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How to Calculate Planarity Restraints

BY A. G. URZHUMTSEV

Research Computing Center, USSR Academy of Sciences, Pushchino, Moscow region, 142292 *USSR*

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Abstract

Planarity of some atomic groups is one of the important stereochemical features of a model under refinement. A planarity restraint is usually included in the functional to be minimized. A new method of *analytical* calculation of the exact gradient value is suggested for the standard function [Schomaker, Waser, Marsh & Bergman (1959). *Acta Cryst.* **12**, 600-604] which controls planarity in the most direct way. This approach makes it possible to refine the optimum plane orientation at the same time as atomic coordinates.

I. Introduction

The procedure for atomic model refinement in protein crystallography is (or may be reduced to) a minimization of some functional. This functional is usually a sum of simple criteria, each of which is responsible for a special type of restraint. One of the most important stereochemical restraints imposed on a number of atomic groups is a planarity restraint. It usually consists of items of the same type, each of which is a function of the coordinates of the atoms which should lie on the plane. The function value increases with planarity distortion.

Various approaches are known to define such a function. In one of them planarity is controlled by means of bond lengths, bond angles *etc.* (Waser, 1963; Levitt & Lifson, 1969; Hermans & McQueen, 1974; Ten Eyck, Weaver & Matthews, 1976; Chambers & Stroud, 1977). Another method is the introduction of one (Dodson, Isaacs & Rollett, 1976) or two (French, 1975; Tomlin, 1987) dummy atoms at a distance from the best plane through a group of atoms and changing the distances between atoms of the group and the dummy atoms. The third approach (used, for example, in a program by Hendrickson & Konnert, 1980) is based on the calculation of a root-mean-square deviation of atoms from the best plane (Schomaker *et al.*, 1959). This approach seems the most suitable of the three, since the two others define planarity requirements in a less direct way and are not always effective (the latter was demonstrated by Haneef, Moss, Stanford & Borkakoti, 1985). But one should keep in mind when dealing with the last method that it requires the calculation of the best plane parameters. Usually, they are determined with the iterative procedure of Frazer, Duncan & Collar (1938), and the best plane orientation is difficult to refine. To avoid the problem of the choice of the best plane, Haneef *et al.* (1985) suggested a new variant of this approach that does not need optimal plane parameters and makes use of a very simple criterion.

In spite of the evident advantages, the criterion of Haneef *et al.* (1985) has an important feature: it distorts the atomic group, forcing atoms to move towards the centre of the group. This effect is explained in the present work. Of course, other functionals, *e.g.* bond-length restraints, prevents the group from collapsing, but we could not then clearly recognize which functional is responsible for planarity only

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and which is responsible for another restraint. This is therefore not a good method both for comprehension and for some practical studies. So the problem was to combine the directness of the standard criterion (Schomaker *et al.*, 1959) with the possibility of the exact calculation of its gradient.

II. The general method of planarity optimization

1. *The problem of planarity optimization*

Suppose there are N atoms with coordinates $\{\mathbf{r}_j\} = \{x_j, y_j, z_j\}$, $j = 1, \ldots, N$. The equation of a plane may be defined by the unit vector $\mathbf{n}$, $|\mathbf{n}| = 1$, which is perpendicular to the plane, and by a point $\mathbf{m}$ belonging to the plane. The root-mean-square displacement of atoms from the plane is

$$\left(1/N \sum_{j=1,\ldots,N} [(\mathbf{r}_j - \mathbf{m})^T \mathbf{n}]^2\right)^{1/2}, \tag{1}$$

where $\mathbf{a}^T$ means the transposed column vector $\mathbf{a}$. Hence, the function

$$F(\{\mathbf{r}_j\}) = \min_{\mathbf{m},\mathbf{n},|\mathbf{n}|=1} \sum_{j=1,\ldots,N} [(\mathbf{r}_j - \mathbf{m})^T \mathbf{n}]^2 \tag{2}$$

