The atom-to-plane distances $\mathbf{d}$ of the n atoms defining the plane are dependent on the least-squares adjustments of the plane parameters $\Delta\mathbf{n}$ through the relationship,

$$\mathbf{d} = \mathbf{d}^{(0)} - \mathbf{Y}\Delta\mathbf{n}, \tag{4}$$

where

$$\tilde{\mathbf{d}} \equiv (d_1 d_2 \ldots d_n), \tag{5}$$

$$\tilde{\mathbf{Y}} \equiv (\mathbf{y}_1\, \mathbf{y}_2 \ldots \mathbf{y}_n), \tag{6}$$

and $\mathbf{d}^{(0)}$ denotes the distances before adjustments. Substituting the least-squares solution [equations (20a) and (23) of paper I]

$$\Delta\mathbf{n} = {}^{n}\mathbf{M}\tilde{\mathbf{Y}}\mathbf{W}\mathbf{d}^{(0)} \tag{7}$$

into (4), we obtain the relationship

$$\mathbf{d}\tilde{\mathbf{d}} = \mathbf{d}^{(0)}\tilde{\mathbf{d}}^{(0)} - \mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}}\mathbf{W}\mathbf{d}^{(0)}\tilde{\mathbf{d}}^{(0)} - \mathbf{d}^{(0)}\tilde{\mathbf{d}}^{(0)}\,\mathbf{W}\mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}} + \mathbf{Y}\Delta\mathbf{n}\Delta\tilde{\mathbf{n}}\tilde{\mathbf{Y}}, \tag{8}$$

where $\mathbf{W}$ is the weight matrix defined by

$$\mathbf{W} = {}^{d}\mathbf{M}_0^{-1}. \tag{9}$$

The error matrix for $\mathbf{d}$ can readily be obtained from (8) with the aid of (9) as

$$\begin{aligned} {}^{d}\mathbf{M}_1 &= {}^{d}\mathbf{M}_0 - \mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}}\mathbf{W}\,{}^{d}\mathbf{M}_0 - {}^{d}\mathbf{M}_0\,\mathbf{W}\mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}} + \mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}} \\ &= {}^{d}\mathbf{M}_0 - \mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}}. \end{aligned} \tag{10}$$

The diagonal element of ${}^{d}\mathbf{M}_1$ is the variance of the atom-to-plane distance of the plane-defining atom,

$$\sigma_1^2(d_i) = ({}^{d}\mathbf{M}_0)_{ii} - \tilde{\mathbf{y}}_i\,{}^{n}\mathbf{M}\mathbf{y}_i. \tag{11}$$

It should be noted that (11) is the same as (1) except that the sign of the second term is reversed.

Expression (11) may be checked for a three-atom plane. In this case reference must be made to the elimination method of paper II. It can generally be shown that

$$\mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}} = \mathbf{Y}_e\,{}^{p}\mathbf{M}\tilde{\mathbf{Y}}_e, \tag{12}$$

where $\mathbf{Y}_e$ is the derivative matrix [equation (12) of paper II] after one of the plane parameters has been eliminated, and ${}^{p}\mathbf{M}$ is the error matrix for the remaining three plane parameters which is given by

$${}^{p}\mathbf{M} = (\tilde{\mathbf{Y}}_e\,\mathbf{W}\mathbf{Y}_e)^{-1}. \tag{13}$$

Now, since $\mathbf{Y}_e^{-1}$ is defined for a three-atom plane, (12) together with (13) gives

$$\mathbf{Y}\,{}^{n}\mathbf{M}\tilde{\mathbf{Y}} = \mathbf{W}^{-1} = {}^{d}\mathbf{M}_0, \tag{14}$$

that is, from (10),

$${}^{d}\mathbf{M}_1 = 0, \tag{15}$$

for a three-atom plane, which is the expected result.

The Fortran program BP70 of paper II has been modified according to (11) for the plane-defining atoms.

A simple example of a four-atom group will serve for illustration. The four atoms are located at A(1,0,0), B(0,1,0), C(−1,0,0) and D(0,−1,0·01) in a Cartesian coordinate system in Å units, with a common isotropic standard deviation of 0·01 Å. If we define a plane with three atoms A, B and C, the plane evidently coincides with the x,y plane through the origin, and atom D not defining the plane is out of the plane by 0·01 Å, with the standard deviation σ_2 of (1) of 0·02 Å; atom D is coplanar within the standard deviation.

On the other hand, if we define a plane with all the four atoms, the best plane inclines by 0·29 (57)° from the x,y plane, with the origin-to plane distance of 0·0025 (50) Å. Atoms A and C, and B and D are out of the plane by 0·0025 Å in opposite directions, with a common standard deviation σ_1 of equation (11) of 0·005 Å; the four atoms are again planar within the standard deviations.

$$\chi^2 \equiv \sum [d_i/\sigma_1(d_i)]^2 \tag{16}$$

for the four atoms is 1·00 for one degree of freedom, which also confirms the planarity. However, such statistical tests based on the ratios d/σ must be used with caution, because any groups of atoms would hardly be planar, if the atomic positions are determined with very high precision. In other words, the atom-to-plane distances themselves are also important to test planarity (*e.g.* d less than ±0·005 Å).

