IMPROPER AXIS OF SYMMETRY

Improper Axis of Symmetry

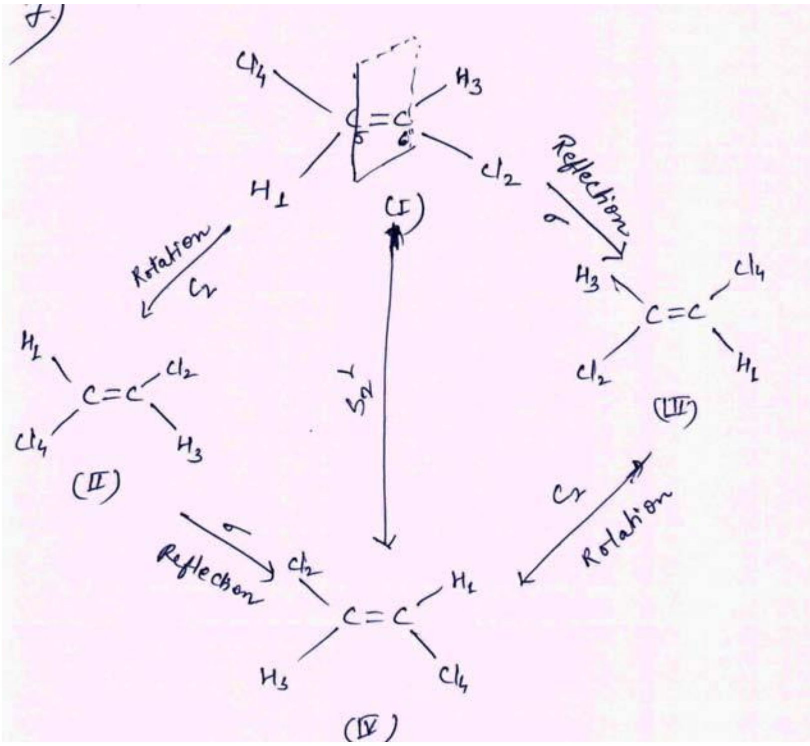
An improper axis of rotation is said o exist when rotation about an axis followed by a reflection in a plane perpendicular to the axis of rotation results in an equivalent or identical configuration or in other words we can say that it is an imaginary axis on which the molecule has to be rotated and then reflected on a plane perpendicular to the rotation axis to get an equivalent or identical configuration.

The improper axis of rotation is represented by S_n. The operations generated by it are represented by S_n^m, where

n = order of axis and

m= no. of times the operation is being performed.

This symmetry element can be best understood by considering the following example of trans dichloro ethene. Carrying out a C_2 operation about an axis passing through the C=C bond gives configuration II which is then followed by reflection in a plane perpendicular to axis of rotation gives configuration IV which is equivalent to I. We perform the same operations but this time in reverse manner. First we reflect the molecule in a plane described above. This results in configuration III which after rotation about the axis along the C=C and again gives configuration IV. These combined operations are shown in figure.



From the above figure it is concluded that "whether we perform C_2 operation first than the σ or we perform σ first and then C_2 operation, the result is same.

$$\sigma . C_2 = C_2 . \sigma$$

So either rotation followed by reflection or reflection followed by rotation will give the same results. The order of operation is important the operation is always carried out from right to left as indicated by arrow. On comparing II and III with I, we find that neither II nor III is equivalent to I and hence neither C_2 nor σ is a symmetry operation but configuration IV is equivalent to I and hence the combination of C_2 and σ is a symmetry operation. Thus the improper axis in the above example of trans dichloro ethylene is represented by S_2. The BF_3 molecule has C_3 axis and he molecular plane lying perpendicular to it makes the improper axis to exist automatically. The improper axis is co-linear with C_3 axis. Thus the improper axis in BF_3 is represented as S_3.

The element S_n^m generates a set of operations $S_n^1\, S_n^2\, S_n^3$..... but whether $S_n^m = E$ or not, depends upon on *n* being even or odd. We shall now discuss these 2 cases.

Let us consider the operations generated by S_n axis with *n* even say S_4. It should be mention that an element of symmetry is said to generate as many operations as necessary to get an identical configuration. Now we write the operations generated by S_4 in the following way.

$$S_4^1 = C_4^1 . \sigma^1 = S_4^1$$

$$S_4^2 = C_4^2 . \sigma^2 = C_2^1 . E = C_2^1 \quad \{\text{because } \sigma^2 = E \text{ and } C_4^2 = C_2^1\}$$

$$S_4^3 = C_4^3 . \sigma^3 = S_4^3$$

$$S_4^4 = C_4^4 . \sigma^4 = E$$

Thus the operations generated by S_4 axis have S_4^1, C_2^1, S_4^3 and E. In these operations we have C_2 and E which are the operations generated by a C_2 axis. This means that we have a C_2 axis co-linear with the S_4 axis.

Let us now consider S_n axis with *n* odd say an S_3 axis, and the operations generated by this axis are as follows:

$$S_3^1 = C_3^1 . \sigma^1 = S_3^1$$

$$S_3^2 = C_3^2 . \sigma^2 = C_3^2 . E = C_3^2$$

$$S_3^3 = C_3^3 . \sigma^3 = E . \sigma = \sigma \quad \{\text{because } \sigma^3 = \sigma\}$$

$$S_3^4 = C_3^4 . \sigma^4 = C_3^4 . E = C_3^1 \quad \{\text{because } C_n^{m+1} = C_n^1 \text{ and } \sigma^4 = E\}$$

$$S_3^5 = C_3^5 . \sigma^5 = S_3^5$$

$$S_3^6 = C_3^6 . \sigma^4 = C_3^3 . E = E.E = E \quad \{\text{because } C_n^{m+3} = C_n^3\}$$

Thus an S_3 axis has generated S_3^1, C_3^1, C_3^2, S_3^5, σ and E operations.

From the above examples we note that-

- An S_3 axis has generated six operations and in general an S_n axis with *n* odd will generate 2*n* operations.

- An S_4 axis has generated 4 operations so in general an S_n axis with n even will generate n operations.