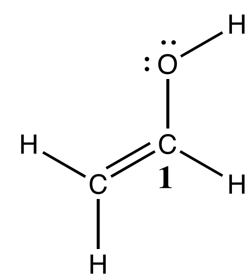
Chemistry 2000 Spring 2019 Test 1
Version B SOLUTIONS

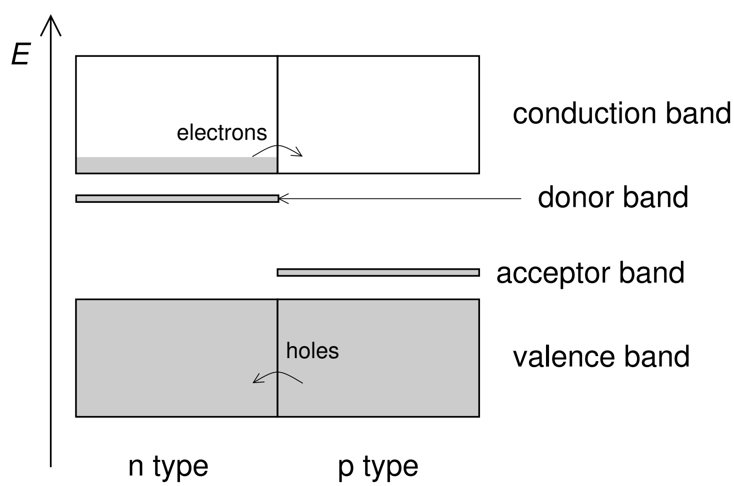
1. (a)



(b) According to valence-bond theory, the hybridization of carbon **1** is **sp^2** while the hybridization of the oxygen atom is **sp^3**.

(c) According to valence-bond theory, the hydrogen-oxygen sigma bond is made by overlapping an oxygen **sp^3** orbital with a hydrogen **1s** orbital. [2 marks]

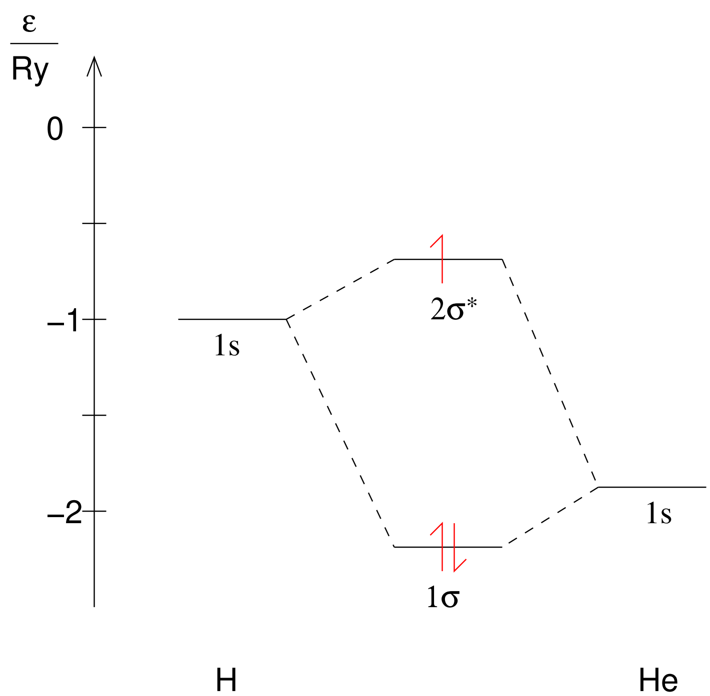
2. (a)



(b) In the case of a light-emitting diode, electrons are supplied to the **n** side of the junction. Light is emitted when the electrons go from the **conduction** band to the **valence** band at **the interface separating the n- and p-type seconductors (the p-n junction)**.

