disposent en couches successives perpendiculairement à l'axe **a***, l'enchaînement à l'intérieur d'une couche se faisant par mise en commun des sommets et alignement suivant une arête. On passe d'une couche à la suivante par une rotation de 90° autour de l'axe **a**, de l'ensemble de la couche (Fig. 2). Ce genre d'enchaînement se rencontre de façon générale dans les structures tétraédriques déficitaires de type MX_2 (Hulliger, 1976). Ces couches sont reliées par des atomes de potassium situés sur des droites parallèles aux arêtes du tétraèdre $[Ga_4S_{10}]$.

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Structure of Beryllium–Rhenium $Re_{0{\cdot}92}Be_{16}$

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Abstract. $M_r = 315{\cdot}5$, cubic, $F\bar{4}3m$, $Z = 1$, $a = 5{\cdot}875\ (2)$ Å, $V = 202{\cdot}8\ (2)$ Å^3, $D_x = 2{\cdot}58$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 14{\cdot}5$ mm^{-1}, $F(000) = 133\ (1)$, $T = 295$ K, $R = 0{\cdot}038$ for 79 reflections. In this intermetallic compound the Re positions are only partially occupied. The Be atom is in a nominally 12-coordinate environment. The structure is well described as composed of Be tetrahedra which share vertices. The mostly vacant Re sites are in uninterrupted channels through the Be network.

Introduction. Intermetallic compounds of Be occur in variety and have relatively low X-ray absorption coefficients. Consequently, these compounds are uniquely suited to the study of metal bonding through critical analysis of charge density distribution as obtained from X-ray diffraction experiments. As part of a systematic study of Be alloys we have determined the structure of $Re_{0{\cdot}92}Be_{16}$.

Experimental. A mixture of Re and Be in a 1:26 atomic ratio was pressed into a pellet. The pellet was then melted under an inert atmosphere in a copper-hearth tungsten-arc furnace. When the sample was remelted to ensure homogeneity, the pellet shattered. The fragments were searched for suitable crystals. Computer-controlled four-circle diffractometer (Syntex $P\bar{1}$, Mo $K\alpha$ radiation). Irregular crystal ~0·1 mm on an edge. Lattice parameters determined by least-squares refinement on the 2θ values of 15 reflections in the range $23° < 2\theta < 40°$. Intensity data measured only for positive indices in the ranges $h \le 13$, $k \le 9$, $l \le 13$. Standard reflections 400, 040, 224: sample standard deviations less than 3% of I. 215 intensities measured (max. $\sin\theta/\lambda = 1{\cdot}18$ Å^{-1}), yielding 79 unique reflections; two reflections unobserved $[I < 3\sigma(I)]$. Lorentz, polarization and empirical absorption (North, Phillips & Mathews, 1968) corrections; max. absorption correction 0·9986, min. 0·9284 using *SDP* (Enraf–Nonius, 1979) package. $R_{\rm int}$ for merging equivalent reflections 0·015. Positional parameter for Be, anisotropic thermal parameters for all atoms and occupancies of the Re atoms were refined by a full-matrix least-squares method minimizing $\sum w(|F_o| - |F_c|)^2$ using *SHELX*76 (Sheldrick, 1978); $w = 1/\sigma^2(F)$; $R = 0{\cdot}038$; $R_w = 0{\cdot}034$. Final parameter shift-to-error ratios all $<0{\cdot}2$. Final difference Fourier synthesis extremes $+4{\cdot}5$, $-3{\cdot}7$ e Å^{-3}. Anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974).

Discussion. The final structural parameters are given in Table 1;* a list of selected interatomic distances is given in Table 2.

The Re atomic positions both have identical site symmetry and nearly identical stereochemistry. Fig. 1 shows the nominal coordination around an Re atom. The Be framework around each Re atom is in the form of a 12-apex truncated tetrahedron. If all Re positions were fully occupied, as shown in Fig. 1, there would be

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39252 (2 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atomic positions and thermal parameters*

E.s.d.'s are given in parentheses.

	Re(*a*)	Re(*c*)	Be
x	0·0	0·25	0·622 (1)
y	0·0	0·25	$(=x)$
z	0·0	0·25	$(=x)$
Site occupancy	0·129 (2)	0·102 (2)	1·0
U_{11}	0·0038 (4)	0·0151 (9)	0·0059 (6)
U_{22}	$(=U_{11})$	$(=U_{11})$	$(=U_{11})$
U_{33}	$(=U_{11})$	$(=U_{11})$	$(=U_{11})$
U_{12}	0·0	0·0	−0·0002 (6)
U_{13}	0·0	0·0	$(=U_{12})$
U_{23}	0·0	0·0	$(=U_{12})$

Table 2. *Interatomic distances* (Å) *for* $Re_{0\cdot92}Be_{16}$

E.s.d.'s are given in parentheses.

