(9) **Today**

4.1 Symmetry elements and Operations

4.2 Point Groups

Next Class (10)

4.1 Symmetry elements and Operations

4.2 Point Groups

(11) **Second Class from Today**

4.3 Character Tables

Third Class from Today (12)

Test 1

Why care about symmetry?

Infrared Spectroscopy - vibrations that change the dipole of a molecule absorb infrared light

Raman Spectroscopy - vibrations that change the polarizability of a molecule are Raman active

Formation of molecular orbitals requires the interaction of atomic orbitals with the appropriate symmetry

Electronic transitions are also ruled by symmetry

Symmetry operations are the motions: rotation, reflection, etc

Symmetry elements are the thing about which the motion occurs: the axis of rotation, the plan of reflection

Symmetry operations of a molecule are those motions which when performed produce a result indistinguishable from the original

E no change is made to the molecule

multiply the coordinates of every atom by 1

Rotation occur about an axis (element)

indicates a rotation operation

C_n

Where n = 360° / (degrees through which the object is rotated)

If rotating by 120° then $n = \frac{360}{120} = 3$

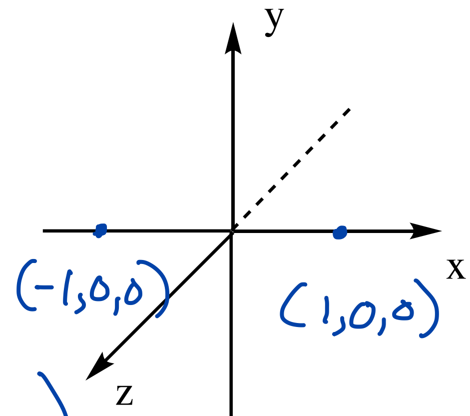
C_3 is a 120° rotation

Reflection (operation) through a plane (element)

more on this shortly

σ_h horizontal ($\perp$ to the principal axis)

σ_v vertical ($\parallel$ to the principal axis)



σ_d dihedral (a type of vertical mirror plane)
($\parallel$ to principal axis and bisecting 2 C_2 axes)

reflections only change 1 position

front/back

σ_{yz} the (1,0,0) would become (-1,0,0)
(1,1,0) would become (-1,1,0)

Inversion (operation) through a point (element)

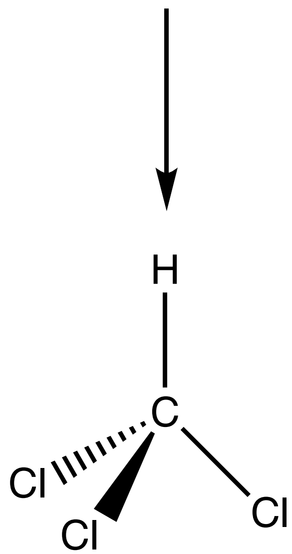
i all atoms move through the center point to a position equaly distant to the starting position

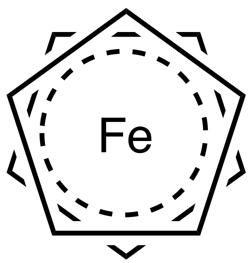
S_n

Where n = 360° / (degrees through which the object is rotated)

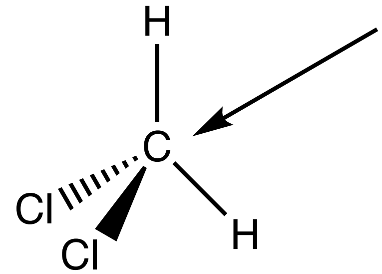
First rotate by $360°/n$ degrees
and reflect through a mirror plane $\perp$ to
the axis of rotation

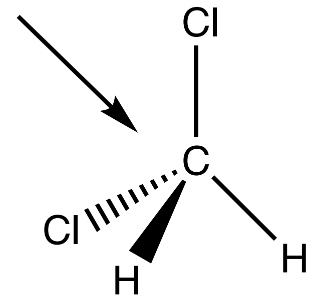
Look along bonds



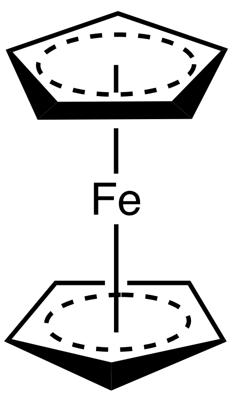


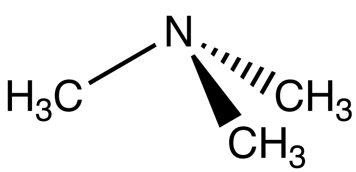
Look along lines that bisect bond angles

