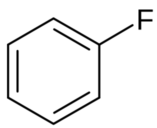
2. Point groups

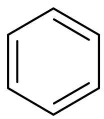
- all possible combinations of symmetry operations:
  - not all combinations are possible



C_2
2 σ_v

The combination C_2, 2 σ_v, i is not possible here or ever!

  - some combinations follow naturally



C_6
...

Part of ... has to be a C_2 and a C_3, both are colinear to C_6!

Point groups in the Schoenflies system

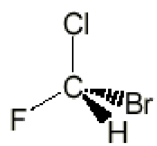
- C: point groups with only one symmetry axis (except for C_1, C_s, C_i)
- D: point groups with nC_2 axes perpendicular to the principal axis
- T, O, I: higher order point groups

Point groups continued

➡ C_1

- symmetry element: E only

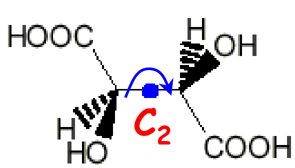
C_1



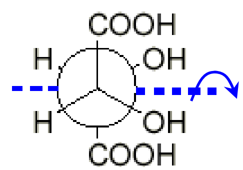
➡ C_n

- symmetry element: one C_n only

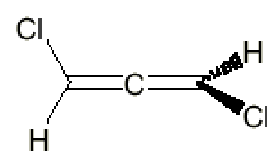
C_2

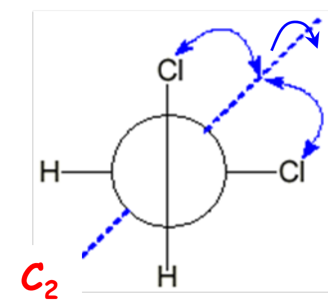


C_2

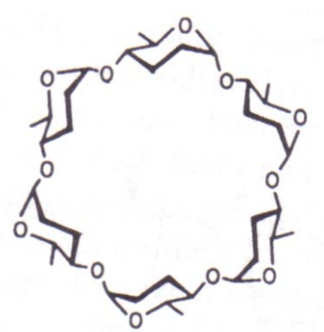


C_2



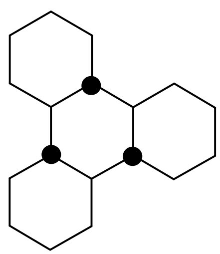


C_6



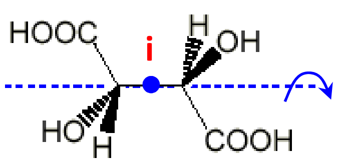
Point groups continued

- D_n
  - symmetry elements: C_n , n $C_2 \perp$ to C_n

D_3  C_3 3 C_2

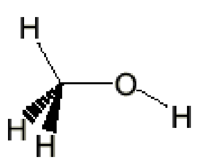
D_2 : twisted (< 90°) ethene

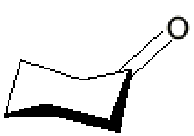
- C_i (or S_2)
  - symmetry element: *i* only

C_i S_2 

We will not cover the other S_{2n} groups.

- C_s
  - symmetry element: σ only

C_s 

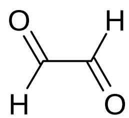
C_s 

Point groups continued

C_{nh}

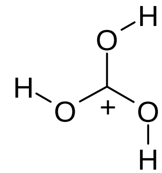
- symmetry elements: C_n , σ_h , [i]

C_{2h}



C_2
σ_h
i

C_{3h}

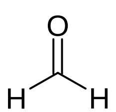


C_3
σ_h

C_{nv}

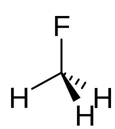
- symmetry elements: C_n , n σ_v

C_{2v}

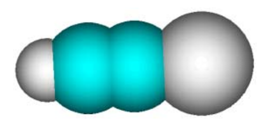


C_2
2 σ_v

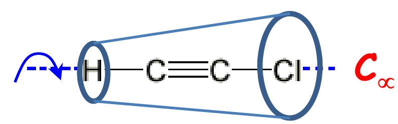
C_{3v}



C_3
3 σ_v



$C_{\infty v}$



C_∞
∞ σ_v

$C_{\infty v}$ is "conical" symmetry.

$H-C \equiv C-CH_3$

What about these? Linear?

