tetraedrischer Koordination derart, dass jedes Tetraeder mit einer Seitenfläche in einer Bandebene und die vierte Ecke in dem anderen Band des Bandpaares liegt. Dabei gehören die drei Kanten der in einer Bandebene liegenden Tetraederseite drei verschiedenen Koordinationsdreiecken an, d.h. die Cu-Atome des Bandes liegen in den Schwerpunkten gerade jener Dreiecke, die nicht Seitenflächen von Koordinations-Tetraedern sind. Die Koordinationspolyeder erklären sehr gut das Nadelwachstum. Oftedal (1932) beobachtete beim Covellin ebenfalls eine Dreieckskoordination. Dort bilden diese Dreiecke jedoch parallele Ebenen durch den ganzen Kristall, während hier parallele Bänder vorliegen, die nur in einer Richtung unendlich ausgedehnt sind. Es ist zu vermuten, dass durch diesen Unterschied die unterschiedliche Kristallform erklärt werden könnte. Covellin bildet nämlich Plättchen, während Betechtinit nadelförmig wächst. Die Bindungskräfte im Dreieck dürften stärker als die im Tetraeder sein, da die Cu–S-Abstände im Dreieck im Mittel kleiner sind als im Tetraeder.

Die auf Grund der Struktur geänderte Bruttoformel wurde durch eine nachträgliche sorgfältig durchgeführte chemische Analyse bestätigt: $Pb_2(Cu,Fe)_{21}S_{15}$.

Mit dieser Bruttoformel ergibt sich die Röntgendichte zu 5,73 g.cm.$^{-3}$.

Wir danken Herrn Prof. Dr. A. Schüller für die Anregung zu dieser Arbeit sowie für die Überlassung des Materials. Ein grosser Teil der Rechenarbeiten wurde von Frau Lindow ausgeführt.

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Laves Phase Compounds of Rare Earths and of Hafnium with Noble Metals

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The compounds $ScIr_2$, YAl_2, YRh_2, YIr_2, YPt_2, $LaRu_2$, $LaRh_2$, $LaOs_2$, $LaIr_2$, $LaPt_2$, $CeRu_2$, $CeRh_2$, $CeOs_2$, $CeIr_2$, $PrRu_2$, $PrRh_2$, $PrOs_2$, $PrIr_2$, $PrPt_2$, $NdRu_2$, $NdRh_2$, $NdIr_2$, $NdPt_2$, $GdRh_2$, $GdIr_2$, and $GdPt_2$ are cubic Laves phases, $MgCu_2$ structure (*C*15). The space group is O_h^7–$Fd3m$ with 8 formula weights in the unit cell. Lattice constants for these compounds are reported.

The compounds $HfRe_2$, $HfOs_2$, $ScRu_2$, $ScOs_2$, YRu_2, YRe_2, YOs_2, $PrOs_2$, $NdOs_2$, $SmOs_2$, $GdRu_2$, $GdOs_2$, $ErRu_2$, $LuRu_2$, and $LuOs_2$ are hexagonal Laves phases, $MgZn_2$ structure (*C*14). The space group is D_{6h}^4–$P6_3/mmc$ with 4 formula weights in the unit cell. Lattice constants are reported. Both the cubic and hexagonal Laves phases were determined by the powder diffraction method.

The superconducting transition temperatures for $ScRu_2$, $ScOs_2$, $ScIr_2$, YRu_2, YRe_2, YOs_2, YIr_2, YPt_2, $LaRu_2$, $LaOs_2$, $CeRu_2$, $LuOs_2$, $HfRe_2$ and $HfOs_2$ are reported. Ferromagnetic transition temperatures are given for the praseodymium, neodymium and gadolinium compounds and for $SmOs_2$.

The investigation of superconductivity and ferromagnetism in Laves phase compounds has continued (Matthias & Corenzwit, 1957; Matthias & Bozorth, 1958) and new compounds of rare earths and of hafnium with noble metals have been prepared. These are $ScRu_2$, $ScOs_2$, $ScIr_2$, YRu_2, YRh_2, YRe_2, YOs_2, YIr_2, YPt_2, $LaRu_2$, $LaRh_2$, $LaOs_2$, $LaIr_2$, $LaPt_2$, $CeRu_2$, $CeRh_2$, $CeOs_2$, $CeIr_2$, $PrRu_2$, $PrRh_2$, $PrOs_2$, $PrIr_2$, $PrPt_2$, $NdRu_2$, $NdRh_2$, $NdOs_2$, $NdIr_2$, $NdPt_2$, $SmOs_2$, $GdRu_2$, $GdRh_2$, $GdOs_2$, $GdIr_2$, $GdPt_2$, $ErRu_2$, $LuRu_2$, and $LuOs_2$. A YAl_2 compound was also prepared. The hafnium compounds include $HfRe_2$ and $HfOs_2$. The superconductivity and ferromagnetism of the ruthenium compounds of Sc, Y, La, Ce, Pr, Nd and Er is discussed in the paper by Matthias, Suhl & Corenzwit (1958).

