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MULTIPLICATION OF SIMPLIFIED MATRIX SYMBOLS

PART III

A b s t r a c t. Simplified matrix symbols of symmetry operations can be easily multiplied using a numerical multiplication table presented in the paper.

INTRODUCTION

Multiplication tables for symmetry elements coexisting with a 6-fold and with a 4-fold axis have been presented in foregoing papers /Nedoma *et al.*, 1979, 1980/. In the present paper the possibility of further simplification of the graphical form of these tables will be discussed.

NUMERICAL MULTIPLICATION TABLE

Let us write explicitly all matrices contained in both multiplication tables published in foregoing papers /Table 1/. Each matrix is written below its simplified symbol. In the left corner of each field - near the simplified symbol - the matrix written on this field is arbitrarily labelled with a number contained between 1 and 32.

With aid of this table each symmetry operation can be described using three different notations: by the matrix written explicitly, by the corresponding simplified matrix symbol or by the number of the matrix.

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Table 1 — Symmetry matrices

No. / symbol	matrix
1 1/MNP/	$\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}$
2 2/100/	$\begin{bmatrix}1&0&0\\0&\bar1&0\\0&0&\bar1\end{bmatrix}$
3 2/010/	$\begin{bmatrix}\bar1&0&0\\0&1&0\\0&0&\bar1\end{bmatrix}$
4 2/001/	$\begin{bmatrix}\bar1&0&0\\0&\bar1&0\\0&0&1\end{bmatrix}$
5 2/110/	$\begin{bmatrix}0&1&0\\1&0&0\\0&0&\bar1\end{bmatrix}$
6 2/1-10/	$\begin{bmatrix}0&\bar1&0\\\bar1&0&0\\0&0&\bar1\end{bmatrix}$
7 2/101/	$\begin{bmatrix}0&0&1\\0&\bar1&0\\1&0&0\end{bmatrix}$
8 2/10-1/	$\begin{bmatrix}0&0&\bar1\\0&\bar1&0\\\bar1&0&0\end{bmatrix}$
9 2/011/	$\begin{bmatrix}\bar1&0&0\\0&0&1\\0&1&0\end{bmatrix}$
10 2/01-1/	$\begin{bmatrix}\bar1&0&0\\0&0&\bar1\\0&\bar1&0\end{bmatrix}$
11 2/√3 10/	$\begin{bmatrix}\tfrac12&\tfrac{\sqrt3}{2}&0\\\tfrac{\sqrt3}{2}&-\tfrac12&0\\0&0&\bar1\end{bmatrix}$
12 2/√3-10/	$\begin{bmatrix}\tfrac12&-\tfrac{\sqrt3}{2}&0\\-\tfrac{\sqrt3}{2}&-\tfrac12&0\\0&0&\bar1\end{bmatrix}$
13 2/1√3 0/	$\begin{bmatrix}-\tfrac12&\tfrac{\sqrt3}{2}&0\\\tfrac{\sqrt3}{2}&\tfrac12&0\\0&0&\bar1\end{bmatrix}$
14 2/1-√3 0/	$\begin{bmatrix}-\tfrac12&-\tfrac{\sqrt3}{2}&0\\-\tfrac{\sqrt3}{2}&\tfrac12&0\\0&0&\bar1\end{bmatrix}$
15 3/001/	$\begin{bmatrix}-\tfrac12&-\tfrac{\sqrt3}{2}&0\\\tfrac{\sqrt3}{2}&-\tfrac12&0\\0&0&1\end{bmatrix}$
16 3/00-1/	$\begin{bmatrix}-\tfrac12&\tfrac{\sqrt3}{2}&0\\-\tfrac{\sqrt3}{2}&-\tfrac12&0\\0&0&1\end{bmatrix}$
17 3/111/	$\begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}$
18 3/-1-1-1/	$\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}$
19 3/1-1-1/	$\begin{bmatrix}0&0&\bar1\\\bar1&0&0\\0&1&0\end{bmatrix}$
20 3/-11-1/	$\begin{bmatrix}0&0&1\\\bar1&0&0\\0&\bar1&0\end{bmatrix}$
21 3/-1-11/	$\begin{bmatrix}0&0&\bar1\\1&0&0\\0&\bar1&0\end{bmatrix}$
22 3/-111/	$\begin{bmatrix}0&\bar1&0\\0&0&1\\\bar1&0&0\end{bmatrix}$
23 3/1-11/	$\begin{bmatrix}0&\bar1&0\\0&0&\bar1\\1&0&0\end{bmatrix}$
24 3/11-1/	$\begin{bmatrix}0&1&0\\0&0&\bar1\\\bar1&0&0\end{bmatrix}$
25 4/001/	$\begin{bmatrix}0&\bar1&0\\1&0&0\\0&0&1\end{bmatrix}$
26 4/00-1/	$\begin{bmatrix}0&1&0\\\bar1&0&0\\0&0&1\end{bmatrix}$
27 4/010/	$\begin{bmatrix}0&0&1\\0&1&0\\\bar1&0&0\end{bmatrix}$
28 4/0-10/	$\begin{bmatrix}0&0&\bar1\\0&1&0\\1&0&0\end{bmatrix}$
29 4/100/	$\begin{bmatrix}1&0&0\\0&0&\bar1\\0&1&0\end{bmatrix}$
30 4/-100/	$\begin{bmatrix}1&0&0\\0&0&1\\0&\bar1&0\end{bmatrix}$
31 6/001/	$\begin{bmatrix}\tfrac12&-\tfrac{\sqrt3}{2}&0\\\tfrac{\sqrt3}{2}&\tfrac12&0\\0&0&1\end{bmatrix}$
32 6/00-1/	$\begin{bmatrix}\tfrac12&\tfrac{\sqrt3}{2}&0\\-\tfrac{\sqrt3}{2}&\tfrac12&0\\0&0&1\end{bmatrix}$

