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ORIENTED SYMMETRY ELEMENTS IN SPACE
PART 1. ABBREVIATED SYMBOLS

Abstract. Abbreviated symbols of the general type

$$n\left(\begin{array}{c|c} M & A \\ N & B \\ P & C \end{array}\right) \quad \text{and} \quad n\left(\frac{M\ N\ P}{x_0\ y_0\ z_0}\right)$$

for describing oriented symmetry elements in space are defined.

INTRODUCTION

In the series of foregoing papers published in this journal (1980—1983) the problems of coexistence of oriented point symmetry elements have been discussed in terms of abbreviated matrix symbols. Now an attempt will be made to enlarge these symbols in such a manner to discuss the problems of oriented symmetry elements coexisting in space.

GENERAL REMARKS

As demonstrated earlier each point symmetry operation can be described using one of two possible abbreviated symbols:

$n(MNP)$ for usual rotation axes
$\bar{n}(MNP)$ for inversion axes

Using the generalized matrix we can always pass from an abbreviated symbol to the corresponding matrix and vice-versa. Let us consider now a symmetry operation coexisting with a translation. The symmetry operation can be written in form of a matrix with elements a_{ij} and the translation can be given as a vector T with components $T_x T_y T_z$.

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If we transform the coordinates of a point x, y, z using firstly the matrix with elements a_{ij} and performing then the translation T we obtain three coordinates of a new point which corresponds to the point with coordinates x, y, z.

$$x' = a_{11} \cdot x + a_{12} \cdot y + a_{13} \cdot z + T_x$$
$$y' = a_{21} \cdot x + a_{22} \cdot y + a_{23} \cdot z + T_y$$
$$z' = a_{31} \cdot x + a_{32} \cdot y + a_{33} \cdot z + T_z$$

If we perform firstly the translation and then the transformation described by a_{ij} we obtain other values x', y', z':

$$x' = a_{11} \cdot x + a_{12} \cdot y + a_{13} \cdot z + a_{11} \cdot T_x + a_{12} \cdot T_y + a_{13} \cdot T_z$$
$$y' = a_{21} \cdot x + a_{22} \cdot y + a_{23} \cdot z + a_{21} \cdot T_x + a_{22} \cdot T_y + a_{23} \cdot T_z$$
$$z' = a_{31} \cdot x + a_{32} \cdot y + a_{33} \cdot z + a_{31} \cdot T_x + a_{32} \cdot T_y + a_{33} \cdot T_z$$

In both cases the resulting matrix has the general form:

$$\begin{Vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{Vmatrix}$$

For describing symmetry operations in space we must therefore use matrices of the general type written above (the so called "3×4" — matrices).

Transforming the coordinates of a point x, y, z using firstly the matrix A with elements a_{ij} and acting then on the resulting coordinates with an other matrix B with elements b_{ij} we obtain new coordinates $x'y'z'$ given by the formulae:

$$x' = c_{11} \cdot x + c_{12} \cdot y + c_{13} \cdot z + b_{11} \cdot a_{14} + b_{12} \cdot a_{24} + b_{13} \cdot a_{34} + b_{14}$$
$$y' = c_{21} \cdot x + c_{22} \cdot y + c_{23} \cdot z + b_{21} \cdot a_{14} + b_{22} \cdot a_{24} + b_{23} \cdot a_{34} + b_{24}$$
$$z' = c_{31} \cdot x + c_{32} \cdot y + c_{33} \cdot z + b_{31} \cdot a_{14} + b_{32} \cdot a_{24} + b_{33} \cdot a_{34} + b_{34}$$

where the matrix with elements c_{ij} (matrix C) fulfils the matrix equation $C = B \cdot A$.

