

heated to its melting point and quenched to room temperature. A change was noticed in the powder photograph, which although not leading to a change in symmetry indicated changes in lattice constants. These were calculated and differed in the following way from the original: a - and c -axes were each reduced by about 0.02 Å. The treatment had been rather drastic and as the analyses did not indicate an impurity which could have caused this, the change was not clearly understood. More recently, the YFeO_3 was made by J. P. Remeika both by the original method (Remeika, 1956) and by a modification of that method. These gave patterns and lattice constants not like the original, but rather like the melted and quenched sample. Subsequently, a very pure ceramic sample was made by D. W. Mitchell by a co-precipitation technique as has been used by Mitchell to prepare rare earth garnets (see for example Gillo & Geller, 1958). This sample also gives a pattern much the same as the first melted and quenched sample and the more recent specimens made by Remeika.

Table 1. Powder diffraction data for YFeO_3 , CrK radiation

Index	d_o	d_c	I	Index	d_o	d_c	I
110)	3.811*	{3.839	vwv	303}	1.443	{1.445	$m-s$
002)		{3.801		133}		{1.444	
111	3.409	3.427	$m-s$	232}	1.412	{1.413	
020	2.784	2.796	m	115}		{1.413	vwv
112	2.688	2.701	vs	313}	1.398	{1.399	
200	2.630	2.640	$m-s$	040}		{1.398	vwv
021	2.616	2.624	$w-m$	322	1.386	1.387	vwv
211	2.272	2.277	$w-m$	041	1.374	1.375	$w-m$
022	2.247	2.252	vw	224	1.350	1.350	s
202	2.162	2.168	w	025	1.3362	1.3356	vwv
113	2.108	2.115	$w-m$	400	1.3206	1.3199	$w-m$
122	2.066	2.072	vwv	042	1.3115	1.3120	w
220	1.915	1.919	$m-s$	215	1.2826	1.2823	vwv
004	1.898	1.900	m	006)	1.2672	{1.2669	w
023	1.875	1.877	$w-m$	411}		{1.2666	
221	1.856	1.861	m	331	1.2618	1.2619	$m-s$
213	1.735	1.737	vwv	043	1.2240	1.2240	w
301)		{1.714		241	1.2195	1.2194	$m-s$
222)	1.710	{1.713	s	332	1.2126	1.2127	$w-m$
131)		{1.712		116	1.2031	1.2031	s
311	1.637	1.639	vw	420	1.1936	1.1936	$w-m$
132	1.594	1.595	m	225	1.1916	1.1918	$m-s$
024	1.571	1.572	m	421	1.1791	1.1791	m
204	1.541	1.542	m	242	1.1750	1.1749	$w-m$
312	1.534	1.536	s	305)	1.1502	{1.1505	s
				135}		{1.1498	

* Broad.

The powder pattern reported here (Table 1) is that of the specimen made by Mitchell. The lattice constants are:

$$a = 5.280, b = 5.592, c = 7.602 \text{ all } \pm 0.003 \text{ \AA}.$$

The volume of the unit cell is 224.5 Å³ and the X-ray density, 5.71 g.cm.⁻³. The pseudocell dimensions are:

$$a (= c) = 3.845, b = 3.801, \beta = 93.3^\circ.$$

The 'minimum average interionic distances' (see Geller & Wood, 1956, and Geller, 1957a) in YFeO_3 are:

$$\text{Y}^{3+}-\text{Y}^{3+}=3.828, \text{Y}^{3+}-\text{O}^{2-}=2.708, \text{Fe}^{3+}-\text{O}^{2-}=1.914 \text{ \AA}.$$

The effect on the calculated relative ionic sizes (Geller, 1957b) is negligible ($\leq 0.001 \text{ \AA}$).

Because the repetition of the original procedure produced crystals with the unit cell and pattern given here, it appears that the presence of lead could not be the cause of the difference.* Furthermore, analysis of the original material did not indicate an impurity of any amount which could cause such a significant difference. We therefore do not really know the cause, but believe that the pattern given in Table 1 is the one which should be used.

Several of the other orthoferrites were prepared again by Remeika's modified method and no differences found between the more recent powder patterns and those given in the paper by Geller & Wood (1956). It is also noteworthy that the new lattice constants allow YFeO_3 to fit better into the scheme of the perovskite-like crystals. For example, the difference in pseudocell axes $|a-b|$ is 0.044 Å with $\beta = 93.3^\circ$ (see Geller, 1957a, p. 246).

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* We had indicated earlier that the Pb probably did not enter the structure.

Notes and News

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