Electronic Absorption

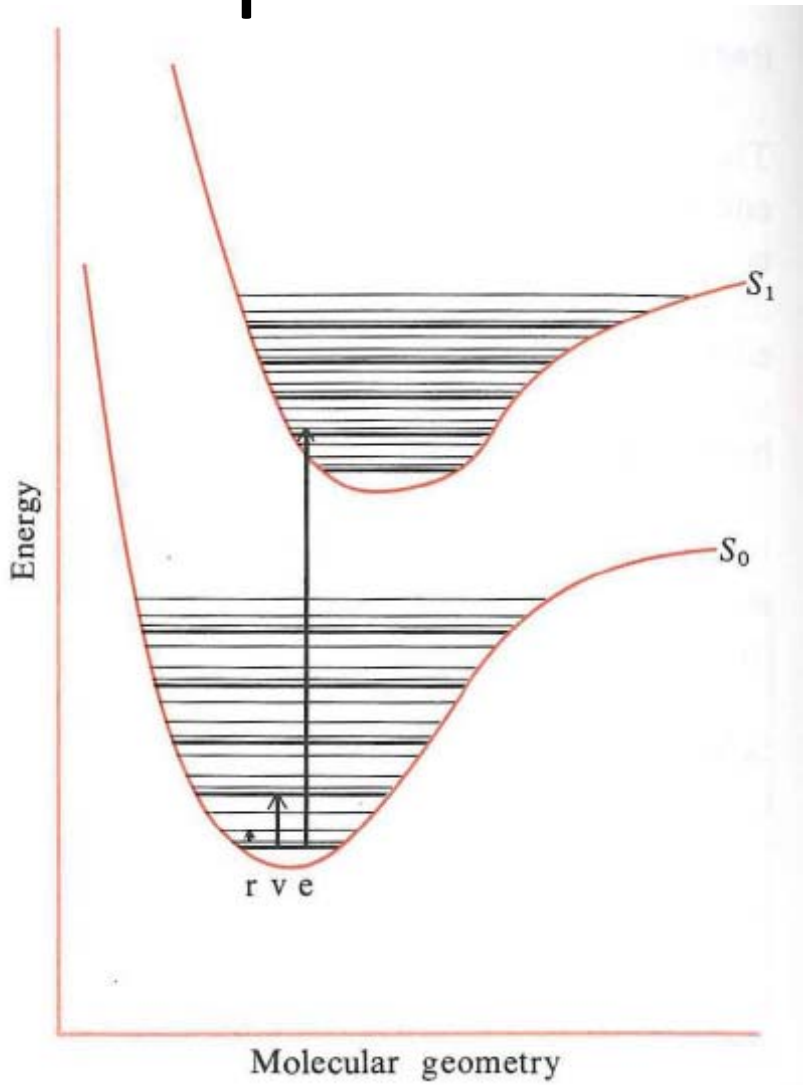


Figure 7-1

Energy levels of a small molecule. Selected rotational sublevels of the vibrational levels of each of two electronic states are shown. Transitions corresponding to electronic (e), vibrational (v), and rotational (r) spectra are indicated.

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 362

Electromagnetic Spectrum

You should know this!

Table 7-1

Biologically useful spectroscopic regions

Typical wavelength (cm)	Approximate energy (kcal mole^{-1})	Spectroscopic region	Techniques and applications
10^{-11}	3×10^{8}	γ-Ray	Mössbauer
10^{-8}	3×10^{5}	X-ray	X-ray diffraction, scattering
10^{-5}	3×10^{2}	Vacuum UV	Electronic spectra
3×10^{-5}	10^{2}	Near UV	Electronic spectra
	Carbon–carbon bond energy		
6×10^{-5}	5×10^{3}	Visible	Electronic spectra
10^{-3}	3×10^{0}	IR	Vibrational spectra
	RT at ambient temperature		
10^{-2}	3×10^{-1}	Far IR	Vibrational spectra
10^{-1}	3×10^{-2}	Microwave	Rotational spectra
10^{0}	3×10^{-3}	Microwave	Electron paramagnetic resonance
10	3×10^{-4}	Radio frequency	Nuclear magnetic resonance

