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A Set of Effective Coordination Number (12) Radii for the β-Wolfram Structure Elements

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A set of effective coordination number (12) radii is derived from the known compounds of 'β-wolfram' structure from which the lattice constants of the compounds are reproduced to within ±0·03 Å. In several cases there are significant differences between the CN(12) radii here derived and those given by Pauling and Wells. Crystallographic data are given on all the known compounds with β-W structure, including three not heretofore reported. It is found that Pauling's resonating-valence-bond theory of metals does not apply to this series of compounds.

Introduction

To date,* thirty-two intermetallic compounds with the β-wolfram structure† (Fig. 1) are known. This structure is favorable to superconductivity, a fact established by Hardy & Hulm (1954) and by Matthias, who has discovered eleven of the compounds shown in Table 1 (see references *a*, *b*, *c* of Table 1). In particular Nb_3Sn (Matthias, Geballe, Geller & Corenzwit, 1954) has the highest superconducting transition temperature, 18·05±0·1° K., known to date. An examination of the compounds crystallizing with the β-W structure has produced a list of effective 12-coordination radii for the elements involved from which the lattice constants of these compounds may be reproduced to within ±0·03 Å.

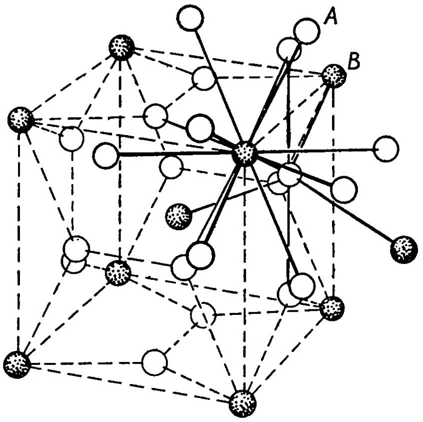

Fig. 1. The β-W structure.

Discussion

The β-W structure belongs to space group O_h^3–$Pm3n$. Two types of sites are occupied by the atoms in the A_3B compounds (Fig. 1): the A atoms occupy positions 6(*c*): $\pm(\frac{1}{4}, \frac{1}{2}, 0; \circlearrowleft)$; the B atoms occupy positions 2(*a*): $(0, 0, 0;\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The A atoms have an effective coordination number of 14 whereas that of the B atoms is 12. Each A atom is coordinated to two A atoms at the distance $\frac{1}{2}a_0$, $(A\text{–}A)_1$; to 8 A atoms at distance $\frac{1}{4}a_0\sqrt{6}$, $(A\text{–}A)_2$; and to 4 B atoms at distance $\frac{1}{4}a_0\sqrt{5}$, $(B\text{–}A)$. Each B atom is coordinated to twelve A atoms at the distance $(B\text{–}A)$. These distances are listed in Table 1 together with the measured lattice constants and those derived from the 12-coordination radii given in Table 2. The derived lattice constants are obtained by adding the radii of the two atoms in the compound and multiplying this sum by $4/\sqrt{5}$.

It is seen (Table 1) that only in the case of Cr_3Ir is the difference between the measured and derived lattice constants as large as 0·03 Å. In this case a homogeneity range has been reported by Raub (1954) and the value taken for the 75 atomic % Cr compound has been obtained by interpolation.

Although an exhaustive survey has not been made, such excellent agreement obtained from a specialized set of radii does not appear to be the rule. Except for the Cr_3Ir, the discrepancies are within the rounding-off

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* This is the date of the revision. At the time of the first writing 29 compounds were reported. The paper by Greenfield & Beck (1956, see Table 1) appeared after the first writing.

† See also Hägg & Schönberg (1954), who show that W_3O has a completely disordered β-W structure and argue that β-W itself does not exist.

