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MULTIPLICATION OF SIMPLIFIED MATRIX SYMBOLS

PART I

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Abstract. A multiplication table for symmetry operations coexisting with a sixfold axis is presented. The simplified matrix symbol corresponding to the matrix resulting from two coexisting symmetry operations can be found immediately in the *multiplication table*.

INTRODUCTION

Each point symmetry operation met with in crystallography can be described in terms of the well-known matrix notation or with aid of the simplified notation of the type $n(MNP)$ introduced in one of the foregoing papers (Nedoma 1975).

Both these notations have their advantages and disadvantages:

MATRIX NOTATION

Advantages

1. Two matrices describing two symmetry operations can be immediately multiplied using simple rules of matrix multiplication to obtain the resulting matrix.

2. A matrix describing a given point symmetry operation can be directly used to transform the coordinates of a chosen point in space.

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Disadvantages

1. A matrix corresponding to a given point symmetry operation can not be written immediately, each of its elements must be previously calculated. Generally speaking these calculations are not always easy to be performed.

2. The deciphering of a given matrix can be sometimes difficult. Having a matrix (for instance that resulting from matrix multiplication) we do not always immediately see what symmetry operation it describes.

3. Two matrices can be always multiplied, but in crystallography the multiplication is allowed only in cases of coexisting point symmetry operations. Having two matrices describing two point symmetry operations we do not always directly see whether these operations do coexist with each other i.e. whether the multiplication is allowed.

SIMPLIFIED NOTATION OF THE TYPE $n(MNP)$

Advantages

1. The simplified symbol corresponding to a concrete point symmetry operation can be writen immediately.

2. Each simplified symbol can be deciphered without any difficulties.

3. Calculating the E-value ($E = M_1M_2 + N_1N_2 + P_1P_2$) and comparing it with those allowed for two given simplified symbols we can immediately see whether the corresponding operations do coexist with each other *i.e.* whether the multiplication of the matrices is allowed.

Disadvantages

1. The simplified symbols can not be multiplied directly. They must be firstly converted into the corresponding matrices (with aid of the generalized matrix introduced previously). The matrices yield after multiplication the resulting matrix which must be deciphered to be converted into its simplified symbol.

2. The simplified symbol can not be used directly to transform the coordinates of a point in space. To perform this transformation the simplified symbol must be firstly traduced into the corresponding matrix.

In the present and in following papers an attempt will be made to eliminate the first of both mentioned disadvantages of the simplified notation and to overcome the difficulties connected with multiplication of simplified matrix symbols.

POINT SYMMETRY OPERATIONS COEXISTING WITH A SIXFOLD ROTATION AXIS

Let us consider a sixfold rotation axis passing in space through the point 0, 0, 0 along the z-axis of the system of coordinates.

Using the simplified notation we can write for this operation the symbol $6(001)$.

With aid of the table of allowed E-values (Nedoma, Bolek 1976) we can immediately see that operation $6(001)$ can coexist with following operations only:

$$6(001) \text{ or } 6(00\bar{1})$$
$$3(001) \text{ or } 3(00\bar{1})$$
$$2(001) \text{ or } 2(MN0)$$

For sake of convenience let us choose $M = 0 \quad N = 1$.

The multiplication table containing the operations $6(001)$, $6(00\bar{1})$, $3(001)$, $3(00\bar{1})$ and $2(001)$ has been already discussed in the foregoing paper (Nedoma, Pobożniak 1977). The table must be now enlarged to include additionally the operation $2(010)$.

Performing all matrix multiplications and traducing the resulting matrices into their simplified symbols we obtain the multiplication table given in Table 1.

All operations dealt with in this paper can be written either in the usual matrix form or in the form of simplified symbols as follows:

$$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = 6(001) \qquad \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = 6(00\bar{1})$$

$$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = 3(001) \qquad \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} = 3(00\bar{1})$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = 2(001) \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = 1(MNP)$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(010) \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(100)$$

$$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(1\sqrt{3}\,0) \qquad \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(1-\sqrt{3}\,0)$$