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 350

Example: Formaldehyde

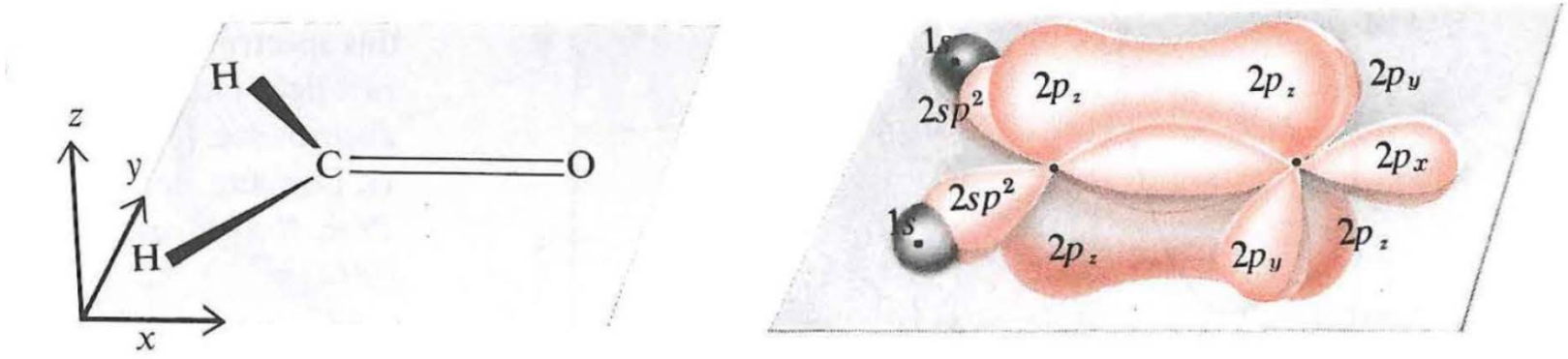


Figure 7-6

The formaldehyde molecule and a schematic diagram of its bonding.

- Carbon Orbitals:
  - 3 *sp* orbitals
  - 1 p_x orbital (p_x)
- Oxygen Orbitals:
  - p_z, p_x orbital
  - Nonbonding (filled) p_y orbital

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 370

Example: Formaldehyde

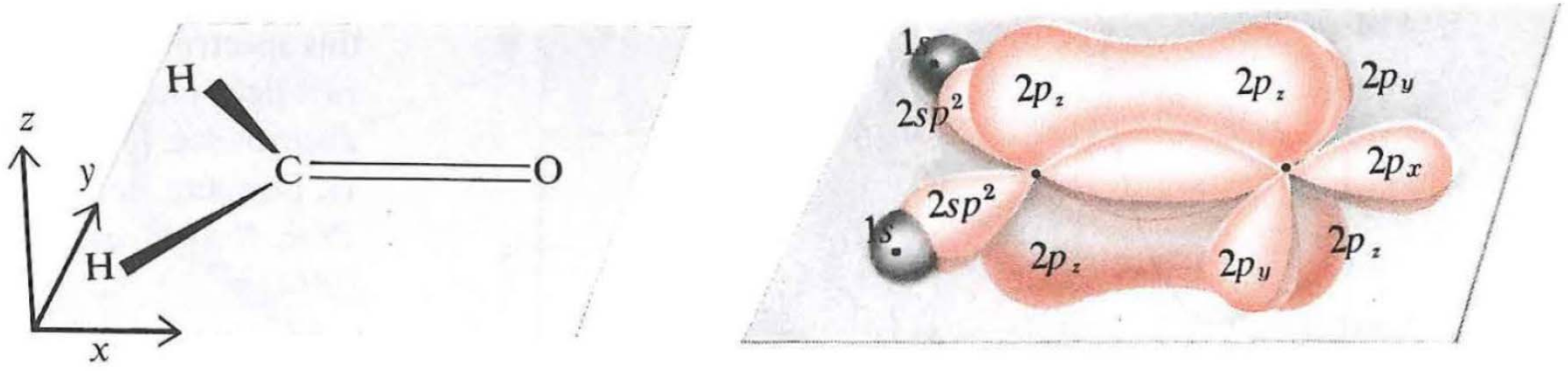


Figure 7-6

The formaldehyde molecule and a schematic diagram of its bonding.

