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COEXISTENCE OF SYMMETRY ELEMENTS IN TERMS OF ABBREVIATED MATRIX SYMBOLS PART II

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Abstract. Three different tables of allowed E-values ($E = M_1M_2 + N_1N_2 + P_1P_2$) for coexisting point symmetry operations $n_1(M_1N_1P_1)$ and $n_2(M_2N_2P_2)$ can be reduced to one table valid for all rotation, inversion and mirror axes.

INTRODUCTION

Simple rotation and inversion axes discussed in the first part of this paper (Nedoma, Bolek 1977) were chosen in such a way that their simplified symbols could be noted as $n(001)$ or $\bar{n}(001)$ respectively. The groups of symmetry operations derived for these axes can be generalized for all possible positions of these axes in space.

TRANSFORMATION $001 \rightarrow MNP$

Let us write the matrix transforming the coordinates $0,0,1$ into M,N,P (the values M,N,P fulfill as usually the condition $M^2 + N^2 + P^2 = 1$). The transformation $001 \rightarrow MNP$ can be treated e.g. as a rotation written shortly as $\alpha(M_xN_x0)$ (Fig. 1).

For M_x and N_x (Fig. 2) we can write:

$$\frac{M_x}{\sqrt{M_x^2 + N_x^2}} = \sin\varphi \qquad\qquad \frac{-N_x}{\sqrt{M_x^2 + N_x^2}} = \cos\varphi$$

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On the other hand we have:

$$\sin\varphi = \frac{N}{\sqrt{M^2+N^2}} \qquad \cos\varphi = \frac{M}{\sqrt{M^2+N^2}}$$

Taking into account the fact that $M_x^2 + N_x^2 = 1$ we obtain

$$M_x = \frac{N}{\sqrt{M^2+N^2}} \qquad N_x = \frac{-M}{\sqrt{M^2+N^2}}$$

For the rotation angle α we can write (Fig. 1)

$$\cos\alpha = \frac{P}{\sqrt{M^2+N^2+P^2}} \qquad \sin\alpha = \frac{\sqrt{M^2+N^2}}{\sqrt{M^2+N^2+P^2}}$$

From the point M_xN_x0 the rotation transforming the coordinates $0,0,1$ into M,N,P is seen as a right one. As demonstrated before there are two ways of using the generalized matrix in such cases: to introduce $-\alpha$ instead of α, or to change simultaneously all signs of M,N,P into opposite ones. Taking into account that $M^2+N^2+P^2=1$ and changing the sign of α we obtain the matrix:

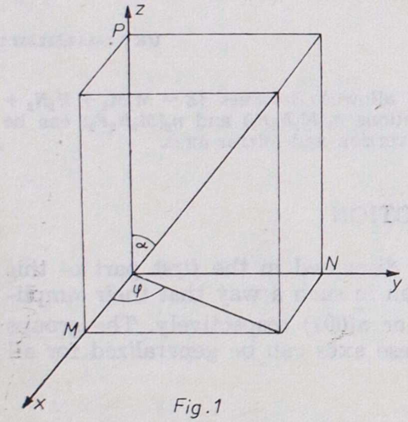

Fig. 1

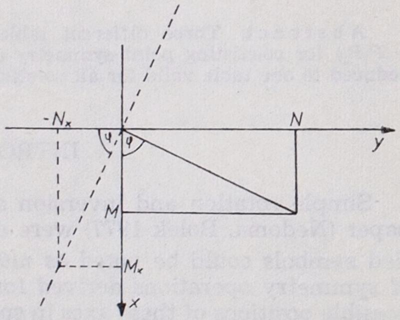

Fig. 2

$$\left\|\begin{matrix} \frac{N^2}{1+P}+P & \frac{-MN}{1+P} & M \\ \frac{-MN}{1+P} & \frac{M^2}{1+P}+P & N \\ -M & -N & P \end{matrix}\right\|$$

Transforming all coordinates appearing in the equation:

$$\{6(001)\times 6(001)\} = \begin{matrix} 6(001) & 3(001) & 2(001) \\ 6(001) & 3(001) & 1(MNP) \end{matrix}$$

with aid of the matrix derived above we obtain

$$\{6(MNP)\times 6(MNP)\} = \begin{matrix} 6(M,N,P) & 3(M,N,P) & 2(M,N,P) \\ 6(-M,-N,-P) & 3(-M,-N,-P) & 1(M,N,P) \end{matrix}$$

