Table 2. *New structure types*

α-VIr

Orthorhombic, space group $Cmmm\,(D_{2h}^{19})$; $N=8$ atoms per cell.

V in $4(g)\pm(x, 0, 0)$; $x\sim 0{\cdot}28$;
Ir in $4(j)\pm(0, y, \frac{1}{2})$; $y\sim 0{\cdot}22$.

β-Ta(Pd, Rh)$_3$

Rhombohedral, space group $R\bar{3}m\,(D_{3d}^{5})$; $N=36$ atoms per hexagonal cell; stacking sequence: *ababcbcac*, *ababcbcac*.

Ta in $3(a)$ $(0, 0, 0)$;
$6(c)\pm(0, 0, z)$; $z_c\sim\frac{2}{9}$;
$Pd_{0\cdot72}Rh_{0\cdot28}$ in $9(e)$ $(\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ \frac{1}{2}, \frac{1}{2}, 0)$;
$18(h)\pm(x, \bar{x}, z;\ x, 2x, z;\ 2\bar{x}, \bar{x}, z)$;
$x\sim\frac{1}{2}$; $z_h\sim\frac{2}{9}$.

γ-Ta(Pd, Rh)$_3$

Hexagonal, space group $P6_3/mmc\,(D_{6h}^{4})$; $N=40$ atoms per unit cell; stacking sequence: *abcbcacbcb*, *abcbcacbcb*.

Ta in $2(b)\pm(0, 0, \frac{1}{4})$;
$2\times4(f)\pm(\frac{1}{3}, \frac{2}{3}, z;\ \frac{2}{3}, \frac{1}{3}, \frac{1}{2}+z)$; $z_{f_1}\sim\frac{3}{20}$;
$z_{f_2}\sim-\frac{1}{20}$;
$Pd_{0\cdot67}Rh_{0\cdot33}$ in $6(h)\pm(x, 2x, \frac{1}{4};\ 2\bar{x}, \bar{x}, \frac{1}{4};\ x, \bar{x}, \frac{1}{4})$; $x_h\sim\frac{1}{2}$;
$2\times12(k)\pm(x, 2x, z;\ 2\bar{x}, \bar{x}, z;\ x, \bar{x}, z;$
$\bar{x}, 2\bar{x}, \frac{1}{2}+z;\ 2x, x, \frac{1}{2}+z;\ \bar{x}, x, \frac{1}{2}+z)$;
$x_{k_1}\sim-\frac{1}{6}$; $z_{k_1}\sim\frac{3}{20}$;
$x_{k_2}\sim\frac{1}{6}$; $z_{k_2}\sim-\frac{1}{20}$.

ing lines. Error limits are $<5{\cdot}10^{-4}$, except for β-TaNi$_3$ and Ta(Pd$_{0.67}$Rh$_{0.33}$)$_3$, where they are $2{\cdot}10^{-3}$, and $1{\cdot}10^{-3}$, respectively. Table 1 lists the new intermediate phases, including again a layer structure symbol as introduced previously (Giessen & Grant, 1964). Table 2 presents three new structure types.

In addition to the phases listed in Table 1, ordered WIr$_3$ of the MgCd$_3$ type probably exists, but this could not be proved conclusively owing to the similar scattering powders of W and Ir. The structure of α-VIr is related to $B2$-CsCl by a distortion of the atom positions and approximate doubling of two $B2$-cell edges. Most of the ternary AB$_3$ phases of the types Ta(Pd$_x$,Rh$_{1-x}$)$_3$ and Ta(Pd$_x$,Ru$_{1-x}$)$_3$ are related in such a fashion that a similar valence electron concentration in both series causes identical structures to appear; in this context the occurrence of Ta(Pd$_{0.5}$Ru$_{0.5}$)$_3$ with the $L1_2$-AuCu$_3$ structure of TaRh$_3$ is remarkable. The significance of the valence electron concentration in relation to the structure type is also borne out by the occurrence of (Ta$_{0.5}$Al$_{0.5}$)Ni$_3$ with the TiNi$_3$ structure, where equal parts of Ta and Al substitute for Ti.