may be taken as a planarity restraint, where the minimum is considered with respect to all possible planes. Then planarity optimization for a group of atoms with coordinates $\{\mathbf{r}_j\}$ would mean the minimization of the function

$$F(\{\mathbf{r}_j\}) \to \min_{\{\mathbf{r}_j\}}. \tag{3}$$

2. *The best-plane determination*

We denote by $\mathbf{m}_*$ and $\mathbf{n}_*$ the value of the parameters $\mathbf{m}$ and $\mathbf{n}$ of the best plane for a given set of atoms, *i.e.* ones minimizing the sum in (2) for a given $\{\mathbf{r}_j\}$. A well known geometric fact is that

$$\mathbf{m}_* = 1/N \sum_{j=1,\ldots,N} \mathbf{r}_j, \tag{4}$$

i.e. $\mathbf{m}_*$ is the centroid of a system of points with coordinates $\{\mathbf{r}_j\}$. Hence, the replacement of variables

$$\mathbf{r}_j \to \mathbf{q}_j = \mathbf{r}_j - 1/N \sum_{j=1,\ldots,N} \mathbf{r}_j \tag{5}$$

reduces (2) to a simpler function:

$$f(\{\mathbf{q}_j\}) = \min_{\mathbf{n},|\mathbf{n}|=1} \sum_{j=1,\ldots,N} [\mathbf{q}_j^T \mathbf{n}]^2$$
$$= \sum_{j=1,\ldots,N} [\mathbf{q}_j^T \mathbf{n}_*(\{\mathbf{q}_j\})]^2. \tag{6}$$

To determine the optimal vector $\mathbf{n}_*$ of the normal, Schomaker *et al.* (1959) used a very simple *iterative* procedure of Frazer *et al.* (1938) which gives a *numeric* answer. This is an effective approach but it leads to some problems when $f(\{\mathbf{q}_j\})$ is minimized. Gradient methods are usually used for atomic model refinement and the gradient of the function f should be calculated. However, the derivatives of the $\mathbf{n}_*(\{\mathbf{q}_j\})$ are difficult to calculate when using an iterative procedure, and usually only partial derivatives of the function f with respect to $\mathbf{q}_j$ are calculated. This means that vector $\mathbf{n}_*$ is a constant when calculating the gradient of $f(\{\mathbf{q}_j\})$ and the plane orientation is not refined during the minimization step.

3. *The approach by Haneef et al.* (1985)

The sum in (6), the minimum of which is equal to zero, may be rewritten as

$$\sum_{j=1,\ldots,N} [\mathbf{q}_j^T \mathbf{n}]^2 = \mathbf{n}^T V \mathbf{n}, \tag{7}$$

where

$$V = V(\{\mathbf{q}_j\}) = \sum_{j=1,\ldots,N} [\mathbf{q}_j \mathbf{q}_j^T]. \tag{8}$$

The right-hand side of (7) is equal to zero if and only if the determinant of matrix V is also equal to zero:

$$\sum_{j=1,\ldots,N} [\mathbf{q}_j^T \mathbf{n}]^2 = 0 \leftrightarrow \det V(\{\mathbf{q}_j\}) = 0. \tag{9}$$

Proceeding from this fact, Haneef *et al.* (1985) suggested the following form for the minimization problem (3):

$$f_V(\{\mathbf{q}_j\}) = \det V(\{\mathbf{q}_j\}) \to \min_{\{\mathbf{q}_j\}}. \tag{10}$$

Such a replacement of the function to be minimized looks attractive since it makes the determination of the best plane unnecessary and greatly simplifies the calculation of the new functional and its gradient.

