- in a mixture of compounds, relative peak intensity indicates the number of components, by measuring the absorbance of several concentrations and using the Beer-Lambert Law to determine the  $\epsilon$  for the electronic transition.
- for single compounds it indicates the kind of electronic transition involved

## Electronic structure

- electrons orbit around the nucleus and their energy is quantised i.e. related to the radius of the orbit by giving it a principal quantum number 'n'.
- when the atom absorbs light the electron jumps to a higher energy.
- the jump is related to frequency and wavelength of the light absorbed by  $\Delta E$  = h  $\nu$  = he /  $\lambda$
- if there is light with a frequency to correspond to the energy change between the inner orbit and outer orbit, that light will be absorbed
- three p orbitals for each principal quantum number : px, py, pz
- molecular orbitals form by combining atomic orbitals together
- the angular momentum dictates the orbital shape
- $sp^3 orbitals = s+p_x+p_y+p_z$  (tetrahedral shape)



## **Transitions**

- $\pi$  to  $\pi^*$  transitions lie in the UV range (200-300nm) for simple organic molecules.
- $\lambda_{max} = 163 \text{ nm in ethene}$
- orbitals can interact along the polyunsaturated chain.
- transition shifts to longer wavelength as chain length increases. 30nm per additional C=C bond.
- $\pi$  to  $\pi^*$  energy is smaller as there are more bonding and anti bonding energy levels in the same space.
- the transition will move to smaller energy

## <u>Benzene</u>

- sp<sup>2</sup> hybridised planar molecule
- $\lambda_{max} = 203$  nm (between this and 295 if there are substituents)