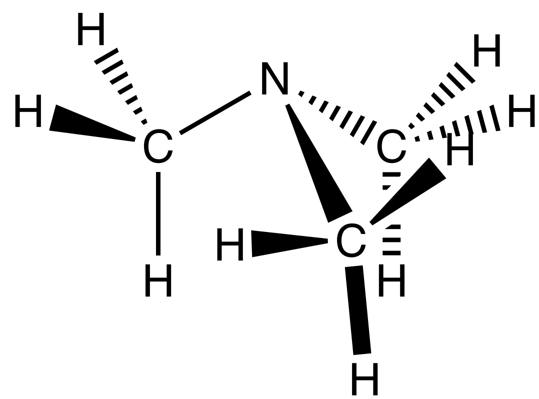




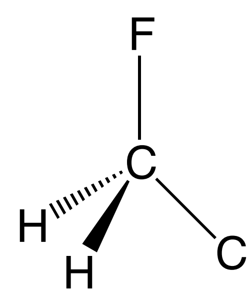
Used simplified structures

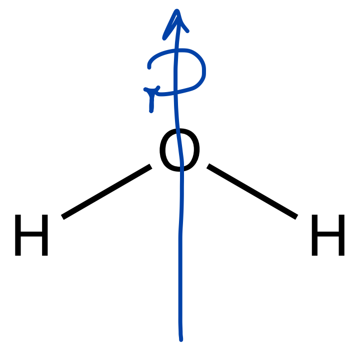




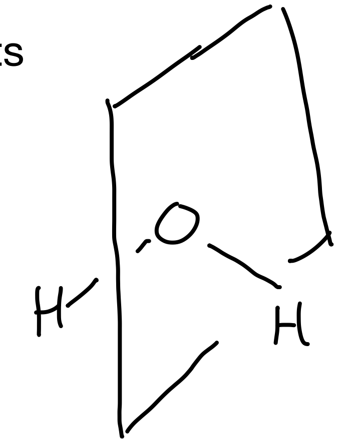


Put Dissimilar Atoms in a Plane or Line

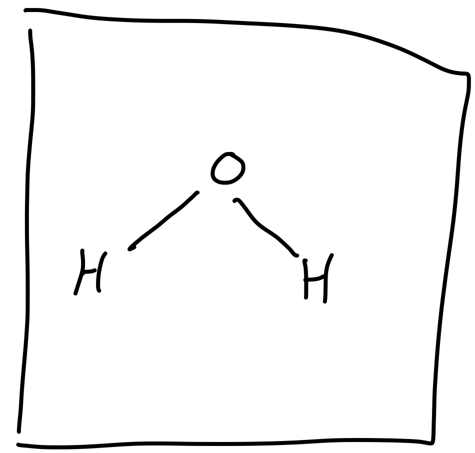




C_2



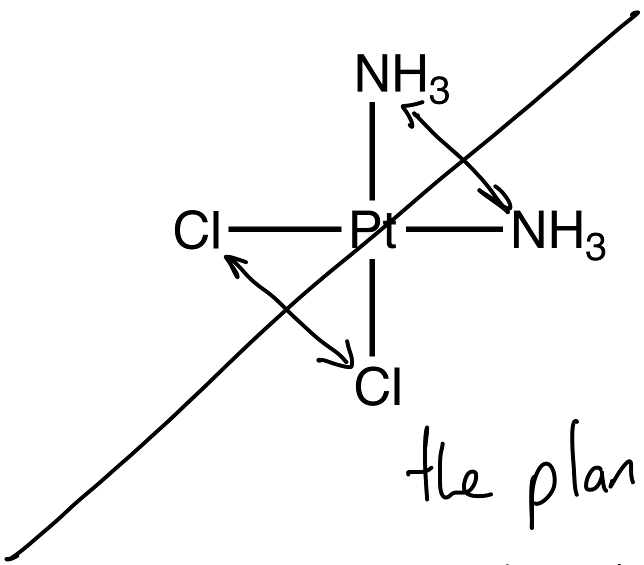
σ_v



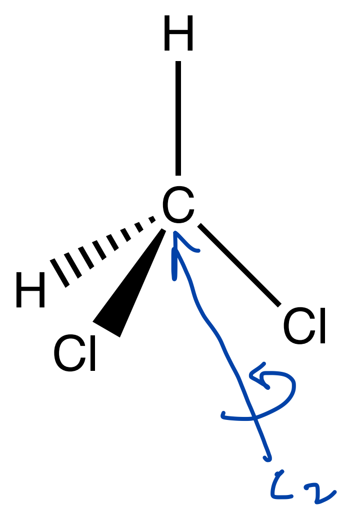
σ_v

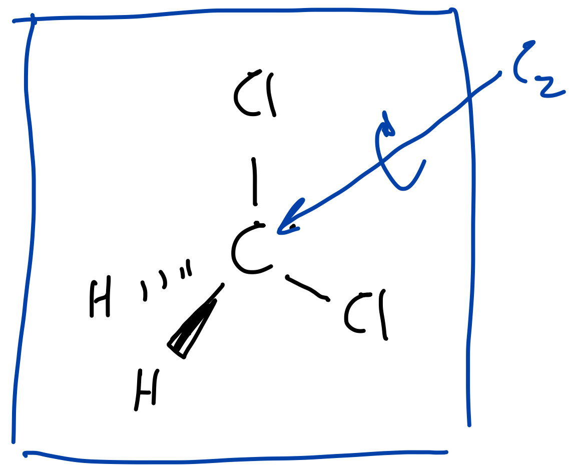
the plane of the screen

vertical mirror plane

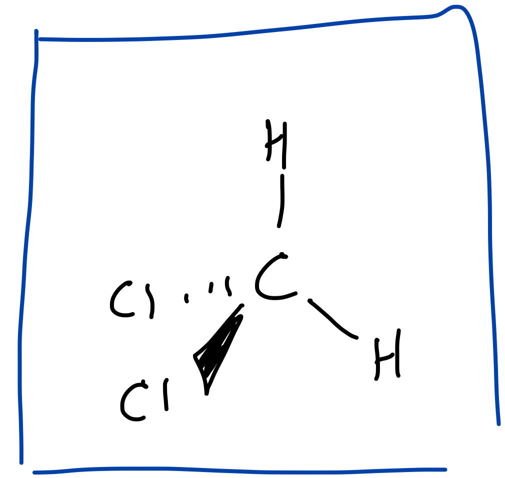


the plane the atoms are in

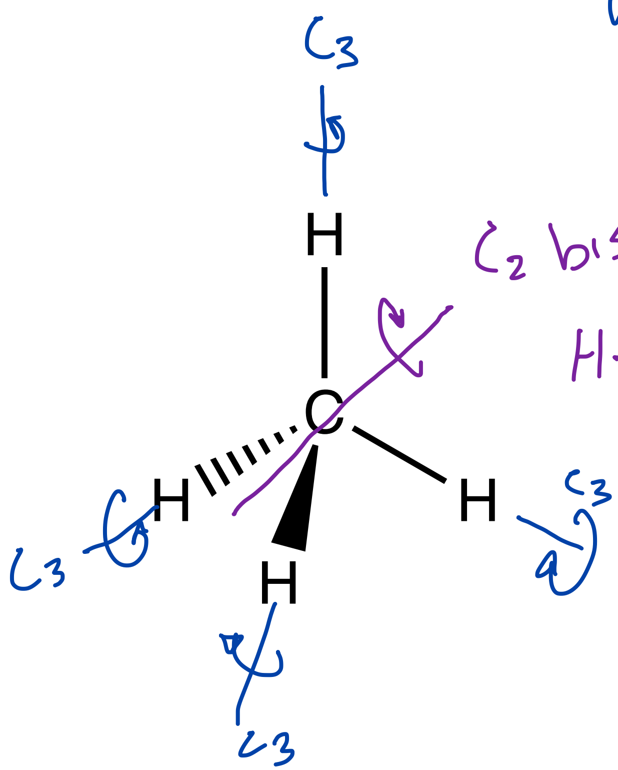




σ_v plane of the screen



σ_v plane of the screen



C_2 bisecting each H–C–H angle (3)

6 σ_d's

+ 6 S_4 operations

In mathematics, a group is a **set** combined with an **operation** that has the specific mathematical properties properties

the operation combines any two elements of the set to form a third element which is part of the original set

other ways of saying this:
a set must be closed under the operation
there must be closure with respect to the operation

operating on elements of the set must satisfy the associative property

there must be an identity element in the set that when operated on by the operation along with any element of the set returns the original element

the operation in the set must be invertible; that is, the set must contain elements such that the operation on two elements in the set produce the identity element

It is a collection of symmetry operations with at least one fixed point that satisfies the criteria of being a mathematical "group"

C_{2v}

The set is the set of symmetry operations.
The operation is the symmetry operations operating on each other.

$C_2 \times \sigma_{v(xz)} = \sigma_{v(yz)}$ $\quad$ $C_2 \times \sigma_{v(yz)} = \sigma_{v(xz)}$ $\quad$ $\sigma_{v(xz)} \times \sigma_{v(yz)} = C_2$

$C_2 \times (\sigma_{v(xz)} \times C_2) = \sigma_{v(xz)}$ $\quad$ $(C_2 \times \sigma_{v(xz)}) \times C_2 = \sigma_{v(xz)}$

$$E \times C_2 = C_2$$

$$C_2 \times C_2 = E$$