GROUP THEORY

NO - 9

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POINT GROUPS
(PART TWO)
DIHEDRAL POINT GROUPS
D_{nd} and D_{nh}

DIHEDRAL POINT GROUPS – D_{nd} and D_{nh}

5) D_{nd} POINT GROUP

Elements of the D_{nd} point group

- The elements of the D_{nd} point group are
- E,
- C_n, C_n^2, C_n^3, ... C_n^{n-1},
- n C_2 perpendicular to C_n
- S_{2n}, S_{2n}^3, S_{2n}^5, S_{2n}^7,... S_{2n}^{2n-1} and
- n σ_d planes

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- n C_2 perpendicular to C_n
- S_{2n} , S_{2n}^3, S_{2n}^5, S_{2n}^7,... S_{2n}^{2n-1} and
- n σ_d planes

D_{2d} POINT GROUP

- The elements of the D_{nd} point group are
- E,
- C_n, C_n^2, C_n^3, ... C_n^{n-1},
- n C_2 perpendicular to C_n
- S_{2n}, S_{2n}^3, S_{2n}^5, S_{2n}^7,... S_{2n}^{2n-1} and
- n σ_d planes

- The elements of the D_{2d} point group are
- E
- C_2
- 2 C_2 perpendicular to C_2
- S_4, S_4^3 ($S_{2n}^{2n-1} = S_4^{4-1} = S_4^3$)
- 2 σ_d planes

The elements of the D_{2d} point group are

E, C_2, 2 C_2 perpendicular to C_2, S_4, S_4^3 and 2 σ_d planes (8 elements)

Classes within the D_{2d} point group

- The 8 elements of the D_{2d} point group are
  - E, C_2, 2 C_2 perpendicular to C_2 , S_4, S_4^3 and 2 σ_d planes

- These elements according to classes are
  - E
  - C_2
  - 2 C_2 perpendicular to C_2
  - S_4, S_4^3
  - 2 σ_d planes

The elements of the D_{2d} point group are usually written as

$$E, C_2, 2C_2', 2S_4, \text{and } 2\sigma_d$$

- Order of the D_{2d} point group = 8
- Number of classes = 5

D_{3d} POINT GROUP

- The elements of the D_{nd} point group are
- E,
- C_n, C_n^2, C_n^3, ... C_n^{n-1},
- n C_2 perpendicular to C_n
- S_{2n}, S_{2n}^3, S_{2n}^5, S_{2n}^7,... S_{2n}^{2n-1} and
- n σ_d planes

- The elements of the D_{3d} point group are
- E
- C_3, C_3^2
- 3 C_2 perpendicular to C_3
- S_6, S_6^3, S_6^5

  S_6^3 may be written in another form

  $S_6^3 = C_6^3 \sigma^3 = C_2 \sigma = S_2 = i$
- $3\sigma_d$ planes

The elements of the D_{3d} point group are

E, C_3, C_3^2, $3C_2$ perpendicular to C_3, S_6, S_6^5, i and 3 σ_d planes (12 elements)

Classes within the D_{3d} point group

- The 12 elements of the D_{3d} point group are
  - E, C_3, C_3^2, $3C_2$ perpendicular to C_3, S_6, S_6^5, i and $3\sigma_d$ planes

- These elements according to classes are
  - E
  - C_3, C_3^2
  - $3C_2$ perpendicular to C_3
  - S_6, S_6^5
  - i
  - $3\sigma_d$ planes

The elements of the D_{3d} point group are usually written as

$$E, 2C_3, 3C_2, 2S_6, i \text{ and } 3\sigma_d$$

- Order of the D_{3d} point group = 12
- Number of classes = 6

D_{5d} POINT GROUP

- The elements of the D_{nd} point group are
- E,
- C_n, C_n^2, C_n^3, ... C_n^{n-1},
- n C_2 perpendicular to C_n
- S_{2n}, S_{2n}^3, S_{2n}^5, S_{2n}^7,... S_{2n}^{2n-1} and
- n σ_d planes

- The elements of the D_{5d} point group are
- E
- C_5, C_5^2, C_5^3, C_5^4
- 5 C_2 perpendicular to C_5
- S_{10}, S_{10}^3, S_{10}^5, S_{10}^7, S_{10}^9

  S_{10}^5 may be written in another form

  $S_{10}^5 = C_{10}^5 \sigma^5 = C_2 \sigma = S_2 = i$
- 5 σ_d planes

The elements of the D_{3d} point group are

E, C_5, C_5^2, C_5^3, C_5^4, 5 C_2 perpendicular to C_5, S_{10}, S_{10}^3, S_{10}^7, S_{10}^9, i and 5 σ_d planes (20 elements)

Classes within the D_{5d} point group

- The 20 elements of the D_{5d} point group are
  - E, C_5, C_5^2, C_5^3, C_5^4, 5 C_2 perpendicular to C_5, S_{10}, S_{10}^3, S_{10}^7, S_{10}^9, i and 5 σ_d planes

