deduce $\varrho(r)$ from *oriented* preparations of tobacco mosaic virus (Franklin & Holmes, 1958; see for general aspects Vainshtein, 1966).

The expression used by Franklin & Holmes is

$$\varrho(r)=2\pi\int_0^{s_{max}} F(s)J_0(2\pi sr)s\mathrm{d}s \qquad (1)$$

where $F(s)$ is the continuous cylindrically symmetrical equatorial structure factor of the rod (with amplitude and phase) and J_0 is a zero order Bessel function. To apply this equation to the scattering by a dilute solution it is necessary to establish the relationship between $F(s)$ and the observed intensity of scattering by the solution $I(s)$.

This relationship is presented by Burge & Draper (1967) for the special cases of long rigid rods with $\varrho(r)=$ constant, e^{-ar^2}, $r^2e^{-ar^2}$. These results imply the general result

$$I(s) \propto \frac{1}{s}|F(s)|^2 . \qquad (2)$$

Thus equation (1) becomes

$$\varrho(r) \propto \int_0^{s_{max}} [I(s)]^{1/2}J_0(2\pi sr)s^{3/2}\mathrm{d}s \qquad (3)$$

which is essentially the equation of Fedorov & Aleshin (1966).

The necessary conditions for the validity of equation (3) are those for equation (2). These are: (i) $s \gg 1/L$ with L the rod length; the problem of extrapolating $sI(s)$ to zero scattering angle has been considered by Luzzati (1960). (ii) The scattering corresponds entirely (in practice predominantly) to $F(s)$, *i.e.* at a given radius the cylindrically symmetrical rod density is assumed to be constant along its length.

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The application of direct methods to centrosymmetric structures containing heavy atoms.

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For those reflexions of which the sign is determined by a relatively small number of heavy atoms, the known heavy-atom contribution is subtracted from the observed structure factor to obtain the magnitude and the sign of the light-atom contribution. Thereafter the signs of the reflexions that do not have appreciable heavy atom contributions are found using the triple product sign relationship.

As the solution of structures with a relatively small number of heavy atoms is straightforward in most cases, direct methods of sign determination have been used only rarely for these structures. It will be shown in this communication that the solution can easily be obtained by using the well-known triple product sign relationship

$$S_{\mathbf{h}+\mathbf{h}'} \sim S_{\mathbf{h}} \, . \, S_{\mathbf{h}'} . \qquad (1)$$

The procedure described below is similar to the method used by Subramanian (1967) to solve a structure in projection. It is assumed that the positions of the heavy atoms are known and that there is a sufficient number of reflexions whose signs are determined by the heavy atoms. These reflexions do not obey the probability relation (1). On subtracting the heavy atom contribution from the observed structure factors of these reflexions, one obtains the *magnitude* and the *sign* of the light atom contributions for these reflexions. Thereafter one can solve the remaining light atom structure by applying equation (1) to obtain the signs of the reflexions that do not have appreciable contributions from the heavy atoms.

The procedure was used to solve the structure of the complex $Au[S_2C_2(CN)_2]_2Au[S_2CN(C_4H_9)_2]_2$ (to be published). The space group was found to be $P2_1/c$, with two formula units per unit cell. The reflexions hkl ($h=2n$, $k+l=2n$) were all very strong and the gold atoms were placed at the (special) positions 000, $\frac{1}{2}00$, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and $0\frac{1}{2}\frac{1}{2}$. 1337 observed 'strong' reflexions (with equal positive contributions from the gold atoms) and 538 observed 'weak' reflexions (without any contributions from the gold atoms) were used.

The first step was a calculation of the Wilson plot. The following expression (Parthasarathy, 1966) was used:

$$\langle I\rangle_{\mathbf{h}} = K_L\langle\textstyle\sum_i^L f_i^2 \exp(-2B_L \sin^2\theta/\lambda^2)\rangle_{\mathbf{h}} + K_H\langle|F_H|^2 \exp(-2B_H \sin^2\theta/\lambda^2)\rangle_{\mathbf{h}} \qquad (2)$$

where $I=(K|F_{obs}|^2)$ is the observed intensity on a relative scale, $K=K_L=K_H$ is the scale factor, $\sum^L$ denotes a summation over all light atoms in the unit cell, F_H is the heavy atom contribution to the structure factor and B_L and B_H are the overall temperature factor parameters of the light and heavy atoms respectively. The average is taken over reflexions $\mathbf{h}$ within a given $\sin\theta$ interval.

For the 'weak' reflexions ($F_H=0$) the second term in equation (2) vanishes and a Wilson plot for these reflexions gave the scale factor K_L (1·29) and the value of B_L (3·24 Å^2). On substituting these results in equation (2) a Wilson plot for the 'strong' reflexions gave the scale factor K_H (1·26) and the value of B_H (2·91 Å^2). A small difference in K_L and K_H will not effect the following steps.

The second step is the calculation of the normalized structure factors E. The formulae normally used for the calculation of E values do not make sense for a structure containing heavy atoms. For the corresponding light atom

structure the E values, E_L, are defined by:

$$E_L = F_L(\varepsilon\sum_i^L f_i^2)^{-1/2} \exp(B_L \sin^2\theta/\lambda^2) \quad (3)$$

where F_L is the light atom contribution to the structure factor and, for space group $P2_1/c$, $\varepsilon=2$ for $h0l$ and $0k0$ reflexions and $\varepsilon=1$ for all other reflexions (Hauptman & Karle, 1953).