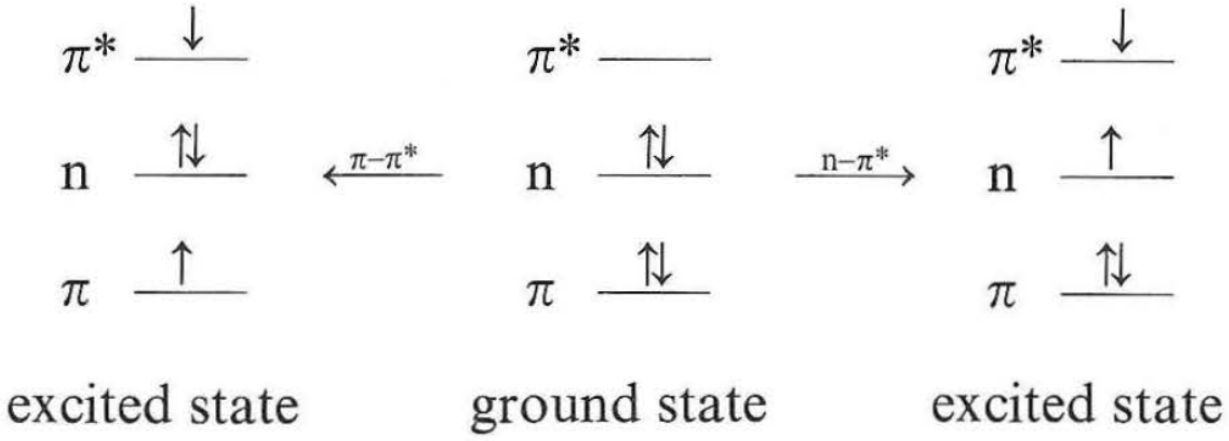
C(sp) + O(p_x) → σ bonding (no node)

C(p_z) + O(p_z) → π bonding (axial node)

O(p_y) → nonbonding

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 370

Example: Formaldehyde



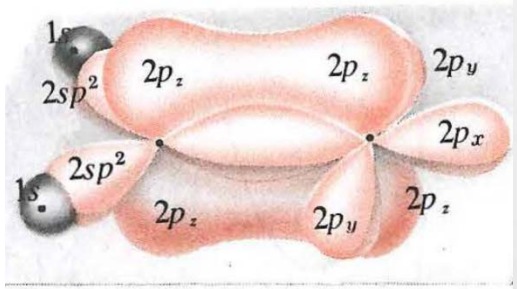
C(*sp*) + O(p_x) → σ bonding (no node)

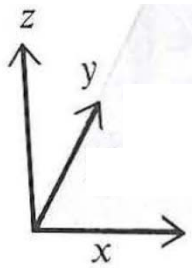
C(p_z) + O(p_z) → π bonding (axial node)

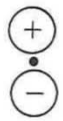
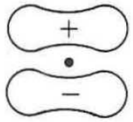
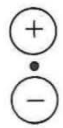
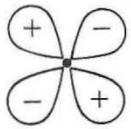
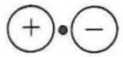
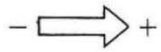
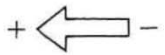
O(p_y) → nonbonding

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 370

Example: Formaldehyde





Function:	Viewed along: x axis	Viewed along: y axis	Symmetry reflected through: xy	xz	yz
Molecular orbitals					
π			Odd	Even	Even
π^*			Odd	Even	Odd
n			Even	Odd	None
Dipole operators					
$\underset{\sim}{\mu}_x$			Even	Even	Odd
$\underset{\sim}{\mu}_y$			Even	Odd	Even
$\underset{\sim}{\mu}_z$			Odd	Even	Even

