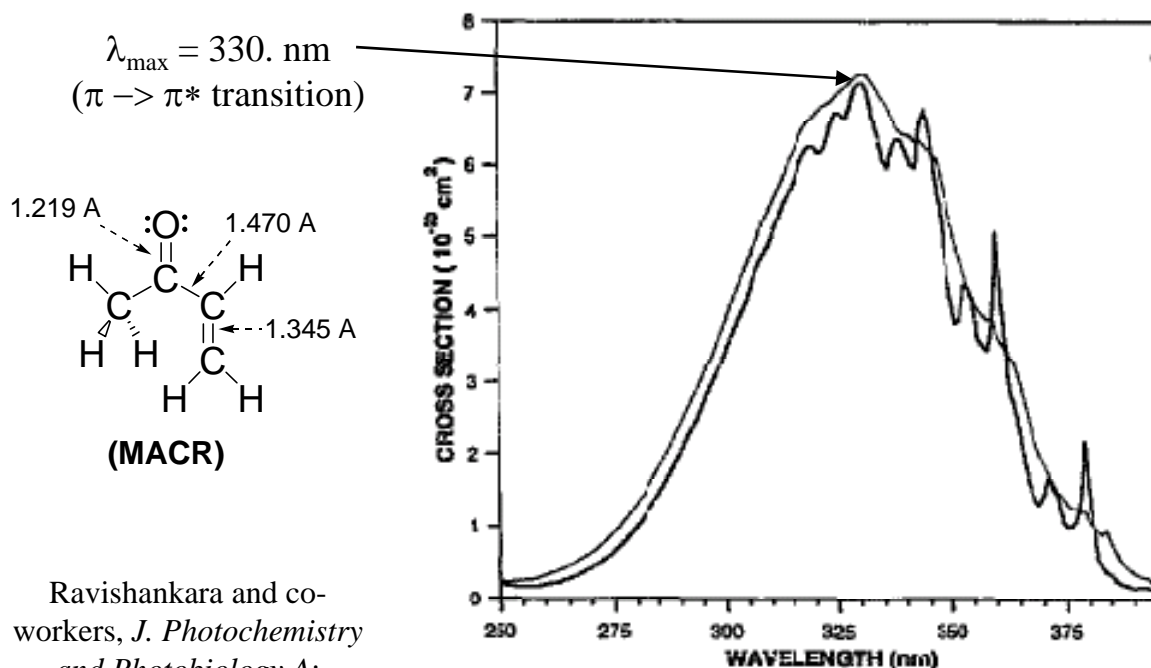


## Modeling the UV Absorption Spectrum of Methacrolein



Ravishankara and co-workers, *J. Photochemistry and Photobiology A: Chemistry* **1997**, *110*, 1.

Fig. 2. Absorption spectra of MVK (—) and MACR (---) at 298 K.

## Free Electron Molecular Orbital Model:

- (1) Pi electrons behave like particles in a 1-dimensional box ( $\pi$  MO's and particle in a box eigenfunctions have the same nodal patterns).
- (2) The length of the box is (more or less) the distance between the most separated conjugated atoms.
- (3) Each wavefunction "holds" (describes) two pi electrons of opposite spin (that is, obeys the Pauli exclusion principle).
- (4) The pi electronic ground state obeys the aufbau principle.
- (5) The longest wavelength peak in the UV/visible absorption spectrum corresponds to a transition between the  $\pi$  HOMO and the  $\pi^*$  LUMO.