The 'strong' reflexions have positive structure factors and we have $F_L = F_{obs} - F_H$; the magnitude and the sign of the E_L value is obtained by equation (3). This resulted in 365 signed E_L values, with $|E_L| > 1{\cdot}3$. For the 'weak' reflexions we have $|F_L| = |F_{obs}|$ and only the magnitude of the E_L value is obtained. This resulted in 270 reflexions with $|E_L| > 1{\cdot}3$.

The third step is the application of equation (1) to obtain the signs of the 'weak' reflexions. When several interactions of the type $(\mathbf{h}+\mathbf{h}')=(\mathbf{h})+(\mathbf{h}')$ occur for $|E_L| > 1{\cdot}3$, where both $S_{\mathbf{h}}$ and $S_{\mathbf{h}'}$ are known, several predictions of the sign $S_{\mathbf{h}+\mathbf{h}'}$ are obtained by application of (1). These predictions should be reasonably consistent before $S_{\mathbf{h}+\mathbf{h}'}$ is considered to be determined and singly occurring interactions should never be trusted. We have followed a procedure similar to the sign correlation procedure (Beurskens, 1963). The origin was partly fixed by the choice of the gold atom positions and further determined by assigning arbitrary signs to two 'weak' reflexions: 221 ($|E_L| = 4{\cdot}0$) and $34\bar{8}$ ($|E_L| = 2{\cdot}9$). We define the following sets of reflexions, all with $|E_L| > 2{\cdot}0$:

$\mathbf{h}_1$ are 'strong' reflexions, hkl ($h=2n$, $k+l=2n$).
$\mathbf{h}_2$ are the two origin determining choices.
$\mathbf{h}_3$ are the reflexions $\mathbf{h}_1+\mathbf{h}_2$ and $\mathbf{h}_2+\mathbf{h}_2'$.
$\mathbf{h}_4$ are the reflexions $\mathbf{h}_1+\mathbf{h}_3$, $\mathbf{h}_2+\mathbf{h}_3$ and $\mathbf{h}_3+\mathbf{h}_3'$.

The application of equation (1) on only reflexions $\mathbf{h}_1$ cannot give new signs; together with the reflexions $\mathbf{h}_2$ probable signs for 36 reflexions $\mathbf{h}_3$ were calculated. Upon entering $\mathbf{h}_3$ in equation (1), many reflexions take part in the calculations and consequently the sign of one reflexion $\mathbf{h}_4$ will often be found from several independent sign relations (1). Signs were calculated for 48 reflexions $\mathbf{h}_4$; of these the signs of 24 reflexions were determined by at least five consistent relations (1) and accepted to be correct. Although some of the signs for reflexions $\mathbf{h}_3$ may be incorrectly determined, it is highly improbable that all reflexions $\mathbf{h}_3$ used for the sign determination of one reflexion $\mathbf{h}_4$ are incorrect. The intermediate results for $\mathbf{h}_3$ and the rest of $\mathbf{h}_4$ were rejected.

Continued application of equation (1) on 365 'strong' reflexions, 2 reflexions $\mathbf{h}_2$ and 24 reflexions $\mathbf{h}_4$ resulted in the sign determination of 158 more 'weak' reflexions with $|E_L| > 1{\cdot}3$. A Fourier synthesis revealed the positions of all of the light atoms, except the hydrogen atoms.

Calculations were performed using computer programs written by R. Dewar and A. Stone, modified by one of the authors (JHN).

The above described procedure may be generalized for heavy atoms on general positions. In this case there also exist reflexions with intermediate heavy atom contributions. For these reflexions $|F_L| = ||F_{obs}| \pm |F_H||$ and the lowest F_L value is taken to avoid incorrect sign indications. In our opinion this procedure is well suited to an automatic solution of structures containing heavy atoms.

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Resonance effects in low and high energy electron diffraction by crystals. Erratum.

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Corrections to a previous paper [*Acta Cryst.* (1970). A**26**, 60] are given.

The following corrections should be made in our paper of the above title (Miyake & Hayakawa, 1970).

P. 64, col. 1, line 15 from bottom: For 'lowest Bragg reflexion 004.' read 'lowest Bragg reflexions 004 and 006.'.

P. 64, col. 1, line 14 from bottom: For 'as an extra peak caused by' read 'as the 006 peak influenced by'.

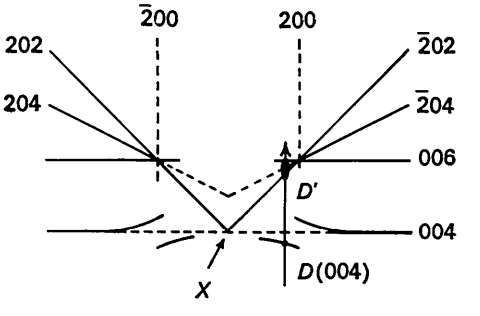
Fig. 10 (facing p. 64): The vertical dotted line (D) should be displaced by 5 mm to the right.

P. 65, Fig. 11(a): The reflexion indices should be corrected as follows:

for 006 read 008
for 008 read 0010
for 0010 read 0012
for 0012 read 0014.

P. 65, Fig. 11(b), lines 4–5 of the legend: For 'The peak D is the non-Bragg reflexion caused by' read 'The peak D' is the 006 reflexion influenced by'.

P. 66. Fig. 12: This should be replaced by



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