Re(*a*)–12 Be	2·440 (7)	Be–3 Be′	2·03 (1)
4 Re(*c*)	2·544 (1)	3 Be″	2·12 (1)
Re(*c*)–12 Be	2·431 (7)	3 Re(*c*)	2·431 (7)
4 Re(*a*)	2·544 (1)	3 Re(*a*)	2·440 (7)

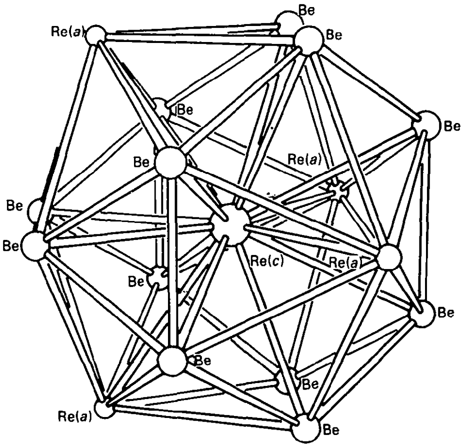

Fig. 1. The nominal coordination environment of an Re(*c*) atom.

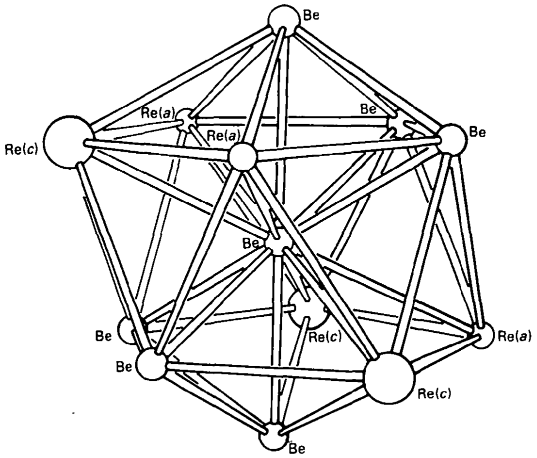

Fig. 2. The nominal 12 coordination of a Be atom.

an Re atom capping each of the four hexagonal faces formed by Be atoms.

Fig. 2 shows the nominal icosahedral coordination around each Be atom. The Be network is built up of corner-sharing tetrahedra, which define an opposing pair of triangular faces in each icosahedron.

$Re_{0\cdot92}Be_{16}$ has the same structure type as $AuBe_5$ (Misch, 1935). The differences between the compounds arise in the $(a{:}0,0,0)$ and the $(c{:}\frac{1}{4},\frac{1}{4},\frac{1}{4})$ positions. $AuBe_5$ was reported to have four Au in $(a{:}0,0,0)$ and four Be in $(c{:}\frac{1}{4},\frac{1}{4},\frac{1}{4})$ while $Re_{0\cdot92}Be_{16}$ has both positions partially occupied by Re atoms. If each Re position were fully occupied, and a Be had coordinates $(\frac{5}{8},\frac{5}{8},\frac{5}{8})$, the structure would be centrosymmetric in $Fd\bar{3}m$ and the same as that reported for $NbBe_2$ by Sands, Zalkin & Krikorian (1959).

Because approximately seven out of eight Re sites are vacant, the interatomic distances calculated from the structure model must be interpreted carefully. In particular, it is quite unlikely that any Re atom has its full complement of four Re neighbors. Consequently, almost every Re atom, more probably an Re(*c*) atom in view of its larger thermal parameters, can move preferentially in the direction of an unoccupied neighboring site and it is not certain that any two Re atoms in the crystal are well described as having the reported interatomic distance of 2·544 (1) Å.

Each Be atom has six near neighbors of Be atoms (Sands, Zalkin & Krikorian, 1959) in fully occupied sites. The Be atoms are in tetrahedra which share vertices in such a way that the tetrahedra themselves are arranged in larger tetrahedra in the crystalline array. The geometry of this structure of Be atoms does not allow for any substantial variation with the variable placement of Re atoms in their mostly unoccupied sites. The Be–Be interatomic distances, in contrast to those involving Re, are probably not subject to substantial artificiality arising from partial occupancy of the Re sites.

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