All the compounds except $SmOs_2$ were prepared by heating stoichiometric amounts of the elements in an arc furnace in a helium or argon atmosphere. The $SmOs_2$ compound was prepared by powder metallurgy. X-ray diffraction powder photographs were taken of the resulting product using a Norelco camera of 114·6 mm. diameter and Cu *K*-radiation unless otherwise noted.

In most cases the reaction product was pure. The patterns of the ruthenium and osmium compounds include lines from these elements. Some of the patterns also indicate the presence of the rare earth oxide or nitride.

Relative intensities for each of the compounds were calculated by means of the expression:

$$I \propto p|F_{hkl}|^2(1+\cos^2 2\theta)/(\sin^2\theta\cos\theta)$$

where p is the multiplicity factor, $F(hkl)$ is the structure amplitude and the remaining term is twice the Lorentz and polarization factor. The scattering factors for all the elements except those for scandium and aluminum were obtained from the paper by Thomas & Umeda (1957). The factors for scandium were taken from the *International Tables* (1935) and for aluminum from the paper by Viervoll & Øgrim (1949). Dispersion corrections from Dauben & Templeton (1955) were applied.

Cubic Laves phase compounds

The X-ray powder diffraction patterns of $ScIr_2$, YAl_2, YRh_2, YIr_2, YPt_2, $LaRu_2$, $LaRh_2$, $LaOs_2$, $LaIr_2$, $LaPt_2$, $CeRu_2$, $CeRh_2$, $CeOs_2$, $CeIr_2$, $PrRu_2$, $PrRh_2$, $PrOs_2$, $PrIr_2$, $PrPt_2$, $NdRu_2$, $NdRh_2$, $NdIr_2$, $NdPt_2$, $GdRh_2$, $GdIr_2$, and $GdPt_2$, were indexed on a cubic lattice.* The lattice constants and superconducting or ferromagnetic transition temperatures are given in Table 1. The approximate densities of $LaIr_2$ and YPt_2 were determined by the pycnometric method and from these, the number of formula weights per unit cell was calculated to be 7·9, ~ 8. The YPt_2 compound contained 17·39 wt.% yttrium which corresponds to $Y_{0\cdot92}Pt_2$. The powder patterns are all very similar to that of $CaRh_2$ previously determined as the $MgCu_2$ (*C*15 type) structure by Wood & Compton (1958).

Table 1. *Lattice constants, interatomic distances, and transition temperatures for cubic Laves phases*

Compound	a_0 (Å) (±0·001 Å)	Interatomic distances (Å) *A–A*	*B–B*	*A–B*	Transition temperature (°K.)
$ScIr_2$	7·348	3·182	2·598	3·046	1·03 sc.
YAl_2	7·860	3·403	2·778	3·259	—
YRh_2	7·459	3·230	2·637	3·092	—
YIr_2	7·500*	3·248	2·651	3·110	2·18 sc.
YPt_2	7·590	3·286	2·683	3·147	1·57 sc.
$LaRu_2$	7·702	3·335	2·723	3·193	1·63 sc.
$LaRh_2$	7·646	3·311	2·703	3·170	—
$LaOs_2$	7·737	3·350	2·735	3·208	6·5 sc.
$LaIr_2$	7·686	3·328	2·717	3·187	—
$LaPt_2$	7·774†	3·366	2·748	3·223	—
$CeRu_2$	7·535	3·263	2·664	3·124	4·9 sc.
$CeRh_2$	7·538	3·264	2·665	3·125	—
$CeOs_2$	7·593	3·288	2·684	3·148	—
$CeIr_2$	7·571	3·278	2·676	3·139	—
$PrRu_2$	7·624	3·301	2·695	3·161	40 fm.
$PrRh_2$	7·575	3·280	2·678	3·140	8·6 fm.
$PrOs_2$	7·663	3·318	2·709	3·177	>35 fm‡
$PrIr_2$	7·621	3·300	2·694	3·160	18·5 fm.
$PrPt_2$	7·709	3·338	2·725	3·196	7·9 fm.
$NdRu_2$	7·614	3·297	2·692	3·157	35 fm.
$NdRh_2$	7·564	3·275	2·674	3·136	8·1 fm.
$NdIr_2$	7·605	3·293	2·688	3·153	11·8 fm.
$NdPt_2$	7·694	3·332	2·720	3·190	6·7 fm.
$GdRh_2$	7·514	3·254	2·656	3·115	>77 fm.
$GdIr_2$	7·550	3·269	2·669	3·130	>77 fm.
$GdPt_2$	7·637	3·307	2·700	3·166	>77 fm.