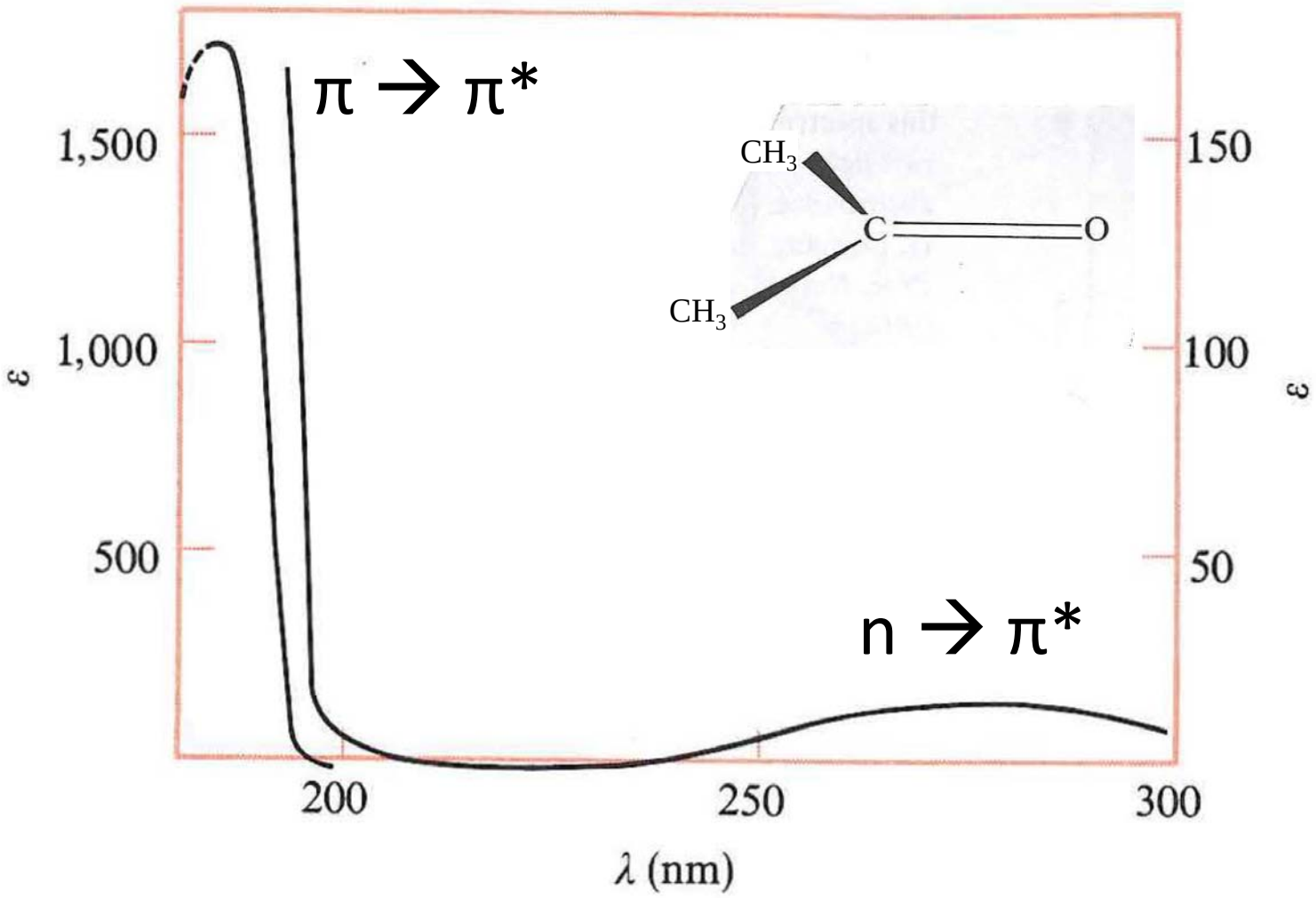
bond center

Figure 7-7

The symmetry of molecular orbitals and dipole operators of formaldehyde.

From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 370, 373

Acetone Spectrum



From *Biophysical Chemistry, Part II*
Cantor & Schimmel, Chapt. 7, p. 374