4. *Comparison of the functionals*

Let λ_1, λ_2 and λ_3 denote the eigenvalues of the matrix V defined in (8) and $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ denote the corresponding normalized eigenvectors ($|\mathbf{v}_j| = 1$ for $j = 1, 2, 3$). The eigenvalues are non-negative, $0 \le \lambda_1 \le \lambda_2 \le \lambda_3$, since the matrix is symmetric and positively defined. Because of the orthogonality of eigenvectors, any unit vector $\mathbf{n}$ may be written as the sum

$$\mathbf{n} = \alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \alpha_3 \mathbf{v}_3 \tag{11}$$

with

$$\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1 \tag{12}$$

and (6) with (7) taken into account becomes

$$f(\{\mathbf{q}_j\}) = \min_{\alpha_1,\alpha_2,\alpha_3} [\alpha_1^2 \lambda_1(\{\mathbf{q}_j\})$$
$$+ \alpha_2^2 \lambda_2(\{\mathbf{q}_j\}) + \alpha_3^2 \lambda_3(\{\mathbf{q}_j\})]. \tag{13}$$

Here the minimization in (13) with respect to α_1, α_2, α_3 under condition (12) means the search for the best plane. This minimum which is λ_1 can be achieved at $\alpha_1 = 1$, $\alpha_2 = 0$, $\alpha_3 = 0$, *i.e.* when $\mathbf{n}$, the normal vector

to the plane, is an eigenvector of matrix V corresponding to its smallest eigenvalue. So the problem of optimization (3) is reduced to the problem of minimization of the smallest eigenvalue of matrix V (Schomaker *et al.*, 1959; Urzhumtsev, Lunin & Vernoslova, 1989):

$$f(\{\mathbf{q}_j\}) = \lambda_1(\{\mathbf{q}_j\}) \to \min_{\{\mathbf{q}_j\}}. \qquad (14)$$

Also it follows from (13) that the eigenvalues λ_1, λ_2 and λ_3 are characteristics of the degree of planarity of the atomic group along the eigenvectors of matrix V: λ_1 corresponds to the 'best' direction, λ_3 to the 'worst' direction and λ_2 to a third direction perpendicular to them.

Since the determinant of the matrix V may be calculated as

$$\det V = \lambda_1\lambda_2\lambda_3, \qquad (15)$$

it can be seen that the minimization (10) proposed by Haneef *et al.* (1985) optimizes planarity along 'all directions at a time', not along the 'best' direction. In other words, the 'volume' of the system of points is minimized and points move towards the centre of mass. It is easy to see that this is not quite the task we have stated above. This also explains why it is not necessary now to calculate the best plane.

III. Analytical calculation of the standard planarity criterion

1. *Analytical calculation of the smallest eigenvalue*

Since it has been proved that problems (3) and (14) are the same, the *analytical* method of $\lambda_1(\{\mathbf{q}_j\})$ calculation could eliminate the principal shortcoming of the criterion (2) in gradient calculation.

The set of eigenvalues of matrix V defined in (8) may be determined from the equation

$$\det[V - \lambda E] = 0, \qquad (16)$$

where E is a unit matrix. If we denote $\mathbf{q}_j = \{X_j, Y_j, Z_j\}$, the eigenvalues are roots of

$$\lambda^3 + a\lambda^2 + b\lambda + c = 0, \qquad (17)$$

where

$$a = -S_{XX} - S_{YY} - S_{ZZ} \qquad (18a)$$

$$b = \det\begin{pmatrix} S_{XX} & S_{XY} \\ S_{YX} & S_{YY} \end{pmatrix} + \det\begin{pmatrix} S_{YY} & S_{YZ} \\ S_{ZY} & S_{ZZ} \end{pmatrix} + \det\begin{pmatrix} S_{XX} & S_{XZ} \\ S_{ZX} & S_{ZZ} \end{pmatrix} \qquad (18b)$$

$$c = -\det\begin{pmatrix} S_{XX} & S_{XY} & S_{XZ} \\ S_{YX} & S_{YY} & S_{YZ} \\ S_{ZX} & S_{ZY} & S_{ZZ} \end{pmatrix} \qquad (18c)$$