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Magnétoélectricité et pyroconductivité.

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Abstract

Magnetoelectric classes in which the magnetoelectric tensor is non-symmetrical allow the existence of spontaneous electrical currents.

Les 58 classes magnétoélectriques ont été énumérées par Indenbom (1960; voir aussi Cracknell, 1975), qui a précisé la forme du tenseur magnétoélectrique dans chacune d'elles. La théorie des représentations permet d'obtenir simplement ces résultats (Bertaut, 1968; Sivardière & Waintal, 1969; Sivardière, 1969).

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Par ailleurs Ascher (1965) a énuméré les 31 classes 'pyroconductives' décrivant le symétrie ponctuelle des cristaux porteurs de courants électriques spontanés **j**. On remarque que ces 31 classes sont comprises dans les 58 classes magnétoélectriques (au contraire les 31 classes pyroélectriques et les 31 classes pyromagnétiques ne sont pas toutes magnétoélectriques): les tenseurs magnétoélectriques Q_{ij} correspondants sont non symétriques. Dans les autres classes magnétoélectriques, les tenseurs magnétoélectriques sont symétriques.

Cette propriété s'interprète aisément. Dans une classe pyroconductive, un vecteur de Poynting $\mathbf{E} \times \mathbf{B}$ construit à partir d'un champ électrique **E** et d'un champ magnétique **B** est invariant. En effet $\mathbf{E} \times \mathbf{B}$ et **j** se transforment de la même manière dans les opérations $\bar{1}$ (centrosymétrie) et $1'$ (renversement du temps).

Considérons alors une classe magnétoélectrique. Si le tenseur Q_{ij} correspondant est symétrique, on ne peut former aucun invariant magnétoélectrique antisymétrique du type $E_iB_j - E_jB_i$ $(i,j = x,y,z)$, donc on ne peut construire aucun vecteur $\mathbf{E} \times \mathbf{B}$ ou **j** invariant: la classe considérée n'est pas pyroconductive.

Considérons maintenant une classe magnétoélectrique dans laquelle le tenseur Q_{ij} n'est pas symétrique. On peut alors isoler la partie antisymétrique de Q_{ij} et former des invariants antisymétriques du type $E_iB_j - E_jB_i$. Par suite, la classe considérée est pyroconductive.

Ainsi dans la classe $4/m'$, le tenseur **Q** a la forme:

$$\begin{pmatrix} Q_{11} & Q_{12} & 0 \\ -Q_{12} & Q_{11} & 0 \\ 0 & 0 & Q_{33} \end{pmatrix},$$

d'où l'unique invariant antisymétrique $E_xB_y - E_yB_x = (\mathbf{E} \times \mathbf{B})_z$. Cette classe autorise donc l'existence de courants spontanés parallèles à l'axe z.

De même dans la classe $2'/m$, **Q** a la forme:

$$\begin{pmatrix} 0 & 0 & Q_{13} \\ 0 & 0 & Q_{23} \\ Q_{31} & Q_{32} & 0 \end{pmatrix}$$

(en choisissant l'axe binaire parallèle à Oz), d'où les invariants antisymétriques $E_xB_z - E_zB_z = (\mathbf{E} \times \mathbf{B})_y$ et $E_yB_z - E_zB_y = (\mathbf{E} \times \mathbf{B})_x$. Cette classe autorise donc l'existence de courants spontanés parallèles au plan xy.

En conclusion, les classes magnétoélectriques dans lesquelles le tenseur **Q** n'est pas symétrique sont pyroconductives: la forme de **Q** indique la direction des courants spontanés autorisés.

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Rapid comparison of protein structures.

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Abstract

An unusually fast method of superposing two sets of atomic coordinates for related molecular structures by least squares is described. It exploits the special nature of the problem and uses the method of conjugate gradients. The calculation takes about 0·003 s and is fast enough to be used in on-line graphics systems.

The object of this paper is to describe a very fast and simple iterative method for calculating the rigid-body rotations which are needed to match protein structures to one another. The analysis of structures often requires two sets of coordinates for a group of atoms to be compared by finding the rigid-body rotation and translation which matches them as closely as possible. This least-squares fitting approach has been used to compare closely-related proteins (Freer, Kraut, Robertus, Wright & Xuong, 1970; Huber, Epp, Steigemann & Formanek, 1971; Lesk & Chothia, 1980) or different functional forms of the same molecule (Baldwin & Chothia, 1979); to assess the validity of energy minimization methods (Cohen & Sternberg, 1980); and to superpose repeated structural elements within the same protein (McLachlan, 1972*a*). In simple one-to-one comparisons the time spent in the superposition calculation is unimportant, but more general methods involve multiple comparisons, with a systematic search for fragments of structure anywhere in one protein, *A*, which are similar to any part of a second protein, *B* (Rao & Rossmann, 1973; Rossmann & Argos, 1976, 1977; Remington & Matthews, 1978; McLachlan, 1979). Studies of this kind have been used to assess the significance of structural relationships between proteins which may have descended from a common evolutionary ancestor (Remington & Matthews, 1980; Schulz, 1980).

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