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A GENERALIZED MATRIX OF SYMMETRY ELEMENTS

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Abstract. Each point symmetry operation can be described with an abbreviated symbol $\alpha(D, M, N, P)$ in which

α — angle of rotation (also 0° in the case of mirror planes)
D — + 1 for a simple axis, — 1 for a mirror axis
MNP — coordinates of a point in space fulfilling the condition

$$M^2 + N^2 + P^2 = 1$$

The paper contains a generalized matrix, the elements of which can be easily calculated from data contained in the abbreviated symbol. Formulae for deciphering each given matrix and for writing it in the form of the abbreviated symbol are also given.

INTRODUCTION

Symmetry operations can be described — as known — with the following general matrix:

$$a_{ij} = \left\| \begin{matrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{matrix} \right\| \qquad [1]$$

In the case of operations which transform the coordinates of each point in space (x, y, z) to $(x' \; y' \; z')$ without changing the coordinates of the point (0, 0, 0) the general matrix [1] can be written in the following simpler form:

$$a_{ij} = \left\| \begin{matrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{matrix} \right\| \qquad [2]$$

Using this matrix description of symmetry operations it is sometimes difficult and troublesome to find the proper a_{ij} — values for a given operation. On the other hand, if a matrix describing a symmetry operation is given,

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one can not always easily see from the matrix which symmetry operation it represents. In this paper the possibilities of overcoming these difficulties are discussed.

ANALYSIS OF THE GENERAL MATRIX a_{ij}

Because of the additional condition valid in the crystallography, that the distance between two arbitrary chosen points P and Q must remain unchanged after the transformation of coordinates, the following well known equations must be fulfilled:

$$\begin{aligned} a_{11}^2 + a_{21}^2 + a_{31}^2 &= 1 \\ a_{12}^2 + a_{22}^2 + a_{32}^2 &= 1 \\ a_{13}^2 + a_{23}^2 + a_{33}^2 &= 1 \end{aligned} \qquad [3a]$$

$$\begin{aligned} a_{11}\cdot a_{12} + a_{21}\cdot a_{22} + a_{31}\cdot a_{32} &= 0 \\ a_{11}\cdot a_{13} + a_{21}\cdot a_{23} + a_{31}\cdot a_{33} &= 0 \\ a_{12}\cdot a_{13} + a_{22}\cdot a_{23} + a_{32}\cdot a_{33} &= 0 \end{aligned} \qquad [3b]$$

$$D^2 = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}^2 = 1 \qquad [3c]$$

If $D = 1$ the matrix [2] describes a simple rotation, if $D = -1$ the symmetry operation consists in rotation with simultaneous reflection in a mirror plane perpendicular to the axis of rotation and passing through the point (0, 0, 0). Mirror plane alone can be thus considered as rotation by an angle 0° (or 360°) with simultaneous reflection. Symmetry center can be treated as rotation by 180° with simultaneous reflection.

All matrices of the type [2] fulfilling the conditions [3] consist therefore in rotation (also by the angle of 0°) and differ only from the point of view whether they describe a simple rotation ($D = 1$) or a rotation with simultaneous reflection ($D = -1$).

The position of each simple axis or of a mirror axis will be described in this paper with aid of coordinates M, N, P of a point through which this axis passes. As the axis must pass also through the point (0, 0, 0) the position of the axis in the space is exactly determined when the coordinates M, N, P are known. For sake of convenience the point with coordinates (M, N, P) can be chosen on the surface of a sphere with the radius equal 1. The coordinates M, N, P will fulfill in this case the condition

$$M^2 + N^2 + P^2 = 1$$

Each symmetry operation of the type [2] is clearly determined if the values α, D, M, N, P are given. α denotes the angle of rotation, D — determines the kind of operation (simple rotation or rotation with reflection), M, N, P — describe the position of the axis in the space.

THE GENERALIZED MATRIX

If we introduce the values α, D, M, N, P explicite in the general matrix [2] we obtain a following new matrix:

$$\begin{Vmatrix} M^2R + \cos\alpha & MNR - P\cdot\sin\alpha & MPR + N\cdot\sin\alpha \\ MNR + P\cdot\sin\alpha & N^2R + \cos\alpha & NPR - M\cdot\sin\alpha \\ MPR - N\cdot\sin\alpha & NPR + M\cdot\sin\alpha & P^2R + \cos\alpha \end{Vmatrix} \qquad [4]$$

where $R = D - \cos\alpha$

Substituting corresponding values for α, D, M, N, P we can easily obtain a matrix describing a given symmetry operation. We can thus introduce an abbreviated symbol for each symmetry operation: $\alpha(D, M, N, P)$. Knowing all values which appear in this abbreviated symbol, we can — with aid of the generalized matrix — easily write the matrix representing the given operation.