and S_{XX} denotes $\sum_{j=1,\ldots,N} X_jX_j$, S_{XY} denotes $\sum_{j=1,\ldots,N} X_jY_j$ *etc.* The use of the new variable

$$\mu = \lambda + a/3 \qquad (19)$$

reduces (17) to

$$\mu^3 + g\mu + h = 0 \qquad (20)$$

where

$$g = -a^2/3 + b \qquad (21a)$$

$$h = 2(a/3)^3 - ab/3 + c. \qquad (21b)$$

Since the eigenvalues of the matrix V is real, the roots of (20) may be expressed as (Korn & Korn, 1968)

$$\begin{aligned} \mu_0 &= 2(-g/3)^{1/2}\cos[\alpha/3] \\ \mu_+ &= 2(-g/3)^{1/2}\cos[(\alpha+2\pi)/3] \\ \mu_- &= 2(-g/3)^{1/2}\cos[(\alpha-2\pi)/3] \end{aligned} \qquad (22)$$

where

$$\cos(\alpha) = -\tfrac{1}{2}h(-g/3)^{-3/2}. \qquad (23)$$

Let us choose a value of α in the interval $[0, \pi]$ as a solution of (23). Then it can be seen from the trigonometric circle (Fig. 1) that in all situations root μ_+ is not greater than μ_- and μ_0. Hence,

$$\lambda_1(\{\mathbf{q}_j\}) = \mu_+(\{\mathbf{q}_j\}) - a(\{\mathbf{q}_j\})/3 \qquad (24)$$

and may be calculated *analytically* by (18)-(24). Thus, the full chain of the criterion calculations is

$$\{\mathbf{r}_j\} \xrightarrow{(5)} \{\mathbf{q}_j\} \xrightarrow{(18)} a, b, c \xrightarrow{(21)} g, h \xrightarrow{(23)} \cos(\alpha) \xrightarrow{(22)} \mu_+ \xrightarrow{(24)} \lambda_1. \qquad (25)$$

2. *Gradient calculation*

Gradient calculation for the functional to be minimized is a necessary step of the refinement procedures used nowadays. Since planarity restraint is a

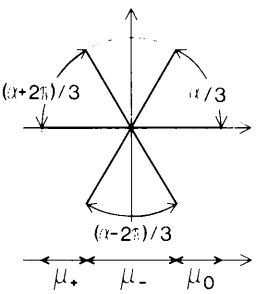

Fig. 1. A schematic diagram of the roots of the reduced third-degree equation $\mu^3 + g\mu + h = 0$:

$\mu_0 = 2(-g/3)^{1/2}\cos[\alpha/3]$;

$\mu_+ = 2(-g/3)^{1/2}\cos[(\alpha+2\pi)/3]$;

$\mu_- = 2(-g/3)^{1/2}\cos[(\alpha-2\pi)/3]$.

Here $0 \le \alpha(g, h) \le \pi$.

component of the functional, its gradient should also be calculated.

It follows from the fast differentiation algorithm (Kim, Nesterov & Cherkasskiy, 1984; Lunin & Urzhumtsev, 1985) that the gradient of an arbitrary functional depending on *any number of variables* may be calculated using practically the same time as is needed to compute the function itself. Besides, no difference approaches are needed in this case and the calculated gradient value is *exact*, not *approximate*. This is performed by 'reversing' the chain of the functional calculations, *i.e.* by calculating at each step the gradient with respect to the variables in the preceding step of the functional calculation.

