 Nb:	2.53 ₇ ; 2.65 ₇ ; 2.82 ₃
-6 As _I :	3.23 ₉ ; 3.25 ₈ ; 3.45 ₂ ; 3.46 ₈ ; 3.79 ₄ ; 3.96 ₂
-5 As _{II} :	2.44 ₆ ; 2.84 ₂ (2); 3.382 ₃ (2)

Interatomic distances in NbSb_2 (Å)

Nb-3 Nb:	3.24; 3.631 ₉ (2)
-5 Sb _I :	2.91 (2); 2.94 (2); 2.97
-3 Sb _{II} :	2.84; 2.85 (2)
Sb _I -5 Nb:	2.91 (2); 2.94 (2); 2.97
-5 Sb _I :	3.25; 3.28 (2); 3.631 ₉ (2)
-6 Sb _{II} :	3.60 (2); 3.77 (2); 3.96; 4.20
Sb _{II} -3 Nb:	2.84; 2.85 (2)
-6 Sb _I :	3.60 (2); 3.77 (2); 3.96; 4.20
-5 Sb _{II} :	2.72; 3.07 (2); 3.631 ₉ (2)

each of the triangular faces of the prism. The As_I (Sb_I) atoms are surrounded by five near niobium neighbours in a distorted square pyramidal arrangement and by one close As_I (Sb_I) neighbour located across the base of the pyramid. The As_{II} (Sb_{II}) atoms are coordinated to three As_{II} (Sb_{II}) atoms and three niobium atoms. The arrangement of the As_{II} (Sb_{II}) atoms produces alternately longer and shorter As_{II}-As_{II} (Sb_{II}-Sb_{II}) distances. The short distance, which indicates that bonding exists between the metalloid atoms, is one of the most interesting features of these structures.

The relationships between the NbAs_2 -type structure and the structures of other MX_2 compounds containing a transition element (here limited to the subgroup IV, V and VI elements) in combination with a pnictogen (*i.e.* a group V element) are conveniently discussed in terms of the general $(8-N)$ rule. The connection between valence, crystal chemistry and semiconductivity (see *e.g.* Mooser & Pearson (1960), Hulliger & Mooser (1963) and Pearson (1964)) is described by:

$$(n_e + b_a - b_c)/n_a = 8$$

where per formula unit n_e is the number of valence electrons, b_a is the number of valence electrons involved in anion-anion bond formation, b_c is the

Table 4. *Attempted correlation of valence and crystal structure of some MX₂ compounds by the general (8-N) rule*

Compound	Structure type	n_e/n_a	b_a/n_a	b_c/n_a	Anion substructure
TiSb ₂ *	CuAl ₂	7	1		X-X pairs
ZrAs ₂ †	PbCl ₂	7	$\frac{1}{2}$	$-\frac{1}{2}$	X _I -X _I pairs
ThAs ₂ * ThSb ₂ *	Cu ₂ Sb	7		-1	
VSb ₂ *	CuAl ₂	$7\frac{1}{2}$	1	$\frac{1}{2}$	X-X pairs
NbAs ₂ NbSb ₂	NbAs ₂	$7\frac{1}{2}$	$\frac{1}{2}$		X _{II} -X _{II} pairs
CrSb ₂ *	Marcasite	8	1	1	X-X pairs
MoP ₂ § WP ₂ §	MoP ₂	8	1	1	X _I -X _{II} pairs
UP ₂ * UAs ₂ * USb ₂ * UBi ₂ *	Cu ₂ Sb	8			

* Pearson (1958).

† Trzebiatowski, Weglowski & Lukaszewics (1958).

‡ Jeitschko & Nowotny (1962).

§ Rundqvist & Lundström (1963).

number of valence electrons involved in cation-cation bonds (together with any unshared electrons on the cations) and n_a the number of anions.

A complete test of the rule on a given compound necessitates knowledge of (i) valence (n_e), (ii) crystal structure (b_a and b_c) and (iii) filling of valence band (*i.e.* occurrence of semiconductivity). When two of these factors are known the rule might be used to predict the third. The rule is normally used as a criterion for occurrence of semiconductivity in a compound whose detailed crystal structure and valences are known. Although the application of the general (8-N) rule to describe transition metal compounds may be doubtful, many compounds containing transition metals are semiconductors and satisfy the rule with a reasonable valence.

Table 4 shows the partition of n_e/n_a (based on valences corresponding to the group numbers), b_a/n_a (according to the crystal structures) and b_c/n_a (assuming the general (8-N) rule satisfied) for the considered MX₂ compounds. The general (8-N) rule appears to be satisfied for TiSb₂, NbAs₂, NbSb₂, UP₂, UAs₂, USb₂ and UBi₂. For VSb₂, CrSb₂, MoP₂ and WP₂ with positive b_c/n_a values a decreased metal valence, *i.e.* localized electrons on the metal atoms, would have to be assumed to comply with the rule. For ZrAs₂, HfAs₂, ThAs₂ and ThSb₂ the negative b_c/n_a ratios show that the metal valence would have to be increased to agree with the rule. To increase the valence, electrons must be excited from energetically lower orbitals of the metal atoms.

As no satisfactory electrical and only very few magnetic data are available for these compounds a complete test cannot be performed. Two unpaired *d*-electrons in CrSb₂ (Haraldsen, Rosenqvist & Grøn-vold, 1948) and none in NbAs₂ and NbSb₂ (Furuseth & Kjekshus, 1964) account satisfactorily for the b_c/n_a values listed in Table 4. Further consideration will have to await more experimental data.

It is interesting to compare the CuAl₂, PbCl₂, NbAs₂, MoP₂ and marcasite types of structure. As seen from Table 4 the five structures have in common the feature of X-X pairs. In the CuAl₂ and marcasite structures, where the X atoms are crystallographically equivalent, all the X atoms occur in pairs. In the MoP₂ structure the same situation arises because X-X pairs occur between the two crystallographically

different X_I and X_{II} atoms. In the PbCl₂ and NbAs₂ structures, where the pairing takes place between only one of the crystallographically equivalent X atoms, only half of the X atoms form pairs.

It is instructive to compare the projections of these five structures shown in Figs. 3-7. A comparison of these figures shows the resemblance between the structures. The metal and metalloid sublattices are similar in the projections, but differ somewhat in the third dimension. By squeezing, twisting and changing of height the metalloid sublattice is altered to produce the correct number of X-X pairs in the various structures. It is also interesting to follow the change in coordination of the metalloid atoms around the metal atoms in these structures. The coordination polyhedron gradually changes from a distorted anti-prism in the CuAl₂ type structure *via* prismatic coordinations in the PbCl₂, NbAs₂ and MoP₂ types of structures to that of an octahedron in the marcasite type structure.

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