In-Class Problems / Self-study Problems / Test Preparation: Lecture 1

- **In-Class P1** What is the principle axis for PCl_5?
  - the principle axis is the highest Cn axis, ie the axis with the largest n, thus the C_3 axis is the principle axis

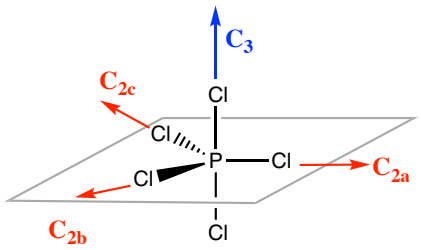
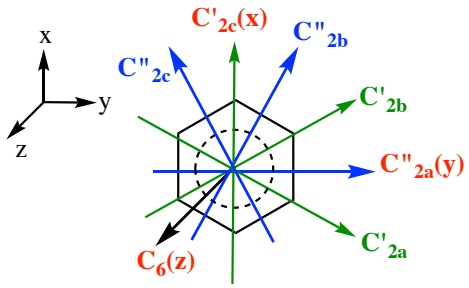
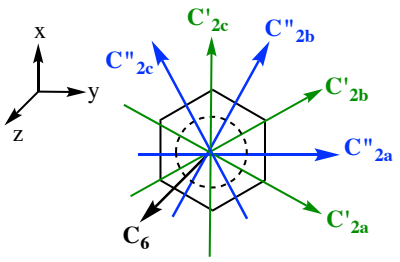


Figure 1 PCl_5 rotation axes

- **In-Class P2** Add the cartesian labels to the relevant axes shown on benzene in **Figure 2**





C_6 comes out of the page
C'_2 go through atoms
$C"_2$ go through bonds

Figure 2 benzene rotation axes

- **In-Class P3** Determine the point group of NH_3
  - NH_3 is trigonal pyramidal
  - symmetry elements for NH_3 are E, C_3, and $3\sigma_v$ planes, **Figure 3**
  - use the flow chart
    1. is the molecule linear? NO
    2. is the molecule T_d or O_h? NO
    3. is there a principle C_n axis? YES (C_3 so n=3)
    4. are there nC_2 perpendicular to the principle axis (ie 3C_2 axes)? NO
    5. is there a σ_h? NO
    6. are there nσ_v? YES (n=3)
  - therefor the point group of **NH_3 is C_{3v}**

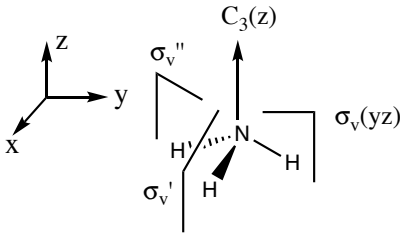


Figure 3 symmetry elements NH_3

- **Q1** find, draw and label all the rotation axes for the square planar $[PtCl_4]^{2-}$ molecular ion
  - see **Figure 4**
  - C_4 is the prinicple axis so defines the z-axis position
  - C_2 and C_4 are coincident, ie in the same place
  - there are two **types** of C_2 axis, ones that go through bonds and ones that go between bonds, different types of axis are labelled with single/double primes
  - only the C_2' axes lie along cartesian axes

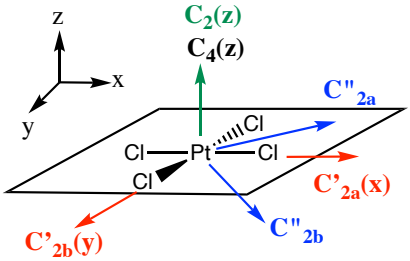


Figure 4 rotation axes for $[PtCl_4]^{2-}$

- **Q2** find, draw and label all the rotation axes and reflection planes for the trigonal planar BH_3 molecule
  - see **Figure 5**
  - diagrams must be clear, you don't need to fit all of the operations on a single diagram
  - you can put some operations on a "side on" diagram and some on an "in-plane" diagram
  - mirror planes can also be represented by a "partial" plane as shown

