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COEXISTENCE OF SYMMETRY ELEMENTS IN TERMS OF ABBREVIATED MATRIX SYMBOLS

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Abstract. Two symmetry operations described by abbreviated symbols $\alpha(D_1M_1N_1P_1)$ and $\beta(D_2M_2N_2P_2)$ can coexist only when $E = M_1M_2 + N_1N_2 + P_1P_2$ assumes one of "allowed" values. "Allowed" E-values for given α and β rotation angles are presented in tables.

INTRODUCTION

Each symmetry operation met with in crystallography 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,
$M\ N\ P$ — coordinates of a point in space fulfilling the condition $M^2 + N^2 + P^2 = 1$ (the axis passes through points *0, 0, 0* and M, N, P).

Using the generalized matrix introduced in the foregoing paper (Nedoma 1975)

$$\begin{matrix} M^2R + \cos\alpha & MNR - P\sin\alpha & MPR + N\sin\alpha \\ MNR + P\sin\alpha & N^2R + \cos\alpha & NPR - M\sin\alpha \\ MPR - N\sin\alpha & NPR + M\sin\alpha & P^2R + \cos\alpha \end{matrix}$$

where:

$R = D - \cos\alpha$

all elements of the matrix corresponding to a given abbreviated symbol can be easily calculated.

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For two generalized matrices given by abbreviated symbols $\alpha(D_1M_1N_1P_1)$ and $\beta(D_2M_2N_2P_2)$ a third resulting matrix $\gamma(D_3M_3N_3P_3)$ can be always derived by simple matrix multiplication. The resulting angle of rotation γ must assume however — as all rotation angles in crystallography — only allowed values (60°, 90°, 120°, 180°, 360°). Two arbitrary chosen matrices can be thus always multiplied, but the resulting matrix must not always denote a symmetry operation met with in crystallography.

Using matrix notation it is not easy to see immediately whether the multiplication of two given matrices leads to a matrix of a symmetry operation allowed in crystallography i.e. it is not easy to decide whether two given matrices describe two coexisting symmetry operations. The aim of the present paper was to discuss the coexistence of symmetry elements in terms of abbreviated symbols introduced previously (Nedoma 1975).

COEXISTENCE OF TWO SYMMETRY OPERATIONS

Let us consider two symmetry operations $\alpha(D_1M_1N_1P_1)$ and $\beta(D_2M_2N_2P_2)$. The elements appearing in matrices describing these operations will be denoted a_{ij} and b_{ij} respectively. As demonstrated previously (Nedoma 1975) the γ-angle of the third symmetry operation c_{ij} derived by matrix multiplication can be calculated from the general equation

$$\cos\gamma = \frac{S_3 - D_3}{2}$$

where:

$S_3 = c_{11} + c_{22} + c_{33}$

c_{ij} = denotes the elements of the resulting matrix $\gamma(D_3M_3N_3P_3)$.

The value of the determinant D_3 can be obtained — as known — by simple multiplication of determinants D_1 and D_2:

$$D_3 = D_1 \cdot D_2$$

The matrix elements c_{11}, c_{22} and c_{33} can be calculated by matrix multiplication using the notation of generalized matrix.

$$\begin{aligned} c_{11} = {} & (M_1^2 R_1 + \cos\alpha)(M_2^2 R_2 + \cos\beta) + \\ & + (M_1N_1R_1 - P_1\sin\alpha)(M_2N_2R_2 + P_2\sin\beta) + \\ & + (M_1P_1R_1 + N_1\sin\alpha)(M_2P_2R_2 - N_2\sin\beta) \end{aligned}$$

$$\begin{aligned} c_{22} = {} & (M_1N_1R_1 + P_1\sin\alpha)(M_2N_2R_2 - P_2\sin\beta) + \\ & + (N_1^2 R_1 + \cos\alpha)(N_2^2 R_2 + \cos\beta) + \\ & + (N_1P_1R_1 - M_1\sin\alpha)(N_2P_2R_2 + M_2\sin\beta) \end{aligned}$$

$$\begin{aligned} c_{33} = {} & (M_1P_1R_1 - N_1\sin\alpha)(M_2P_2R_2 + N_2\sin\beta) + \\ & + (N_1P_1R_1 + M_1\sin\alpha)(N_2P_2R_2 - M_2\sin\beta) + \\ & + (P_1^2 R_1 + \cos\alpha)(P_2^2 R_2 + \cos\beta) \end{aligned}$$