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MX$_4$ compounds of alkaline earth metals with IIIB group elements.

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In the course of a study on the equilibrium diagrams of alkaline earth metals with the elements of the IIIB group of the periodic system, intermediate phases of the type MX$_4$ have been found in the systems Ca–Ga, Sr–Ga, Ba–Ga, Ba–In, Ba–Tl.

The gallium alloys were prepared by fusion under argon atmosphere in Phytagoras and those of indium and thallium in sealed iron crucibles. The chemical analysis showed that the compositions of the specimens were in agreement (±1 %) with the stoichiometric values. The (Ca, Sr, Ba)Ga$_4$ compounds are grey and brittle; BaIn$_4$ and BaTl$_4$ are white and rather soft. These MX$_4$ phases, except BaTl$_4$ (whose different structure type was not determined), show the tetragonal $D1_3$ structure type ($I4/mmm-D_{4h}^{17}$) known so far for aluminum compounds (Andress & Alberti, 1935; Nowotny & Wesenberg, 1939; Nowotny, Wormnes & Mohrnheim, 1940, 1942). The atomic positions are: $[0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}]+$: $2M(0,0,0)$; $4X'\pm(0,0,z)$; $4X''(0,\frac{1}{2},\frac{1}{4})(\frac{1}{2},0,\frac{1}{4})$; (M = alkaline earth atom). The unit cell is shown in Fig. 1.

The powder patterns obtained with the Straumanis method using copper $K\alpha$ radiation gave the values of the lattice constants recorded in Table 1. The best agreement of the observed intensities with those calculated for z between

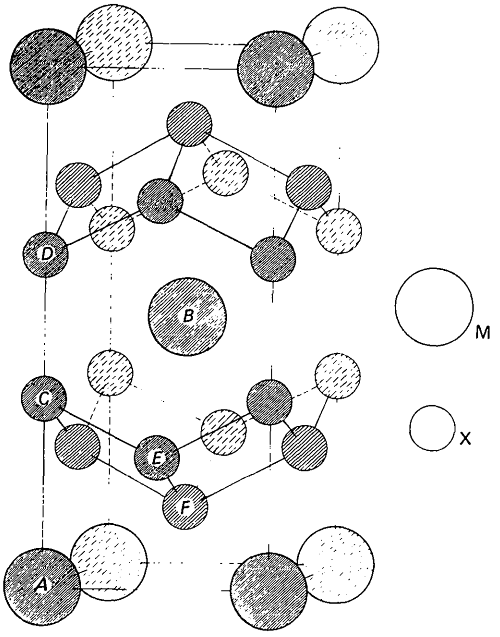

Fig. 1. Unit cell of MX$_4$ (M = Ca, Sr, or Ba; X = Ga, In or Tl).

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Table 1. *Lattice constants and interatomic distances* (Å) *for the compounds examined having the* $D1_3$ *structure type*

Compound	a_0	c_0	c/a	z	d_{AC}	d_{BC}	$d_{AE}=d_{BE}$	d_{CD}	d_{CE}	$R_m^{[12]}+R_x^{[8]}$
$CaGa_4$	4·370	10·65	2·44	0·379	4·04	3·35	3·44	2·58	2·58	3·33
$SrGa_4$	4·437	10·70	2·41	0·378	4·05	3·40	3·48	2·61	2·61	3·48
$BaGa_4$	4·560	10·81	2·37	0·377	4·08	3·49	3·53	2·66	2·66	3·56
$BaIn_4$	4·930	11·90	2·41	0·382	4·55	3·76	3·86	2·81	2·92	3·74

0·775 and 0·785 was found for the values shown in Table 1. The z parameters for the gallium compounds correspond to the relation $d_{CD}=d_{CE}$ (Fig. 1); while for $BaIn_4$ the best z value is somewhat greater (0·382) than the one corresponding to this condition (0·378). Table 1 also contains the interatomic distances, following the letters marked in Fig.1.