As it can be seen the resulting matrix can be easily obtained by usual matrix multiplication if both matrices to be multiplied are written in the form "4×4".

$$\begin{Vmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ 0 & 0 & 0 & 1 \end{Vmatrix} \times \begin{Vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

The resulting matrices in both cases discussed above can be now obtained directly by matrix multiplication:

$$\begin{Vmatrix} 1 & 0 & 0 & T_x \\ 0 & 1 & 0 & T_y \\ 0 & 0 & 1 & T_z \\ 0 & 0 & 0 & 1 \end{Vmatrix} \times \begin{Vmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & a_{23} & 0 \\ a_{31} & a_{32} & a_{33} & 0 \\ 0 & 0 & 0 & 1 \end{Vmatrix} = \begin{Vmatrix} a_{11} & a_{12} & a_{13} & T_x \\ a_{21} & a_{22} & a_{23} & T_y \\ a_{31} & a_{32} & a_{33} & T_z \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

and

$$\begin{Vmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & a_{23} & 0 \\ a_{31} & a_{32} & a_{33} & 0 \\ 0 & 0 & 0 & 1 \end{Vmatrix} \times \begin{Vmatrix} 1 & 0 & 0 & T_x \\ 0 & 1 & 0 & T_y \\ 0 & 0 & 1 & T_z \\ 0 & 0 & 0 & 1 \end{Vmatrix} = \begin{Vmatrix} a_{11} & a_{12} & a_{13} & T'_x \\ a_{21} & a_{22} & a_{23} & T'_y \\ a_{31} & a_{32} & a_{33} & T'_z \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

where

$$T'_x = a_{11} \cdot T_x + a_{12} \cdot T_y + a_{13} \cdot T_z$$
$$T'_y = a_{21} \cdot T_x + a_{22} \cdot T_y + a_{23} \cdot T_z$$
$$T'_z = a_{31} \cdot T_x + a_{32} \cdot T_y + a_{33} \cdot T_z$$

The matrices "3×3" contained in the matrices "4×4" are multiplied exactly in the same manner as in the case of point groups.

Let us limit ourselves to the case when $D = 1$ and introduce the following abbreviated symbol

$$n\begin{pmatrix} M & a_{14} \\ N & a_{24} \\ P & a_{34} \end{pmatrix} \quad \text{for} \quad \begin{Vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

The matrix "3×3" is described with the usual symbol $n(MNP)$. The values MNP are written this time vertically for reasons to be clear later. The right column in the symbol contains the values $a_{14} a_{24} a_{34}$.

Using the methods discussed in foregoing papers we can always write an abbreviated symbol for a given matrix and vice-versa.

EXAMPLE 1

Write an abbreviated symbol for the matrix

$$\begin{Vmatrix} 0 & \bar{1} & 0 & 5 \\ 1 & 0 & 0 & 6 \\ 0 & 0 & 1 & 7 \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

The matrix "3×3" contained in this matrix can be described with the symbol 4(001), then the full abbreviated symbol corresponding to the given matrix is

$$4\begin{pmatrix} 0 & 5 \\ 0 & 6 \\ 1 & 7 \end{pmatrix}$$

EXAMPLE 2

Write the matrix corresponding to the abbreviated symbol

$$3\begin{pmatrix} 1 & 2 \\ 1 & 6 \\ 1 & 1 \end{pmatrix}$$

We write the matrix "3×3" corresponding to the symbol 3(111) and "enlarge" it to

$$\begin{Vmatrix} 0 & 0 & 1 & 2 \\ 1 & 0 & 0 & 6 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

Each symmetry axis described with the symbol $n(MNP)$ passes through the origin of the system of coordinates.

Let us assume now that the symmetry axis must not pass through the point 0, 0, 0 but that it can pass through an arbitrary chosen point with coordinates $x_0 y_0 z_0$. What matrix will describe the action of such a symmetry operation on a point x, y, z?

If we shift all points in space according to the formulae:

$$X = x - x_0 \qquad Y = y - y_0 \qquad Z = z - z_0$$

the point xyz will coincide with the origin of coordinates.

