

# Spectroscopy

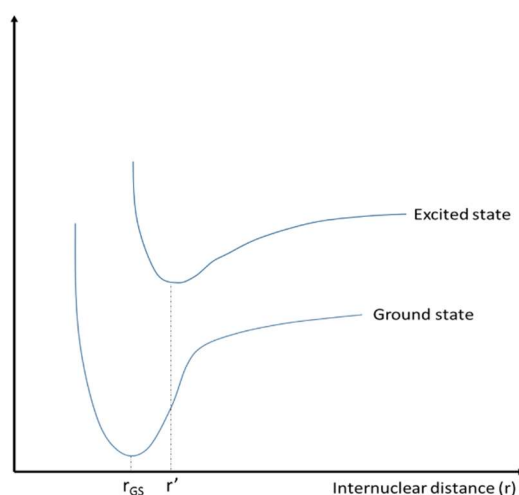
## Corrections Chapter 5

1. The electronic configuration of the CO molecule is described by following MOs:  $KK(3\sigma)^2(4\sigma^*)^2(1\pi)^4(5s)^2$ . The first excited state is described by:  $KK(3\sigma)^2(4\sigma^*)^2(1\pi)^4(5s)^1(2\pi^*)^1$

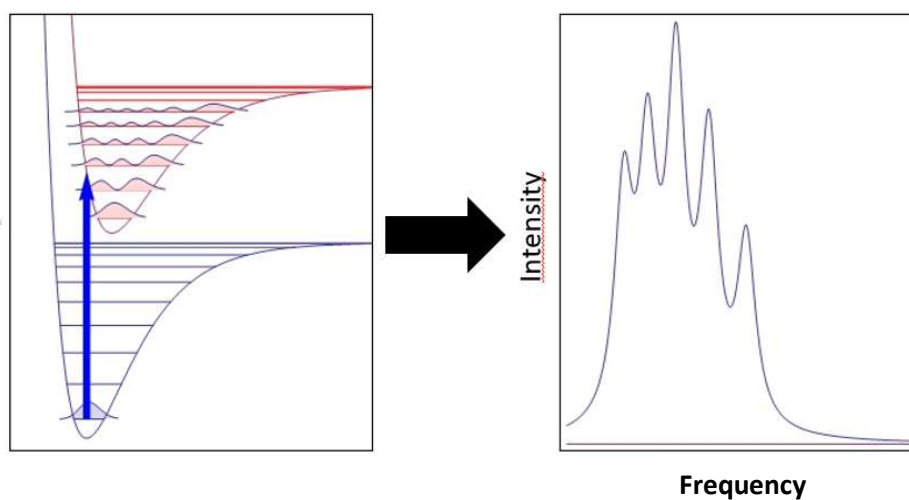
a. Discuss the changes in bond strength and bond length associated with the electronic excitation.

As one can see from the electronic configuration, one of the electrons that was in the  $5s$  orbital in the ground state is promoted to a  $2\pi^*$  orbital in the excited state, which is an anti-bonding orbital. In other words, the bond order is lower in the excited state than in the ground state. Therefore, the bond weakens and the bond length will be higher in the excited state.

b. Sketch the corresponding potential energy curves.



c. Sketch the vibrational structure observable in the spectrum for this electronic transition.



Since the excited state has an equilibrium distance higher than the ground state, following the Franck-Condon principle we can expect that the best overlap with the ground state wave function will be to states that have larger numbers of vibrational quanta. If we zoom in each vibrational transition, we should see the P and R branches but not the Q branch since it is a diatomic molecule.

d. Sketch the rotational structure observable in the spectrum for this electronic transition.

Since  $r_{v'} > r_v''$ , then  $B_{v'} < B_v''$ , the rotational spectrum will have a band head in the R branch, so it would be something like:

