

This parameter  $r$  contains only experimentally determined quantities. Physically it represents the ratio of the average heights at the end points  $\pm V$  to the average height over the entire range  $-V \leq v \leq V$ . Hence it will obviously be less than unity for all cases of interest.

Equation (4) now yields immediately

$$c = c_1 / (1 - r). \quad (5)$$

This expression gives the true centroid  $c$  in terms of experimentally known quantities without the need of successive approximations. If data are recorded at reasonably closely spaced abscissa intervals, the integrals in equations (1) and (4) can, of course be replaced by the corresponding sums. Furthermore the zeroth approximation and the range may usually be chosen so as to eliminate the use of fractional abscissa intervals at the end points.

While the above derivation involves certain approximations, the resulting errors will normally be small. It can be shown that the fractional error in  $c$  will usually be of the order of  $(c/w)^2 + |sc/w|$ , where  $w$  is the full width of the profile at half intensity and  $s$  is the index of asymmetry as defined by Sauder (1966). In our error calculations we employed the model given by equation (II. 9) of Thomsen & Yap (1968), which we termed an 'asymmetric witch'. For this model, with  $s = 0.25$ ,  $c = 0.05 w$ , and a total truncation range of only  $2w$ , we compute a fractional error of 0.5% in  $c$ . For wider truncation ranges the error becomes still smaller.

Very recently Wilson (1967) published a paper which also includes a treatment of the statistical errors in the centroid, median, and peak. Aside from superficial aspects, his results for centroid and median differ from ours in one significant respect, *i.e.* he ignores any statistical error in the determination of the truncation limits. Clearly, if we use the centroid definition recommended by Taylor, Mack & Parrish, the random intensity fluctuations responsible for the statistical error in  $c_1$  also produce an error in the truncation limits. For this case, it can be shown (Thomsen &

Yap, 1968) that the net effect is to multiply Wilson's error by a factor  $(1-r)^{-1}$ . Another interesting consequence of employing the Taylor, Mack & Parrish definition is to eliminate any error due to uncertainty in the correction for a constant background.

Admittedly the factor  $(1-r)^{-1}$  is quite close to unity ( $\sim 1.05$ ) for the large truncation ranges generally used by crystallographers. However, if we consider a Lorentzian profile with a truncation range of twice the full width, this factor increases the error by more than 50%. Other methods of truncation also involve additional statistical error, although the analysis may be less straightforward. Similar considerations apply to the median.

It should also be noted that Wilson's equation (27) (for the standard deviation of the peak as determined by a parabolic fit) is dimensionally correct only if the quantity  $I$  in his equation (26) represents counts rather than intensity (counts per unit time). With this modification it becomes a special case of our result for a polynomial fit. Wilson (1965) had previously derived this equation with all terms properly defined, but neglected to transform the notation when quoting it in his recent paper.

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### Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (G. Boom, Laboratorium voor Fysische Metaalkunde der Rijksuniversiteit, Universiteitscomplex Paddepoel, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.*

## International Union of Crystallography

### Structure Reports

The Executive Committee has pleasure in announcing that Volume 22 of *Structure Reports*, covering the literature for 1958, was published in August. Volume 23 (1959) had been published earlier. Volumes 24 (1960), 26 (1961), 27 (1962) and Volume 25 (the cumulative index for 1951-60) are now with the press and will be ready in 1968-69.

Volumes 22, 24 and 26 each consist of 800-900 pages. Their prices are (Netherlands Guilders) f140 (or at present rates of exchange \$39 or £16.8s.). The price of Volume 25 (Index) will be f90 (\$25.00 or £10.10s.).

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livered immediately, and Volumes 24 and 25 as soon as printed.

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## International Union of Crystallography

### **Eighth General Assembly and International Congress of Crystallography.**

#### **Exhibition of Photographs**

During the Eighth General Assembly and International Congress of Crystallography, 13–21 August 1969, Stony Brook, U.S.A., an Exhibition of Photographs of Crystallographic Interest will be organized by the Union's Commission on Crystallographic Apparatus. The first Exhibition was held during the previous Congress in Moscow, 1966, and attracted an international response with exhibits of high quality and both scientific and aesthetic appeal. The Commission on Crystallographic Apparatus has, therefore, decided to organize a similar exhibition during the forthcoming Congress and invites crystallographers and others to participate actively by submitting suitable prints for display.

The exhibition will be divided into two sections:

- (a) photographs of crystals;
- (b) photographs of diffraction patterns from crystals.

The prints should be mounted on standard photographic mounting board (no glass or wooden framing) and may be accompanied by explanatory material if desired. Neither mounted print nor explanatory material should separately exceed 2000 cm<sup>2</sup> in area (40×50 cm format preferred). Each print must have a caption and exhibitor's name and address. Exhibitors may submit more than one print.

The photographs will be judged (by a small committee) in terms of aesthetic appeal rather than technical interest or importance and the best photographs will be awarded certificates of merit and, if possible, published in a suitable journal.

Intending exhibitors (who need not be participants in the Congress) are requested to write to Prof. F. H. Herbstein, Department of Chemistry, Israel Institute of Technology, Haifa, Israel, before 1 March 1969, submitting small prints of their proposed entries. Immediately after that date they will be notified whether their contributions are suitable for the exhibition. Contributions will not be returned unless specific arrangements are made with the organizers; contributors attending the Congress will have to remove their own exhibits.