We can therefore write

$$X' = a_{11}\cdot X + a_{12}\cdot Y + a_{13}\cdot Z$$
$$Y' = a_{21}\cdot X + a_{22}\cdot Y + a_{23}\cdot Z$$
$$Z' = a_{31}\cdot X + a_{32}\cdot Y + a_{33}\cdot Z$$

Substituting

$$X' = x' - x_0 \qquad Y' = y' - y_0 \qquad Z' = z' - z_0$$

we obtain

$$x' = a_{11}\cdot x + a_{12}\cdot y + a_{13}\cdot z + (1 - a_{11})\cdot x_0 - a_{12}\cdot y_0 - a_{13}\cdot z_0$$
$$y' = a_{21}\cdot x + a_{22}\cdot y + a_{23}\cdot z - a_{21}\cdot x_0 + (1 - a_{22})\cdot y_0 - a_{23}\cdot z_0$$
$$z' = a_{31}\cdot x + a_{32}\cdot y + a_{33}\cdot z - a_{31}\cdot x_0 - a_{32}\cdot y_0 + (1 - a_{33})\cdot z_0$$

To write such a matrix the matrix elements a_{ij} for the "3×3" matrix and the values $x_0 y_0 z_0$ must be known.

Let us introduce for this matrix the following abbreviated symbol containing all informations needed:

$$n\begin{pmatrix} M\ N\ P \\ \hline x_0\ y_0\ z_0 \end{pmatrix}$$

Knowing this symbol we can immediately write the corresponding matrix: We write firstly the "3×3" matrix for the symbol $n(MNP)$ and then calculate the elements of the fourth column according to formulae

$$a_{14} = (1 - a_{11})\cdot x_0 - a_{12}\cdot y_0 - a_{13}\cdot z_0$$
$$a_{24} = -a_{21}\cdot x_0 + (1 - a_{22})\cdot y_0 - a_{23}\cdot z_0$$
$$a_{34} = -a_{31}\cdot x_0 - a_{32}\cdot y_0 + (1 - a_{33})\cdot z_0$$

EXAMPLE 3

Write the matrix corresponding to the abbreviated symbol $2\begin{pmatrix} 0 & 1 & 1 \\ \hline 3 & 2 & 8 \end{pmatrix}$

We have

$$2(011) = \begin{Vmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{Vmatrix}$$

$$a_{14} = 2\cdot x_0 \qquad a_{24} = y_0 - z_0 \qquad a_{34} = -y_0 + z_0$$
$$a_{14} = 6 \qquad a_{24} = -6 \qquad a_{34} = 6$$

The matrix has the form

$$\begin{Vmatrix} -1 & 0 & 0 & 6 \\ 0 & 0 & 1 & -6 \\ 0 & 1 & 0 & 6 \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

STANDARDIZATION OF THE SYMBOL $N\begin{pmatrix} M\ N\ P \\ \hline x_0\ y_0\ z_0 \end{pmatrix}$

The axis passes not only through the point $x_0 y_0 z_0$: all points with coordinates

$$x_t = x_0 + M\cdot t \qquad y_t = y_0 + N\cdot t \qquad z_t = z_0 + P\cdot t$$

lay also on the axis. Each of them can be chosen to describe the position of the axis in space. This means that for each arbitrary chosen t-value the points with coordinates $x_t y_t z_t$ should lead to the same matrix.

Let us check this supposition for a_{14}

$$a_{14} = (1 - a_{11})\cdot x_t - a_{12}\cdot y_t - a_{13}\cdot z_t$$

After substitution and rearrangement we obtain

$$a_{14} = (1 - a_{11})\cdot x_0 - a_{12}\cdot y_0 - a_{13}\cdot z_0 + t\cdot(M - M\cdot a_{11} - N\cdot a_{12} - P\cdot a_{13})$$

Substituting for $a_{11} a_{12} a_{13}$ their values from the generalized matrix we can easily state that for $D = 1$ the expression in parentheses is always equal zero. Thus independently of t for all points with coordinates $x_t y_t z_t$ fulfilling the parametric equation of the straight line coinciding with the axis the same matrix is obtained.

