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On the unit cell of $YCrO_3$.

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A finely powdered sample of $YCrO_3$ was recently prepared in these laboratories by Mr John T. Looby. Measurement of the X-ray powder pattern (Cu $K\alpha$ radiation) of this new compound revealed several relationships of the form $k_1q_1 = k_2q_2$, where the k's are integers and the q's are $\sin^2\theta$ values (Hesse, 1948). Examples are:

$$0{\cdot}0831 \fallingdotseq 2\times0{\cdot}0417;$$
$$0{\cdot}1283 \fallingdotseq 4\times0{\cdot}0320;$$
$$0{\cdot}2081 \fallingdotseq 5\times0{\cdot}0417;$$
$$0{\cdot}1751 \fallingdotseq 8\times0{\cdot}0219.$$

The values for k_2—2, 4, 5, 8—suggested that the crystals were tetragonal, but several attempts to index the photograph on the basis of a tetragonal unit cell failed. This was taken to mean that the squares of the lengths of at least two of the cell edges were sufficiently close to being commensurate, and the cell angles sufficiently close to 90°, to simulate the symmetry of the tetragonal system.

The Goldschmidt tolerance factor for yttrium chromium oxide is about 0·86 and would indicate an orthorhombic (or possibly monoclinic) distortion of the cubic idealized perowskite structure (Wells, 1950). Indeed, when the photograph was viewed uncritically, the lines seemed to form clusters in such a way as to resemble the photograph of a simple cubic compound. If the second strong cluster corresponded to the cubic 110 reflection, the cell would

Table 1. *Monoclinic indexing of* $YCrO_3$

	$\sin^2\theta$		
I	Obs.*	Calc.	*hkl*
vvw	0·0190	0·0195	$\bar{1}01$
vvw	0·0219	0·0217	101
w	0·0320	0·0322	111
m	0·0417	0·0418	020
		0·0411	200
vw	0·0452	—	—
s	0·0518	0·0516	210
		0·0521	120
vw	0·0637	0·0640	211
		0·0635	121
vw	0·0673	0·0677	220β
s	0·0782	0·0780	$\bar{2}02$
vvs	0·0831	0·0829	220
s	0·0865	0·0866	202
m	0·0888	0·0885	$\bar{2}12$
w	0·0972	0·0971	212
vw	0·1063	0·1060	301
vw	0·1111	0·1100	$\bar{3}11$
m	0·1161	0·1164	311
		0·1157	131
m^-	0·1203	0·1198	$\bar{2}22$
m	0·1283	0·1284	222
m	0·1354	0·1351	230
w^+	0·1415	0·1414	$\bar{3}21$
w	0·1478	0·1478	321
		0·1475	231
s	0·1643	0·1645	400
m^+	0·1676	0·1672	040
m^-	0·1722	0·1720	$\bar{2}32$
m	0·1751	0·1750	410
		0·1757	$\bar{3}03$
vw	0·1804	0·1807	232
		0·1810	$\bar{4}11$
vw	0·1970	0·1972	$\bar{4}02$
vw	0·2005	0·2000	331
s	0·2081	0·2083	240
		0·2076	$\bar{4}12$
w	0·2130	0·2124	$\bar{4}21$
		0·2140	402
w^+	0·2247	0·2244	412
vvw	0·2301	—	—
vw	0·2341	0·2340	332
m^+	0·2389	0·2390	$\bar{4}22$
m^+	0·2458	0·2452	$\bar{2}42$
s	0·2555	0·2558	422
		0·2548	$\bar{4}13$
m^+	0·2913	0·2912	$\bar{4}32$
vw	0·3014	0·3024	250
vw	0·3122	0·3122	$\bar{4}04$
		0·3114	423
w^+	0·3227	0·3226	$\bar{4}14$
m^+	0·3317	0·3317	440
vvw	0·3383	0·3384	$\bar{4}33$
		0·3378	$\bar{4}41$
		0·3392	252
w	0·3462	0·3462	441
		0·3458	404
w	0·3552	0·3562	414
		0·3562	$\bar{5}31$
vw	0·3669	0·3672	351
		0·3666	531
w	0·3811	0·3812	442
		0·3817	$\bar{5}32$
		0·3805	610
w	0·4088	0·4090	$\bar{6}12$
w^+	0·4175	0·4173	260
w	0·4247	0·4242	540
		0·4255	$\bar{2}61$
		0·4238	602
vw	0·4336	0·4342	612
vw	0·4420	0·4423	$\bar{5}24$
		0·4425	504
w	0·4594	0·4594	533
		0·4584	$\bar{4}25$
w	0·4642	0·4642	630
vw	0·4762	0·4759	542
		0·4758	$\bar{3}61$
		0·4752	452
w	0·4927	0·4926	$\bar{6}32$
		0·4920	613
w	0·5124	0·5120	070
		0·5130	444
w	0·5194	0·5198	$\bar{6}14$
w	0·5733	0·5734	$\bar{4}62$
		0·5734	$\bar{4}54$
		0·5743	$\bar{7}03$
m^-	0·5917	0·5910	642
m^-	0·6020	0·6016	624
		0·6014	722

* 114·6 mm. diameter Philips camera.

have an edge of about 3·8 Å. The number of lines actually observed up to $\sin\theta = 0\cdot8$ was roughly five times the number a 4 Å cubic cell could have produced in this interval. At higher values of $\sin\theta$ the lines were too diffuse to measure or even count.

