

Table 1. *Lattice constants and interatomic distances (Å) for the compounds examined having the D1₃ 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 BaIn₄ 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.

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Crystal structures of some equi-atomic gadolinium compounds*. By KARL A. GSCHNEIDNER, JR, † *University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.*

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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

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† Present address: Department of Metallurgy and Institute for Atomic Research, Iowa State University, Ames, Iowa, U.S.A.

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 D1₃ 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 MX₄ phase having the D1₃ structure type only when $R_m/R_x \geq 1.4$.

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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 $\phi \tan \phi$ 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, B2 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.

Table 1. *Lattice parameters and structural data for some GdM compounds, where M is Al, Cu, Rh, Ag or Au*

Compound	Lattice constant	Structure type	Reference
GdAl	$a = 3.7208 \pm 0.0002 \text{ \AA}$	CsCl + 2nd phase	(a)
GdAl	$a = 9.274 \pm 0.007$ $b = 7.679 \pm 0.008$ $c = 5.584 \pm 0.003$	CeAl	This paper
GdCu	$a = 3.505$	CsCl	(b)
GdCu	$a = 3.503 \pm 0.001$	CsCl	(a)
GdCu	$a = 3.5020 \pm 0.0004$	CsCl	This paper
GdRh	$a = 3.4425 \pm 0.0006$	CsCl	This paper
GdAg	$a = 3.66$	CsCl	(c)
GdAg	$a = 3.653$	CsCl	(d)
GdAg	$a = 3.6476 \pm 0.0008$	CsCl	(a)
GdAg	$a = 3.6491 \pm 0.0002$	CsCl	This paper
GdAu	$a = 3.593 \pm 0.002$	CsCl + 2nd phase	(e)
GdAu	$a = 3.6009 \pm 0.0008$ $a = 4.522 \pm 0.005$ $b = 10.826 \pm 0.008$ $c = 4.734 \pm 0.004$	CsCl and CrB	This paper This paper

(a) Baenziger & Moriarty (1961). (b) Dwight (1959a). (c) Dwight (1959b). (d) Iandelli (1960). (e) Chao, Luo & Duwez (1963).

Examination of the published literature indicates that the rare earth-aluminum compounds, RAl, crystallize with either b.c.c., CsCl type or one of two different orthorhombic structures, *i.e.* CeAl type, which belongs to the space group $Cmc2_1$ (van Vucht, 1957) or CrB type found for YAl (Dagerhamn, 1963). All the lines in the GdAl powder pattern could be indexed on the basis of the CeAl type orthorhombic structure. Although Baenziger & Moriarty (1961) found some b.c.c. lines in their complex X-ray pattern for GdAl while none were found in this research, this does not necessarily indicate that one of the results is incorrect. The difference could be explained by the existence of a high-temperature b.c.c. phase retained upon quenching by Baenziger & Moriarty (1961) but not retained in this research because of either too slow a cooling rate during quenching or too low an annealing temperature, *i.e.* below the orthorhombic \rightleftharpoons b.c.c. transition temperature.

Chao, Luo & Duwez (1963) found that when GdAu was very rapidly quenched, only the b.c.c. lines were observed, but when this compound was slowly cooled both the complex and b.c.c. lines were obtained. No other literature data

are available concerning the structures of the complex phase of any of the rare-earth-gold equi-atomic compounds. All the lines, other than those which were indexed as b.c.c., CsCl type, could be indexed as orthorhombic CrB, B_f type.

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Infinite slit height corrections in small angle X-ray scattering*. By B. CHU and D. M. TAN CRETU, *Chemistry Department, The University of Kansas, Lawrence, Kansas, U.S.A.*

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The problem of correcting for the effect of beam height on scattering curves, which will be referred to as 'unsmearing' (Entschmierung), has been considered by many authors (Guinier & Fournet, 1947a, b, 1955; DuMond, 1947; Shull & Roess, 1947; Yudowitch, 1949; Franklin, 1950; Kratky, Porod & Kahovek, 1951; Schmidt, 1955; Gerold, 1957; Kratky, Porod & Skala, 1960; Schmidt & Hight, 1960; Heine & Roppert, 1962; Heine, 1963; Kent & Brumberger, 1964; Rausell-Colom, 1963). However, numerical calculations are tedious without the aid of a computer and col-

limation correction has often become a time-consuming obstacle for beginners in small-angle X-ray scattering work. It is therefore of interest to point out the simplicity of Schmidt's method (Schmidt & Hight, 1960) which has the advantage of eliminating the need for numerical differentiation or functional fitting of the experimental curve. Furthermore, for an infinitely long and negligibly wide primary beam, his approximate method is applicable to all slit collimated cameras provided that the requirement for infinite slit height approximation is satisfied.

For slits of negligible width and infinite height, the experimental scattered intensity $F(h)$ for a scattering angle h is related to the perfect collimation scattered intensity $I(h)$

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