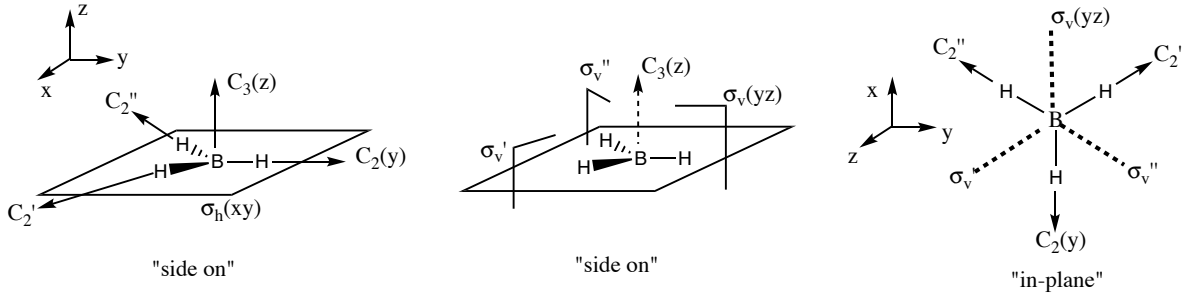


Figure 5 mirror planes and rotation axes for BH_3

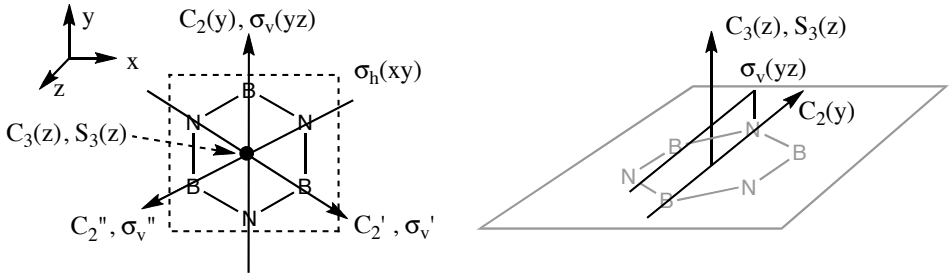
- **Q3** identify the shape of the following molecules if they have a center of inversion, if the inversion point lies on an atom, identify that atom. (a)CO_2 (b)$SiCl_4$ (c) SF_6 (d) NH_3 (e) benzene
  - (a) CO_2 is linear, yes, inversion point lies on the C atom
  - (b) $SiCl_4$ is tetrahedral, no inversion point
  - (c) SF_6 is octahedral, yes, inversion point lies on the S atom
  - (d) NH_3 is trigonal pyramidal, no inversion point
  - (e) benzene is hexagonal planar, yes, inversion point lies in the center of the ring

- **Q4** determine the point group of BH_3
  - BH_3 is trigonal planar
  - all of the symmetry elements are shown above in **Figure 5**
  - use the flow chart
    1. is the molecule linear? NO
    2. are there 2 or more C_n n>2? NO
    3. is there a princile C_n axis? YES (C_3 so n=3)
    4. are there nC_2 perpendicular to the principle axis (ie 3C_2 axes)? YES
    5. is there a σ_h? YES
  - therefor the point group of the molecule is D_{3h}

- **Q5** determine the point group of the following molecules (* = more challenging)

a)	SH_2	C_{2v}	
b)	CO_2	$D_{\infty h}$	
c)	$POCl_3$	C_{3v}	
d)	trans-N_2F_2	C_{2h}	
e)	CCl_4	T_d	
f)	$[PtCl_4]^{2-}$	D_{4h}	
g)	CHFClBr	C_1	
h)	hydrazine N_2H_4	C_2	
i)	*cyclohexane (chair)	D_{3d}	https://www.chemtube3d.com/sym-d3dcyclohexane/
j)	*cyclohexane (boat)	C_{2v}	https://www.chemtube3d.com/sym-cyclohexaneboat/
k)	*benzene	D_{6h}	https://www.chemtube3d.com/symbenzened6h/

- **Q6** On a sketch of borazine illustrate and label the symmetry elements of the D_{3h} point group
  - put in the axial definition, note the z axis is coming out of the page in the first diagram because it has to align with the C_3 axis, **Figure 6**
  - don't crowd your diagrams, use two or three if that will make things clear!



σ_v planes lie perpendicular to the page
and pass through the C_2 axes
S_3 axis is coincident with the C_3 axis

Figure 6 symmetry elements sketched on a molecule of borazine