PG SEMISTR II, UNIT III, SYMMETRY ELEMENTS

BY

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SubGroups

A subgroup is a self-contained group of elements residing within a larger group.

$$\frac{h \text{ (order of main group)}}{g \text{ (order of subgroup)}} = k \text{ (integer)}$$

G_6	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

G_3	E	D	F
E	E	D	F
D	D	F	E
F	F	E	D

Classes

Assume that A and X are elements of a group and we perform the following operation:

$$X^{-1}AX = B$$

Where B is another element in the group. B is then called the similarity transform of A by X. If this relationship holds, then A and B are said to be conjugate.

The following is true for elements that are related by similarity transforms:

1) Every element is conjugate with itself

$$A = X^{-1}AX$$

(X may be equal to the identity element E)

2) If A is conjugate with B, then B is conjugate with A

Thus, if we have:

$$X^{-1}AX = B$$

Then there must exist another element Y such that:

$$Y^{-1}BY = A$$

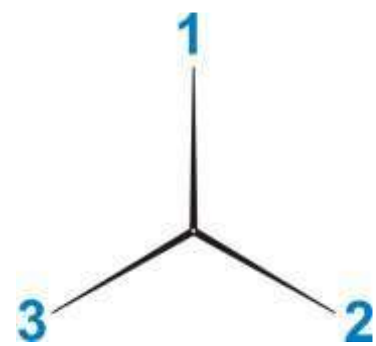
3) Finally, if A is conjugate to both B and C, then B and C must also be conjugate to each other.

A group of elements that are conjugate to one another is called a Class of Elements.

To determine which elements group together to form a class you have to work out all the similarity transforms for each element in the group. Those sets of elements that transform into one another are then in the same class.

Consider the C_{3v} symmetry point group "matrix":

C_{3v}	E	C_3	C_3^2	σ_v^1	σ_v^2	σ_v^3
E	E	C_3	C_3^2	σ_v^1	σ_v^2	σ_v^3
C_3	C_3	C_3^2	E	σ_v^2	σ_v^3	σ_v^1
C_3^2	C_3^2	E	C_3	σ_v^3	σ_v^1	σ_v^2
σ_v^1	σ_v^1	σ_v^2	σ_v^3	E	C_3	C_3^2
σ_v^2	σ_v^2	σ_v^3	σ_v^1	C_3^2	E	C_3
σ_v^3	σ_v^3	σ_v^1	σ_v^2	C_3	C_3^2	E



Lets determine the classes of symmetry operations for this point group. Lets start with the similarity transforms for the vertical mirror planes:

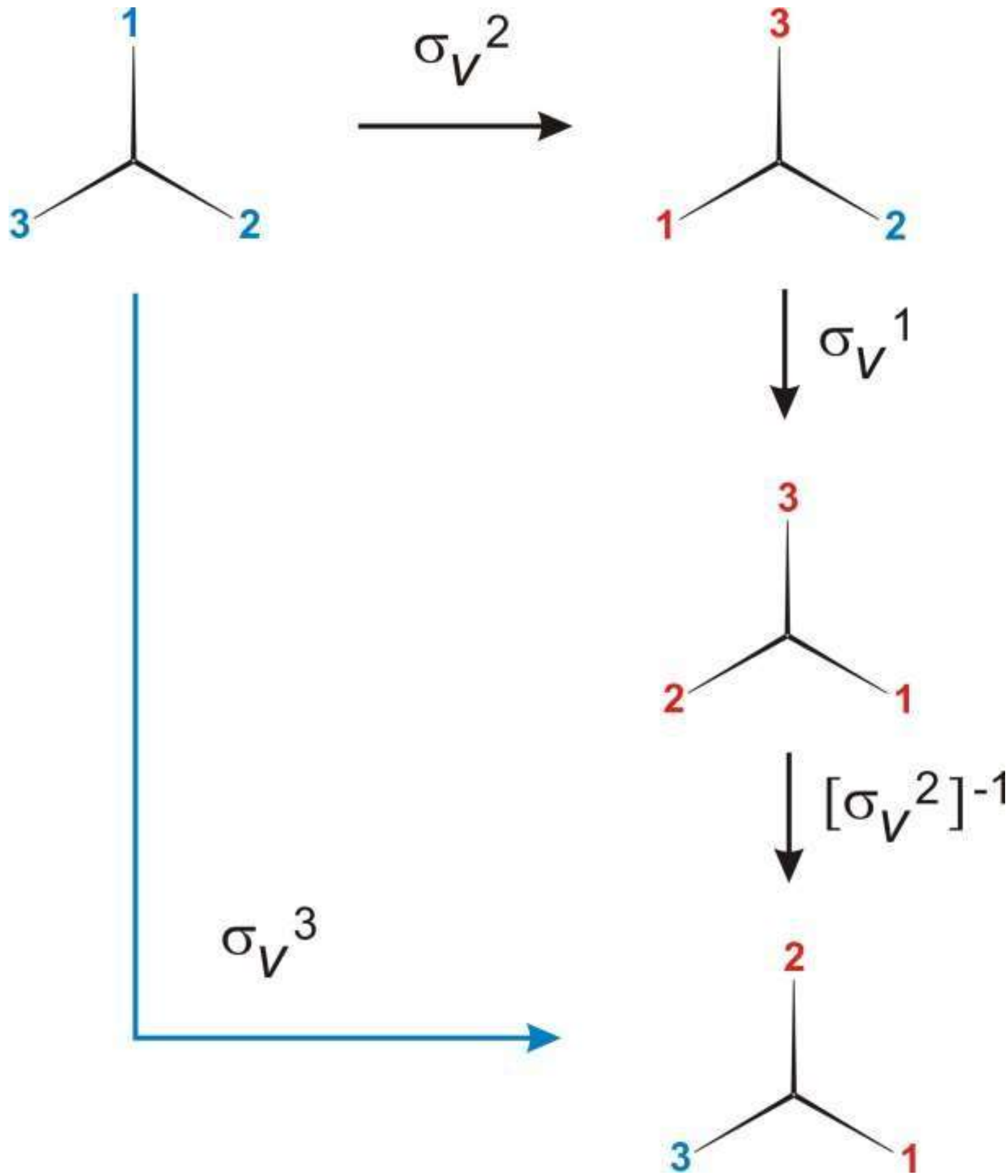
$$\sigma_v^1 \, \sigma_v^1 \, [\sigma_v^1]^{-1} = \sigma_v^1$$