By the way of illustration let us describe a 4-fold symmetry axis along the x-axis of the coordinate system:

in matrix notation

$$\begin{bmatrix}1&0&0\\0&0&\bar1\\0&1&0\end{bmatrix}$$

in simplified notation *4/100/*

in numerical notation *29*

Multiplication tables for symmetry elements coexisting with a 6-fold and with a 4-fold axis can be reduced to one numerical Table 2.

The product of multiplication of two symmetry elements can be directly read in the multiplication Table 2.

Let us multiply e.g. the following two matrices:

$$\begin{bmatrix}1&0&0\\0&0&\bar1\\0&1&0\end{bmatrix}\times\begin{bmatrix}\bar1&0&0\\0&0&1\\0&1&0\end{bmatrix}=\begin{bmatrix}\bar1&0&0\\0&\bar1&0\\0&0&1\end{bmatrix}$$

The resulting matrix has been obtained by direct matrix multiplication.

In simplified matrix symbols the same multiplication can be noted

    4/100/ x 2/011/ = 2/001/

The resulting matrix symbol has been directly read in one of the two multiplication tables published in foregoing papers.

Numerical multiplication table

(Table 2 — 32 × 32 numerical multiplication table. First column gives the row index; the top row gives the column index 1–32. Blank regions in the original are left empty.)