Table 1. *Interatomic distances and lattice constants of β-wolfram structures*

All values in Ångström units

Compound	$(B–A)$	$(A–A)_1$	$(A–A)_2$	Measured a_0	Derived a_0	$\|\Delta a_0\|$	Ref.*
Nb_3Ir	2·869	2·566	3·143	5·131	5·13	0·00	*a*
Nb_3Pt	2·880	2·577	3·155	5·153	5·17	0·02	*a*
Nb_3Os	2·862	2·561	3·136	5·121	5·13	0·01	*a*
Nb_3Au	2·91	2·605	3·19	5·21	5·22	0·01	*b*
Nb_3Sn	2·956	2·645	3·238	5·289	5·29	0·00	*a*
Nb_3Rh	2·859	2·558	3·132	5·115	5·13	0·01	*p*
Ta_3Sn	2·949	2·638	3·231	5·276	5·28	0·00	*a*
V_3Ir	2·674	2·393	2·930	4·785	4·78	0·01	*c*
V_3Pt	2·692	2·408	2·949	4·815	4·81	0·01	*c*
V_3Au	2·73	2·44	2·99	4·88	4·87	0·01	*b*
V_3Co	2·613	2·338	2·863	4·676	4·67	0·01	*d*
V_3Ni	2·632	2·355	2·884	4·710	4·70	0·01	*m*
V_3Si	2·640	2·361	2·892	4·722	4·70	0·02	*e*
V_3Ge	2·666	2·385	2·920	4·769	4·76	0·01	*f*
V_3Sn	2·759	2·468	3·023	4·94	4·94	0·00	*a*
V_3Rh	2·665	2·384	2·919	4·767	4·77	0·00	*p*
V_3As	2·66	2·37	2·91	4·75	4·75	0·00	*o*
Mo_3Ir	2·776	2·482	3·040	4·965	4·96	0·01	*g*
Mo_3Os	2·780	2·487	3·045	4·973	4·96	0·01	*g*
Mo_3Si	2·734	2·445	2·995	4·890	4·88	0·01	*h*
Mo_3Ge	2·758	2·467	3·021	4·933	4·94	0·01	*i*
Ti_3Ir	2·799	2·504	3·066	5·007	4·99	0·02	*c*
Ti_3Pt	2·814	2·517	3·082	5·033	5·03	0·00	*j*
Ti_3Au	2·849	2·548	3·121	5·096	5·08	0·02	*j*
Ti_3Hg	2·901	2·595	3·177	5·189	5·19	0·00	*n*
Cr_3Si	2·551	2·282	2·795	4·564	4·58	0·02	*k*
Cr_3Ge	2·584	2·312	2·831	4·623	4·63	0·01	*f*
Cr_3Pt	2·634	2·356	2·885	4·711	4·69	0·02	*l*
Cr_3Ir	2·614	2·339	2·865	4·678	4·65	0·03	*l*
Cr_3Rh	2·603	2·328	2·851	4·656	4·64	0·02	*p*
Cr_3Ru	2·618	2·342	2·868	4·683	4·69	0·01	*l*
Zr_3Hg	3·107	2·779	3·404	5·558	5·56	0·00	*m*

* *a*: Geller *et al.*, 1955; *b*: Wood & Matthias, 1956; *c*: Matthias *et al.*, 1955; *d*: Duwez, 1951; *e*: Wallbaum, 1939; *f*: Wallbaum, 1944; *g*: Raub, 1954; *h*: Templeton & Dauben, 1950; *i*: Searcy *et al.*, 1952; *j*: Duwez & Jordan, 1952; *k*: Borén, 1933; *l*: Raub, 1955; *m*: Rostoker & Yamamoto, 1954: *n*: Pietrokowsky, 1954; *o*: Bachmayer & Nowotny, 1955; *p*: Greenfield & Beck, 1956.

Table 2. CN(12) *radii for metals in β-wolfram structures*

Metal	'β-W' radius	Semi-empirical values	
		Pauling	Wells
Nb	1·51 Å	1·47 Å	1·47 Å
Ta	1·50	1·49	1·47
V	1·31	1·36	1·35
Mo	1·41	1·39	1·40
Ti	1·43	1·47	1·47
Cr	1·24	1·30	1·29
Zr	1·64	1·60	1·60
Rh	1·355	1·34	1·34
Ir	1·36	1·36	1·36
Pt	1·38	1·39	1·39
Au	1·41	1·46	1·44
Os	1·36	1·35	1·35
Co	1·30	1·25	1·25
Ni	1·32	1·25	1·25
Si	1·32	—	1·34*
Ge	1·35	—	1·39
Sn	1·45	—	1·58
Ru	1·38	1·34	1·34
Hg	1·47	1·57	1·55
As	1·34	—	1·34*

* Derived from CN(4) radius by comparison with value for Ge.

error of the calculation. To attempt to push the accuracy further is unjustifiable for two reasons: (1) different investigators have obtained values of lattice constants for the same compound which differ by as much as the deviations shown in Table 1; (2) in most cases it is tacitly assumed that the stoichiometry is correct although no chemical analyses have been made and despite the knowledge that at least some of these systems have homogeneity ranges.

For purposes of comparison the CN(12) radii derived by Pauling (1945) and Wells (1950) are given in Table 2 also. The largest difference between the Pauling and Wells radii of a given element is 0·02 Å. However, there are some very significant differences between the effective CN(12) radii of several of the elements in the β-W structure and the CN(12) radii of either Pauling or Wells, particularly with respect to accurate prediction of lattice constants. For example, suppose one had wished to predict the lattice constants of Ti_3Ir assuming the β-W structure. The Pauling or Wells radii lead to a value of 5·07 Å for the lattice constant, 0·06 Å too large. The value predicted is the one given in Table 1, the values of the Ti and Ir radii having been obtained earlier from a set of radii derived from a smaller number of known compounds. The case of V_3Au is even more vivid. Pauling's radii would give 5·05 Å and Wells' 4·99 Å, 0·16 and 0·10 Å, respectively, too large. Needless to say, in the case of Nb_3Sn, the Wells values would lead to an extremely high value for the lattice constant of Nb_3Sn, 5·46 Å. It is, in fact, rather unfortunate that the lattice constant is not as large as this, because if it were, the temperature of transition to superconductance of this compound would be very high indeed (Matthias, 1953).

The constancy of the B atom radii in these compounds is not surprising because the B atoms have 12 equidistant A atom nearest neighbors (Fig. 1) in all the compounds, i.e. the B atoms may be considered to have pure CN(12).* But the A atoms which have a nominal CN(14) in these compounds do not have a constant CN(14) radius, i.e., if this radius is obtained by averaging the fourteen near neighbor distances. Yet the ECN(12) radii of the A atoms as obtained from the $(B–A)$ distances do show remarkable constancy. This suggests that the $(A–A)_1$ and $(A–A)_2$ distances shift somewhat to accommodate the changing B atom size.

In the paper by Greenfield and Beck (1956), it is stated that the B atoms appear to have only a minor effect on the lattice constants. If this were so, the short $(A–A)_1$ distances should be very nearly constant for a particular A atom. Actually these show variations which are proportional to the changing size of the B atom. Consider, for example, the niobium compounds: the change of (Nb–Nb) from Nb_3Ir to Nb_3Sn is 0·079 Å, corresponding to a difference in lattice constant of 0·158 Å and to a difference in effective CN(12) radii of 0·09 Å. With constant B atom the change in lattice constant is apparently greater, but this comparison is somewhat misleading in that there are three times as many A atoms as B atoms in the cell. What we have to examine is the relative change per atom. We notice the trivial case: when B is constant, and the sizes of the different A atoms are very nearly the same, the lattice constants are very nearly the same, just as when the A atom is constant and the B atoms have very nearly the same size. Compare Nb_3Sn with Ta_3Sn, for example. This case alone is enough to show that the change in A-atom size is no more important than a change in B-atom size. If it were, the lattice constants for Ta_3Sn and Nb_3Sn should be markedly different.

Consider now, as another example, the pairs Nb_3Sn, Nb_3Ir and V_3Sn, V_3Ir. The ratios of the lattice constants are as follows:

Nb_3Sn/V_3Sn	1·07
Nb_3Ir/V_3Ir	1·07
Nb_3Sn/Nb_3Ir	1·03
V_3Sn/V_3Ir	1·03

Referring to Table 2, one sees that the percentage difference in radii is more than twice as large for the A atoms as for the B atoms in these cases. Recalling that there are three times as many A as B atoms in the unit cell, one concludes that a B atom is somewhat more important than an A atom in determining the cell size.

The compounds with β-W structure, though belonging to an apparently simple structure type, do not at this time shed much light on the matter of the valency of the interacting atoms. Direct application of Pauling's resonating-valence-bond theory (Pauling, 1949) leads to the results shown in Table 3. The only result which looks reasonable in the group is that for the valences of V and Pt in V_3Pt. The valences for Nb and V should be 5; for Ir, Pt, Os and Co, 6; for Sn, Si and Ge, 4. If the bond number for each of the twelve equivalent neighbors of a B atom is put equal to $\frac{1}{2}$, as for example in Nb_3Pt, making the valence of Pt 6, then the bond number for the $(Nb–Nb)_1$ becomes greater than 3 if the R_1 for Nb is taken as 1·40 Å, a value not in good agreement with Pauling's value of 1·342 Å. If the R_1 for Pt is taken as 1·36 Å, not in good agreement with Pauling's value of 1·295 Å for Pt, the $(Nb–Nb)_1$ bond number becomes 1·5.