$$\sigma_v^2 \, \sigma_v^1 \, [\sigma_v^2]^{-1} = \sigma_v^3$$

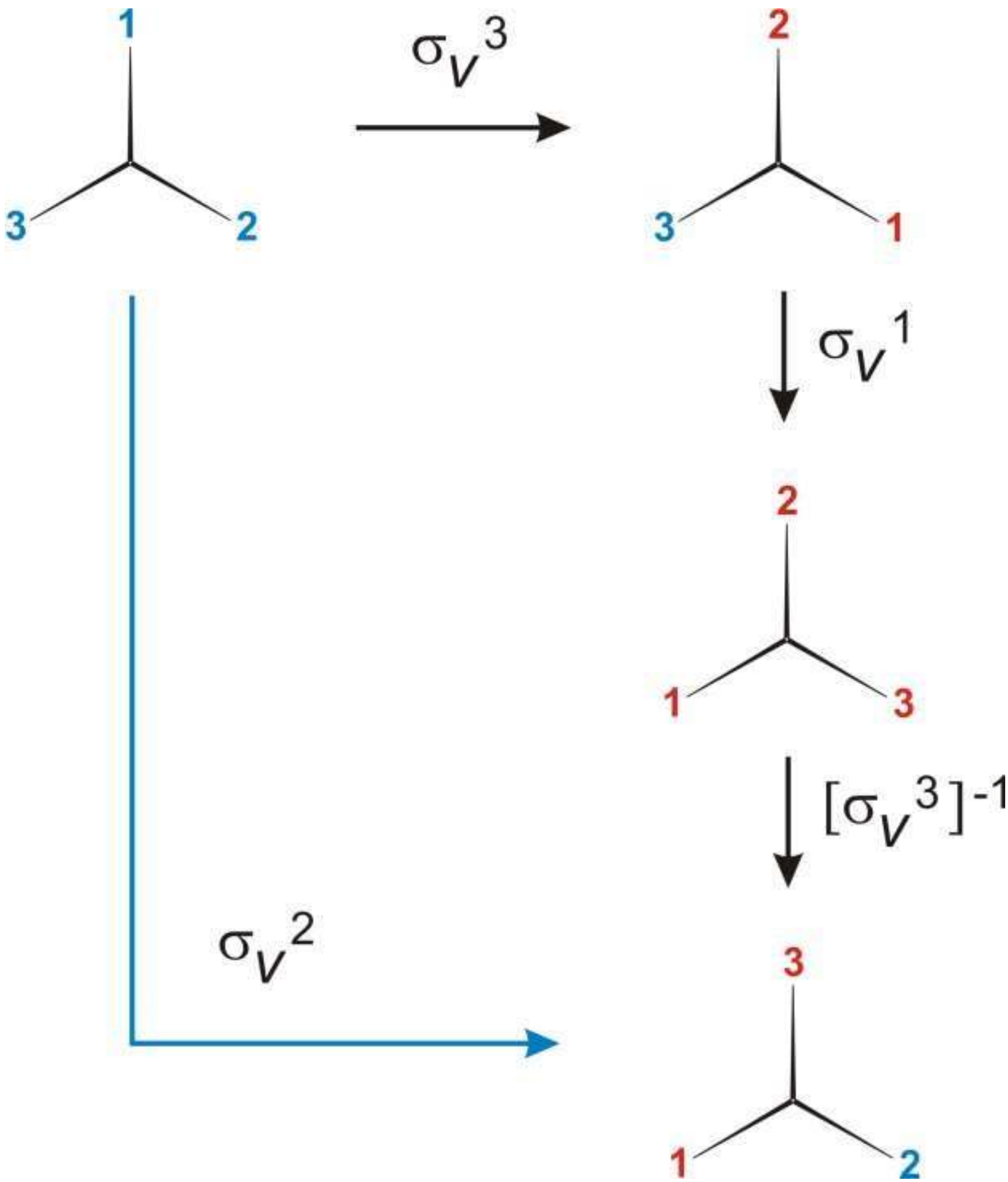
$$\sigma_v^3 \, \sigma_v^1 \, [\sigma_v^3]^{-1} = \sigma_v^2$$

Let's see how this works graphically:

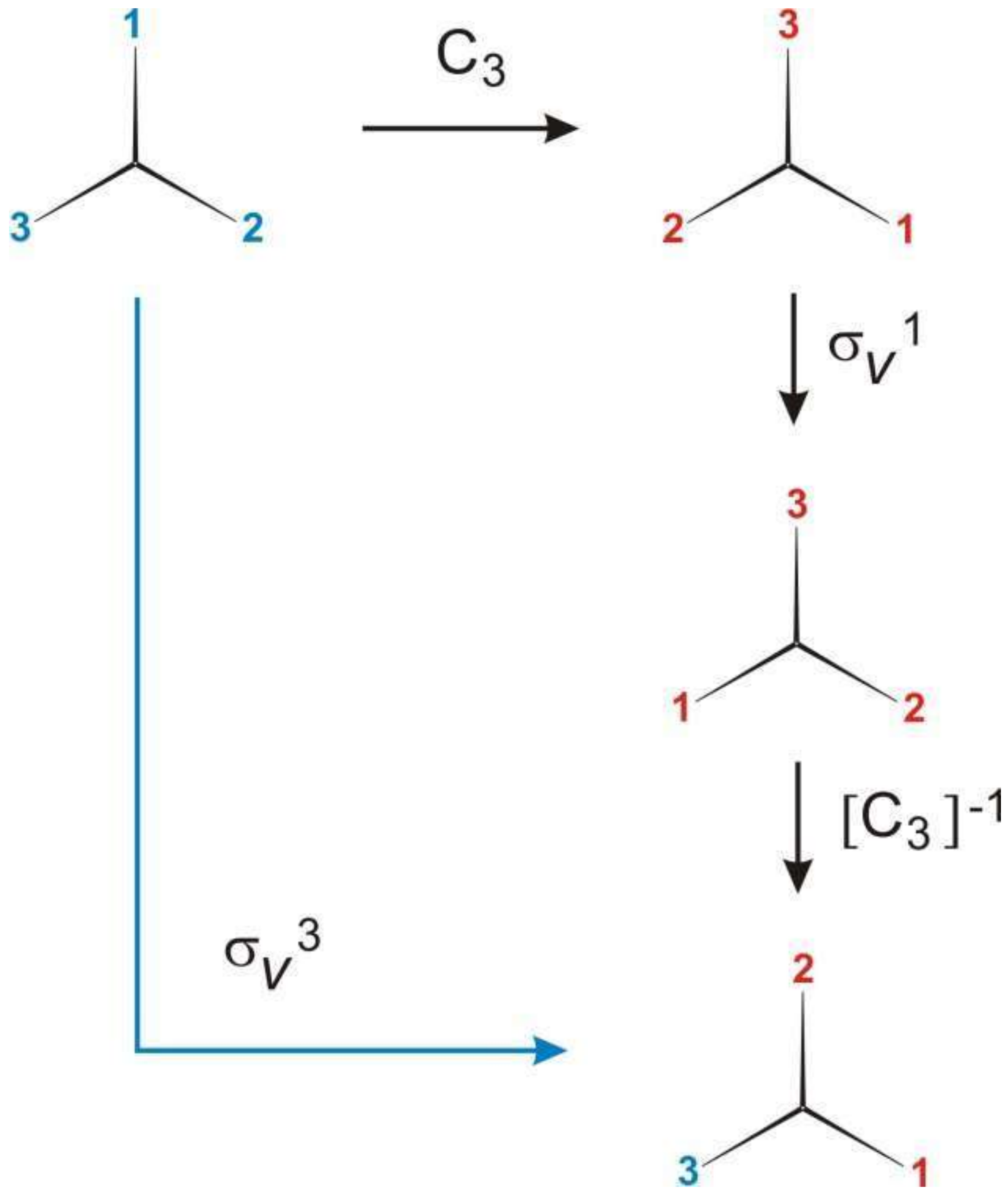
$$\sigma_v^{\ 2}\ \sigma_v^{\ 1}\ [\sigma_v^{\ 2}]^{-1} = \sigma_v^{\ 3}$$



$$\sigma_v^{3}\,\sigma_v^{1}\,[\sigma_v^{3}]^{-1} = \sigma_v^{2}$$



$$\mathbf{C_3}\ \sigma_v^{\ 1}\ [\mathbf{C_3}]^{-1} = \sigma_v^{\ 3}$$



If we continue these similarity transforms we find that the various symmetry operations for C_{3v} break down into the following classes:

E

C_3, C_3^2

σ_v^1, σ_v^2, σ_v^3

If we examine the character tables in Cotton we find that the symmetry operations are listed and grouped together in these very same classes:

C_{3v}	E	$2C_3$	$3\sigma_v$

Corollary: the orders of all the classes must be integral factors of the order of a group.

Order of a point group = # of symmetry operations