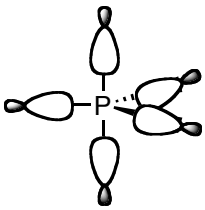
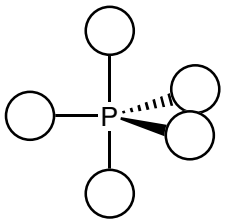
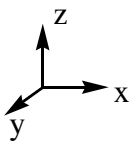
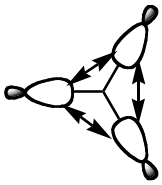
Determine the point group of PL_5. Draw and label the symmetry elements of the point group on a diagram of PL_5. Construct the valence molecular orbital diagram for PL_5 where L is a σ-bonding ligand. Sigma bonding ligands contribute sp type hybrid orbitals, which "look" very much like H 1sAOs to the central element P. Build the MO diagram in two steps, first form an intermediate MO diagram by interacting the equatorial and axial orbital fragments as shown below (diagram to right), then form the final MO diagram combining the L_5 fragment with the P atom. Assume a (single) reference ligand donor orbital lies slightly below the 3pAO of P. In the first instance assume L is a one electron donor ligand (like H) and that no MO mixing occurs. If you have time consider potential mixing within this complex.

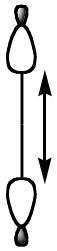








equitorial

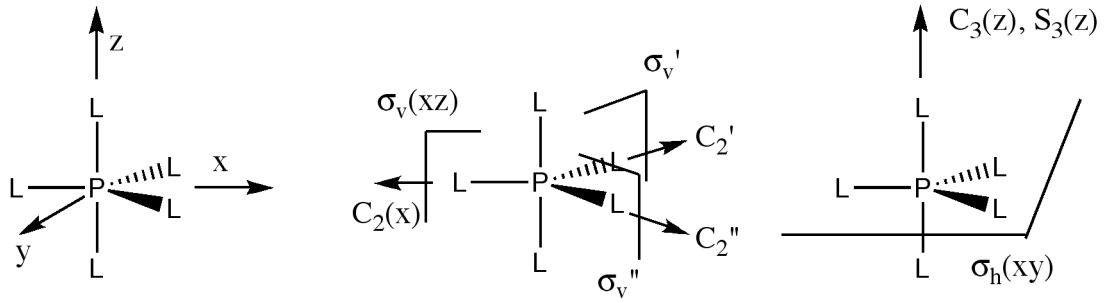


axial

Determine the point group of PF_5. shape has been given, point group is D_{3h} (**1 mark**)

- Draw and label the symmetry elements of the point group on a diagram of PF_5.

the axial system has been defined for you in the question, symmetry operations are:

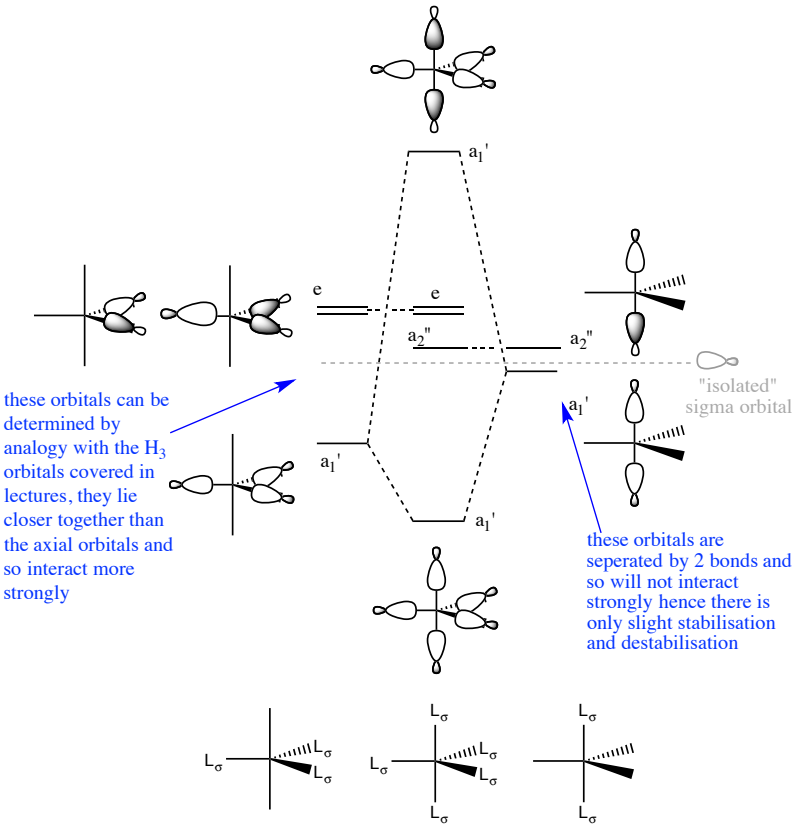


all C_2 axes (**1 mark**)
C_3 and S_3 axes (**1 mark**)
all σ_v and the σ_h planes (**1 mark**)
neat clear diagram (**1 mark**)
using the full notation (ie axial descriptors) (**1 mark**)