Table 3. *Valences of atoms in some β-wolfram structures as computed from Pauling's resonating-valence-bond theory*

Compound (A_3B)	Valence for atom A	Valence for atom B
Nb_3Ir	5·8	4·4
Nb_3Pt	5·9	4·7
Nb_3Os	6·1	4·4
Nb_3Sn	5·0	5·3
V_3Sn	5·4	7·1
V_3Ir	5·7	5·9
V_3Pt	5·1	6·2
V_3Si	5·8	4·7
V_3Ge	5·6	5·3
V_3Co	6·4	5·0

One of the referees of the original manuscript* pointed out in his earlier remarks that the above application of Pauling's theory did not seem to be made in the way suggested by Pauling. The author had not taken into account the probability that 'atoms distribute their d-character differently among the orbitals in bonds to different atoms, so as to increase the single-bond radius for some bonds and to decrease it for others'. If this is done for compounds for which the Pauling valences for the A and B atom are 5 and 6 respectively, things work rather well. For example, for Nb_3Pt each bond from Pt to Nb is taken as a half bond, giving Pt a valence of 6. This also leaves three valences for niobium, since there are four (Nb–Pt)

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* This is not strictly true because the angular relationship is not the same as either in the face-centered or in the hexagonal close-packed cell.

* This revision is essentially unchanged from the original. The main changes involve the recognition of the work of Greenfield & Beck and an elaboration of the thesis that Pauling's resonating-valence-bond theory does not explain the bonding in these compounds.

bonds to a Nb. Assign two to the two short distances and one to the eight long ones. This then gives for the single-bond radii of Nb the three values 1·40, 1·29 and 1·31 Å respectively, or a weighted average of 1·33 Å, which differs by 0·01 Å from the value given by Pauling, but this seems to be very good agreement. The application works equally well for Nb_3Ir and Nb_3Os, but it does not work for many of the other compounds, nor does there seem to be much hope of finding another variation that will improve the situation.

Pauling (1949) gives very lucid arguments as to why Sn cannot have a valence higher than 4. These arguments should presumably be valid for Si and Ge also. For the latter elements some more recent work (Pauling & Pauling, 1956) further establishes this to be the case (although in that paper a valence of 4·60 is obtained for Si when Si is dissolved in Cu: this however is not clarified). If we now consider Nb_3Sn, we must divide the four valencies of Sn among twelve bonds: this gives $n = \frac{1}{3}$ for the Nb–Sn bonds. Thus we have an extra $\frac{2}{3}$ bond to divide up among the remaining Nb–Nb distances. It hardly seems reasonable to make the $(Nb–Nb)_1$ bond numbers $\frac{4}{3}$ since, in Nb_3Sn, $(Nb–Nb)_1$ is the longest of the Nb bonds. The same holds for the longer Nb–Nb distances.

The situation gets worse when the Mo and Cr compounds are considered. According to Pauling (1949), these elements have valence 6. (Cr also has valence 3, but that makes things even worse.) If the *B* atom is sexivalent, there is one extra valence and for Ge and Si $1\frac{2}{3}$ extra valencies left over. Things are not improved when the *A* atom is quadrivalent, as in the cases of the Ti and Zr compounds.

In their recent paper Pauling & Pauling (1956) point out that the valence of As in alloys is 3. This, if applied to V_3As, leaves $1\frac{1}{2}$ valencies for which to account.

Although it is unsound to assign to some of the short $(A–A)_1$ distances bond number 1 and to others a number different from 1, suppose that $n = \frac{3}{2}$ is assigned to the $(Mo–Mo)_1$ in Mo_3Ir. One then obtains for the single-bond radii 1·33, 1·19 and 1·25 Å in the order as given above. The weighted average of these is 1·264 Å, a significant difference of 0·032 Å from Pauling's value.

Thus one must conclude that Pauling's resonating-valence-bond theory for intermetallic compounds does not apply to this series of compounds.

It is not clear as to how one may arrive at rules for predicting with reliability the occurrence of a phase with β-W structure. Of the known compounds (Table 1) the *A* atoms are in Groups IV*a*, V*a*, VI*a* and the *B* atoms come mainly from the transition metals and the Group IV and V*b* metalloids. But not all of the elements in these groups are involved, and of those involved not all the possible combinations yield β-W phases.

Summary

A set of effective coordination number (12) radii has been established for metals in the β-W structure. The *B* atoms appear to have surroundings which are more nearly spherical than are those of the *A* atoms, but sphericity of any of the atoms is not implied. The interesting point is the apparent constancy of the radii in the *A*–*B* interactions. In the structure, although the *A*–*A* interaction must play an important role in determining the cell size, it is apparently unnecessary to consider that interaction in predicting the cell size. That is to say, for a particular compound the equilibrium interatomic distances may be completely determined (within the error stated) from a knowledge of the effective CN(12) radii.