Following this algorithm the gradient of $\lambda(\{\mathbf{r}_j\})$ should be calculated with the 'reversed' chain (25):

$$\nabla_{\mu_+}\lambda_1 \rightarrow \nabla_{\cos(\alpha)}\lambda_1 \rightarrow \nabla_{gh}\lambda_1 \rightarrow \nabla_{abc}\lambda_1 \rightarrow \nabla_{\mathbf{q}}\lambda_1 \rightarrow \nabla_{\mathbf{r}}\lambda_1. \quad (26)$$

Here $\nabla_{\mathbf{x}} f$ means the gradient of the function f calculated with respect to the variables $\mathbf{x}$. Note that to calculate

$$\partial\lambda_1/\partial\cos(\alpha) = [\partial\lambda_1/\partial\mu_+][\partial\mu_+/\partial\cos(\alpha)] \quad (27)$$

in the first step of (26) one may use the transformation

$$d\cos[(\alpha+2\pi)/3]/d\cos(\alpha) = \{d\cos(\alpha)/d\cos[(\alpha+2\pi)/3]\}^{-1} = \tfrac{1}{3}\{4\cos^2[(\alpha+2\pi)/3]-1\}^{-1}. \quad (28)$$

3. *Singular situations*

Roots of equation (20) are real if (Korn & Korn, 1968)

$$R_1 = (g/3)^3 + (h/2)^2 \leq 0 \quad (29)$$

$$R_2 = g \leq 0. \quad (30)$$

When R_1 is small ($R_1 \rightarrow -0$), it is difficult to compute (28) because $R_1 = 0$ yields $\alpha = 0$ and $\cos[(\alpha+2\pi)/3] = \frac{1}{2}$. Besides, if $g \rightarrow -0$ [it follows from (29) that $h \rightarrow 0$ and $R_1 \rightarrow -0$], then problems arise with the calculation of $\cos(\alpha)$ or $\nabla_{gh}\lambda_1$. So, in practical calculations for $R_1 > -\varepsilon$ (ε is some small positive value) we set

$$g = -3[\varepsilon + h^2/4]^{1/3} \quad (31)$$

which gives $R_1 = -\varepsilon < 0$ and $R_2 = g < 0$.

4. *Remark. A linearity criterion of an atomic group*

Following Schomaker *et al.* (1959), we can propose a similar criterion to 'linearize' an atomic group. In terms of the eigenvalues, it states the minimality of the *two* smallest eigenvalues, λ_1 and λ_2, *e.g.*

$$f_1(\{\mathbf{q}_j\}) = \lambda_1(\{\mathbf{q}_j\}) + \lambda_2(\{\mathbf{q}_j\}) \rightarrow \min_{\{\mathbf{q}_j\}}. \quad (32)$$

It is clear from Fig. 1 that λ_1 and λ_2 correspond to μ_+ and μ_-. This shows the possibility of an analytical expression for such a criterion and its gradient.

IV. Model calculations

To test our approach we used a 'tyrosine-type' model structure consisting of eight 'atoms'. The atoms were initially placed in the plane $z = 0$ at a distance of 1·5 Å to form a six-membered ring with an extra couple of atoms connected to two opposite ring atoms (Fig. 2). Then the end atoms, *A* and *H*, were shifted by Δr along the z axis and the ring atoms *B* and *G* were connected to them by a movement of the same amount in the opposite direction. For such a system of points we calculated the gradient of functional f_V proposed by Haneef *et al.* [see (10)] and the gradient of the functional f defined in (14). It may be seen from Table 1 that the stronger the distortion of the plane, the more the criterion f_V forces atoms to move toward the centre (the gradient is opposite to the direction of minimization). In contrast, the gradient of the criterion f calculated with (26) has no noise components until Δr reaches a value of 1·50 Å, after which the atoms begin to pack in a new plane, $y = 0$.

We discuss here only gradient calculation but no test refinement because the latter is connected with a different question of the choice of methods and strategy of minimization. This example has shown that our approach allows one to restrain only what is wanted to be restrained and from this point of view the approach seems preferable to others used nowadays.

