Acta Cryst. (1989). A**45**, 145–146

Correlation between occupancy and temperature factors of solvent molecules in crystal structures of proteins.

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(*Received* 25 *January* 1988; *accepted* 14 *July* 1988)

Abstract

Correlation between occupancy and temperature factors during the refinement of a disordered molecule is discussed on the basis of their effects on an atomic scattering factor curve. When the resolution of the data is limited, occupancy and temperature factors affect scattering-factor curves in a similar fashion, and therefore they are correlated. An examination of this correlation suggests that small deviations (0·1) of occupancy factors from their tentative values may be compensated by suitable changes in temperature factors when the data are limited to medium (2·5 Å) resolution.

The refinement of partially occupied or disordered atoms is becoming increasingly important in macromolecular structure determination. Often both occupancy and temperature factors are refined for atoms suspected of disorder (*e.g.* solvent atoms). Kundrot & Richards (1987) used model calculations to study the results of structure-factor least squares with and without variable occupancy factors. They have concluded that, for data limited to a nominal resolution of not better than 1 Å, it is not appropriate to vary both occupancy and temperature factors for solvent molecules in protein structure refinements. In this note I address the effect of occupancy and temperature factors on the structure factors by examining the way occupancy and temperature factors affect the scattering-factor values and I reach a different conclusion from that of Kundrot & Richards (1987).

The modulus of a structure factor, $|F_h(s)|$, calculated from an atom is given by

$$|F_h(s)| = Qf(s)\exp(-Bs^2),$$

where s is $(\sin\theta)/\lambda$ for the reflection h. B and Q are temperature and occupancy factors of the atom respectively; $f(s)$ is the scattering factor (Freeman, 1962) of the atom at the given value of s. In this expression the occupancy factor appears as a scale factor on the scattering factor, whereas the temperature factor appears in an exponential function involving s. Q changes the 'volume' under the scattering-factor curve and B alters both this 'volume' and the 'shape' of the scattering-factor curve. The question addressed in this paper is: when data are limited to medium resolution, is the change in 'shape' and 'volume' due to B noticeably different from the change in 'volume' alone due to Q? If the data are limited to a narrow range of s, $\exp(-Bs^2)$ may be assumed to be a constant, similar to Q, for all the available diffraction data; obviously, then, both Q and B affect $f(s)$ in a similar fashion and, therefore, Q and B are correlated. The correlation between Q and B, when s spreads over a larger range, is the subject of this paper.

A structure-factor least-squares calculation with B and Q involves obtaining B and Q, which would modify ideal $f(s)$, so as to fit as well as possible to the scattering factor, $f'(s)$, of the atoms in the crystal. Therefore, a refinement of both B and Q may be justified if an $f(s)$ modified by a Q (and B) is different from the $f(s)$ modified by B alone. To study the correlation between the $f(s)$ affected by B or Q, a function R can be defined as

$$R = \sum_{d=d_{\min}}^{d_{\max}} |Qf(s) - f(s)\exp(-Bs^2)| \Big/ \sum_{d=d_{\min}}^{d_{\max}} Qf(s)$$

where d is the Bragg spacing that corresponds to a value of s. The value of R is the difference between the scattering amplitude due entirely to scattering factor and occupancy factor, and that due entirely to scattering factor and thermal parameter, normalized by the scattering factor modified by the occupancy factor. $Qf(s)$ is the scattering factor modified by an occupancy factor of Q and a B of 0, and $f(s)\exp(-Bs^2)$ is the scattering factor modified by an occupancy factor of 1 and a temperature factor of B. The value of R is an agreement factor between the scattering-factor curves, $f(s)$, modified by Q and B separately. If an $f(s)$ can be modified either by $Q = Q'$ or by $B = B'$ to get the same agreement with $f'(s)$ (considered over a given range of s), then R should be zero for $Q = Q'$ and $B = B'$ and in such a situation the scattering factors used in a refinement either with B alone or with B and Q are very similar; therefore, it should be adequate to refine only B (or Q). If, for a particular range of s, $Qf(s)$ for $Q = Q'$ is different from $f(s)\exp(-Bs^2)$ for all values of B, then R

