

SHORT COMMUNICATIONS

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Interpretation of pseudo-extinctions. By HEINZ SCHULZ, *Max-Planck-Institut für Festkörperforschung, 7 Stuttgart 80, Federal Republic of Germany*

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Equations for the interpretation of pseudo- (non-space-group) extinctions are given.

1. Introduction

Pseudo-extinctions are present if reflections allowed by space-group symmetry are found to be extinct in a systematic way (examples are shown in Niggli, 1959*a*; Schulz & Schröder, 1973). Niggli (1959*b*) proposed for the solutions of these pseudo-extinctions the following method: the true elementary cell is reduced in such a way that the pseudo-extinctions become true space-group extinctions for the artificial elementary cell. Afterwards this elementary cell is increased stepwise.

In the following a method which allows all solutions of a pseudo-extinctions rule to be found simultaneously and its limitations are described.

2. Interpretation of pseudo-extinctions

We assume that a crystal contains a translational vector which is not embodied in the translational part of the crystal symmetry. This can be expressed by an elementary cell containing two atoms of the same kind located at the origin of the elementary cell (000) and at $(x = r/s, y = t/u, z = v/w)$; r, s, \dots, w are integers. This atomic arrangement generates extinct layers in reciprocal space, which can be described by the plane equation:

$$P \equiv Ah + Bk + Cl = D \pmod{E}; \quad (1)$$

(hkl) are coordinates in reciprocal space. If reflections are included in these layers, they must fulfil the equation:

$$1 + \exp \left[2\pi i \left(\frac{r}{s} h + \frac{t}{u} k + \frac{v}{w} l \right) \right] = 0. \quad (2)$$

From (2) follows

$$\frac{r}{s} h + \frac{t}{u} k + \frac{v}{w} l = \frac{1}{2} \pmod{1}. \quad (3)$$

Therefore, (1) can be reduced to

$$A'h + B'k + C'l = \frac{1}{2} \pmod{1}. \quad (4)$$

The coefficients (A', B', C') can be written as

$$A' = \frac{r'}{s}, \quad B' = \frac{t'}{u}, \quad C' = \frac{v'}{w}.$$

The solutions of (4) are given by

$$\begin{aligned} \frac{r'}{s} h &= \frac{1}{2} \pmod{1} \\ \frac{t'}{u} k &= \frac{1}{2} \pmod{1} \\ \frac{v'}{w} l &= \frac{1}{2} \pmod{1} \end{aligned} \quad (5)$$

with $x' = r'/s$; $y' = t'/u$; $z' = v'/w < 1$. The coordinates (xyz) are embodied in the solutions $(x'y'z')$.

Example

We assume that an elementary cell contains two atoms occupying the positions $(0,0,0)$ and $(\frac{5}{6}, \frac{3}{8}, 0)$. This arrangement causes the following pseudo-extinctions:

$$h = 0 \pmod{6} \quad k = 4 \pmod{8}$$

and

$$h = 3 \pmod{6} \quad k = 0 \pmod{8}.$$

Layers in reciprocal space containing only these pseudo-extinct reflections can be described by

$$P \equiv 4h + 3k = 12 \pmod{24}.$$

This equation can be reduced to

$$\frac{h}{6} + \frac{k}{8} = \frac{1}{2} \pmod{1}.$$

The solutions are given by

$$\frac{r'}{6} 3 = \frac{1}{2} \pmod{1}, \quad \frac{r'}{6} < 1$$

and

$$\frac{t'}{8} 4 = \frac{1}{2} \pmod{1}, \quad \frac{t'}{8} < 1.$$

It follows that all possible solutions are given by

$$x' = (\frac{1}{6}, \frac{3}{8}, \frac{5}{6}); \quad y' = (\frac{1}{8}, \frac{3}{8}, \frac{7}{8}); \quad z' = 0.$$

3. Application

For the structure determination of $\text{MoO}_2\text{Cl}_2 \cdot \text{H}_2\text{O}$ (Schulz & Schröder, 1973), the solutions of the following pseudo-

extinction have been used: reflections with $k = 2 \pmod{4}$ are extinct. Equation (1) can be written as:

$$k = 2.$$

This can be reduced to

$$\frac{1}{4}k = \frac{1}{2} \pmod{1}$$

and

$$\frac{l'}{4} = \frac{1}{2} \pmod{1}.$$

It follows from (5) that $y' = \frac{1}{4}$ and $\frac{3}{4}$. This means that an atom at (x, y, z) is accompanied by an atom at $(x, y + \frac{1}{4}, z)$ or $(x, y + \frac{3}{4}, z)$.

4. Limitations

The above-mentioned equations can be used if only one translational vector between pairs of atoms is present. Only in simple cases may a limited number of solutions of (5) be helpful for a structure determination. However, errors in space-group determination can be avoided by successful interpretations of pseudo-extinctions.

References

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On the probability of measuring the intensity of a reflexion as negative. By A. J. C. WILSON, *Department of Physics, University of Birmingham, Birmingham B15 2TT, England*

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Infrequently quoted statistical results relating to taxi queues *etc.* are modified to obtain the probability of obtaining an observed number of counts $R_o = T_o - B_o$ when the 'true' numbers of counts are R , T and B for reflexion, total and background respectively and T_o and B_o have the expected Poisson distributions. The expression, valid for negative as well as positive values of R_o , is

$$p(R_o) = \exp\{-(B+T)\} (T/B)^{R_o/2} I_{R_o}\{2(BT)^{1/2}\},$$

where $I_n(x)$ is the hyperbolic Bessel function of the first kind. If the negative values of R_o are included, R_o is an unbiased estimator of R . In no case is $R_o^{1/2}$ an unbiased estimator of $R^{1/2}$, so that Patterson and R_2 methods are preferred to usual electron-density and R_1 methods in structure determination whenever they are appropriate.

In the absence of drift and other disturbing influences, the number of counts recorded during the counting interval used in diffractometers working in the fixed-time mode fluctuates in accordance with the Poisson probability distribution. If the 'true' number of counts to be expected in the interval is N , the probability that the number actually observed will be N_o is given by

$$p(N_o) = \exp(-N) N^{N_o} / N_o!. \quad (1)$$

The quantities p , N and N_o are necessarily non-negative. The intensity of a reflexion, say R , is given by the difference between the 'true' number of counts T expected when the diffractometer is set to receive the reflexion and the 'true' number of counts expected when the diffractometer is set to receive the immediate background:

$$R = T - B; \quad (2)$$

for simplicity it is assumed that the counting times for reflexion and background are the same. The observed values, T_o and B_o , will fluctuate with probabilities given by equations like (1), so that the observed value R_o will sometimes be negative, though the 'true' value R must be zero or positive. What is the probability $p(R_o)$ of obtaining any particular observed difference R_o ? The answer is not well known, and is to be found in comparatively few text-books. For the *sum*

$$S_o = T_o + B_o, \quad (3)$$

the result is immediate: the sum of two Poisson-distributed variables is itself Poisson-distributed, with parameter S equal to the sum of the parameters T and B of its components, but obviously the converse is not true for the *difference*. It is easy to write down a formal expression:

$$p(R_o) = \sum p(B_o)p(T_o), \quad (4)$$

the summation being over all B_o and T_o related by

$$R_o = T_o - B_o. \quad (5)$$

Substitution from equation (1) gives

$$p(R_o) = \sum_{B_o=0}^{\infty} \exp\{-(B+T)\} B^{B_o} T^{B_o+R_o} / B_o! (B_o+R_o)!. \quad (6)$$

The summation was carried out in a special case by Irwin (1937) and in general by Skellam (1946); it results in the Bessel function I_n , related to the ordinary Bessel function J_n in the same way as the hyperbolic functions cosh and sinh are related to the trigonometric functions cos and sin. The required probability distribution for the observed number of counts in a reflexion is thus

$$p(R_o) = \exp\{-(B+T)\} (T/B)^{R_o/2} I_{R_o}\{2(BT)^{1/2}\}. \quad (7)$$

Extensive tables of I_n exist (for example, in Abramowitz & Stegun, 1964). As is fairly obvious intuitively, the mean value