Fig. 1 shows a comparison of the average electron density summed for the backbone atoms and C_β plotted against the sequence numbers before and after the two refinement cycles. There is an obvious improvement in continuity of the electron density along the polypeptide backbone; in addition, the average electron density at each atomic site increased 32% for the backbone atoms and 22% for the side-chain atoms. In spite of the fact that no stereochemical constraints were applied, the bond lengths and bond angles remained relatively unchanged under the above transformation; the average values of the C_α–C′, C′–O and C_α–N bonds are 1·536, 1·218 and 1·466 Å respectively.

The coordinates produced by this procedure have been listed by Richards & Wyckoff (1973) and used by them to prepare full drawings of the structure. They are also on file in the Protein Data Bank, designated set 6D (T. F. Koetzle, Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973).

References

DIAMOND, R. (1971). *Acta Cryst.* A**27**, 436–452.

RICHARDS, F. M. (1968). *J. Mol. Biol.* **37**, 225–231.

RICHARDS F. M. & WYCKOFF, H. W. (1973). *Atlas of Molecular Structures in Biology*, edited by D. C. PHILLIPS & F. M. RICHARDS, Vol. 1. Oxford: Clarendon Press.

WYCKOFF, H. W., TSERNOGLOU, D., HANSON, A. W., KNOX, J. R., LEE, B & RICHARDS, F. M. (1970). *J. Biol. Chem.* **245**, 305–328.

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Single-crystal diffractometer data: economizing in background counting times.

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A method is described for economizing the time spent in background counting during a single-crystal data collection with a computer-controlled diffractometer. The percentage time saved for a reflexion depends on the peak-to-background ratio whereas the fraction of peak counting time spent on the background depends, in addition, on the background level and on the precision required for the reflexion intensity.

It is possible to reduce the total time spent measuring single-crystal intensity data, without sacrificing precision, by economizing on the background counting time. The procedure enables the time allocated to peak and background measurements to be varied so that for a given reflexion the gain in precision obtained by a small increase in peak measurement time off-sets the loss in precision suffered by a larger decrease in the background measurement time. The percentage time saved on a reflexion depends on the peak-to-background ratio. The method is equally applicable to scan-type or peak-height measurements.

It has been shown (Grant, 1973) that single-crystal intensity data can be collected to a prestated counting statistics precision p' on a computer-controlled single-crystal diffractometer. Before each reflexion is measured fully, it is first measured for a short trial time, with equal times q on the peak and background to give counts of I_q and B_q respectively. To give the required precision the total counting times for both peak and background should be $t'=f'q$ where

$$f'=\frac{I_q+B_q}{p'^2(I_q-B_q)^2}\ . \qquad (1)$$

If both peak and background are measured for further times $(f'-1)q$ then the required precision would be obtained and the total time spent on this reflexion would be $2f'q$.

If the diffractometer uses a step-scan technique then the peak is measured for the further time by a step scan in which the time per step is increased by the factor $(f-1)$ over that for the trial step scan. If a continuous scan technique is used then repeated fast scans of the peak for a total time $(f-1)q$ are made, if a fast scan of time q is used for the trial measurement.

It is possible to economize on the time spent on a reflexion, particularly if the peak-to-background ratio is large, by measuring the background for a shorter time than that for the peak without reducing the overall precision of the measurement. If, after the trial time q, the time $t=fq$ is calculated for a precision p better than p', then

$$f=\frac{I_q+B_q}{p^2(I_q-B_q)^2} \qquad (2)$$

and if the peak is measured for a further time $(f-1)q$, the background can be measured for a shorter time without changing the overall precision from p' and peak time will be increased slightly. Under this arrangement the total peak counts expected will be $I=fI_q$ and the total background counts expected will be $B=B_q+(f-1/n)B_q$, where the background subsequent to the trial time is measured for one nth of the remaining peak time.

The precision p' of such a measurement is

$$\frac{\sigma(N)}{N}=\frac{(I+r^2B)^{1/2}}{I-rB}=\frac{(I_q+rB_q)^{1/2}}{f^{1/2}(I_q-B_q)}\ ,$$

where the background is measured for one rth of the total peak time, *i.e.*

$$r=\frac{f}{\left[1+\dfrac{(f-1)}{n}\right]}\ . \qquad (3)$$

Let $p'/p=y$ where $y>1$; then

$$y=\frac{(I_q+rB_q)^{1/2}}{f^{1/2}(I_q-B_q)}\cdot\frac{f^{1/2}(I_q-B_q)}{(I_q+B_q)^{1/2}}=\frac{(I_q+rB_q)^{1/2}}{(I_q+B_q)^{1/2}}\ .$$

Writing this in terms of the peak-to-background ratio $x(=I_q/B_q)$,

$$y=\left(\frac{x+r}{x+1}\right)^{1/2}$$

or

$$r=y^2(x+1)-x\ . \qquad (4)$$

If a suitable value of y can be found, then for a given x, r and hence n can be calculated. That is, the fraction of time to spend on the background, after the trial time, can be deduced.