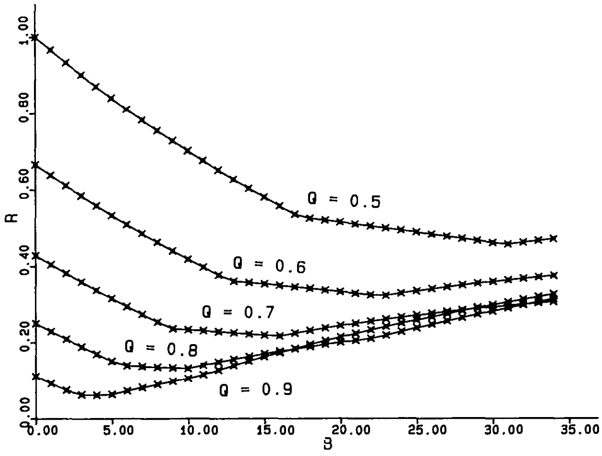

Fig. 1. Differences between the scattering factors modified by Q and B separately. The function R is defined in the text. The summation was performed at Bragg spacings of 10, 5, 3·3 and 2·5 Å and the scattering factor of an oxygen atom was used.

will be non-zero no matter what the value of B, and in such a situation the refinement of B or Q will not use the same modification to the scattering factors and hence the two refinements are different in this respect.

Fig. 1 shows the differences between the scattering factors modified by Q and B separately. For a particular value of Q, B is varied from 0 to 35 Å^2 using a step of 1 Å^2 and the values of R (vertical axis) are plotted. The summation was carried out for Bragg spacings of 10, 5, 3·3 and 2·5 Å; and $f(s)$ of an oxygen atom was used. The graph for $Q = 0{\cdot}9$ goes through a low value around $B = 4$ Å^2, showing that instead of using a Q of 0·9 and a B of 0, one may use a Q of 1·0 and a B of 4 Å^2 to obtain very similar scattering-factor curves out to 2·5 Å. In other words, the scattering-factor curve out to 2·5 Å obtained after refining Q to 0·9 and B to 0 is very similar to the scattering-factor curve obtained by fixing Q at 1·0 and refining B to 4 Å^2. However, the scattering-factor curve used after refining Q to 0·5 and B to 0 is significantly different from the scattering-factor curve used after fixing Q at 1·0 and allowing B to take any possible value.

These graphs reveal that, at medium resolution (to 2·5 Å) for small error in Q (for example, $Q = 1{\cdot}0$ is used instead of $Q = 0{\cdot}9$), there exists a suitable change in the value of B (4 Å^2) for which R is small (0·06). However, for larger errors in Q, R remains rather high for B ranging from 0 to 35 Å^2. Extension of the summation to smaller values of Bragg spacing obviously increases the discrepancy between scattering factors modified independently by Q and B. These graphs show that, at medium resolution (to 2·5 Å), B can modify scattering factors to compensate for a small error in Q, but larger error in Q cannot be accurately compensated for by B. In practice, the need to refine Q arises only for atoms suspected of disorder, and these atoms pose special problems. A disordered atom, unlike the rest of the atoms in the unit cell, may not contribute significantly to the higher-resolution diffraction patterns and hence the structure-factor least squares may tend to wipe out its contribution to higher-resolution reflections. In such situations the existence of higher-resolution data by itself may not suggest the independence of Q and B for disordered atoms. Therefore, for atoms suspected of disorder, it might be expedient to impose the desired constraints through tight restraints on B and Q rather than by elimination of variables (Hendrickson, 1985).

I thank Drs D. R. Davies, E. A. Padlan and S. Sheriff for useful discussions.

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Acta Cryst. (1989). A**45**, 146-148

Electron microscope analyses of domains and discommensurations in ferroelectric Rb_2ZnCl_4. Erratum.

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(*Received* 1 *November* 1988)

Abstract

The following corrections should be made in Tsuda, Yamamoto & Yagi [*Acta Cryst.* (1988). A**44**, 864-870].

(1) 'only two kinds of domain boundaries' in the *Abstract* should be changed to 'two kinds of image contrast of domain boundaries'.

(2) The expressions for h_2, h_4, h_6 in § 4.1 should be replaced by

$$\begin{array}{llll} h_2: & -x & -y & -z+\frac{2}{3} \\ h_4: & -x & -y & -z \text{ (inversion)} \\ h_6: & -x & -y & -z+\frac{1}{3}. \end{array}$$

(3) 'two kinds of DC's showing different contrast' in the second paragraph in § 4.1 should be changed to 'two kinds of DC contrast'.

All relevant information is given in the *Abstract*.

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