

The calculated standard errors may therefore be unrealistically low. (BATT and POST did not report standard errors on the cation-oxygen distances which I have calculated [see below]. In the course of my calculations, I found that the average values of these distances, that they calculated from their parameters, were in error by about one standard deviation. The corrected values are listed in a subsequent table.

The standard errors given by BATT and POST may not even be physically reasonable. At room temperature, yttrium iron garnet is not really cubic even though no significant deviation from cubicity has as yet been observed with x-rays. This means only that the x-ray diffraction technique, as others, has a limit on its "resolving power". Any crystal that has a spontaneous polarization, either magnetic or electric, cannot be cubic. The "easy" direction of magnetization of yttrium iron garnet below its Curie temperature is the [111] direction, therefore indicating that it actually belongs to a rhombohedral space group. This is not of great importance to the determination of the positional parameters inasmuch as it is unlikely that deviations from the cubic space-group positions are quantitatively measurable by known techniques. But that such deviations *may* exist should be recognized.

There is no question that physical measurement techniques other than those of x-ray diffraction "see" the non-cubicity: for example, the existence of the spontaneous magnetization alone (which only requires a small permanent magnet to observe), the optical birefringence observed by DILLON<sup>22</sup>, the Mössbauer spectroscopic investigation of  $\text{Tm}_3\text{Fe}_2\text{Fe}_3\text{O}_{12}$  by COHEN<sup>23</sup>. Of course, no *cubic* Shubnikov group describes a ferroelectric, ferrimagnetic, or ferromagnetic structure<sup>24</sup>.

The three sets of oxygen positional parameters obtained in the three independent investigations of yttrium iron garnet are:

	$x$	$\sigma$	$y$	$\sigma$	$z$	$\sigma$
GELLER and GILLES	-0.0274	0.0009	0.0572	0.0009	0.1495	0.0009
BATT and POST	-0.0269	0.0001	0.0581	0.0003	0.1495	0.0001
EULER and BRUCE	-0.0270	0.0004	0.0569	0.0005	0.1505	0.0005

<sup>22</sup> J. F. DILLON, JR., Optical properties of several ferrimagnetic garnets. *J. Appl. Physics* 29 (1958) 539-541; 1286-1291.

<sup>23</sup> R. L. COHEN, Mössbauer effect in  $\text{Tm}^{159}$  in thulium iron garnet. *Physics Letters* 5 (1963) 177-178.

<sup>24</sup> N. N. NERONOVA and N. V. BELOV, Ferromagnetic and ferroelectric space groups. *Kristallografiya* 4 (1959) 807-812; *Soviet Physics-Crystallography* 4 (1960) 769-774.

These are really all rather close, although because of the large lattice constant, small differences in parameter values may cause substantial differences in interionic distances:

	$\text{Fe}^{3+}(a)-\text{O}^{2-}$	$\sigma$	$\text{Fe}^{3+}(d)-\text{O}^{2-}$	$\sigma$	$\text{Y}^{3+}-\text{O}^{2-}$	$\sigma$
GELLER and GILLES	2.01	0.01	1.88	0.01	2.43 2.37	0.01 0.01
BATT and POST	2.013	0.002	1.881	0.001	2.417 2.365	0.003 0.001
EULER and BRUCE	2.019	0.006	1.866	0.005	2.434 2.356	0.006 0.005

The analogous  $\text{Fe}^{3+}-\text{O}^{2-}$  distances found in gadolinium iron garnet are 2.00 (0.01) and 1.89 (0.01) Å. These, together with the values found for yttrium iron garnet by GELLER and GILLES and by BATT and POST seem to favor the larger tetrahedral  $\text{Fe}^{3+}-\text{O}^{2-}$  distance, that is 1.88 Å rather than 1.87 Å. Yet four out of five  $\text{Fe}^{3+}(d)-\text{O}^{2-}$  values obtained by EULER and BRUCE for the iron garnets are lower: Lu, 1.87 Å; Yb, 1.86 Å; Y, 1.87 Å; Dy, 1.86 Å; and Sm, 1.88 Å. The  $\text{Fe}^{3+}(a)-\text{O}^{2-}$  distances for the same garnets were found to be 2.03 and 2.02 (for two different LuFe garnet specimens), 2.01, 2.02, 2.03, and 2.04 Å, respectively. It would seem that the value in GdFe garnet should lie between those in DyFe and SmFe garnet, but this has not been found to be the case (see Table 2).

Table 2. Cation-oxygen distances in garnets as determined by EULER and BRUCE

	Lu	Yb	Y	Gd	Dy	Sm
$\text{Al}^{3+}(a)-\text{O}^{2-}$	1.94 Å	1.94 Å	1.94 Å	1.94 Å		
$\text{Ga}^{3+}(a)-\text{O}^{2-}$	1.99	2.00	2.00			
$\text{Fe}^{3+}(a)-\text{O}^{2-}$	2.02	2.01	2.02		2.03 Å	2.04 Å
$\text{Al}^{3+}(d)-\text{O}^{2-}$	1.76	1.76	1.76	1.78		
$\text{Ga}^{3+}(d)-\text{O}^{2-}$	1.85	1.84	1.85			
$\text{Fe}^{3+}(d)-\text{O}^{2-}$	1.86	1.87	1.87		1.86	1.88

The  $d-h$  and  $a-h$  distances in the garnets refined by EULER and BRUCE are realistically rounded off to two decimal places in Table 2. These distances do not show a trend, e.g.  $\text{Fe}^{3+}(d)-\text{O}^{2-} = 1.86$  Å in Lu and DyFe garnet while in YbFe garnet it is larger, 1.87 Å. Thus,