- These elements according to classes are
  - E
  - C_5, C_5^3
  - C_5^2, C_5^4
  - 5 C_2 perpendicular to C_5
  - S_{10}, S_{10}^7
  - S_{10}^3, S_{10}^9
  - i
  - 5 σ_d planes

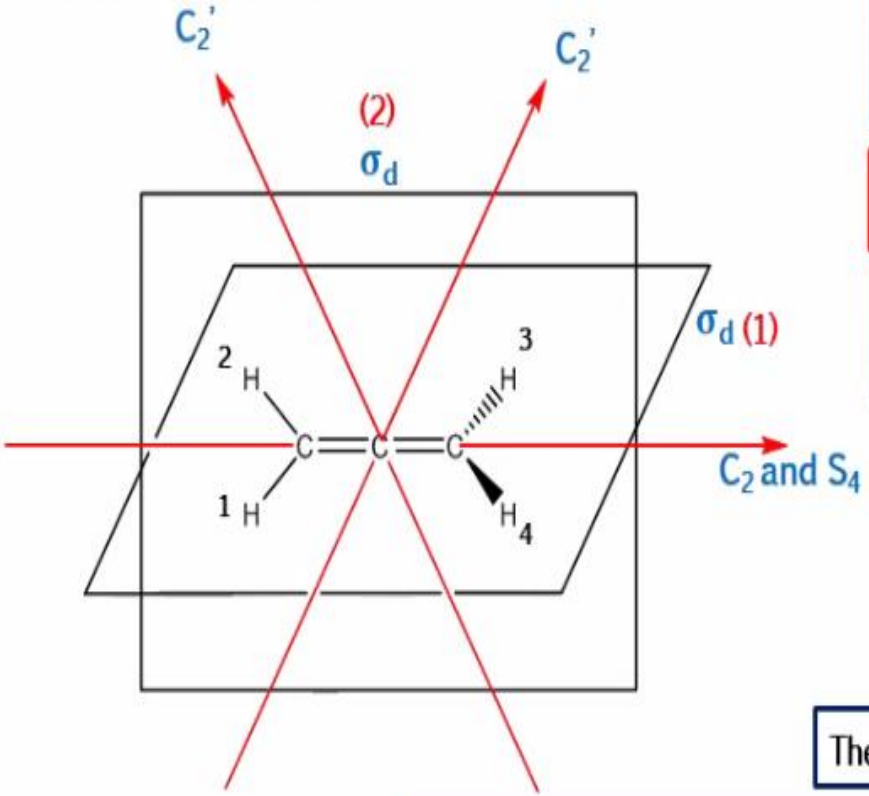
The elements of the D_{5d} point group are usually written as

$E, 2C_5, 2C_5^2, 5C_2, 2S_{10}, 2S_{10}^3$, i and $5\sigma_d$

- Order of the D_{5d} point group = 20
- Number of classes = 8

Allene $H_2C{=}C{=}CH_2$

- D_{2d} Point group



Use a molecular model to visualize the various planes and axes in the allene molecule

The 3 C atoms and H (1) and H (2) are in one plane and H (3) and H (4) are in a perpendicular plane

The C_2 axis passes through the three C atoms

The C_2 axis is also the S_4 axis . Allene was the example for a molecule with S_4 axis. Refer video 3 of 20.

The 2 C_2' axes pass through the second C atom

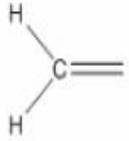
The 2 σ_d s bisect the angle between the 2 C_2' axes.

The σ_d labelled (1) contains the 3 C atoms and H(1) and H(2) and bisects the angle H(3)-C-H(4)

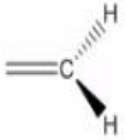
The σ_d labelled (2) contains the 3 C atoms and H(3) and H(4) and bisects the angle H(1)-C-H(2)

An important feature of the D_{nd} point group

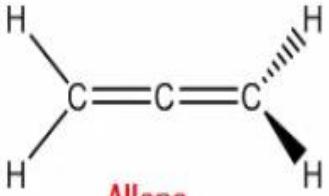
- In allene, there are two C_{2v} fragments



C_{2v} fragment



C_{2v} fragment



Allene

These two fragments are staggered at an angle of 90^0 ie. $180^0/2$

In fact, any molecule belonging to the D_{nd} point group can be regarded as being made of 2 identical fragments of C_{nv} symmetry staggered at an angle of $180^0/n$