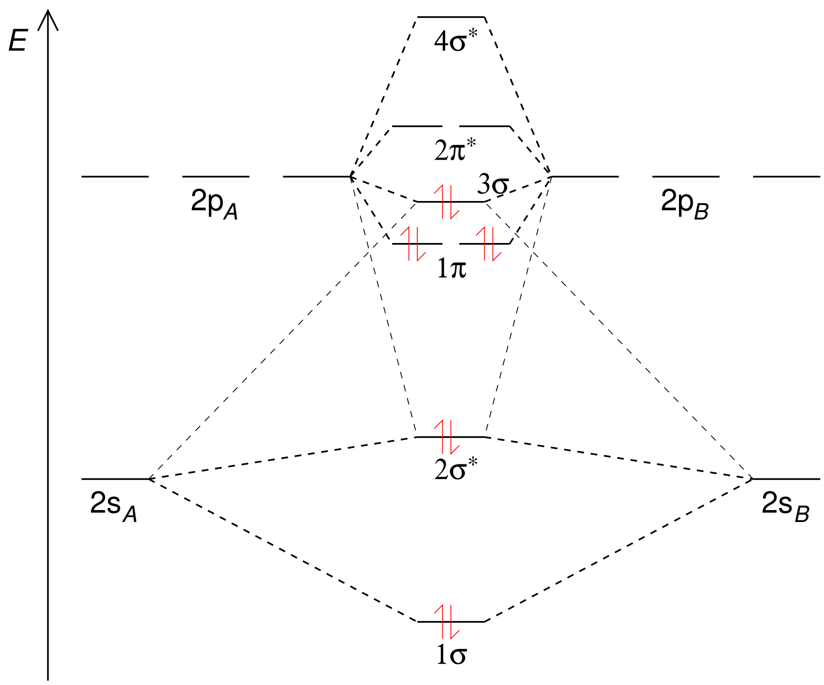
3. Yes, HCl is a greenhouse gas. It has a dipole moment, and this dipole moment will change during a vibration, so it can absorb IR radiation.

4.

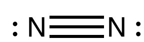


Note that there is more bonding than antibonding character (bond order = $\frac{1}{2}$), so this molecule could exist. Like many other exotic molecules we have seen this term, this one is found in space and can be made in certain experiments.

5. N_2 has 10 valence electrons, and s-p mixing is significant in this molecule, so that the 3σ orbital is above the 1π orbital. The MO diagram is as follows:



The Lewis diagram of nitrogen is of course



The MO diagram predicts a bond order of

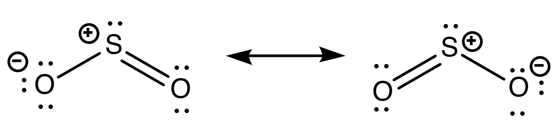
$$\text{bond order} = \frac{1}{2}\{\text{bonding} - \text{anti}\} = \frac{1}{2}(8-2) = 3.$$

This agrees with the Lewis diagram.

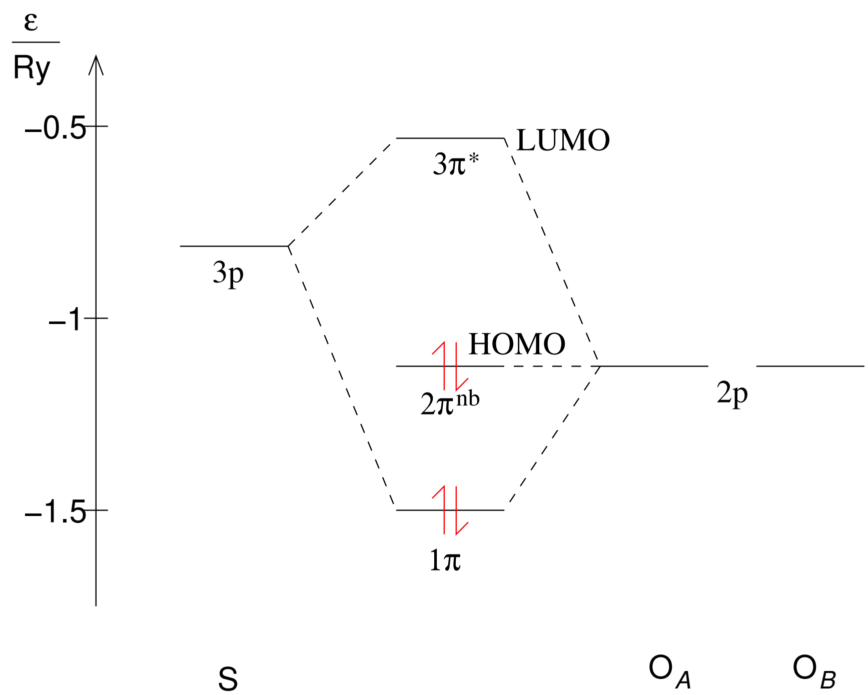
Our rules for counting π electrons in Lewis diagrams would indicate that N_2 has 4 π electrons, which agrees with the number of π electrons in the MO diagram.

