Combining Symmetry Operations (Multiplication)

- ☞ Multiplication of symmetry operations is the successive performance of two or more operations to achieve an orientation that could be reached by a single operation.

- ☞ The order in which successive different symmetry operations are performed can affect the result.

- ☞ Multiplication of symmetry operations is *not* in general commutative, although certain combinations may be.

- ☞ In writing multiplications of symmetry operation we use a "right-to-left" notation:

  $BA = X$ "Doing A then B has the same result as the operation X."

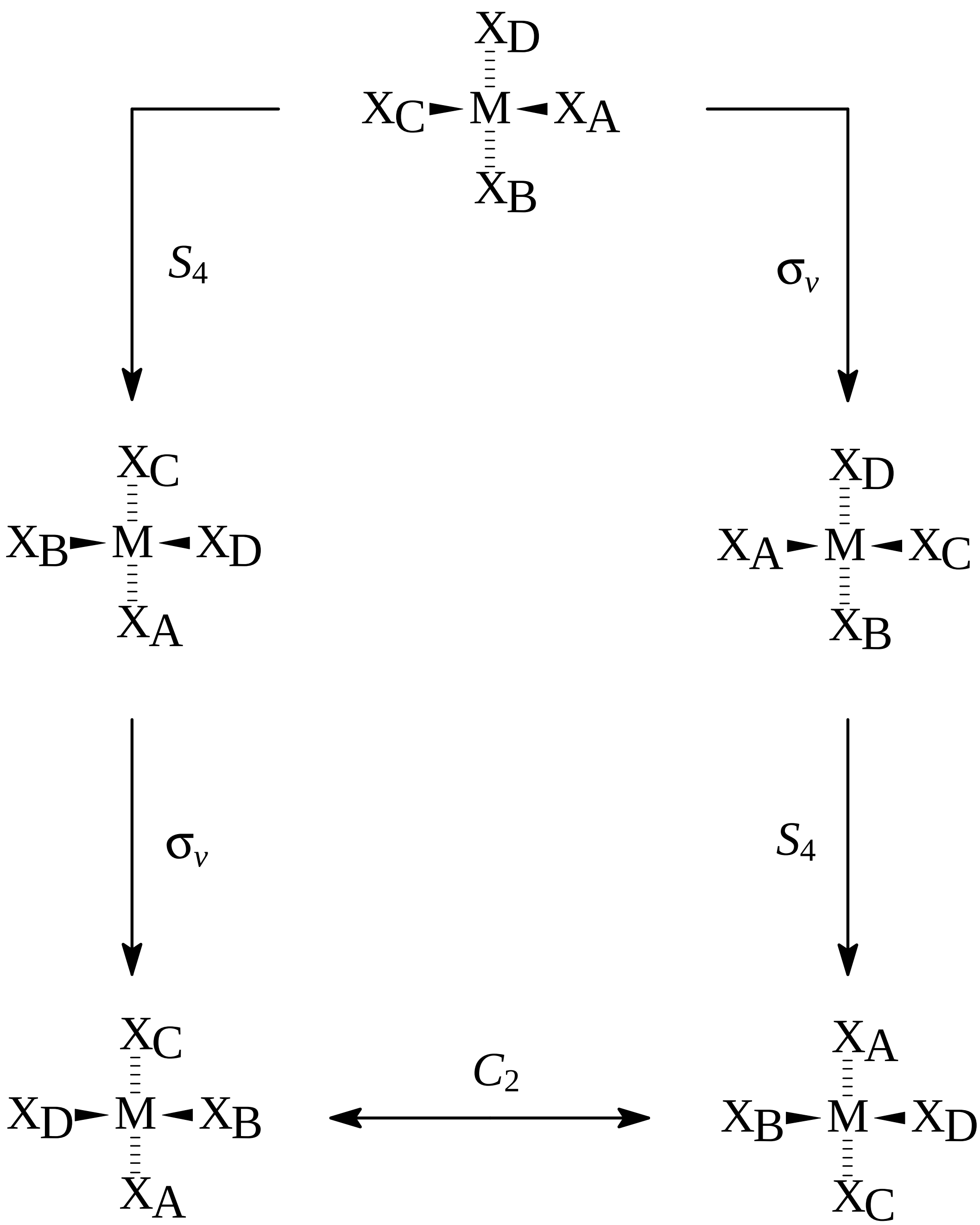
  - ✓ We cannot assume that reversing the order will have the same result.

  - ✓ It may be that either $BA \neq AB$ or $BA = AB$.

- ☞ Multiplication is associative:

$$C(BA) = (CB)A$$

Fig. 1.12 The order of performing S_4 and σ_v, shown here for a tetrahedral MX_4 molecule, affects the result. The final positions in each case are not the same, but they are related to each other by C_2.



