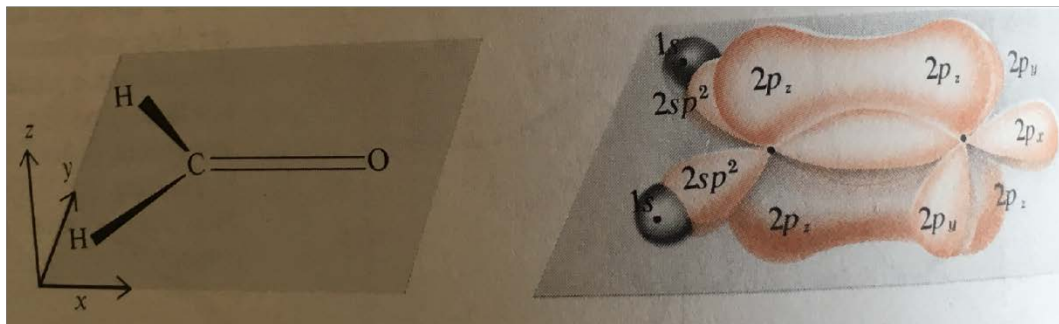


Deadline: lecture Thursday (2017-06-15)

- (7 points) For the formaldehyde molecule (see figure), determine whether the  $n \rightarrow \pi^*$  and the  $\pi \rightarrow \pi^*$  transitions are zero or not zero. Note, you should check the symmetry of the transition dipole moment  $\langle n | \mu_x | \pi^* \rangle$  for every individual coordinate. Sketch the energy levels for the  $n$ ,  $\pi$ , and  $\pi^*$  states with number of electrons with spin before and after the transitions ( $n \rightarrow \pi^*$  and  $\pi \rightarrow \pi^*$ ).

formaldehyde  $\text{H}_2\text{CO}$



- (2 points) Deduce the four wave functions for the  $sp^3$  hybridization with normalization factors.
- (4 points) Estimate the natural lifetimes and decoherence times (with negligible pure dephasing) of the absorption bands of peak 1 (thio acetic acid dimer) and peak 2 (thio acetic acid monomer) from the FWHM. Here, we used Gaussian profiles with  $\Delta \nu = 0.441/(c \cdot \tau)$ , and  $\Delta \nu$  the FWHM in wavenumbers and  $\tau$  the natural lifetime. Time-resolved measurements find two time constants of  $(0.9 \pm 0.1)$  ps and  $(10 \pm 1)$  ps. To which peaks (1 & 2) would you assign the time constants, explain this.

