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## Refined atomic coordinates for the sillimanite structure.

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In the course of a comparison of the structure of mullite (Ďurovič, 1962*a*) with that of sillimanite (Ďurovič, 1962*b*), it was necessary to re-examine the sillimanite structure of Hey & Taylor (1930). One of the main results of the mullite structure analysis was the establishment of statistical occupation of the Al, Si* atomic positions (Fig. 1(*a*)). This statistical occupation was indicated by low peaks in the Fourier projection $\varrho(x, y)$, and confirmed during the refinement.The same result was obtained independently by Sadanaga, Tokonami & Takéuchi (1962). It was therefore desirable to determine whether the sillimanite structure showed a similar effect, especially as the experimental methods used by Hey & Taylor were insufficiently sensitive for this purpose.

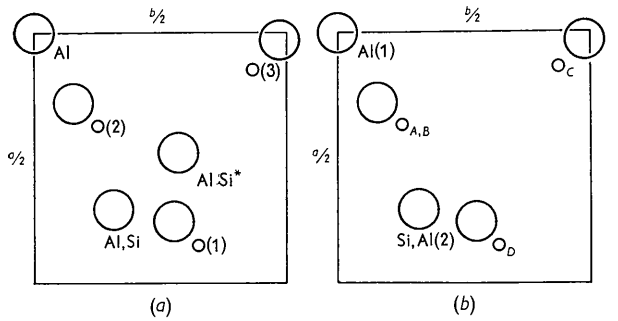


Fig. 1. Atomic positions in the mullite (*a*) and sillimanite (*b*) crystal structures.

For the re-examination crystals of the sillimanite variety xenolite (40·30% $SiO_2$, 59·60% $Al_2O_3$, 0·85% $Fe_2O_3$ and 0·07% $TiO_2$; ideal composition 62·93% $Al_2O_3$) were used. The measured density was $3{\cdot}226 \pm 2$ g.cm.$^{-3}$. The electron-density projection was calculated from 72 independent reflexions observed on Weissenberg photographs taken with Cu radiation. The structure was refined by repeated $F_o - F_c$ syntheses, the final $R$ factor being 0·071 (0·068). The syntheses showed no Al, Si* maximum of the type found in mullite (Fig. 1(*b*)). The final atomic coordinates are compared with those determined by Hey & Taylor in Table 1. The assignment of the $z$ parameters was verified by comparison of observed and calculated values of $F(h0l)$ and $F(0kl)$.

Table 1. *Refined atomic coordinates of sillimanite and those determined originally by Hey & Taylor*

| | This work | | | Hey & Taylor | | |
|---|---|---|---|---|---|---|
| Atoms | $x$ | $y$ | $z$ | $x$ | $y$ | $z$ |
| Al(1) | 0 | 0 | 0 | 0 | 0 | 0 |
| Al(2) | 0·352 ±0·001 | 0·158 ±0·001 | ¾ (¼) | 0·36 | 0·15 | ¾ |
| Si | 0·352 ±0·001 | 0·158 ±0·001 | ¼ (¾) | 0·36 | 0·15 | ¼ |
| $O_A$ | 0·139 ±0·002 | 0·079 ±0·002 | ¼ | 0·15 | 0·07 | ¼ |
| $O_B$ | 0·139 ±0·002 | 0·079 ±0·002 | ¾ | 0·15 | 0·07 | ¾ |
| $O_C$ | 0·025 ±0·002 | 0·490 ±0·002 | ¾ | 0·03 | 0·47 | ¼ |
| $O_D$ | 0·374 ±0·002 | 0·275 ±0·002 | 0 | 0·39 | 0·28 | 0 |

No detailed analysis of the occupation of the tetrahedral positions was possible.

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## The crystal structure of $SnCl_2$. A correction.

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The text of the paper by van den Berg, 1961, contains an error in the interatomic distances of the Sn atom at $z = \frac{1}{4}$ to the Cl atoms in the same plane. These distances should be 3.22, 2.66 and 3.30 Å. The distances in Fig. 1 are correct.

### Reference

BERG, J. M. VAN DEN (1961). *Acta Cryst.* **14**, 1002.