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## Crystal setting.

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In a note on the setting of crystals for X-ray diffraction work by Garaycochea & Cid-Dresdner (1961) a list of references is given 'to help newcomers to X-ray crystallography in finding the most suitable technique for setting crystals for their particular case.' I should like to draw attention to an important paper by Davies (1950) omitted from this list which supersedes the technique of Weisz & Cole (1948) described in detail in Garaycochea & Cid-Dresdner's note.

The Davies technique consists in taking a double-setting photograph, as suggested by Weisz & Cole, but with the arcs at 45° to the incident X-ray beam. In this setting the misalignment in each arc can be related to the separation of crystal reflexions or Laue streaks on one side of the film only. Theoretically the separations should be measured at a Bragg angle of 45° but in practice the values are found to be relatively insensitive to small shifts on either side of this position. The method could therefore be used in the majority of cases mentioned in Garaycochea & Cid-Dresdner's note, without recourse to complex sign conventions. In view of its basic simplicity and general application the Davies technique deserves to be more widely known.

### References

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## The setting of single crystals.

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Garaycochea & Cid-Dresdner (1961) have described a graphical method for setting single crystals when the zero-layer curves are not visible at the two positions with Bragg angle $\theta = 45°$. The idea of a graphical solution is a useful addition to the range of existing techniques of crystal-setting. For example, it can be used when the zero-layer curve is visible on only one side of the film.

However, it is advantageous to set the goniometer arcs at 45° to the X-ray beam, since a particularly simple setting method can then be used in which the zero-layer separation is measured at or near the two positions $\theta = 45°$ (Davies, 1950). If, however, one has set the arcs at 45° and been unable to measure the separation at the two positions $\theta = 45°$, then a graphical solution can still be used. The procedure, which is described below, is similar to that of Garaycochea & Cid-Dresdner but modified to take account of the 45° arc setting.

Let the separation of the zero-layer curves at any Bragg angle $\theta$ be $\Delta_1$ if on the left-hand side of the film, and $\Delta_2$ if on the right. The $\Delta$ are positive where the upper curve is the more intense. Let $i_1$ and $i_2$ be the angular corrections required on the two arcs, being positive if anti-clockwise. The orientation of the two arcs is best described by supposing the X-ray beam to travel from north to south; then for the longer exposure arc No. 1 faces north-west and arc No. 2 faces south-west. On a graph of $i_2$ against $i_1$ construct the 45° lines $i_1 = i_2$ and $i_1 = -i_2$. It will be convenient to work in degrees if the goniometer arcs are so graduated. For each measured value $\Delta_1$ of the layer curve separation construct the line which has intercepts

$$\frac{180}{\pi} \cdot \frac{\Delta_1}{2R(1-\cos 2\theta)}$$

degrees along the $i_1$-positive direction of $i_1 = i_2$, and

$$\frac{180}{\pi} \cdot \frac{\Delta_1}{2R \sin 2\theta}$$

degrees along the $i_1$-positive direction of $i_1 = -i_2$.

For separations $\Delta_2$ interchange subscripts 1 and 2 in the preceding instruction. Construct several such lines. Their common intersection gives the required arc corrections in sign and magnitude.

The advantages of the 45° arc setting have been confirmed by Kennard (1961). The object here has been to combine it with the graphical method of solution, so that one may always use a single procedure for taking the diffraction pattern, and then choose whichever method of interpretation is appropriate.

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