It is worth pointing out the high coordination around the larger atoms of the lattice may contribute to the stability of this structure. In fact, each alkaline earth atom (M) is surrounded by 18 atoms of other element (X): it has 8 nearest neighbours, 8 others are somewhat farther removed, and 2 are at a still greater distance. The X atoms are of two different types: one type is in contact with 5 X atoms and with 4 atoms of the alkaline earth element; the other is in contact with 4 X atoms and 4 alkaline earth atoms.

If we consider the isomorphous compounds of the alkaline earth metals Ca, Sr and Ba, the influence of the 'size factor' in the formation of this structure can be evaluated from the ratio of the atomic radii R_m and R_x. Quantitative information obtained from a comparison of the atomic radii R_m and R_x taken by Laves (1956) (see the last column of Table 1) can only be approximate, because proper corrections of the atomic sizes for the effective coordination number would have to be made.

Table 2. *Values of the ratio* R_m/R_x (M = Ca, Sr, Ba; X = Al, Ga, In, Tl)

Only group (*A*) corresponds to the existence of the $D1_3$ structure type

Ba/Ga	1·62	(*A*)	Sr/In	1·35	(*B*)
Ba/Al	1·57		Ba/Tl	1·31	
Sr/Ga	1·56		Sr/Tl	1·27	
Sr/Al	1·51		Ca/In	1·25	
Ca/Ga	1·45		Ca/Tl	1·17	
Ba/In	1·42				
Ca/Al	1·41				

However, the sequence of the values of the atomic radii ratio R_m/R_x reported in decreasing order in Table 2 shows the existence of the MX_4 phase having the $D1_3$ structure type only when $R_m/R_x \geq 1{\cdot}4$.

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Crystal structures of some equi-atomic gadolinium compounds*.

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In a program dealing with the properties of 4*f* and 5*f* transition metals and alloys a number of equi-atomic alloys of gadolinium were prepared; specifically, they were GdAl, GdCu, GdRh, GdAg and GdAu. At the time this work was initiated the crystal structures of GdAl (Baenziger & Moriarty, 1961), GdCu (Dwight, 1959*a*; Baenziger & Moriarty, 1961) and GdAg (Dwight, 1959*b*; Iandelli, 1960; Baenziger & Moriarty, 1961) had been reported in the literature. Since then data have also been published for GdAu (Chao, Luo & Duwez, 1963). The results obtained in this study are in reasonable agreement with the previously published data, except for GdAl.

The alloys were prepared by arc-melting together weighed amounts of the two components. X-ray samples taken from the arc-cast buttons were sealed in evacuated Pyrex capillary tubes and heat treated for 15 min at 500 °C and then water quenched. The X-ray pattern of the GdRh sample obtained in this manner was quite poor. A second heat treatment of 15 min at 550 °C, however, was sufficient to provide sharp back-reflection doublets. The powder patterns were taken by using a 114·59 mm diameter Debye–Scherrer camera and filtered copper radiation. The lattice constants for the b.c.c., CsCl type compounds of GdCu, GdRh and GdAg were calculated from $K\alpha_1$ and $K\alpha_2$ doublets in the back-reflection region by using a φ tan φ extrapolation method. For GdAl and GdAu the lattice constants were obtained by the Nelson–Riley extrapolation method.

The X-ray patterns of GdCu, GdRh and GdAg were easily indexed as b.c.c., CsCl, *B*2 type compounds and contained no extra lines. The lattice parameters of these compounds, which were corrected for refraction, are summarized in Table 1. The powder patterns of GdAl and GdAu were quite complex, which is in agreement with previous data. In the case of GdAl the lines for the b.c.c. phase reported by Baenziger & Moriarty (1961) could not be identified in the powder pattern. For GdAu, however, it was possible to identify most of the b.c.c., CsCl type lines in the complex pattern, which is in accord with the results of Chao, Luo & Duwez (1963). The non-cubic phase in both the GdAl and GdAu powder patterns was indexed as having an orthorhombic structure. These results are discussed below and the lattice parameters are summarized in Table 1.

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