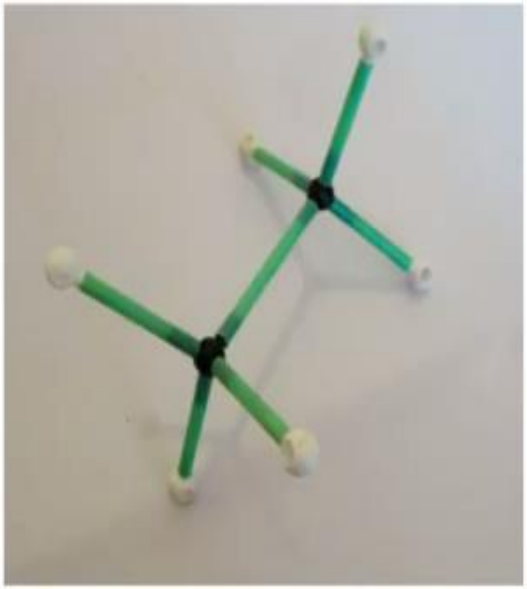
D_{3d} POINT GROUP

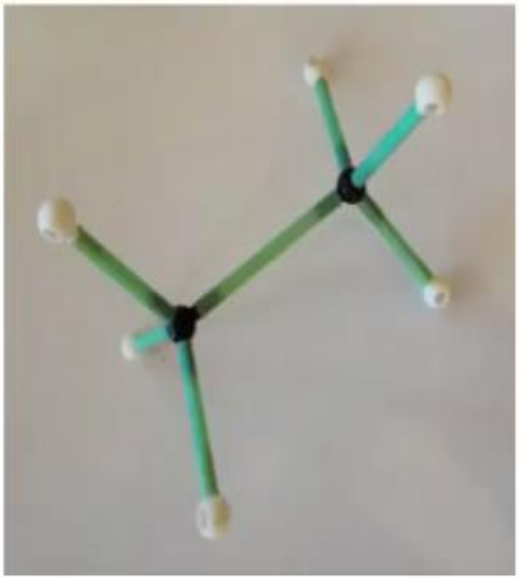
- A D_{2d} molecule like allene consists of two identical fragments of C_{2v} symmetry staggered at an angle of $180^0/2 = 90^0$

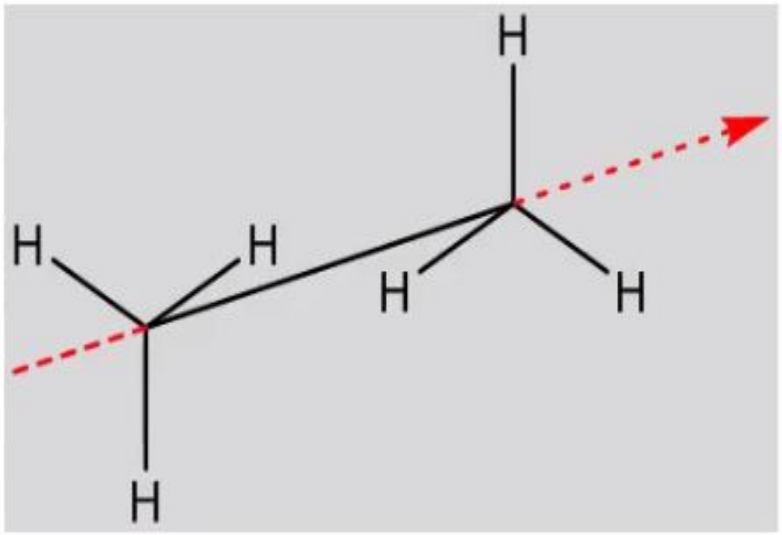
- A D_{3d} molecule should consist of two identical fragments of C_{3v} symmetry staggered at an angle of $180^0/3 = 60^0$

The molecule which comes to our mind immediately is the staggered ethane (which was the example for a molecule with S_6 axis in the video 3 of 20)

- D_{3d} Point group







There are 2 CH_3 fragments and each fragment is pyramidal like NH_3 and hence of C_{3v} symmetry

The C_3 axis passes through the two C atoms

The C_3 axis is also the S_6 axis .

The 3 C_2 axes pass through a point midway between the 2 C atoms

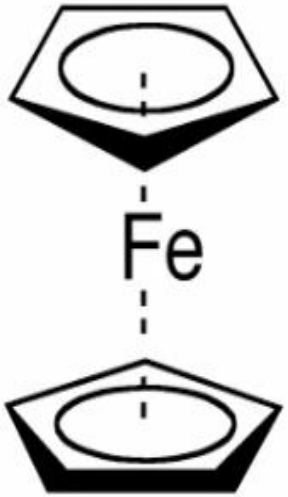
The 3 σ_d s bisect the angle between the C_2 axes.

Each σ_d plane passes through the 2 C atoms and 2 H atoms, one from each C atom

D_{5d} POINT GROUP

- A D_{5d} molecule should consist of two identical fragments of C_{5v} symmetry staggered at an angle of $180^0/5 = 36^0$

Example: Staggered Ferrocene



Visualize all the 20 symmetry operations of staggered ferrocene

An important note:

Always remember ALLENE, STAGGERED ETHANE and STAGGERED FERROCENE as typical examples of D_{nd} point group.

The D_{nd} symmetry is perhaps the most difficult one to recognize easily.

Continued.....