* Lattice constant ranged from 7·500 to 7·520 Å in a single melt.

† Lattice constant ranged from 7·763 to 7·774 Å in a single melt.

‡ Melt also contained hexagonal Laves phase.

sc. = superconducting.

fm. = ferromagnetic.

This structure belongs to space group O_h^7–$Fd3m$ and the unit cell contains twenty-four atoms. The formula is AB_2 in which the $8A$ atoms occupy position (*a*): $0, 0, 0$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; f.c. and the $16B$ atoms are in position (*d*): $\frac{5}{8}, \frac{5}{8}, \frac{5}{8}$; $\frac{5}{8}, \frac{7}{8}, \frac{7}{8}$; $\frac{7}{8}, \frac{5}{8}, \frac{7}{8}$; $\frac{7}{8}, \frac{7}{8}, \frac{5}{8}$; f.c. The $MgCu_2$ structure determined by Friauf (1927*a*) has been described by Laves (1939, 1956), and by Schulze (1939). Each *A* atom is coordinated to four *A* atoms at $0\cdot4330a_0$ and to twelve *B* atoms at $0\cdot4146a_0$. Each *B* atom is coordinated to six *B* atoms at $0\cdot3535a_0$ and to six *A* atoms at $0\cdot4146a_0$. The calculated interatomic distances are given in Table 1.

Relative intensities for each of the compounds were calculated on the basis of this structure and results for $CeIr_2$ are given in Table 2, together with visually estimated intensities. The low intensity of the low angle lines is probably due to absorption. The good agreement between the observed and calculated intensities confirmed the $MgCu_2$ structure for these compounds.

In the case of the $LaPt_2$ a discrepancy between calculated and observed intensities was noted. The observed intensity of reflections due to scattering from the lanthanum atoms alone, that is, the {220}, {422}, {620}, {642}, {660}, {822}, and {664} reflections were considerably weaker than the calculated values. The Norelco diffractometer was used to obtain a quantitative measurement of the intensities. The intensity data are given in Table 3 together with the structure factor expressions. Chemical analysis of a sample gave 25·03 wt.% lanthanum which corresponds to $La_{0\cdot95}Pt_2$ The lattice constant ranged from 7·763 to 7·774 Å. A satisfactory explanation of the discrepancy between the intensities cannot be offered at this time.

The $PrOs_2$ melt contains both the cubic and hexagonal Laves phases. The data for the hexagonal form is given in Table 4.

Hexagonal Laves phase compounds

The X-ray powder diffraction patterns of $HfRe_2$, $HfOs_2$, $ScRu_2$, $ScOs_2$, YRu_2, YRe_2, YOs_2, $PrOs_2$, $NdOs_2$, $SmOs_2$, $GdRu_2$, $GdOs_2$, $ErRu_2$, $LuRu_2$, and $LuOs_2$ taken with Cr *K*-radiation were indexed on a hexagonal lattice using the Bond chart (Azároff & Buerger, 1958). The lattice constants, and transition

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* The result for $LaOs_2$ is due to Dr W. H. Zachariasen.