The best value of y is the one that gives the maximum fractional saving in time for the reflexion. With this procedure of unequal peak and background times, the total time spent in the reflexion is $[f+(f-1)n/+1)q$ and the time saved compared to the equal peak and background time procedure for the same precision p' is

$$2f'q-\left(f+\frac{f-1}{n}+1\right)q$$

and the fractional time saved is

$$T_s=\frac{2f'-\left(f+\frac{f-1}{n}+1\right)}{2f'}$$

$$=1-\frac{y^2}{2}-\frac{y^2}{2n}+\frac{1}{2f'n}-\frac{1}{2f'}\ .$$

From equations (3) and (4)

$$T_s=1-\frac{y^2}{2}-\tfrac{1}{2}\frac{y^2}{\{y^2(x+1)-x\}}$$

and T_s depends on the choice of y and the peak to background ratio x.

The maximum value of T_s is obtained from

$$-y+\frac{xy}{\{y^2(x+1)-x\}^2}=0 \qquad (5)$$

and the values of interest are those for which both x and y are greater than 1.

If y_s^2 is the solution of (5)

$$y_s^2=\frac{x\pm\sqrt{x}}{(x+1)}$$

and only the positive square-root is of interest.

That such a value of y_s^2 gives a maximum fractional saving in time can be shown easily.

In terms of I_q and B_q the value of y to use is given by

$$y_s^2=\frac{I_q+\sqrt{I_qB_q}}{(I_q+B_q)}\ . \qquad (6)$$

Table 1 shows the values of y_s^2 for various peak-to-background ratios.

Table 1. *Values of y_s^2 for various peak to background ratios*

x	1·0	2·0	5·0	10·0	20·0	50·0
y_s^2	1·0	1·15	1·21	1·20	1·17	1·09

Table 2. *Values of y_s, r and T_s for various peak-to-background ratios*

x	y_s	r	T_s (%)
1·0	1·000	1·000	0·00
1·2	1·021	1·095	0·20
1·5	1·043	1·224	1·01
2·0	1·066	1·414	2·85
5·0	1·098	2·236	12·73
10·0	1·093	3·162	21·25
20·0	1·079	4·472	28·70
50·0	1·057	7·071	36·13

As x tends to 1, y_s^2 also tends to 1, making both r and n unity also; or as would be expected, there is no saving in time as the background should be measured for the same time as the peak for these very weak reflexions.

Values of y_s, r and T_s (expressed as a percentage) are given in Table 2.

It should be noted that the percentage time saving is independent of the precision required. The value of n calculated from an observed x will depend both on p' and the background count.

For

$$n=\frac{(y_s^2f'-r)}{(y_s^2f'-1)}$$

and

$$f'=\frac{(x+1)}{p'^2B_q(x-1)^2}$$

Table 3 shows the values of n calculated for $B_q=50$ and $x=5{\cdot}0$ for various values of p'.

Table 3. *Values of n for various values of the precision p'*

$B_q=50$, $x=5{\cdot}0$, $y_s=1{\cdot}098$, $r=2{\cdot}236$, $T_s=12{\cdot}73$ %

p' (%)	0·5	1·0	2·0	5·0	7·5	10·0
n	2·24	2·26	2·37	4·23	−2·18*	—†

* $f'>1$, but n is negative; no further background measurement after the trial time.

† $f'<1$, the reflexion is satisfactorily measured during the trial time.

With this technique, the sequence for the measurement of a reflexion is:

(i) Measure both the peak and background for equal trial times q and obtain the values I_q and B_q.

(ii) For the required precision p' calculate f' from (1). If $f'<1$, no further measurements are required, the trial time measurements giving sufficient precision.

(iii) From (6) calculate y_s and then from (2) calculate f.

(iv) From (4) calculate r, and then from (3) find n.

(v) Since $f>f'$ and $f'>1$ for these reflexions, it is possible for n to be negative. For this group of reflexions the background is sufficiently well represented by B_q but the peak is measured for a further time $(f-1)q$.

(vi) Usually, however, n will be positive and for these reflexions the peak is measured for a further time $(f-1)q$ and the background for a further time $(f-1/n)q$, to give the precision required.

As described previously (Grant, 1973) controlling conditions can be applied to very weak reflexions by imposing a maximum counting time for any reflexion. Also, modified values of I_q and B_q can be used to ensure that the probability of reaching the required precision is increased. The amount of time saved by the introduction of this method of data collection will depend on the crystal under investigation and the distribution of peak-to-background ratios among the reflexions.

The greatest percentage saving on individual reflexions is on those with large x, but these will usually be measured for a short time anyway, but the method does allow data to be collected to a given precision in less time than formerly and this should recommend its use.

Reference

GRANT, D. F. (1973). *Acta Cryst.* A**29**, 216–217.