Reprinted from Acta Crystallographica, Vol. 18, Part 6 June 1965

PRINTED IN DENMARK

LAP ALAMOS

AUG 21 1965

1- gadolinium 2- rare earths 3- metals

## Acta Cryst. (1965). 18, 1082

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.

## (Received 17 November 1964)

In a program dealing with the properties of 4f and 5f 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, 1959a; Baenziger & Moriarty, 1961) and GdAg (Dwight, 1959b; 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

\* Work performed under the auspices of the U.S. Atomic Energy Commission.

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