Table 2. *Comparison of calculated with observed intensities, visually estimated*

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

Cubic Laves phase

Indices *hkl*	$CeIr_2$ *d* (Å)	Relative intensity obs.	Relative intensity calc.
111	4·311	*w*	169
220	2·660	*w–m*	189
311	2·270	*vs*	1000
222	2·176	*s*	502
400	1·888	*w–m*	96
331	1·734	*w*	42
422	1·540	*w–m*	68
511, 333	1·473	*s*	318
440	1·336	*s*	289
531	1·276	*w–m**	30
620	1·194	*vw*	29
533	1·153	*m*	113
622	1·139	*m–s*	189
444	1·090	*w–m**	23
551, 711	1·059	*vw*	19
642	1·011	*w*	41
553, 731	0·9845	*s*	253
800	0·9454	*w–m*	67
733	0·9249	n.obs.	8
660, 822	0·8918	*w*	31
555, 751	0·8735	*s*	216
662	0·8681	*m–s*	163
840	0·8458	*m*	74
753, 911	0·8304	*w–m*	35
664	0·8066	*m–s**	33
931	0·7936	*vs*	357

Hexagonal Laves phase

Indices *hk·l*	$GdOs_2$ *d* (Å)	Relative intensity obs.	Relative intensity calc.
10·0	4·575	*vw*	207
00·2	4·374	*vvw*	98
10·1	4·040	*vvw*	79
11·0	2·651	*w*	175
10·3	2·477	*s*	566
20·0	2·301	*vvw*	85
11·2	2·277	*vs*	1000
20·1	2·227	*vs*	969
00·4	2·208	*m*	273
20·2	2·038	*m–s*	323
10·4	1·990	*w–m*	164
20·3	1·812	*w–m*	123
21·0	1·742	*vw*	32
30·0	1·539	*vw*	29
21·3	1·499	*m*	221
00·6	1·472	*w**	39
30·2	1·452	*m*	228
10·6	1·401	*m–s*	22
20·5			313
21·4	1·367	*m*†	95
22·0	1·330	*m–s*	276
11·6	1·287	*vvw*	21
31·0	1·274	*vvw*	12
22·2			19
20·6	1·241	*w–m*	137
10·7	1·218	*vvw*	26
31·3	1·174	*w–m*	95

* β line coincident. † Os line coincident.

$GdOs_2$—To conserve space, calculated intensities below 1·3 are omitted.

n. obs. = not observed.

Table 3. *Comparison of calculated with observed intensities of* $LaPt_2$

hkl	Calc.	Obs.	$\|F\|^2$
111	163	167	*a*
220	184	100	*b*
311	1000	785	*c*
222	497	458	*d*
400	97	142	*e*
331	40	79	*a*
422	70	42	*b*
511, 333	324	330	*c*
440	294	276	*f*
531	30	109	*a*
620	30	n. obs.	*b*
533	116	127	*c*
622	193	239	*d*
444	23	64	*e*
551, 711	18	54	*a*
642	40	n. obs.	*b*
553, 731	248	248	*c*
800	65	58	*f*
733	8	n. obs.	*a*
660, 822	29	n. obs.	*b*
555, 751	198	251	*c*
662	146	176	*d*
840	62	158	*e*
753, 911	28	79	*a*
664	27	n. obs.	*b*
931	254	221	*c*
844	562	585	*f*

a. $|F|^2 = 2(4f_{La} - 5{\cdot}656f_{Pt})^2$.
b. $|F|^2 = (8f_{La})^2$.
c. $|F|^2 = 2(4f_{La} + 5{\cdot}656f_{Pt})^2$.
d. $|F|^2 = (16f_{Pt})^2$.
e. $|F|^2 = (8f_{La} - 16f_{Pt})^2$.
f. $|F|^2 = (8f_{La} + 16f_{Pt})^2$.

temperatures are given in Table 4. Pycnometric densities of YOs_2 and $ScRu_2$ indicated that the unit cell contains four formula weights. The $ScRu_2$ compound contained 20·93 wt.% scandium which corresponds to $Sc_{1.2}Ru_2$. The powder patterns are very similar to those of $ZrOs_2$ and $ZrRe_2$ which have been identified by Wallbaum (1942) as hexagonal Laves phases with the $MgZn_2$ (*C*14 type) structure.

The space group for this structure is D_{6h}^4–$P6_3/mmc$ with twelve atoms per unit cell. The atoms are located as follows:

4*A* in (*f*): $\frac{1}{3}, \frac{2}{3}, z;\ \frac{2}{3}, \frac{1}{3}, \bar{z};\ \frac{2}{3}, \frac{1}{3}, \frac{1}{2}+z;\ \frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z;$
$z = \frac{1}{16}$.
2*B* in (*a*): $0, 0, 0;\ 0, 0, \frac{1}{2}$.
6*B* in (*h*): $x, 2x, \frac{1}{4};\ 2\bar{x}, \bar{x}, \frac{1}{4};\ x, \bar{x}, \frac{1}{4};\ \bar{x}, 2\bar{x}, \frac{3}{4};$
$2x, x, \frac{3}{4};\ \bar{x}, x, \frac{3}{4};\ x = -\frac{1}{16}$.