×	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
2	1	4	3	26	25	27	28	10	9	12	11	14	13	22	18	6	5	28	29	12	11											
3	4	1	2	25	26	8	7	30	29	15	16	31	32	11	12	21	22	20	19	17	18	24	23	5	6	28	27	10	9	13	14	
4	3	2	1	6	5	29	30	14	13	12	11	32	31	23	17	21	20	24	18	22	26	25	8	7	9	10	16	15				
5	25	26	6	1	4	22	23	20	19													30	27	10	9	29	7	8	28	2	3	18	24	21	17
6	26	25	5	4	1	24	21	17														10	8	30	29	9	28	7	2	3	23	22	19
7	28	8	27	19	21	1	3	24	22													26	29	5	25	6	10	30	9	20	17	4
8	27	7	28	20	17	3	1	23	18													6	10	25	5	26	29	9	30	19	21	2
9	10	29	30	23	24	21	20	1	2													28	25	8	7	26	5	6	18	22	19	17
10	9	30	29	22	18	19	17	2	1													8	6	7	28	27	5	26	25	24	23	21
11	31	16	14								1	15	32	4	12	3															2	13
12	32	15	13								16	1	4	31	3	11															14	2
13	15	32	12								31	4	1	16	2	14															11	3
14	16	31	11								4	32	15	1	13	2															3	12
15	13	12	32								3	11	14	2	16	1															4	31
16	14	11	31								12	3	2	13	1	15															32	4
17	21	19	20	28	30	10	26	6									18	1	24	22	23	4	2	3	7	27	9	29	5	25		
18	25	24	22	29	10	25	6	27	8								1	17	3	4	2	20	21	19	30	9	26	5	28	7		
19	20	17	21	7	27	10	30	25	5								23	4	22	24	18	1	3	2	28	8	29	9	6	26		
20	19	21	17	8	28	29	9	5	25								24	3	23	18	22	3	2	4	1	28	30	10	25	5		
21	17	20	19	27	9	29	6	26									3	21	1	2	4	19	17	20	9	30	6	25	27	8		
22	24	23	18	10	29	5	26	28	7								3	21	1	2	4	19	17	20	9	30	6	25	27	8		
23	18	22	24	9	30	26	5	8	27								4	19	2	1	3	21	20	17	10	29	5	6	7	28		
24	22	18	23	30	9	6	25	7	28								2	20	4	3	1	17	19	21	29	10	7	8	27	26		
25	5	6	26	3	2	18	24	19	20								9	28	29	30	10	8	7	27	4	1	22	23	17	21		
26	6	5	25	2	3	23	22	17	21								29	7	9	10	30	27	28	8	1	4	24	18	19	20		
27	8	28	7	21	19	2	4	18	23								5	30	26	6	25	9	10	29	21	19	1	3	23	18		
28	7	28	21	17	19	2	4	22	24								25	9	6	26	5	30	10	29	21	19	1	3	23	18		
29	30	9	10	18	22	20	21	4	3								7	26	8	27	28	25	6	5	23	24	17	19	2	1		
30	29	10	9	24	23	17	19	3	4								27	5	28	7	8	6	25	26	22	18	20	21	1	2		
31	11	14	16								13	2	3	12	4	32															15	1
32	12	13	15								2	14	11	3	31	4															1	16

Using the matrix numbers introduced in Table 1 the same multiplication can be noted shortly as 29 x 9 = 4. This "equation" must be - of course - read as follows: matrix 29 multiplied by matrix 9 gives matrix 4.

In the case of inversion axes we could write for instance 29 x $\bar9$ = 29 x 29 x $\bar1$ = 4 x $\bar1$ = $\bar4$.

The same Table 2 gives thus the possibility of multiplying not only all matrices included in the Table 1 but also all matrices of inversion axes corresponding to those included in the table.

The practical use of the multiplication Table 2 will be evident in solving the following problem: find all symmetry elements generated by a 3-fold axis along x and by a 2-fold axis along y.

The simplified symbols of both generating axes are 3/001/ and 2/010/; in numerical notation Table 1/ 15 and 3. Let us construct the following table

$$
\begin{array}{c|cc}
 & 15 & 3 \\
\hline
15 & & \\
3 & &
\end{array}
$$

All symbols appearing in the table must be multiplied by each other. Using the numerical multiplication table we can "fill" easily the table

$$
\begin{array}{c|cc}
 & 15 & 3 \\
\hline
15 & 16 & 12 \\
3 & 11 & 1
\end{array}
$$

In the result of multiplification new operations 16, 12, 11 have appeared. They must be also multiplied by all operations already known to belong to the group. We must therefore enlarge the table

$$
\begin{array}{c|ccccc}
 & 15 & 3 & 16 & 12 & 11 \\
\hline
15 & 16 & 12 & & & \\
3 & 11 & 1 & & & \\
16 & & & & & \\
12 & & & & & \\
11 & & & & &
\end{array}
$$