The sum $S_3 = c_{11} + c_{22} + c_{33}$ is thus given by the following formula

$$\begin{aligned} S_3 = {} & (M_1M_2 + N_1N_2 + P_1P_2)^2 R_1R_2 - 2(M_1M_2 + N_1N_2 + \\ & + P_1P_2)\sin\alpha\sin\beta + R_1\cos\beta + R_2\cos\alpha + 3\cos\alpha\cdot\cos\beta \end{aligned}$$

Introducing for the sake of simplification the symbol

$$E_{1,2} = M_1M_2 + N_1N_2 + P_1P_2$$

we can write for $\cos\gamma$ the following equation

$$\begin{aligned} 2\cos\gamma = {} & E_{1,2}^2 R_1R_2 - 2\cdot E_{1,2}\sin\alpha\cdot\sin\beta + R_1\cdot\cos\beta + R_2\cos\alpha + \\ & + 3\cdot\cos\alpha\cdot\cos\beta - D_1D_2 \end{aligned}$$

Introducing for R_1 and R_2 their general values $D_1 - \cos\alpha$ and $D_2 - \cos\beta$, respectively, we obtain finally

$$\begin{aligned} & E_{1,2}^2 (D_1 - \cos\alpha)\cdot(D_2 - \cos\beta) - 2E_{1,2}\cdot\sin\alpha\cdot\sin\beta + D_1\cos\beta + \\ & + D_2\cos\alpha - D_1D_2 + \cos\alpha\cdot\cos\beta - 2\cos\gamma = 0 \end{aligned} \qquad [1]$$

This equation being symmetrical with respect to $\alpha(D_1M_1N_1P_1)$ and $\beta(D_2M_2N_2P_2)$, holds for both matrix multiplications

$$\alpha(D_1M_1N_1P_1)\cdot\beta(D_2M_2N_2P_2) \text{ and } \beta(D_2M_2N_2P_2)\cdot\alpha(D_1M_1N_1P_1)$$

All values appearing in abbreviated symbols must be therefore chosen in a way ensuring that the resulting $\cos\gamma$ will assume one of allowed values

$$\left(1, \frac{1}{2}, 0, -\frac{1}{2}, -1\right)$$

We can discuss the equation [1] from an other point of view. We can choose arbitrarily three allowed values for α, β and γ, combine them with D_1, D_2 and D_1D_2-values and try to answer the question whether it is possible to find such $E_{1,2}$-values which would fulfill the equation [1]. If this equation can not be solved for given α, β, γ, D_1D_2-values we must come to the conclusion that the chosen α and β values can never lead to the required resulting γ-operation at no E-value i.e. that there is no position of these α and β rotation axes in space which could ensure that the γ-axis resulting from matrix multiplication will rotate the space by an angle allowed in crystalography.

There is an additional condition to be fulfilled if two symmetry axes passing through the point 0, 0, 0 shall coexist in space. If $\alpha(D_1M_1N_1P_1)$ coexists with $\beta(D_2M_2N_2P_2)$ an other axis $\beta(D_2M_4N_4P_4)$ obtained by rotating the $\beta(D_2M_2N_2P_2)$ around the $\alpha(D_1M_1N_1P_1)$-axis must coexist with them in space. The coordinates $M_4N_4P_4$ can be easily calculated from equations:

$$\begin{aligned} M_4 &= a_{11}M_2 + a_{12}N_2 + a_{13}P_2 \\ N_4 &= a_{21}M_2 + a_{22}N_2 + a_{23}P_2 \\ P_4 &= a_{31}M_2 + a_{32}N_2 + a_{33}P_2 \end{aligned}$$

The new derived $\beta(D_2M_4N_4P_4)$-axis must coexist with the $\beta(D_2M_2N_2P_2)$-axis. For this coexistence we can write the following equation (analogous to the equation [1])

$$E_{2,4}^2\cdot(D_2 - \cos\beta)^2 - 2E_{2,4}\sin^2\beta + 2D_2\cos\beta - 1 + \cos^2\beta - 2\cos\varepsilon = 0 \qquad [2]$$

where

$E_{2,4} = M_2M_4 + N_2N_4 + P_2P_4$

ε — angle of rotation resulting from matrix multiplication $\beta(D_2M_2N_2P_2)\cdot\beta(D_2M_4N_4P_4)$.