The $MgZn_2$ structure was determined by Friauf (1927*b*) and has been described by Laves & Löhberg (1934). Each *A* atom is coordinated to one *A* atom at the distance $(A\text{–}A)_1$ and to three *A* atoms at the distance $(A\text{–}A)_2$. Each *B* atom of the first kind (at $0, 0, 0$; $0, 0, \frac{1}{2}$) is coordinated to six *B* atoms of the second kind at the distance $(B\text{–}B)_2$ while each *B* atom of the second kind is coordinated to two *B* atoms of the same kind at the distance $(B\text{–}B)_1$. Each *A* atom is sur-

Table 4. *Lattice constants, interatomic distances and transition temperatures of hexagonal Laves phases*

	Lattice constants										
Compound	a_0 (Å) ($\pm$0·002)	c_0 (Å) ($\pm$0·002)	Axial ratio c/a	P* $(A\text{–}A)_1$ (Å)	Q $(A\text{–}A)_2$ (Å)	$D\text{–}D$ $(B\text{–}B)_1$ (Å)	$C\text{–}D$ $(B\text{–}B)_2$ (Å)	$M\text{–}C$ $(A\text{–}B)_1$ (Å)	$M\text{–}D$ $(A\text{–}B)_2$ (Å)	$M\text{–}D$ $(A\text{–}B)_3$ (Å)	Transition temperature (°K.)
$HfRe_2$	5·239	8·584	1·638	3·219	3·209	2·620	2·625	3·072	3·075	3·080	4·8 sc.
$HfOs_2$	5·184	8·468	1·633	3·176	3·174	2·592	2·592	3·039	3·040	3·040	2·69 sc.
$ScRu_2$	5·119	8·542	1·669	3·203	3·143	2·560	2·597	3·003	3·020	3·052	1·67 sc.
$ScOs_2$	5·179	8·484	1·638	3·182	3·172	2·590	2·595	3·037	3·040	3·044	4·6 sc.
YRu_2	5·256	8·792	1·673	3·297	3·227	2·628	2·670	3·084	3·103	3·139	1·52 sc.
YRe_2	5·396	8·819	1·634	3·307	3·305	2·698	2·699	3·164	3·165	3·166	1·83 sc.
YOs_2	5·307	8·786	1·656	3·295	3·255	2·654	2·678	3·113	3·124	3·144	4·7 sc.
$PrOs_2$	5·368	8·945	1·666	3·354	3·295	2·684	2·720	3·149	3·165	3·196	>35 fm.
$NdOs_2$	5·368	8·926	1·663	3·347	3·294	2·684	2·717	3·149	3·164	3·191	27·5 fm.
$SmOs_2$	5·336	8·879	1·664	3·330	3·275	2·668	2·702	3·130	3·145	3·174	34 fm.†
$GdRu_2$	5·271	8·904	1·689	3·339	3·240	2·636	2·696	3·094	3·120	3·172	>77 fm.
$GdOs_2$	5·319	8·838	1·662	3·314	3·264	2·660	2·690	3·120	3·134	3·160	>77 fm.
$ErRu_2$	5·227	8·780	1·680	3·292.	3·211	2·614	2·663	3·067	3·089	3·132	13 fm.
$LuRu_2$	5·204	8·725	1·676	3·272	3·196	2·602	2·648	3·054	3·074	3·114	—
$LuOs_2$	5·254	8·661	1·648	3·248	3·221	2·627	2·643	3·081	3·089	3·103	3·49 sc.

* Notation used by Berry & Raynor (1953).

† Transition temperature measured by R. M. Bozorth.

rounded by three B atoms of the first kind at $(A\text{–}B)_1$ and nine of the second kind. The calculated interatomic distances are given in Table 4.

Relative intensities for each of the compounds were computed on the basis of this structure and results for $GdOs_2$ are given in Table 2. The low value for the observed intensities for reflections at low angles is probably due to absorption. The observed intensities were estimated visually from powder patterns taken with Cu K-radiation. The good agreement between calculated and observed intensities indicated that the $MgZn_2$ structure is correct.

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