Table 1

Multiplication of simplified matrix symbols

1(M,N,P)	6(0,0,1)	6(0,0,−1)	3(0,0,1)	3(0,0,−1)	2(0,0,1)	2(0,1,0)	2(1,0,0)	$2(\sqrt{3},1,0)$	$2(1,\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	$2(1,-\sqrt{3},0$
6(0,0,1)	3(0,0,1)	1(M,N,P)	2(0,0,1)	6(0,0,−1)	3(0,0,−1)	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},1,0)$	$2(1,\sqrt{3},0)$	2(0,1,0)	2(1,0,0)	$2(\sqrt{3},-1,0$
6(0,0,−1)	1(M,N,P)	3(0,0,−1)	6(0,0,1)	2(0,0,1)	3(0,0,1)	$2(1,\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	2(1,0,0)	$2(\sqrt{3},1,0)$	$2(1,-\sqrt{3},0)$	2(0,1,0)
3(0,0,1)	2(0,0,1)	6(0,0,1)	3(0,0,−1)	1(M,N,P)	6(0,0,−1)	$2(\sqrt{3},-1,0)$	$2(1,\sqrt{3},0)$	2(0,1,0)	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},1,0)$	2(1,0,0)
3(0,0,−1)	6(0,0−1)	2(0,0,1)	1(M,N,P)	3(0,0,1)	6(0,0,1)	$2(\sqrt{3},1,0)$	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	2(1,0,0)	2(0,1,0)	$2(1,\sqrt{3},0)$
2(0,0,1)	3(0,0,−1)	3(0,0,1)	6(0,0,−1)	6(0,0,1)	1(M,N,P)	2(1,0,0)	2(0,1,0)	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	$2(1,\sqrt{3},0)$	$2(\sqrt{3},1,0)$
2(0,1,0)	$2(1,\sqrt{3},0)$	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},1,0)$	$2(\sqrt{3},-1,0)$	2(1,0,0)	1(M,N,P)	2(0,0,1)	3(0,0,1)	6(0,0,1)	3(0,0,−1)	6(0,0,−1)
2(1,0,0)	$2(\sqrt{3},-1,0)$	$2(\sqrt{3},1,0)$	$2(1,-\sqrt{3},0)$	$2(1,\sqrt{3},0)$	2(0,1,0)	2(0,0,1)	1(M,N,P)	6(0,0,−1)	3(0,0,−1)	6(0,0,1)	3(0,0,1)
$2(\sqrt{3},1,0)$	2(1,0,0)	$2(1,\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	2(0,1,0)	$2(1,-\sqrt{3},0)$	3(0,0,−1)	6(0,0,1)	1(M,N,P)	6(0,0,−1)	3(0,0,1)	2(0,0,1)
$2(1,\sqrt{3},0)$	$2(\sqrt{3},1,0)$	2(0,1,0)	2(1,0,0)	$2(1,-\sqrt{3},0)$	$2(\sqrt{3},-1,0)$	6(0,0,−1)	3(0,0,1)	6(0,0,1)	1(M,N,P)	2(0,0,1)	3(0,0,−1)
$2(\sqrt{3},-1,0)$	$2(1,-\sqrt{3},0)$	2(1,0,0)	2(0,1,0)	$2(\sqrt{3},1,0)$	$2(1,\sqrt{3},0)$	3(0,0,1)	6(0,0,−1)	3(0,0,−1)	2(0,0,1)	1(M,N,P)	6(0,0,1)
$2(1,-\sqrt{3},0)$	2(0,1,0)	$2(\sqrt{3},-1,0)$	$2(1,\sqrt{3},0)$	2(1,0,0)	$2(\sqrt{3},1,0)$	6(0,0,1)	3(0,0,−1)	2(0,0,1)	3(0,0,1)	6(0,0,−1)	1(M,N,P)

$$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(\sqrt{3}\ 1\ 0) \qquad \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix} = 2(\sqrt{3}\ \bar{1}\ 0)$$

The multiplication table for point symmetry operations coexisting with a fourfold axis will be discussed in the second part of this paper.

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MNOŻENIE UPROSZCZONYCH SYMBOLI MACIERZOWYCH

Streszczenie

W pracy przedstawiono *tabliczkę mnożenia* dla operacji symetrii współistniejących z osią sześciokrotną. Uproszczony symbol macierzowy odpowiadający macierzy wynikającej z mnożenia dwóch współistniejących z sobą operacji symetrii znaleźć można bezpośrednio w *tabliczce mnożenia.*

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УМНОЖЕНИЕ СОКРАЩЕННЫХ МАТРИЧНЫХ СИМВОЛОВ

Резюме

В работе приведена таблица умножения для операций симметрии сосуществующих с шестикратной осью вращения. Сокращенный символ матрицы получаемой в результате умножения сосуществующих друг с другом операций можно найти непосредственно в таблице.