THE AMERICAN MINERALOGIST, VOL. 49, SEPTEMBER-OCTOBER, 1964

CRYSTALLOGRAPHIC DATA FOR RARE-EARTH ALUMINUM GARNETS

C. B. RUBINSTEIN AND R. L. BARNS, *Bell Telephone Laboratories, Inc., Murray Hill, New Jersey.*

The rare-earth aluminum garnets may be represented by the general formula $R_3Al_2Al_3O_{12}$, in which R represents the rare-earth ion. This note presents the indexed x-ray powder data and indices of refraction for

Table 1. X-Ray Powder Data for Rare Earth Aluminum Garnets, CuKα (λ = 1.5418Å) Radiation.

		TbAlG		DyAlG		HoAlG		ErAlG		TmAlG	
hkl	I visual	d (Å) obsd	d (Å) calcd	d (Å) obsd	d (Å) calcd	d (Å) obsd	d (Å) calcd	d (Å) obsd	d (Å) calcd	d (Å) obsd	d (Å) calcd
211	9	4.910	4.929	4.912	4.916	4.895	4.903	4.886	4.891	4.883	4.881
220	4	4.267	4.269	4.255	4.257	4.240	4.247	4.232	4.236	4.225	4.227
321	7	3.217	3.227	3.216	3.218	3.209	3.210	3.199	3.202	3.196	3.196
400	6	3.016	3.019	2.999	3.011	3.000	3.003	2.990	2.995	2.985	2.989
420	10	2.691	2.700	2.691	2.693	2.687	2.686	2.679	2.679	2.671	2.674
422	4	2.456	2.465	2.458	2.458	2.451	2.452	2.445	2.446	2.442	2.441
521	5	2.197	2.204	2.198	2.199	2.192	2.193	2.186	2.187	2.183	2.183
611,532	6	1.953	1.959	1.952	1.953	1.948	1.948	1.941	1.944	1.938	1.940
631	3	1.780	1.780	1.775	1.775	1.770	1.771	1.768	1.767	1.762	1.763
444	4	1.743	1.743	1.736	1.738	1.733	1.734	1.728	1.729	1.726	1.726
640	5	1.671	1.674	1.668	1.670	1.665	1.666	1.661	1.661	1.658	1.658
721,633,552	3	1.642	1.643	1.639	1.639	1.634	1.634	1.629	1.630	1.627	1.627
642	4	1.610	1.613	1.609	1.609	1.604	1.605	1.600	1.601	1.598	1.598
732,651	2	1.532	1.533	1.527	1.529	1.524	1.525	1.520	1.522	1.517	1.519
800	3	1.508	1.509	1.505	1.505	1.501	1.501	1.496	1.498	1.494	1.495
840	1	1.349	1.350	1.345	1.346	1.342	1.343	1.338	1.340	1.336	1.337
842	3	1.315	1.317	1.313	1.314	1.309	1.311	1.307	1.307	1.304	1.305
921,761,655	1	1.301	1.302	1.298	1.298	1.295	1.295	1.291	1.292	1.288	1.289
664	1	1.287	1.287	1.283	1.283	1.279	1.280	1.277	1.277	1.275	1.275
1040,864	3	1.120	1.121	1.118	1.118	1.115	1.115	1.113	1.112	1.110	1.110
1121,1051,963	1	1.076	1.076	1.074	1.073	1.070	1.070	1.067	1.067	1.065	1.065
880	2	1.067	1.067	1.064	1.064	1.062	1.062	1.059	1.059	1.057	1.057
1222,1064	1	.9788	.9793	.9768	.9767	.9744	.9742	.9722	.9718	.9699	.9698
1244	1	.9103	.9101	.9077	.9077	.9054	.9053	.9037	.9031	.9015	.9013
1260,1084	3	.9004	.8999	.8976	.8976	.8960	.8952	.8936	.8930	.8917	.8912
1440,1282	2	.8298	.8292	.8271	.8270	.8250	.8249	.8228	.8229	.8212	.8212
1442,1266,10104	1	.8214	.8215	.8193	.8194	.8172	.8172	.8152	.8152	.8136	.8136
1521,1453,1365	1	.7961	.7961	.7940	.7940	.7920	.7920	.7900	.7900	.7883	.7884
11103,1097											
1532,1196	1	.7826	.7826								
12100,1286	8	.7730	.7730								

terbium, dysprosium, holmium, erbium and thulium aluminum garnets which will be hereafter referred to as TbAlG, DyAlG, HoAlG, ErAlG and TmAlG. The description of the magneto-optical properties of these materials will be published elsewhere by Rubinstein, Van Uitert and Grodkiewicz.

The powder diffraction photographs were taken with a Straumanis-type Norelco camera of 114.6 mm diameter using CuKα radiation and a Ni filter. Corrections were made for film shrinkage. The data so obtained are given in Table 1.

The lattice parameters used to calculate the spacings reported in Table 1 are given in Table 2. A conservative estimate of the error for the lattice parameter gives 3σ limits of ± 0.003 Å. In addition, the color,

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]
	Colorless			
TbAlG	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.

The authors wish to thank D. J. Nitti for taking the photographs and L. G. Van Uitert and W. H. Grodkiewicz for growing the crystals (to be published). We also wish to thank S. Geller for many useful discussions.

REFERENCES

BERTAUT, F. AND F. FORRAT (1956) *Compt. Rend.* **243,** 1219–1222.

THE AMERICAN MINERALOGIST, VOL. 49, SEPTEMBER–OCTOBER, 1964

DERIVING THE FORMULA OF A MINERAL FROM ITS CHEMICAL ANALYSIS

GABRIELLE DONNAY, *Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C.*

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