Performing the multiplications we receive the table

$$
\begin{array}{c|ccccc}
 & 15 & 3 & 16 & 12 & 11 \\
\hline
15 & 16 & 12 & 1 & 11 & 3 \\
3 & 11 & 1 & 12 & 16 & 15 \\
16 & 1 & 11 & 15 & 3 & 12 \\
12 & 3 & 15 & 11 & 1 & 16 \\
11 & 12 & 16 & 3 & 15 & 1
\end{array}
$$

No new symmetry elements have appeared, the possibility of further generation is closed. The group generated by elements 15, 3 consists thus of elements 15, 3, 11, 12, 16, 1 or in simplified matrix notation of the elements

3/001/, 2/010/, 2/$\sqrt{3}$ 1 0/, 2/$\sqrt{3}$ $\bar{1}$ 0/, 3/00$\bar{1}$/, 1/MNP/

or in explicite matrix form

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

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

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

Let us solve now an other problem connected with the above one. The oriented symmetry elements 3/001/ and 2/010/ have generated all symmetry elements listed above. The derivated elements are also exactly oriented in space. Whole the group can be thus called an oriented group of symmetry elements. What will be the oriented symmetry elements generated by oriented elements 3/001/ and 2/100/? We could of course repeat the same steps as above but we can also proceed in an other manner. If we rotate all rigid system of oriented symmetry elements generated by 3/001/ and 2/010/ around the z axis to place the 2/010/ axis along the x axis /the rotation must be made by 90°/ we obtain the "old" group in the required new orientation. Performing the multiplication

$$
\begin{bmatrix}
0 & 1 & 0 \\
\bar{1} & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}
\times
\begin{bmatrix}
M \\
N \\
P
\end{bmatrix}
$$

where M N P denotes all values appearing in parenthesis in simplified symbols of the "old" oriented group we obtain directly the "new" group generated by 3/001/ and 2/100/.

Deriving an oriented group of symmetry elements in a given orientation with aid of the multiplication table we can thus easily pass to an other orientation of the group in space and write the simplified symbols of elements belonging to the group in other orientation. Making use of the generalized matrix we can pass to corresponding matrices describing the new obtained group.

Several fields of the multiplication table remain empty. This means that the elements belonging to these fields /in the corresponding column and row/ can not be multiplied with aid of the multiplication table: either they do not coexist with each other or their product has

not been included in the Table 1. Let us consider for instance the multiplication 4/100/ x 6/001/ or in numerical form 29 x 31. A 4-fold axis does not coexist with a 6-fold axis. The multiplication can not be performed as the resulting matrix would not have any crystallographic meaning. In the case of multiplication 6 x 15 there is also an empty field instead of resulting product. Passing to simplified symbols we can write 2/1$\bar{1}$0/ x 3/001/. The E value calculated for these symbols amounts to 0 i.e. we have to do with a 2-fold axis perpendicular to a 3-fold axis. The product of these matrices does exist but the resulting matrix has not been included in the Tables 1 and 2. To derive the group an other orientation of these axes in space must be chosen e.g. 3/001/, 2/010/- these both axes being also perpendicular to each other. After having derived this oriented group of symmetry elements we can pass to the former orientation proceeding as above.

R E F E R E N C E S

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MNOŻENIE UPROSZCZONYCH SYMBOLI MACIERZOWYCH

Cz. III

S t r e s z c z e n i e

Uproszczone symbole macierzowe operacji symetrii można z łatwością mnożyć przy pomocy numerycznej "tabliczki mnożenia" przedstawionej w pracy.

Юзеф НЕДОМА, Павел ШРАЙНЕР

УМНОЖЕНИЕ СОКРАЩЕННЫХ МАТРИЧНЫХ СИМВОЛОВ

ЧАСТЬ 3

Р е з ю м е

Сокращенные матричные символы операций симметрии можно легко умножать при помощи нумерической таблицы умножения приведенной в статье.