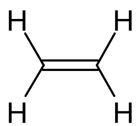
$H_2C=C=CH_2$

Point groups continued

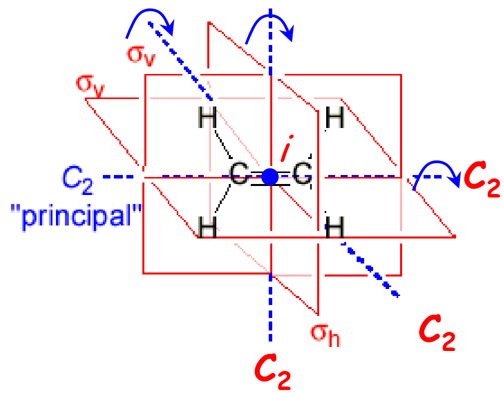
➡ D_{nh}

- symmetry elements: C_n , n C_2 ⊥ to C_n , σ_h , n σ_v , [i]

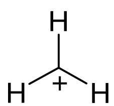
D_{2h}



$3\ C_2$
$2\ \sigma_v$
σ_h
i

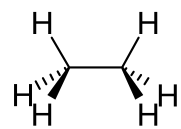


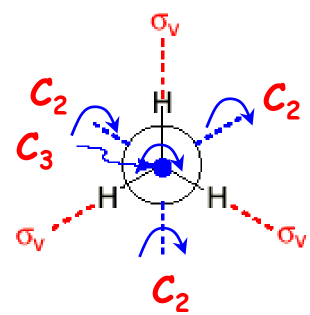
D_{3h}



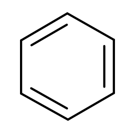
C_3
$3\ C_2$
$3\ \sigma_v$
σ_h

D_{3h}



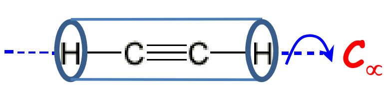


D_{6h}



C_6
(C_3, C_2)
$6\ C_2$
$6\ \sigma_v$
σ_h
i

$D_{\infty h}$



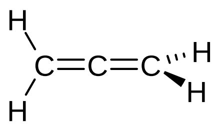
C_∞
$\infty\ C_2$
$\infty\ \sigma_v$
σ_h
i

$D_{\infty h}$ is "cylindrical" symmetry.

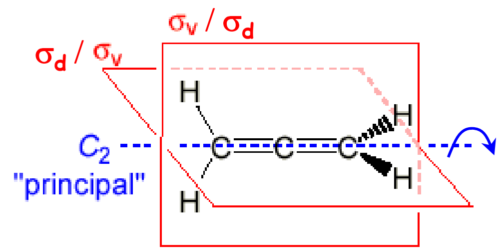
Point groups continued

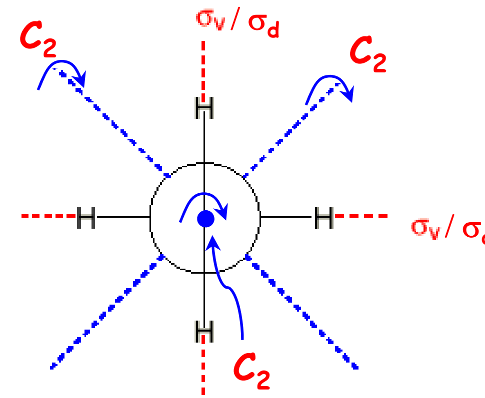
➡ D_{nd}

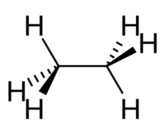
- symmetry elements: C_n , n C_2 ⊥ to C_n , n σ_d (or "σ_v"), [i]

D_{2d} 

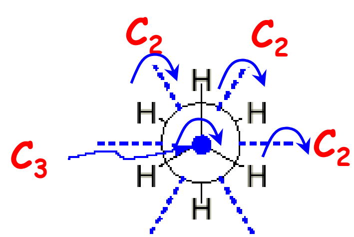
3 C_2
2 σ_d

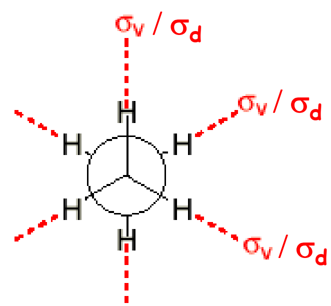




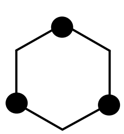
D_{3d} 

C_3
3 C_2
3 σ_d
i





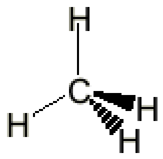
σ_d: These σ_v do not contain the remaining C_2 axes, but they bisect the angle formed by the C_2 axes: they are "diagonal" instead of "vertical".

D_{3d} 

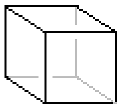
Point groups continued

➡ T_d, O_h, I_h

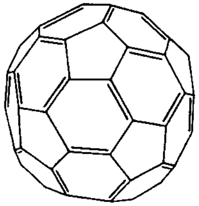
- refer to the Platonic solids
- tetrahedral, octahedral (or cubic), icosahedral symmetry



CH_4



C_8H_8



C_{60}

In all of the point groups above:

We do not need to analyse for S_n specifically, the analysis can be done without.

Chiral point groups

- point groups that contain chiral molecules
- C_1, C_n, D_n: contain only proper symmetry axes
  and are "dissymmetric"
- all other point groups include a reflection element (σ or S_2)
  and are "symmetric"

("asymmetric" is the lack of symmetry and is reserved for C_1)

Bottom line(s):

A chiral molecule has no symmetry, or has only symmetry axes!

A chiral molecule cannot belong to a symmetric point group!

Point group identification scheme