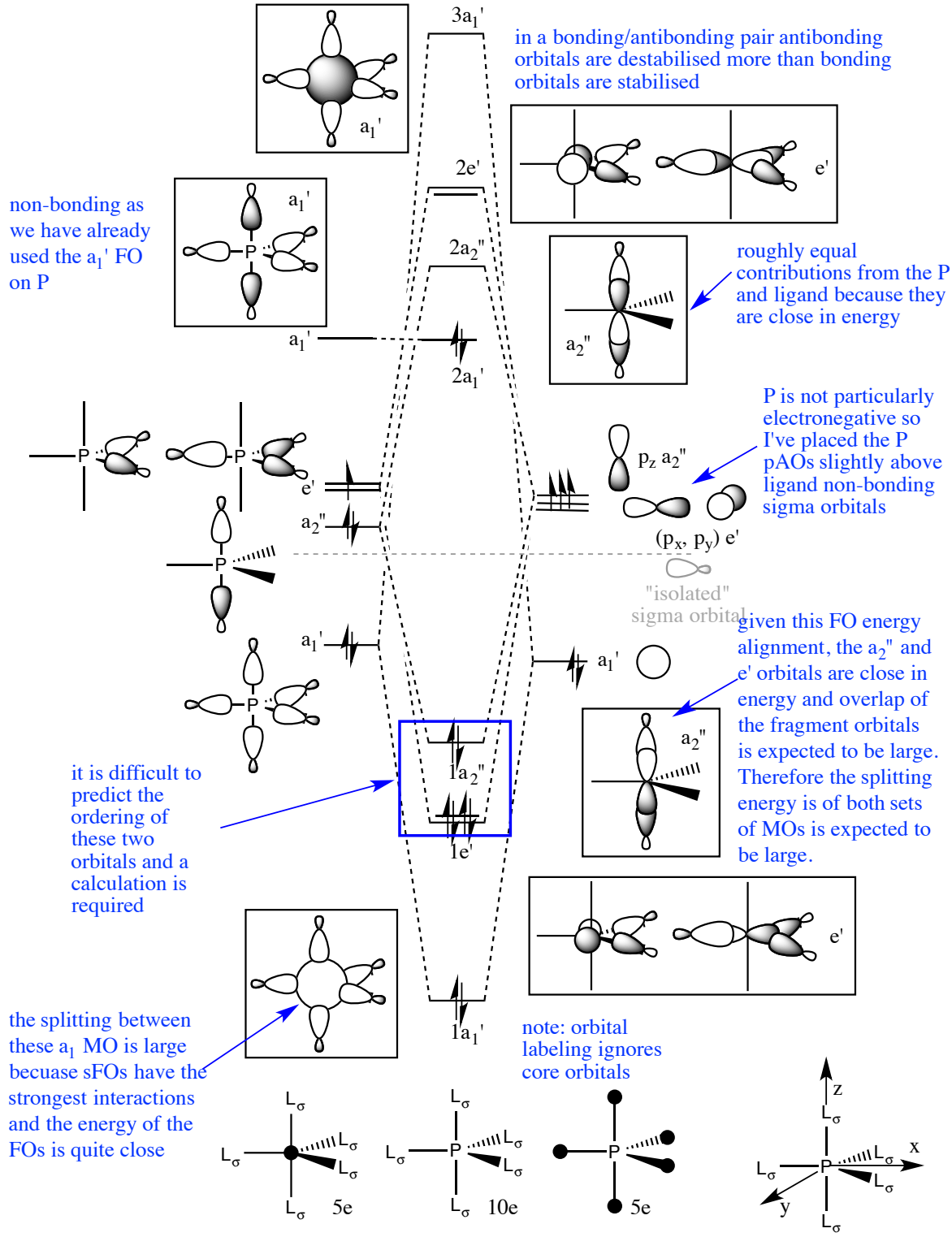
- Forming a MO diagram

1. determine the molecular shape and identify the point group of the molecule
2. define the axial system find all of the symmetry operations on the molecule
3. identify the chemical fragments, and put them along the bottom of the diagram
4. determine the energy levels and symmetry labels of the fragment orbitals
5. combine fragment orbitals of the same symmetry, estimate the splitting energy and draw in the MO energy levels and MOs (in pencil!)
6. determine the number of electrons in each fragment and hence the central MO region, add them to the diagram
7. identify if any MO mixing occurs, determine the mixed orbitals and redraw the MO diagram with shifted energy levels and the mixed MOs
8. use the MO diagram check-list!
9. analyse the MO diagram

- the intermediate MO diagram shown below



- the full MO diagram including annotations is shown below



marks:
1 axial system defined in correct alignment
1 fragments and molecule on diagram, placeholders present
2 depicting and labelling FOs
2 energy level placement FOs
2 for shapes of MOs
1 correct symmetry labels MOs
2 MO energies roughly right
1 correct electronic configuration
3 for a selection of annotations related to MOs and energies
---
15 total

- If you have time consider potential mixing within this complex.
    - mixing could conceivably occur between the $2a_1'$ and $3a_1'$ MOs because they are close in energy, one orbital is non-bonding, and one orbital is occupied while the other is unoccupied. However, this is unlikely to occur because the net interactions are destabilising as shown below (and actually these orbitals contain the same equatorial fragment orbital component, and MOs with the same fragment components do not mix)