The following observations were sufficient to select a unit cell. The 'cubic 200' reflection was split into two lines with the one of smaller Bragg angle more intense than the other; this was accounted for by assuming the a and c axes about equal and the b axis somewhat shorter. The 'cubic 110' reflection appeared split into four lines consisting of one line and a close doublet on opposite sides of a very strong line; these were accounted for by also taking β different from 90°. Weak lines corresponding to spacings greater than 4 Å were present; these were accounted for by doubling the cell edges. The resulting cell had the following dimensions:

$$a \risingdotseq c = 7\cdot61\pm0\cdot01,\quad b = 7\cdot54\pm0\cdot01\ \text{Å};\quad \beta = 92^\circ\ 56'\pm6'.$$

All but two very weak lines were indexable with this cell. Indices were assigned on the basis of Bragg-angle agreement with no consideration as to the possible space group. Except for 504 and 070, however, all the indices are consistent with $P2_1/n$. Both of these exceptions are ambiguous, and, in view of the discussion by Vousden (1951), should be considered less probable than their listed alternates (Table 1).

If a is not exactly equal to c (they are not likely to differ by more than 0·015 Å however), the crystals are probably monoclinic. If a is exactly equal to c, choosing the diagonals of the a–c face as new a and c axes results in a cell which is orthogonal, B centered, and has cell edges of 10·49, 7·54 and 11·04 Å. This cell would imply that the crystals are orthorhombic. The orthorhombic a and c axes could be halved if the monoclinic cell were end centered, but the 332 and $\bar{5}24$ or 504 reflections, both very weak, prevent this possibility.

Another possibility is that the cell is similar to that of $NaNbO_3$ (Vousden, 1951). In this case we would expect the dimensions of the orthorhombic cell to be 5·24, 15·08 and 5·52 Å. If one takes into account the ambiguities in some of the indexing, no reflections prevent this possibility. In fact, this cell could also account for the two previously non-indexed reflections. A decision as to which unit cell is correct, as well as any detailed evaluation of the structure, will probably have to await the growing of satisfactory single crystals.

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A rapid numerical method of calculating structure factors.

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Simple, rapid methods of calculating structure factors usually depend on the use of some geometrical, mechanical or electrical analogue. The methods of Vand (1948), Llewellyn (1951), Phillips (1952), Stanley (1952) and Grenville-Wells (1954) all suffer from some disadvantages such as limited accuracy, the necessity of preparing preliminary tables of $(hx+ky)$, or the inconvenience of the presentation of the result as the length of a line or the deflection of a galvanometer. Numerical methods for calculating the product $\substack{\cos\\ \sin}(hx)\substack{\cos\\ \sin}(ky)$ are convenient only when a single product is required. The method here described is more accurate than most analogue devices and is numerical.

The basis of the method is a single table of values of $\cos x$ at intervals of 0·001 in x, arranged in a rectangular array so that successive rows overlap. In the present table each value of $\cos x$ is contained in a rectangle 1·0 cm. × 0·5 cm. and the values of x in successive rows run thus:

$$0\cdot000\text{–}0\cdot040,\ 0\cdot020\text{–}0\cdot060,\ 0\cdot040\text{–}0\cdot080,\ \ldots,\ 0\cdot980\text{–}0\cdot020,$$
$$0\cdot000\text{–}0\cdot040,\ 0\cdot020\text{–}0\cdot060,\ \ldots,\ 0\cdot980\text{–}0\cdot020\,.$$

Positive and negative values of $\cos x$ are distinguished by the use of different coloured inks and the values of x for both $\sin x$ and $\cos x$ are marked along the edges of the table. This type of arrangement of four complete cycles is necessary in order that the masks, described below, can be moved over the table and the correct relationship between the positions of the values of $\cos x$ preserved. The particular arrangement is flexible and the present table, which can be mounted on a board 18 in. × 20 in., has been designed for convenient desk use.

Masks are prepared, which cover the area of one cycle of the table, from which are cut rectangular holes 1·0 cm. × 0·5 cm. at positions corresponding to ky. One mask is required for each value of y punched with holes corresponding to successive orders of k up to, say, 20, and the holes are marked with the values of k. On the scale proposed the masks are approximately quarto size.

To use the method a table of values of hx is prepared for each atom and the appropriate mask for the y value of the first atom is selected. The mask is placed with the zero-order hole at 000 in the table. The values of $\cos ky$ appear in the holes marked k from 0 to 20. These values are conveniently noted on a recording adding machine. The mask is then moved until the zero-order hole is at x in the table when all the values of $\cos(x+ky)$ appear in the holes marked k and are similarly recorded. This procedure is repeated with the zero-order hole at $2x$, $3x$, etc. until all the values of $\cos(hx+ky)$ have been recorded. Negative values of k can be obtained by punching

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