Table 1

Coexistence of two symmetry axes for $D_1 = 1$; $D_2 = 1$

cos β / cos α	$\frac{1}{2}$		0		$-\frac{1}{2}$		-1	
	E	cos γ	E	cos γ	E	cos γ	E	cos γ
$\frac{1}{2}$	-1	1			-1	$\frac{1}{2}$	1	$-\frac{1}{2}$
	1	$-\frac{1}{2}$			1	-1	-1	$-\frac{1}{2}$
							0	-1
0			-1	1	$-\frac{1}{\sqrt{3}}$	0	1	0
			0	$-\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	-1	-1	0
			1	-1			$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$
							$-\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$
							0	-1
$-\frac{1}{2}$	-1	$\frac{1}{2}$	$-\frac{1}{\sqrt{3}}$	0	-1	1	1	$\frac{1}{2}$
	1	-1	$\frac{1}{\sqrt{3}}$	-1	1	$-\frac{1}{2}$	-1	$\frac{1}{2}$
					$-\frac{1}{3}$	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}$	0
					$\frac{1}{3}$	-1	$-\sqrt{\frac{2}{3}}$	0
							$\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$
							$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$
							0	-1
-1	1	$-\frac{1}{2}$	1	0	1	$\frac{1}{2}$	1	1
	-1	$-\frac{1}{2}$	-1	0	-1	$\frac{1}{2}$	-1	1
	0	-1	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}$	0	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$
			$-\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$-\sqrt{\frac{2}{3}}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{1}{2}$
			0	-1	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	0
					$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	0
					0	-1	$\frac{1}{2}$	$-\frac{1}{2}$
							$-\frac{1}{2}$	$-\frac{1}{2}$
							0	-1

Table 2

Coexistence of two symmetry axes for $D_1 = 1$; $D_2 = -1$

cos β / cos α	$-\frac{1}{2}$		0		$\frac{1}{2}$		1	
	E	cos γ	E	cos γ	E	cos γ	E	cos γ
$\frac{1}{2}$	1	$\frac{1}{2}$			-1	1	0	1
	-1	-1			1	$-\frac{1}{2}$	1	$\frac{1}{2}$
							-1	$\frac{1}{2}$
0			-1	1	$-\frac{1}{\sqrt{3}}$	1	0	1
			0	$\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$
			1	-1			$-\frac{1}{\sqrt{2}}$	$\frac{1}{2}$
							1	0
							-1	0
$-\frac{1}{2}$	-1	1	$-\frac{1}{\sqrt{3}}$	1	$-\frac{1}{3}$	1	0	1
	1	$-\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	0	-1	$\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{2}$
					$\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{2}$
					1	-1	$\sqrt{\frac{2}{3}}$	0
							$-\sqrt{\frac{2}{3}}$	0
							1	$-\frac{1}{2}$
							-1	$-\frac{1}{2}$
-1	0	1	0	1	0	1	0	1
	1	$\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
	-1	$\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$
			1	0	$\sqrt{\frac{2}{3}}$	0	$\frac{1}{\sqrt{2}}$	0
			-1	0	$-\sqrt{\frac{2}{3}}$	0	$-\frac{1}{\sqrt{2}}$	0
					1	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$-\frac{1}{2}$
					-1	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	$-\frac{1}{2}$
							1	-1
							-1	-1

