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The crystal structures of Nb_3Au and V_3Au.

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Recently Geller, Matthias & Goldstein (1955) described several new intermetallic compounds with the 'β-wolfram' structure ($A15$) (*Strukturbericht*, 1937) discovered in the search for superconductors with high transition temperatures. Two new compounds have now been added to the list: Nb_3Au and V_3Au. Nb_3Au becomes superconducting at 11·5° K. and V_3Au is not superconducting above 1·1° K. One other gold compound has been reported to have the β-wolfram structure. This is Ti_3Au, reported by Duwez & Jordan (1952).

The compounds Nb_3Au and V_3Au resulted from the reaction of stoichiometric quantities of niobium powder and gold wire and of massive vanadium and gold wire in a helium arc furnace. The temperature of the reaction is not known, but the sample was certainly heated to above 2000° C. Each charge was fused three times to promote homogeneity.

X-ray diffraction powder photographs were taken of the resulting product, using a Norelco camera of 114·6 mm. diameter and Cu K radiation. The patterns were indexed on a primitive cubic cell with the lattice constants given in Table 2. Reflections of the type (hhl) with l odd are absent. In addition, reflections (410), (430), (531), (621) and (540) are absent. The possibility that compounds with the β-wolfram structure would result from the fusion of these elements in the appropriate proportions had been anticipated, and the close similarity between these powder patterns and those of the compounds reported by Geller *et al.*, indicated that they are isostructural. The absences are those appropriate to the β-wolfram structure. This structure belongs to space group O_h^3–$Pm3n$ with two atoms of one type in position 2(a): (0, 0, 0), ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) and six atoms of the other type in positions 6(c): $\pm(\frac{1}{4}, 0, \frac{1}{2}; \circlearrowright)$. Alternatively, these six atoms may be placed in 6(d): $\pm(\frac{1}{4}, \frac{1}{2}, 0; \circlearrowright)$ and the resulting structure would be the same. The twofold and sixfold positions of space group T_d^4–$P43n$ are the same as those of space group O_h^3–$Pm3n$. The higher-symmetry space group is chosen.

Table 1. *Comparison of calculated with observed intensities, visually estimated*

(vs = very strong; s = strong; m = medium; w = weak)

	Nb_3Au		V_3Au	
hkl	Obs.	Calc.$_{(ord.)}$	Obs.	Calc.$_{(ord.)}$
110	m	25	m–s	47
200	s	46	m	27
210	s–vs	56	w	12
211	vs	100	s	60
220	vw	4	vw	7
310	w	6	vw	10
222	vvw	0·8	Abs.	0·4
320	m	11	Abs.	2
321	s	49	m	29
400	m	13	vw	6
411, 330	vw–w	4	vw	6
420	m	14	vw	9
421	m	10	Abs.	2
332	m	12	vw	8
422	vvw	2	vvw	3
510, 431	w	8	vw	11
520, 432	m	11	vvw	3
521	m–s	21	w	17
440	m	14	vw	8
530, 433	vvw	3	vw	8
600, 442	m	16	w	16
610	w	5	Abs.	2
611, 532	m–s	40	s	52

Note.—The two films were not comparable with each other in intensity; the 'observed' intensities are therefore on different scales.

Table 2

		Interatomic distances (Å)		
Compound	a_0 (Å)	B–A	$(A$–$A)_1$	$(A$–$A)_2$
Nb_3Au	5·21±0·01	2·91	2·61	3·19
V_3Au	4·88±0·01	2·73	2·44	2·99

Each B atom is surrounded by 12 A atoms at a distance B–A; each A atom is at distance $(A$–$A)_1$ from an A atom on either side of it, $(A$–$A)_2$ from eight other A atoms, and B–A from four B atoms which surround it in a distorted tetrahedron.

Relative intensities for each of these compounds were computed on the basis of the above structure, using the formula

$$I \propto p|F_{hkl}|^2 \frac{1+\cos^2 2\theta}{\sin^2\theta \cos\theta} \times 10^{-5},$$

where p is the multiplicity factor, F_{hkl} the structure amplitude, and the remaining term is twice the combined Lorentz and polarization factors. James & Brindley's (1931) scattering factors were used for gold and vanadium, and the Thomas–Fermi factors from the *International Tables* (1935) for niobium.

The results are shown in Table 1, compared with the observed intensities, visually estimated. The agreement is so close that the β-wolfram structure is indicated both for V_3Au and for Nb_3Au. The fact that the (110) reflection in both cases is somewhat weaker than indicated by calculation is interpreted as due to absorption.

In each pattern two 'very very weak' extra lines were observed. The d values for those in the Nb_3Au pattern were 2·42 and 2·24 Å; for those in the V_3Au pattern, 2·28 and 1·44 Å. These lines are not the strongest lines for any of the following substances: Nb, Au, V, Nb_2O_5, V_2O_3, V_2O_5. Their origin is unexplained.

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