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## A note on the crystal structure of $CaF_2 . 5Al_2O_3$.

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It has been pointed out by Günther, Anderson & Perlitz (1950), and by Günther & Perlitz (1952) that in phosphors of the aluminium oxide–calcium fluoride type activated with manganese and baked in air at temperatures between 1300 and 1450° C., the bearer of luminescence is an intermediate phase close to the composition $CaF_2 . 5Al_2O_3$. As it was impossible to obtain single crystals of this phase, powder photographs taken with Cr $K$ radiation in Debye–Scherrer cameras of 57·3 mm. diameter were used to deduce its crystal structure.

It was noticed that the diffraction pattern of this phase was rather similar to those of $PbO . 6Fe_2O_3$ and of $3CaO . 16Al_2O_3$ and $3SrO . 16Al_2O_3$ investigated by Adelsköld (1938) and by Lagerqvist, Wallmark & Westgren (1937) respectively. This is brought out by comparing sequences for strong and medium reflexions in the diffraction patterns of $PbO . 6Fe_2O_3$, $3SrO . 16Al_2O_3$, and $CaF_2 . 5Al_2O_3$, as listed in Table 1. The first column

Table 1. *Sequences of strong and medium reflexions*

| *hkl* | $PbO . 6Fe_2O_3$ | $3SrO . 16Al_2O_3$ | $CaF_2 . 5Al_2O_3$ |
|---|---|---|---|
| 110 | 0·223 | — | 0·223 |
| 107 | 0·253 | 0·250 | 0·249 |
| 114 | 0·280 | 0·280 | 0·281 |
| 203 | 0·328 | — | — |
| 204 | — | 0·358 | — |
| 0,0,10 | — | | — |
| 205 | 0·386 | 0·388 | 0·385 |
| 206 | 0·426 | 0·428 | 0·424 |
| 217 | 0·694 | 0·700 | 0·694 |
| 0,0,14 | — | | — |
| 304 | 0·723 | 0·730 | — |
| 2,0,11 | 0·733 | | 0·730 |
| 220 | 0·886 | 0·894 | 0·891 |
| 1,0,16 | 1·000 | — | — |
| 2,0,14 | | 1·000 | 1·000 |
| 317 | — | 1·145 | 1·139 |
| — | — | — | 1·275 |

of the table contains indices of reflexions listed by Adelsköld and/or by Lagerqvist *et al.*; the second and third columns contain sequences formed by $\sin^2\theta$ values of strong and medium reflexions in the patterns of $PbO . 6Fe_2O_3$ and $3SrO . 16Al_2O_3$, respectively, on the basis of $\sin^2\theta_{1,0,16+2,0,14}$ and $\sin^2\theta_{2,0,14}$ respectively equal to 1; the last column contains the corresponding sequence in the pattern of $CaF_2 . 5Al_2O_3$.

Comparing the last sequence with the two previous ones, all listed reflexions of $CaF_2 . 5Al_2O_3$ except the last were indexed in accordance with the first column. With these indexed reflexions to start with, all the 61 reflexions observed in the diffraction pattern of $CaF_2 . 5Al_2O_3$, except three outermost weak ones, could be accounted for on the basis of the hexagonal quadratic form

$$\sin^2\theta = 0{\cdot}04280[\tfrac{4}{3}(h^2+k^2+hk)+0{\cdot}06454l^2]$$

for the $\alpha$-reflexions, i.e. by a hexagonal lattice with

$$a = 5{\cdot}529 \text{ Å} \quad \text{and} \quad c = 21{\cdot}79 \text{ Å}.$$

The 47 observed $\alpha$-reflexions, their relative intensities estimated by visual inspection, and corresponding interplanar distances are summarized in Table 2.

Table 2. *Interplanar distances, estimated intensities, and indices of reflexions for* $CaF_2 . 5Al_2O_3$.

| $d$ (Å) | $I/I_1$ | *hkl* | $d$ (Å) | $I/I_1$ | *hkl* |
|---|---|---|---|---|---|
| 5·451 | 20 | 004 | 1·672 | 50 | 215 |
| 4·723 | 30 | 101 | 1·672 | | 0,0,13 |
| 4·358 | 40 | 005 | 1·610 | 40 | 2,0,10 |
| 4·023 | 40 | 103 | 1·591 | 40 | 301 |
| 3·620 | 35 | 104 | 1·568 | 70 | 217 |
| 3·232 | 30 | 105 | 1·526 | 90 | 2,0,11 |
| 3·104 | 30 | 007 | 1·507 | 40 | 218 |
| 2·766 | 60 | 110 | 1·460 | 20 | 306 |
| 2·714 | 50 | 008 | 1·446 | 40 | 2,0,12 |
| 2·616 | 80 | 107 | 1·429 | 30 | 1,1,13 |
| 2·458 | 80 | 114 | 1·382 | 100 | 220 |
| 2·387 | 20 | 201 | 1·372 | 30 | 2,0,13 |
| 2·372 | 30 | 108 | 1·339 | 20 | 224 |
| 2·328 | 40 | 115 | 1·303 | 70 | 2,0,14 |
| 2·278 | 50 | 203 | 1·280 | 30 | 2,1,12 |
| 2·199 | 50 | 116 | 1·247 | 10 | 316 |
| 2·193 | 20 | 204 | 1·236 | 10 | 1,0,17 |
| 2·174 | | 0,0,10 | 1·231 | 40 | 228 |
| 2·104 | 80 | 205 | 1·221 | 60 | 317 |
| 2·002 | 70 | 206 | 1·193 | 40 | 318 |
| 1·899 | 30 | 207 | 1·181 | 50 | 403 |
| 1·820 | 20 | 119 | 1·172 | 40 | 1,0,18 |
| 1·800 | 30 | 208 | 1·168 | 10 | 404 |
| 1·718 | 40 | 214 | 1·154 | 60 | 3,0,13 |
| 1·701 | 40 | 209 | | | |

The Laue symmetry of $PbO . 6Fe_2O_3$ and $3SrO . 16Al_2O_3$ is $D_{6h}$–6/*mmm*. Assuming the same symmetry for $CaF_2 . 5Al_2O_3$, its space group would be $D^1_{6h}$–$C6/mmm$ or $D^3_{6h}$–$C6/mcm$, as, of reflexions *hhl* even, those for $l$ odd are present, namely 115, 119 and 1,1,13.

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