Table 3

Coexistence of two symmetry axes for $D_1 = -1$; $D_2 = -1$

cos β / cos α	$-\frac{1}{2}$		0		$\frac{1}{2}$		1	
	E	cos γ	E	cos γ	E	cos γ	E	cos γ
$-\frac{1}{2}$	−1	1			−1	$\frac{1}{2}$	1	$-\frac{1}{2}$
	1	$-\frac{1}{2}$			1	−1	−1	$-\frac{1}{2}$
							0	−1
0			−1	1	$-\frac{1}{\sqrt{3}}$	0	1	0
			0	$-\frac{1}{2}$	$\frac{1}{\sqrt{3}}$	−1	−1	0
			1	−1			$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$
							$-\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$
							0	−1
$\frac{1}{2}$	−1	$\frac{1}{2}$	$-\frac{1}{\sqrt{3}}$	0	−1	1	1	$\frac{1}{2}$
	1	−1	$\frac{1}{\sqrt{3}}$	−1	1	$-\frac{1}{2}$	−1	$\frac{1}{2}$
					$-\frac{1}{3}$	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}$	0
					$\frac{1}{3}$	−1	$-\sqrt{\frac{2}{3}}$	0
							$\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$
							$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$
							0	−1
1	1	$-\frac{1}{2}$	1	0	1	$\frac{1}{2}$	1	1
	−1	$-\frac{1}{2}$	−1	0	−1	$\frac{1}{2}$	−1	1
	0	−1	$\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$\sqrt{\frac{2}{3}}$	0	$\frac{\sqrt{3}}{2}$	$\frac{1}{2}$
			$-\frac{1}{\sqrt{2}}$	$-\frac{1}{2}$	$-\sqrt{\frac{2}{3}}$	0	$-\frac{\sqrt{3}}{2}$	$\frac{1}{2}$
			0	−1	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	$\frac{1}{\sqrt{2}}$	0
					$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	$-\frac{1}{\sqrt{2}}$	0
					0	−1	$\frac{1}{2}$	$-\frac{1}{2}$
							$-\frac{1}{2}$	$-\frac{1}{2}$
							0	−1

Introducing for $M_4N_4P_4$ their equivalents we obtain the following equation

$$E_{2,4} = E_{1,2}^2 \cdot R_1 + \cos\alpha \qquad [3]$$

Eliminating $E_{2,4}$ and $E_{1,2}$ from equations ([1], [2], [3]) and basing on the fact that α, β, γ, ε, D_1, D_2 can assume only rational values we can easily demonstrate that the value of

$$\sqrt{2\,(D_1D_2 + \cos\gamma)\cdot(D_1 + \cos\alpha)\cdot(D_2 + \cos\beta)}$$

must be also rational.

If two symmetry axes $\alpha(D_1M_1N_1P_1)$ and $\beta(D_2M_2N_2P_2)$ shall coexist in space (giving the resulting third symmetry operation $\gamma(D_1D_2,\ M_3N_3P_3)$ two following cryteria must be thus fulfilled:

1. The value of $E_{1,2}$ calculated from the equation

$$E_{1,2}^2\,(D_1 - \cos\alpha)\cdot(D_2 - \cos\beta) - 2\,E_{1,2}\sin\alpha\cdot\sin\beta + D_1\cos\beta + D_2\cos\alpha - D_1D_2 + \cos\alpha\cdot\cos\beta - 2\cos\gamma = 0$$

must be real and fulfill the condition $-1 \leqslant E \leqslant 1$

2. The value of

$$\sqrt{2\,(D_1D_2 + \cos\gamma)\cdot(D_1 + \cos\alpha)\cdot(D_2 + \cos\beta)}$$

must be rational.

Assuming all combination of α, β, γ-angles allowed in crystallography we can check — with aid of these both cryteria — whether two axes α and β can lead to a resulting axis γ and at what $E_{1,2}$-value such a coexistence is possible. Excluding all not-allowed combinations we obtain the values presented in tables 1, 2, 3.

REFERENCES

NEDOMA J.,1975: A generalized matrix of symmetry elements. *Miner. Polon.* 6, 1, 83—89.

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WSPÓŁISTNIENIE ELEMENTÓW SYMETRII W ŚWIETLE SKRÓCONYCH SYMBOLI MACIERZOWYCH

Streszczenie

Dwie operacje symetrii opisane za pomocą symboli skróconych $\alpha(D_1M_1N_1P_1)$ i $\beta(D_2M_2N_2P_2)$ mogą współistnieć z sobą wyłącznie wtedy, gdy $E = M_1M_2 + N_1N_2 + P_1P_2$ przybiera jedną z wartości „dozwolonych". „Dozwolone" wartości E dla danych kątów obrotu α i β przedstawiono w tabelach 1 — 3.

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СОСУЩЕСТВОВАНИЕ ЭЛЕМЕНТОВ СИММЕТРИИ В СВЕТЕ СОКРАЩЕННЫХ МАТРИЧНЫХ СИМВОЛОВ

Резюме

Две операции симметрии описываемые сокращенными символами $\alpha(D_1M_1N_1P_1)$ и $\beta(D_2M_2N_2P_2)$ могут сосуществовать лишь при условии что $E = M_1M_2 + N_1N_2 + P_1P_2$ принимает одно из „допустимых" значений. „Допустимые" значения E для углов вращения α и β приведены в таблицах 1 — 3.