Example 1

Let us check the applicability of the generalized matrix in the case of a fourfold axis perpendicular to the x, z — plane of the coordinate system. The rotation angle is equal to 90° ($\cos\alpha = 0$, $\sin\alpha = 1$), D is equal to 1 (the operation being a simple rotation), $R = 1$. The coordinates M, N, P, are 0, 1, 0 the rotation axis being identical with the y-axis of the coordinate system. Substituting we receive the following matrix

$$\begin{Vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{Vmatrix}$$

which means

$$x' = z \qquad y' = y \qquad z' = -x$$

We can thus write

$$90(1,\ 0,\ 1,\ 0) = \begin{Vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{Vmatrix}$$

With aid of the generalized matrix [4] we can thus easily "translate" the abbreviated symbol into the coorersponding matrix.

DECIPHERING OF MATRICES

Let us consider now the vice-versa operation i.e. the "translation" of a given matrix into the abbreviated symbol from which it can be easier seen what kind of operation is described by this matrix. If we denote the sum $a_{11} + a_{22} + a_{33}$ as S, we obtain easily the following expression from which the rotation angle can be calculated

$$\cos\alpha = \frac{S - D}{2}$$

The value $\cos\alpha$ does not change when α changes its sign. Knowing the $\cos\alpha$-value we do not know the sign of the angle. Let us assume that the angle α will be considered to be positive when regarding the point (0, 0, 0) from the point M, N, P, we see the rotation as a left one i.e. performed in the opposite direction than the course of clock hands. Let us further assume that the rotations will be described only in terms of positive values of α.

For M, N, P we obtain from the generalized matrix the following expressions

$$M = \frac{a_{32} - a_{23}}{2 \cdot \sin \alpha} \qquad N = \frac{a_{13} - a_{31}}{2 \cdot \sin \alpha}$$

$$P = \frac{a_{21} - a_{12}}{2 \cdot \sin \alpha}$$

which are valid when $\sin \alpha \neq 0$.

If $\sin \alpha = 0$ the expressions for MNP lose their meaning. In this case we can have to do with two possibilities $\cos \alpha = 1$ or $\cos \alpha = -1$. Taking into account the fact that there exist two kinds of operations with $D = 1$ or $D = -1$ we have to consider the following four possibilities:

1. $D = 1$ $\quad \cos \alpha = 1$
2. $D = 1$ $\quad \cos \alpha = -1$
3. $D = -1$ $\quad \cos \alpha = 1$
4. $D = -1$ $\quad \cos \alpha = -1$

In all these four cases the generalized matrix has the form

$$\begin{Vmatrix} M^2R + \cos \alpha & MNR & MPR \\ MNR & N^2R + \cos \alpha & NPR \\ MPR & NPR & P^2R + \cos \alpha \end{Vmatrix} \qquad [5]$$

because of the fact that $\sin \alpha = 0$. If $\sin \alpha = 0$ the matrix is thus always symmetrical with respect to its chief diagonal

ad 1. $R = D - \cos \alpha = 1 - 1 = 0 \quad \cos \alpha = 1 \quad D = 1$

The generalized matrix has the form

$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix}$$

and describes an operation of identity

$$x' = x \qquad y' = y \qquad z' = z$$

ad 2. $R = D - \cos a = 2 \quad \cos \alpha = -1 \quad D = 1$

The matrix has the form

$$\begin{Vmatrix} 2M^2 - 1 & 2MN & 2MP \\ 2MN & 2N^2 - 1 & 2NP \\ 2MP & 2NP & 2P^2 - 1 \end{Vmatrix} \qquad [6]$$

and describes a twofold axis i.e. a rotation by 180°. The values M^2, N^2 and P^2 can be easily derived from a_{11}, a_{22}, a_{33} respectively. The signs can be assumed in the following maner:

if $M^2 \neq 0$, we chose for M the positive value; the signs for N and P result from the sign of a_{12} and a_{13} respectively;

if $M^2 = 0$, we calculate the N — value and assume it positive. The sign for P results from a_{23}.

