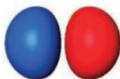
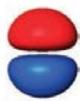
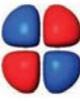


2018 Fall Semester Quiz 3
For General Chemistry I (CH101)

Date: Oct 8 (Mon), Time: 19:00 ~ 19:45

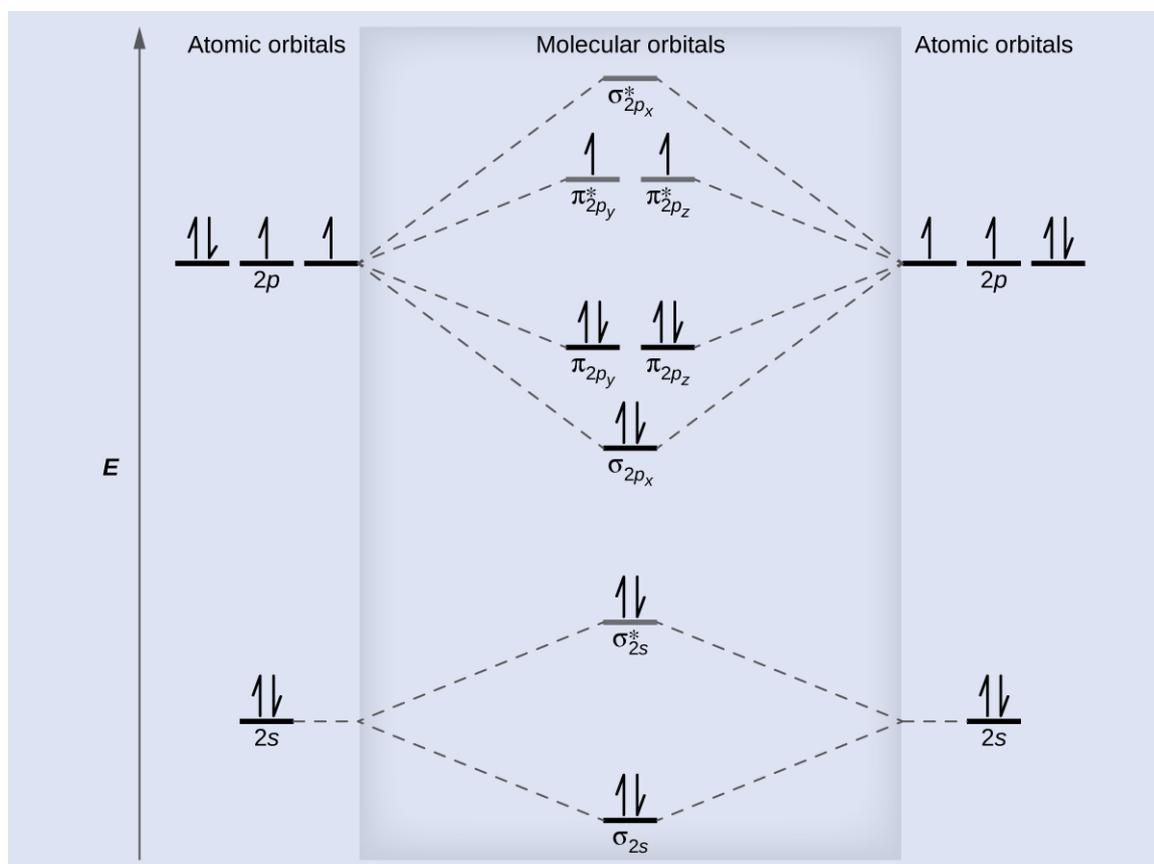
Professor Name	Class	Student I.D. Number	Name

1. (Total 8 pts, 1 pt each) The following figures are wave functions for the first eight energy levels of a H_2^+ molecular ion. Write down the correct labels for each orbital. (Note: (a) is the ground state, and the energies increase in the alphabetical order: (a)<(b)<(c)<...)

	
(a) $1\sigma_g$ OR σ_{g1s}	(b) $1\sigma_u^*$ OR σ_{u1s}^*
	
(c) $2\sigma_g$ OR σ_{g2s}	(d) $2\sigma_u^*$ OR σ_{u2s}^*
	
(e) $1\pi_u$ OR π_{u2p} OR (π_{u2p_x} OR π_{u2p_y})	(f) $3\sigma_g$ OR σ_{g2p} OR σ_{g2p_z}
	
(g) $1\pi_g^*$ OR π_{g2p}^* OR ($\pi_{g2p_x}^*$ OR $\pi_{g2p_y}^*$)	(h) $3\sigma_u^*$ OR σ_{u2p} OR $\sigma_{u2p_z}^*$

2. (Total 12 pts) Consider an O₂ molecule.

(a) (6 pts) Construct the correlation diagram for ground state O₂.



Correct MO diagram +5 pts (labels not required); +2.5 pts for correct MOs from 2s, +2.5 pts for correct MOs from 2p

Correct number of electrons in MO +1 pt

-1 pt for the incorrect energy order of MOs

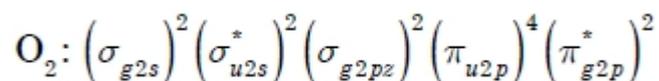
-1 pt for not obeying the Aufbau principle

-1 pt for not obeying the Pauli exclusion principle

-1 pt for not obeying the Hund's rule

-1 pt for any other minor mistakes

(b) (1 pt, no partial pts) Write down the valence electron configuration of ground state O_2 .



