Using this function it is easy to find the best tangential connexion to the high order part of the H scattering curve. One has to leave out as many low-order points of this part as necessary before obtaining a $H^{+\delta}$ curve that crosses the H curve. The results for $\delta = 0{\cdot}3$, $0{\cdot}5$, and $0{\cdot}7$ are summarized in Table 1. The second point of each form factor table is the beginning of the high order part of the H table preserved. The coefficients a_i found from the first three points of each table are compared to those calculated for the first points of the H^{-1} and H tables. Fig. 2 shows the three resulting scattering curves. The scattering factor tables for H and H^{-1} plotted for comparison in Fig. 2 are taken from Vol. III of the *International Tables for X-ray Crystallography* (1962), because the tables in Vol. IV (1974) give poor curves owing to rounding effects.

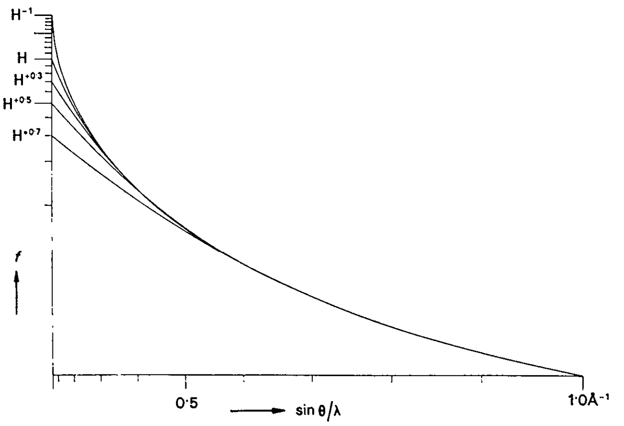

Fig. 2. Scattering factor curves for $H^{+0{\cdot}3}$, $H^{+0{\cdot}5}$, $H^{+0{\cdot}7}$ using high-order tails of the H curve starting at 0·4, 0·5 and 0·6 Å^{-1} respectively and using equation (1) for interpolation.

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A note on two papers by Kuntsevich & Belov.

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1237 four-dimensional space-group types of the 'low-symmetry crystal classes' have been listed by Kuntsevich & Belov [*Kristallografiya* (1971). **16**, 5–17, 268–272]. Comparison of this list with the results of Brown, Bülow, Neubüser, Wondratschek, and Zassenhaus shows that three space-group types are listed twice and one space-group type is missing. The crystal classes considered by Kuntsevich & Belov thus contain 1235 of the 4783 types of space groups of *R*4.

Crystallography in four-dimensional space *R*4 has drawn increasing interest during the last years. Reasons for this may be: possible applications in physics, better insight into dimension-independent features of crystallographic objects, mathematical interest in integer matrix groups, and the availability of large computers for the performance of the necessary calculations.

For the crystal families, crystal systems, crystal classes, and Bravais-types we refer to Wondratschek, Bülow & Neubüser (1971) and the literature quoted there. In a joint project of Brown, Bülow, Neubüser, Wondratschek, and Zassenhaus (referred to as BBNWZ) also a complete list of all affine equivalence classes of space groups of *R*4 was determined, their number being 4783.

Those space groups of *R*4 for which the linear parts of all symmetry operations have order not exceeding two, *i.e.* those corresponding to the triclinic to orthorhombic space groups in *R*3 had been derived and listed by Kunstevich & Belov (1971) (referred to as KB), using geometric arguments. They found 1237 types of such space groups.

Although KB did admirable work, errors are almost unavoidable in computations by hand. There are discrepancies in relation to the tables of BBNWZ, which contain only 1235 affinely-non equivalent space group types of this kind.

A closer inspection shows the following discrepancies. In KB crystal class VIII, X, and XI the KB numbers of space-group types exceed the BBNWZ numbers of space-group types by one, in XV BBNWZ have listed one space-group type more than have KB.

KB characterize their space-group types by certain sets of generators. The symbols used are slightly modified Hermann (1949) symbols. The generating matrices of a representation of each space-group type can be determined easily from these symbols, *e.g.* space-group type VIII, 43

$$A_1 = \left(\begin{array}{cccc|c} \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right) \qquad A_2 = \left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & \frac{1}{4} \\ 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right)$$

and space-group type VIII, 45

$$B_1=\left(\begin{array}{cccc|c}\bar{1}&0&0&0&0\\0&1&0&0&\frac{1}{4}\\0&0&1&0&\frac{1}{4}\\0&0&0&1&\frac{1}{2}\\\hline 0&0&0&0&1\end{array}\right)\qquad B_2=\left(\begin{array}{cccc|c}1&0&0&0&\frac{1}{4}\\0&\bar{1}&0&0&0\\0&0&1&0&\frac{1}{4}\\0&0&0&1&\frac{1}{2}\\\hline 0&0&0&0&1\end{array}\right).$$

With x,y,z,u used as coordinates these matrices give $\bar{x},\frac{1}{4}+y,\frac{1}{4}+z,u$ and $\frac{1}{4}+x,\bar{y},\frac{1}{4}+z,u$ for VIII, 43 or $\bar{x},\frac{1}{4}+y,\frac{1}{4}+z,\frac{1}{2}+u$ and $\frac{1}{4}+x,\bar{y},\frac{1}{4}+z,\frac{1}{2}+u$ for VIII, 45 respectively in the conventional symbols of *International Tables for X-ray Crystallography* (1952).

