

TABLE 2. CRYSTAL PROPERTIES OF THE RARE-EARTH ALUMINUM GARNETS

Sample	Color	Lattice parameter Å	Calculated x -ray density g/cm ³	Index of refraction ²
TbAlG	Colorless			
	Pale yellow ¹	12.074	6.063	1.87 ₂
DyAlG	Pale yellow	12.042	6.193	1.86 ₇
HoAlG	Golden yellow	12.011	6.297	1.85 ₈
ErAlG	Pink	11.981	6.397	1.85 ₇
TmAlG	Pale green	11.957	6.476	1.85 ₅

¹ The pale yellow color exhibited by some samples might be due to lead impurities from the flux in which the crystal was grown.

² Sodium D ($\lambda = 5890$ Å).

x -ray density and index of refraction are also given in Table 2. The index of refraction was determined by means of the Becke line method. An estimate of the probable error for the index is ± 0.002 . All these materials exhibit conchoidal fracture.

The ErAlG lattice parameter agrees with the value 11.98 Å determined by Bertaut and Forrat (1956), but our value for DyAlG differs significantly from their value of 12.06 Å. Unfortunately, no other powder data have been reported, so further comparisons are not possible.

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DERIVING THE FORMULA OF A MINERAL FROM ITS CHEMICAL ANALYSIS

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Hey (1939, 1954) has carefully analyzed the problem of presenting the chemical analysis of minerals. He recommends using the experimentally determined density and cell dimensions, whenever possible, to convert chemical analysis to chemical formula. For the special case of minerals

whose essential crystal structure is *known*, an alternate procedure presents itself, which was not considered by Hey: *the use of the total number of atomic sites per cell*, as found in the structure determination, divided by *Z*, the number of formula units per cell, if desired. This procedure carries the assumption that both omission and addition solid solutions are absent. It has been found advantageous for minerals such as tourmalines, where substitution is so abundant that one should not assume any one crystallographic position to be free of it. The assumption made is, of course, checked in the end, when the observed density is compared with the calculated density, which is based on the derived formula and the cell dimensions. Hey's recommended procedure does not permit this comparison of densities, and although in theory it is just as good to compare the calculated number of atoms per cell with the number required by the structure, in practice this is less satisfactory. The density comparison has become so standard that data compilations such as *Crystal Data* (Donnay, 1963) devote a column to each density. In addition, and more important, the errors inherent in density and cell-dimension determinations, as discussed by Hey (1939, p. 403), are kept out of the formula.

The advantages that this procedure may have for many minerals over the procedures that assume a constant number of certain cations or anions are the following. There is no need to decide each time which elements should be used as the basis of computation. No assumption concerning the formula is "built in" when the formula is derived. The percent error in the conversion factor is minimized by the proposed procedure.

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DISCUSSION OF "PYRRHOTITE MEASUREMENT" BY GROVES AND
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Much interest has been shown in the use of pyrrhotite (Fe_{1-x}S) for geothermometry as described by Arnold (1962) and Arnold and Reichen