Molecular Orbitals:

Example 1: Ethylene



Looking at both sigma and pi bonds

A.O. means atomic orbitals (s, sp², p) M.O. means molecular orbitals (σ , π)

Looking only at the π orbitals:



An electron can be excited from the HOMO to the LUMO using light of a precise wavelength dependent on the energy difference between the two orbitals (since the orbitals are quantized). The electron can go back to it's original orbital and heat (or light) is produced in the process.



As the # of double bonds in the compound increases, decreasing the HUMO-LUMO gap, the energy of the light needed to excite the compound to its excited state is lower.

Once the absorption of light leaves the UV range and into the visible range, the transition becomes visible and the colour of the compound can be seen.



Example 3: 1,3,5,7,9,11-dodecahexaene

Conjugated molecules in vision:



Retinal is combined with the protein opsin in the eye to make rhodopsin, which is a key protein in the mechanism of sight.

Human vision covers the range of 400 nm (4000 Å) to 800 nm (8000 Å), anything outside of these wavelengths is invisible to the naked eye.



The further oxidized form of retinal is retinoic acid. Changing the double bond bearing the carboxylic acid from trans to cis gives the drug Accutane, used to treat acne. (can cause birth defects = teratogen)



E lost as light of longer wave length (potentially now visible) Fluoresence

Light Emission

- 1) Fluorescence
- Absorb UV and emit either UV or Visible
- Short life (singlet state electrons paired)
- 2) Phosphorescence
- Absorb UV and emit UV/Visible
- Long life (triplet state electrons not paired)
- 3) Chemiluminescence
- Reactions that produce light