If $M^2 = 0$ and $N^2 = 0$ we assume for P the value of $+1$.

ad 3. $R = D - \cos \alpha = -2 \quad \cos \alpha = -1 \quad D = -1$

The matrix has the form:

$$\begin{Vmatrix} -2M^2 + 1 & -2MN & -2MP \\ -2MN & -2N^2 + 1 & -NP \\ -MP & -2NP & -2P^2 + 1 \end{Vmatrix} \qquad [7]$$

The values M, N, P are calculated exactly as in the item [2]. The matrix represents a mirror plane.

ad 4. $R = 0 \quad \cos \alpha = -1 \quad D = -1$

The matrix has the form

$$\begin{Vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{Vmatrix}$$

and describes a symmetry center

$$x' = -x \qquad y' = -y \qquad z' = -z$$

In the case of both matrices

$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} \qquad \begin{Vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{Vmatrix}$$

the values MNP can not be evoluated, but are not needed. In the abbreviated form the matrices can be written as 0 (1, MNP) and 180 (-1, MNP).

Example 2

Let us describe the steps needed for deciphering a given matrix, e.g.:

$$\begin{Vmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{Vmatrix}$$

First step: *calculation of D*

As easily seen $D = +1$

conclusion: a simple rotation

Second step: *calculation of cos α* $\quad S = a_{11} + a_{22} + a_{33} = 1$

$$\cos \alpha = \frac{S - D}{2} = 0$$

conclusion: rotation by an angle of 90°

Third step: *calculation of M, N, P*

The matrix being not symmetrical with respect to its diagonal the formulae for M, N, P can be used

$$M = 0 \qquad N = 0 \qquad P = 1$$

Conclusion: the matrix describes an axis of rotation by 90°. The axis is identical with the z-axis of the coordinate system.

Example 3

What kind of symmetry operation is described by the matrix:

$$\begin{Vmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{Vmatrix}$$

As easily seen $D = -1$, we have to do with an axis combined with a simultaneous reflection in a mirror plane perpendicular to it.

$$\cos\alpha = 1 \qquad \sin\alpha = 0$$

$$-2M^2 + 1 = 0 \qquad M^2 = \frac{1}{2} \quad M = \frac{\sqrt{2}}{2}$$

$$-2N^2 + 1 = 1 \qquad N = 0$$

$$-2P^2 + 1 = 0 \qquad P^2 = \frac{1}{2} \quad P = \frac{\sqrt{2}}{2}$$

The abbreviated symbol can be thus written $0\left(-1, \frac{\sqrt{2}}{2}, 0, \frac{\sqrt{2}}{2}\right)$. We have to do with a mirror plane perpendicular to the straight line passing through $\left(\frac{\sqrt{2}}{2}, 0, \frac{\sqrt{2}}{2}\right)$ and (0, 0, 0).

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UOGÓLNIONIA MACIERZ ELEMENTÓW SYMETRII

Streszczenie

Każdą operację symetrii punktowej można opisać za pomocą skróconego symbolu $\alpha(D, M, N, P)$, w którym

α — kąt obrotu (również 0° w przypadku płaszczyzny symetrii)
D — +1 dla zwykłej osi symetrii, −1 dla osi zwierciadlanej
MNP — współrzędne punktu charakteryzujące położenie osi w przestrzeni i spełniające równanie:

$$M^2 + N^2 + P^2 = 1$$

W pracy podano macierz uogólnioną, której elementy można z łatwością obliczyć na podstawie danych występujących w skróconym symbolu. Podano również wzory umożliwiające „rozszyfrowanie" każdej macierzy i napisanie jej w postaci symbolu skróconego.

Иосиф НЭДОМА

ОБОБЩЕННАЯ МАТРИЦА ЭЛЕМЕНТОВ СИММЕТРИИ

Резюме

Любую операцию симметрии можно описать при помощи сокращенного символа α (D, M, N, P) в котором:

α — угол вращения (также 0° в случае плоскости симметрии)
D — +1 для обыкновенной оси вращения, −1 для зеркальной оси вращения
MNP — координаты точки описывающей расположение оси в пространстве, удовлетворяющие уравнению:

$$M^2 + N^2 + P^2 = 1$$

В работе приведена обобщенная матрица элементы которой можно вычислать на основании данных содержащихся в сокращенном символе. Приведены также формулы для „расшифровки" любых матриц и „перевода" их символи сокращенной записи.