It has also been shown that the Pauling resonating-valence-bond theory of intermetallic compounds does not apply to this structure.

Note added in proof, 14 *September* 1956.—Recently, Carpenter & Searcy (1956) reported the existence of Nb_3Ge with the β-W structure and lattice constant 5·168±0·002 Å. The lattice constant predicted for this compound is 5·12 Å, a discrepancy of 0·05 Å, which is indeed very large. Increasing the effective CN(12) radii of either Nb or Ge would result in greater discrepancies than those listed for the compounds involving these atoms. We therefore made melts containing 66·7, 70, and 80 atomic % Nb. In all cases, we obtained at least two phases, one of which was of the β-W type. Moreover, there was no change in lattice constant of the β-W phase, our value being in very close agreement with that of Carpenter & Searcy. However, the melt containing 80 atomic % Nb had least of the extraneous phase or phases, which seems to indicate that the β-W type phase does not have the correct stoichiometry. This, together with the large lattice constant, suggests that some Nb atoms are replacing Ge atoms in the 2(*a*) positions.

In recent work at these Laboratories by Matthias, Wood, Corenzwit & Bala (to be published), four more compounds with β-W structure were discovered, namely Nb_3Sb, V_3Ga, V_3Sb and Mo_3Ga. The lattice-constant values for these lead to the effective CN(12) values of 1·44 Å and 1·37 Å for Sb and Ga respectively. The Ga value is in some doubt because, according to Matthias (private communication), these compounds form only when there is an excess of V or Mo. Also, at least in the V_3Ga case, there is a solution range.

The author wishes to thank Mr H. M. Yates for making the drawing shown in Fig. 1.

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The Crystal Structure of Cyanogen Chloride

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Solid cyanogen chloride, ClCN, at about −30° C. is orthorhombic with $a = 5{\cdot}68$, $b = 3{\cdot}98$, $c = 5{\cdot}74$ Å. The space group is *Pmmn* and there are two molecules per unit cell. The molecules are arranged in infinite linear chains parallel to the *c* axis. The packing of the chains approximates closest packing of cylinders. The distance along a chain between the ends of adjacent molecules is short, only 3·01 Å. This indicates that strong intermolecular attractions exist along the chains. Cyanogen chloride is isostructural with cyanogen bromide.

Introduction

Before this work was begun it was expected that the ClCN molecules would be arranged in linear chains and that an exceptionally strong attraction would act between the chlorine atom of one molecule and the nitrogen atom of another. Evidence for such an attraction came from studies of cyanogen *iodide*: Townes & Dailey (1952) concluded, from the value of the nuclear quadrupole coupling constant of iodine in solid ICN, that the molecules are joined by a bond with about 10% single covalent character. This is consistent with the crystal structure determination of Ketelaar & Zwartsenberg (1939); the iodine atom of one molecule is only about 2·8 Å distant from the nitrogen atom of the next molecule, which is far less than the sum of the van der Waals radii. A similar condition has very recently been found in a crystal structure and quadrupole coupling study of cyanogen bromide (Geller & Schawlow, 1955). The present study of cyanogen chloride was undertaken with the hope that the smaller halogen in this compound would permit accurate interatomic distances to be determined, which was not possible in the cases of the bromide and iodide.

Experimental methods

One sample of cyanogen chloride was kindly provided by The American Cyanamid Company through Dr D. J. Berets. Additional material was prepared by the method of Coleman, Leeper & Schulze (1946). The crude product was agitated with mercury, sodium bicarbonate, and zinc oxide to remove the expected impurities: chlorine, hydrogen chloride, and hydrogen cyanide. It was then dried over calcium chloride, distilled, and sealed into thin-walled Pyrex capillaries. The melting point is −6° C.

Rotation, oscillation, and Weissenberg X-ray photographs were prepared at −30±5° C. with Cu $K\alpha$ or Mo $K\alpha$ radiation. The samples were kept at the desired temperature by directing a stream of cold nitrogen gas over the capillaries.

Single crystals were obtained by melting and refreezing along the length of the capillary (Abrahams, Collin, Lipscomb & Reed, 1950). The crystals showed a strong tendency to grow with the *c* axis parallel to the axis of the capillary. Only once did a crystal grow spontaneously in a different orientation and it was very badly twinned. (Twinning of the crystals occurred very readily on the (110) plane.) It was pos-