Multiplication Tables

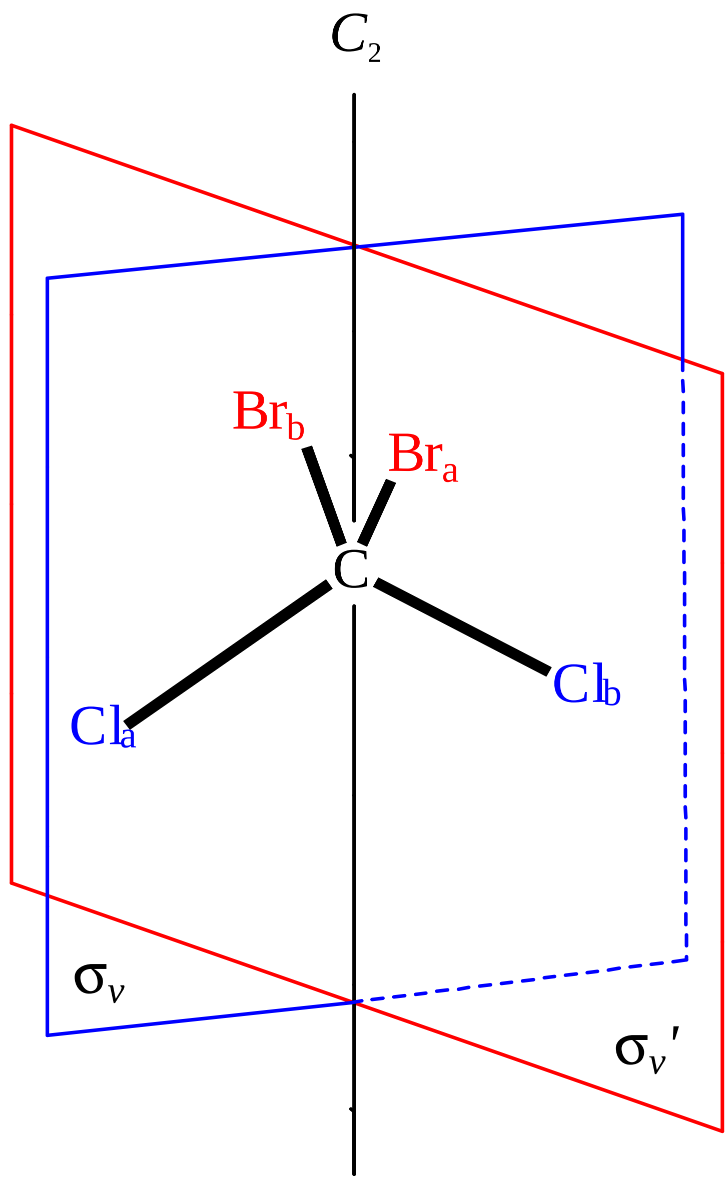
☞ All possible binary combinations of symmetry operations can be summarized in a multiplication table.

	E	A	B	C
E	E	A	B	C
A	A	B	C	E
B	B	C	E	A
C	C	E	A	B

✓ Combination order is "top" then "side"; e.g.,

	E	A	B	C
E	$EE = E$	$EA = A$	$EB = B$	$EC = C$
A	$AE = A$	$AA = B$	$AB = C$	$AC = E$
B	$BE = B$	$BA = C$	$BB = E$	$BC = A$
C	$CE = C$	$CA = E$	$CB = A$	$CC = B$

Fig. 1.13 Symmetry elements of CBr_2Cl_2.



Matrix Notation of the Effects of the Operations

$$[E] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix}$$

$$[C_2] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_b \\ Br_a \\ Cl_b \\ Cl_a \end{bmatrix}$$

$$[\sigma_v] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_b \\ Br_a \\ Cl_a \\ Cl_b \end{bmatrix}$$

$$[\sigma_v'] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_a \\ Br_b \\ Cl_b \\ Cl_a \end{bmatrix}$$

Multiplication Table for the Operations of CBr_2Cl_2

	E	C_2	σ_v	σ_v'
E				
C_2				
σ_v				
σ_v'				

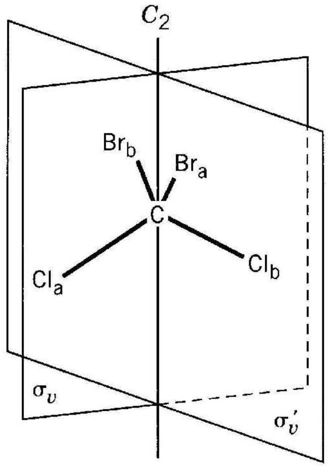
Step 1: Combinations with identity.

	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2			
σ_v	σ_v			
σ_v'	σ_v'			

Step 2: Binary self-combinations.

	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2	E		
σ_v	σ_v		E	
σ_v'	σ_v'			E

Multiplication Table for the Operations of CBr_2Cl_2



Step 3: Mixed binary combinations.

$C_2\sigma_v = ?$

$$[\sigma_v'] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_a \\ Br_b \\ Cl_b \\ Cl_a \end{bmatrix} \qquad [C_2] \times \begin{bmatrix} Br_b \\ Br_a \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_a \\ Br_b \\ Cl_b \\ Cl_a \end{bmatrix}$$

This result is the same as that achieved by σ_v' alone:

$$[\sigma_v] \times \begin{bmatrix} Br_a \\ Br_b \\ Cl_a \\ Cl_b \end{bmatrix} = \begin{bmatrix} Br_b \\ Br_a \\ Cl_a \\ Cl_b \end{bmatrix}$$

✎ $C_2\sigma_v = \sigma_v'$

Complete Multiplication Table

	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2	E	σ_v'	σ_v
σ_v	σ_v	σ_v'	E	C_2
σ_v'	σ_v'	σ_v	C_2	E

General Results:

- ✓ The first row of results duplicates the list of operations in the header row.
- ✓ The first column of results duplicates the list of operations in the label column.
- ✓ Every row shows every operation once and only once.
- ✓ Every column shows every operation once and only once.
- ✓ The order of resultant operations in every row is different from any other row.
- ✓ The order of resultant operations in every column is different from any other column.