Proceeding in the same way in cases of other simple symmetry operations we can write:

$$\begin{array}{llll}
\{4(MNP)\times 4(MNP)\} = & 4(M,N,P) & 2(M,N,P) & \\
 & 4(-M,-N,-P) & 1(M,N,P) & \\
\{3(MNP)\times 3(MNP)\} = & 3(M,N,P) & 1(M,N,P) & \\
 & 3(-M,-N,-P) & & \\
\{2(MNP)\times 2(MNP)\} = & 2(M,N,P) & 1(M,N,P) & \\
\{\bar{6}(MNP)\times \bar{6}(MNP)\} = & \bar{6}(M,N,P) & 3(M,N,P) & \bar{2}(M,N,P) \\
 & \bar{6}(-M,-N,-P) & 3(-M,-N,-P) & 1(M,N,P) \\
\{\bar{4}(MNP)\times \bar{4}(MNP)\} = & \bar{4}(M,N,P) & 2(M,N,P) & \\
 & \bar{4}(-M,-N,-P) & 1(M,N,P) & \\
\{\bar{3}(MNP)\times \bar{3}(MNP)\} = & \bar{3}(M,N,P) & 3(M,N,P) & \bar{1}(M,N,P) \\
 & \bar{3}(-M,-N,-P) & 3(-M,-N,-P) & 1(M,N,P) \\
\{\bar{2}(MNP)\times \bar{2}(MNP)\} = & \bar{2}(M,N,P) & 1(M,N,P) & \\
\{\bar{1}(MNP)\times \bar{1}(MNP)\} = & \bar{1}(M,N,P) & 1(M,N,P) &
\end{array}$$

Each of groups listed above contains always simultaneously both operations $n(MNP)$ and $n(-M,-N,-P)$. Changing the sings of all coordinates appearing in simplified symbols into opposite ones we obtain therefore the same group of symmetry operations. For a group of symmetry operations derived from $n(MNP)$ we can therefore write

$$\{n(MNP)\cdot n(MNP)\} \text{ or } \{n(-M,-N,-P)\cdot n(-M,-N,-P)\}$$

both symbols being equivalent.

Changing the signs only in one symbol in the case of two different coexisting symmetry operations we change also the sign of E. All allowed E-values contained in Tables 1, 2, 3 appear always with both signs.

Introducing the corresponding n-values instead of $\cos\alpha$, substituting inversion axes for mirror axes and ommitting the M,N,P and $-M,-N,-P$ values we can write the following table of allowed (E)-values for two coexisting n_1 and n_2 axes. The table remains unchanged in cases of coexistence $n_1\bar{n}_2$ and $\bar{n}_1\bar{n}_2$ (Table 1).

Table 2 contains the same values written in other form met with in calculating the E-value as $M_1M_2 + N_1N_2 + P_1P_2$.

The E-values can be considered also as cosinus of angles between two coexisting axes. The values of the allowed angles are readily seen from the Table 3.

Table 1

Allowed $|E|$ — values

	6	4	3	2
6	1	—	1	0 1
4	—	0 1	$\frac{1}{\sqrt{3}}$	0 $\frac{1}{\sqrt{2}}$ 1
3	1	$\frac{1}{\sqrt{3}}$	$\frac{1}{3}$ 1	0 $\frac{1}{\sqrt{3}}$ $\sqrt{\frac{2}{3}}$ 1
2	0 1	0 $\frac{1}{\sqrt{2}}$ 1	0 $\frac{1}{\sqrt{3}}$ $\sqrt{\frac{2}{3}}$ 1	0 $\frac{1}{2}$ $\frac{1}{\sqrt{2}}$ $\frac{\sqrt{3}}{2}$ 1

Table 2

Allowed $|E|$ — values

	6	4	3	2
6	1		1	0 1
4		0 1	0.57735	0 0.70711 1
3	1	0.57735	0.33333 1	0 0.57735 0.81650 1
2	0 1	0 0.70711 1	0 0.57735 0.81650 1	0 0.50000 0.70711 0.86602 1

Table 3

Allowed ψ-values calculated from E-values listed in Table 2

$\cos\psi$	ψ	$\cos\psi$	ψ
−1	180°	−0.33333	109°28′16″
1	0°	0.81650	35°15′52″
0	90°	−0.81650	144°44′08″
0.70711	45°	0.86602	30°
−0.70711	135°	−0.86602	150°
0.57735	54°44′08″	0.50000	60°
0.57735	125°15′52″	−0.50000	120°
0.33333	70°31′44″		

REFERENCES

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WSPÓŁISTNIENIE ELEMENTÓW SYMETRII W ŚWIETLE SKRÓCONYCH SYMBOLI MACIERZOWYCH. CZĘŚĆ II

Streszczenie

Trzy różne tabele dozwolonych wartości E ($E = M_1M_2 + N_1N_2 + P_1P_2$) dla współistniejących punktowych operacji symetrii $n_1(M_1N_1P_1)$ oraz $n_2(M_2N_2P_2)$ mogą być sprowadzone do jednej tabeli obejmującej wszystkie osie obrotowe, inwersyjne i zwierciadlane.

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СОСУЩЕСТВОВАНИЕ ЭЛЕМЕНТОВ СИММЕТРИИ В СВЕТЕ СОКРАЩЕННЫХ МАЕРИЧНЫХ СИМВОЛОВ

ЧАСТЬ II

Резюме

Три различных таблицы допускаемых значений E ($E = M_1M_2 + N_1N_2 + P_1P_2$) для сосуществующих элементов симметрии $n_1(M_1N_1P_1)$ и $n_2(M_2N_2P_2)$ можно свести к одной таблице включающей в себя сосуществование всех поворотных, инверсионных и зеркальных осей.