To pass *vice-versa* from the matrix to the symbol we should calculate the $x_0 y_0 z_0$ values knowing the fourth column elements $a_{14} a_{24} a_{34}$. As the number of points laying on the axis is infinite the set of equations can not be solved for $x_0 y_0 z_0$ (the determinant being equal zero). An additional condition is needed to define only one point on the axis which will be used to describe the position of this axis in space.

If the axis does not pass through the point 0, 0, 0 we can always find on it a point for which $M\cdot x_0 + N\cdot y_0 + P\cdot z_0 = 0$

Using this additional equation we can discuss the general symbol

$$n\begin{pmatrix} M\ N\ P \\ \hline x_t\ y_t\ z_t \end{pmatrix}$$

in the following manner.

If $M\cdot x_t + N\cdot y_t + P\cdot z_t = 0$ the symbol can be treated as written in the standardized form

$$n\begin{pmatrix} M\ N\ P \\ \hline x_0\ y_0\ z_0 \end{pmatrix}$$

If $M\cdot x_t + N\cdot y_t + P\cdot z_t \neq 0$ the symbol can be standardized. The equations for $x_t y_t z_t$ are multiplied by M, N, P respectively and added

$$M\cdot x_t + N\cdot y_t + P\cdot z_t = t$$

because of the assumption $M\cdot x_0 + N\cdot y_0 + P\cdot z_0 = 0$ and because of the fact that normalized MNP values fulfil the equation $M^2 + N^2 + P^2 = 1$

Knowing the t value we can calculate the $x_0 y_0 z_0$ values from equations

$$x_0 = x_t - M\cdot t \qquad y_0 = y_t - N\cdot t \qquad z_0 = z_t - P\cdot t$$

EXAMPLE 4

Les us discuss the symbol

$$2\begin{pmatrix} 0 & 1 & 1 \\ \hline 3 & 2 & 5 \end{pmatrix}$$

This symbol describes a twofold axis 2(011) passing through the point 3, 2, 5.

$$M\cdot x_i+N\cdot y_i+P\cdot z_i=\frac{1}{\sqrt{2}}\cdot 2+\frac{1}{\sqrt{2}}\cdot 5=\frac{7}{\sqrt{2}}$$

The symbol can be standardized

$$x_0=3-0 \quad y_0=2-\frac{7}{2}=\frac{-3}{2} \quad z=5-\frac{7}{2}=\frac{3}{2}$$

In standardized form the symbol can be written

$$2\left(\frac{0 \quad 1 \quad 1}{3 \quad -1.5 \quad 1,5}\right)$$

The corresponding matrix has the form

$$\begin{Vmatrix} -1 & 0 & 0 & 6 \\ 0 & 0 & 1 & -3 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 0 & 1 \end{Vmatrix}$$

independently whether we use the $x_i y_i z_i$ or $x_0 y_0 z_0$ values.

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ZORIENTOWANE ELEMENTY SYMETRII W PRZESTRZENI

Część 1. Symbole skrócone

Streszczenie

Zdefiniowano symbole ogólne typu

$$n\begin{pmatrix} M & \vert & A \\ N & \vert & B \\ P & \vert & C \end{pmatrix} \quad \text{i} \quad n\left(\frac{M\;N\;P}{x_0\;y_0\;z_0}\right)$$

opisujące zorientowane elementy symetrii w przestrzeni.

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ОРИЕНТИРОВАННЫЕ ЭЛЕМЕНТЫ СИММЕТРИИ В ПРОСТРАНСТВЕ

Часть 1. Сокращенные символы

Резюме

Определены общие символы типа

$$n\begin{pmatrix} M & \vert & A \\ N & \vert & B \\ P & \vert & C \end{pmatrix} \qquad n\left(\frac{M\;N\;P}{x_0\;y_0\;z_0}\right)$$

описывающие ориентированные элементы симметрии в пространстве.