There is not a clear correspondence between the lone pairs and the MO diagram.

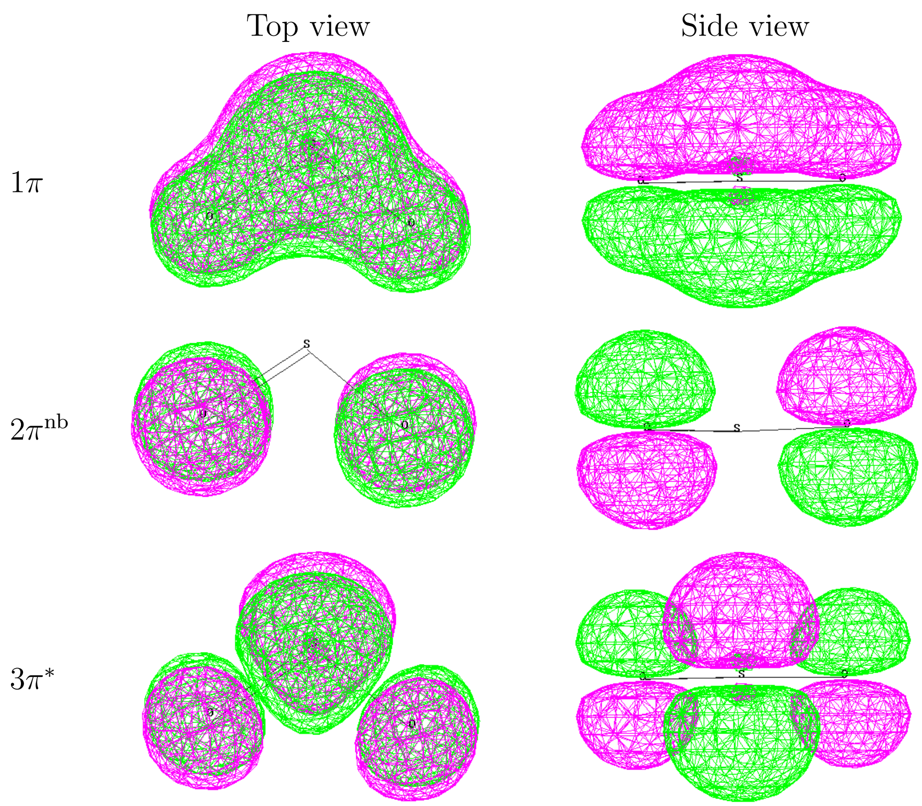
6. (a)



(b) From the Lewis diagram, we count 4 π electrons (two in double bond, one lone pair). The filled MO diagram is therefore the following:



(c)



(d) A Lewis acid accepts electrons into its LUMO, here the $3\pi^*$. The $3\pi^*$ is closest in energy to the sulfur 3p orbital, so it will have a larger contribution from this orbital than from the oxygen 2p orbitals. (Note that the pictures of the $3\pi^*$ above agree with this reasoning.) This would mean that SO_2 would preferentially accept electrons at the sulfur atom.

7. The two lowest-energy peaks correspond to ionization of H_2 to the two lowest vibrational levels of the molecular ion H_2^+. Reading off the graph, we find these ionization energies to be approximately

$$\begin{aligned} & \mathrm{IE}_1 \approx 126\,700\,\mathrm{cm}^{-1}, \\ \text{and} \qquad & \mathrm{IE}_2 \approx 128\,800\,\mathrm{cm}^{-1} \end{aligned}$$

The difference between these two values is the vibrational frequency of H_2^+:

$$\tilde{\nu}(\mathrm{H}_2^+) \approx 128\,800 - 126\,700\,\mathrm{cm}^{-1} = 2100\,\mathrm{cm}^{-1}.$$

The ground-state electronic configuration of H_2 is $(1\sigma)^2$. Ionizing H_2 therefore leaves just one electron in a bonding orbital, so it weakens the bond, which is reflected in the decreased vibrational frequency of the ion. Note, in fact, that the vibrational frequency of H_2^+ is almost exactly half the vibrational frequency of H_2, which makes sense given that, in this very simple molecule, we have lost exactly half of the bonding character by removing an electron from the 1σ orbital.