It is easily verified that the integer matrix

$$T=\left(\begin{array}{cccc|c}1&0&0&0&0\\0&1&0&0&0\\0&0&1&0&0\\0&0&-2&1&0\\\hline 0&0&0&0&1\end{array}\right)$$

transforms the generators A_i into the generators B_i, that is $B_i=T^{-1}A_iT$. Therefore, by changing the basis a_1,a_2,a_3,a_4 to $b_1=a_1$, $b_2=a_2$, $b_3=a_3-2a_4$, $b_4=a_4$, the group VIII, 45 is obtained from VIII, 43. This shows that VIII, 43 and VIII, 45 describe the same space-group type; they are only referred to different coordinate bases. Exactly the same holds for the pairs X, 99 and X, 101 as well as XI, 45 and XI, 46 with the same T as the transforming matrix. As a result of this the entries VIII 45, X 101, and XI 46 have to be removed from the KB Table 4.

On the other hand, KB list in Table 4, crystal class XV, only 62 space-group types, whereas in the BBNWZ computer determination 63 space-group types in this crystal class were found. Here to the F_6 lattice (*U* lattice type of Wondratschek, Bülow & Neubüser, 1971) belong three space-group types of which KB list only two. The space group generated by

$$1122=\left(\begin{array}{cccc|c}1&0&0&0&0\\0&1&0&0&0\\0&0&\bar{1}&0&0\\0&0&0&\bar{1}&0\\\hline 0&0&0&0&1\end{array}\right),\quad 1_{1/2}2_{1/2}1_{1/2}2_{1/2}=\left(\begin{array}{cccc|c}1&0&0&0&\frac{1}{4}\\0&\bar{1}&0&0&\frac{1}{4}\\0&0&1&0&\frac{1}{4}\\0&0&0&\bar{1}&\frac{1}{4}\\\hline 0&0&0&0&1\end{array}\right),$$

$$2_{1/2}1_{1/2}1_{1/2}2_{1/2}=\left(\begin{array}{cccc|c}\bar{1}&0&0&0&\frac{1}{4}\\0&1&0&0&\frac{1}{4}\\0&0&1&0&\frac{1}{4}\\0&0&0&\bar{1}&\frac{1}{4}\\\hline 0&0&0&0&1\end{array}\right)$$

is missing; it should be added under No. 61*a*.

In No. 60 in each set of parallel twofold 'hyper axes' 2211, 2121, 2112, 1212, 1221, and 1122 there occur real rotations. In 61 in three of the six sets of twofold 'hyper axes' there occur real rotations, the other three containing screw rotations only. Finally in 61*a* there are two sets in which real rotations occur, whereas in the other four sets only screw rotations can be found. This shows immediately geometrically that the three space groups considered are non-equivalent (the original derivation by BBNWZ had been an algebraic one).

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A method of obtaining a stereochemically acceptable protein model which fits a set of atomic coordinates.

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A method is proposed by which a protein model with acceptable stereochemistry can be fitted to a set of atomic coordinates. By expressing all constraints in terms of distances between pairs of atoms it is possible to enforce any desired stereochemistry in a physically realistic manner, and at the same time to substantially reduce computing time. Application of the technique to thermolysin is described. The method has been independently developed and applied to insulin by E. J. Dodson, N. W. Isaacs & J. S. Rollett [*Acta Cryst.* (1976). **A32**, 311–315].

The problem of obtaining a model of a protein which is a best fit to a set of observed coordinates and at the same time adheres to a specified stereochemistry has been discussed by a number of authors. In the methods of Diamond (1966) and Warme, Gō & Scheraga (1972), bond lengths and angles are, in general, fixed, and model fitting is achieved by allowing specified dihedral angles to vary. However, in real polypeptides, all bond lengths and angles may deviate somewhat from their idealized values, and in order to obtain a satisfactory representation of a protein it is desirable that such deviations be allowed. Hermans & McQueen (1974) have suggested that such variations from idealized stereochemistry can be incorporated by a method of 'local change' in which one atom is adjusted at a time in a cyclic process. Freer, Alden, Carter & Kraut (1975) have also used, in the refinement of HiPIP, a cyclic refinement of the model in which deviations in bond lengths and angles from their standard values are minimized.