V. Concluding remarks

Different criteria may be used to restrain the planarity of atomic groups. The very convenient criterion by Haneef *et al.* (1985) has a principal shortcoming. In the present paper we have shown that the well known standard criterion (Schomaker *et al.*, 1959) may be rewritten in an analytically tractable form. Although slightly more time consuming than the method of Haneef *et al.* (1985), the present method is free from the defects of the latter while preserving its most

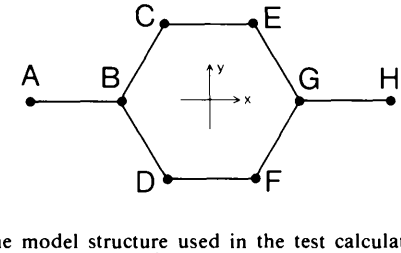

Fig. 2. The model structure used in the test calculations. Interatomic distances are 1·5 Å. The z coordinates are set: for 'atoms' *A* and *H* to $+\Delta\mathbf{r}$, for 'atoms' *B* and *G* to $-\Delta\mathbf{r}$, and for 'atoms' *C*, *D*, *E* and *F* to zero.

Table 1. *Gradients of planarity criteria calculated for the model structure*

Gradients are normalized under $|\nabla F_{A,z}| = 10\,000$. Here *A*, *B*, *C* are different atomic types (Fig. 2).

		A			*B*			*C*		
Δr	Criterion	∇_x	∇_y	∇_z	∇_x	∇_y	∇_z	∇_x	∇_y	∇_z
0·10	f_V*	−484	0	10 000	−242	0	−10 000	−121	775	0
0·25	f_V	−1210	0	10 000	−605	0	−10 000	−303	1 938	0
0·50	f_V	−2424	0	10 000	−1212	0	−10 000	−606	3 876	0
0·75	f_V	−3630	0	10 000	−1815	0	−10 000	−909	5 813	0
1·00	f_V	−4848	0	10 000	−2424	0	−10 000	−1212	7 752	0
1·25	f_V	−6060	0	10 000	−3030	0	−10 000	−1515	9 690	0
1·50	f_V	−7260	0	10 000	−3630	0	−10 000	−1815	11 625	0
0·10–1·25	f†	0	0	10 000	0	0	−10 000	0	0	0
1·50	f‡	0	0	0	0	0	0	0	10 000	0

* $f_V = \lambda_1\lambda_2\lambda_3$ [see (10), (15)].
† $f = \lambda_1$ [see (14)]
‡ Here normalization is under the condition $|\nabla f_{C,z}| = 10\,000$.

important property of an analytical expression in terms of atomic parameters. The exact gradient can also be easily calculated, which makes it possible to refine optimal plane parameters. This method of calculation of this criterion and its gradient may be included in any refinement program.

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Diffraction Streaks from the Chimney Ladder Structure in an $(Sr_{1.5}Ca_{1.5})Cu_{5+\delta}O_y$ Crystal

BY XIAO-JING WU, EIJI TAKAYAMA-MUROMACHI, SHIGERU SUEHARA AND SHIGEO HORIUCHI

National Institute for Research in Inorganic Materials, Tsukuba, Ibaraki, 305, *Japan*

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Abstract

A crystal of $(Sr_{1.5}Ca_{1.5})Cu_{5+\delta}O_y$ has been studied by means of electron diffraction analysis and high-resolution transmission electron microscopy. A chimney ladder structure has been identified in the crystal, which is composed of two sets of incommensurate orthorhombic sublattices L_1 and L_2 with $a = a_1 = a_2 = 1{\cdot}28$, $b = b_1 = b_2 = 1{\cdot}13$, $c_1 = 0{\cdot}390$ and $c_2 = 0{\cdot}275$ nm. Diffraction streaks have been observed in electron diffraction patterns, *i.e.* there is a set of reflection planes parallel to $\mathbf{a}^*\mathbf{b}^*$ related to L_2. A structure model with initial phase disorder has been proposed to explain such diffraction streaks. A mathematical

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