Writing down 2 pi orbitals separately is also fine [e.g. $(\pi_{u2px})^2 (\pi_{u2py})^2 (\pi_{g2px}^)^1 (\pi_{g2py}^*)^1$]

No explanation required; no partial points

(c) (1 pt, no partial pts) Which molecules are diamagnetic: O_2^+ , O_2 , O_2^- , O_2^{2-} ?

b) All of the species except O_2^{2-} should be paramagnetic. A species with an odd number of electrons is automatically paramagnetic. The reason for the paramagnetism of ordinary O_2 is discussed in the text.

No explanation required; no partial points

(d) (2 pts, no partial pts) Give the bond order of each species in (c).

The bond orders of the species are $\frac{5}{2}$ (for O_2^+), 2 (for O_2), $\frac{3}{2}$ (for O_2^-) and 1 (for O_2^{2-}).

No explanation required; no partial points

(e) (2 pts) The energy level order of MOs in O_2 is different from that in N_2 . Explain why.

energies for these two molecular orbitals. A simplified physical interpretation relates this result to the extent to which the 2s and 2p atomic orbitals can mix while contributing to the molecular orbital. The 2s AOs have the right symmetry to mix with 2p AOs to form a σ molecular orbital directed along the z-axis. In the first part of Period 2 the 2s and 2p are sufficiently close in energy that mixing occurs and increases the MO energy. In the latter part the energy separation of 2p and 2s AOs is too great for mixing to occur. Because the 2s and 2p_x and 2p_y AOs do not have the right symmetry to mix and form a π molecular orbital, the energy of the $\pi_{u2p_{x(y)}}$ MO remains nearly constant across the period even when the 2s and 2p AOs are close together in energy.

2s and 2p orbitals can mix -> +1 pt

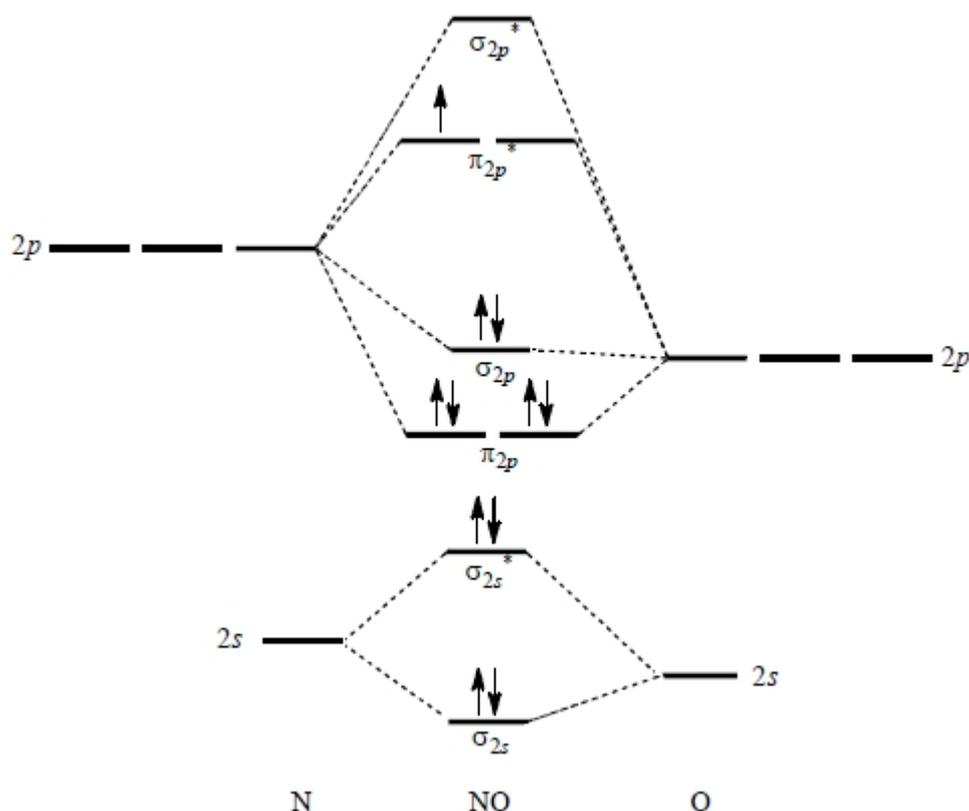
For N_2 , 2s and 2p are sufficiently close (in energy) to mix, and it increases the MO energy -> +0.5 pt

For O_2 , 2s and 2p are not close enough, so the MO energy does not increase as much -> +0.5 pt

If you mention any kind of interaction (mixing or repulsion) between two sigma MOs, full points are given.

3. (Total 11 pts) Consider a NO molecule.

(a) (6 pts) Construct the correlation diagram for ground state NO and give its bond order. Is NO paramagnetic or diamagnetic?



Bond order = 2.5, and NO is paramagnetic. (No explanation required)

Correct correlation diagram +3 pts (labels not required); +1.5 pts for MOs from 2s, +1.5 pts for MOs from 2p

Correct number of electrons in MO +1 pt

Bond order +1 pt

Paramagnetic +1 pt

The orbital potential energy of 2s, 2p orbitals of oxygen must be lower than those of nitrogen. If this is not correctly depicted, -1 pt

-1 pt for the incorrect energy order of MOs

-1 pt for not obeying the Aufbau principle

-1 pt for not obeying the Pauli exclusion principle

-1 pt for not obeying the Hund's rule

-1 pt for any other minor mistakes

(b) (2 pts) Which molecule has a higher ionization energy: NO or CO? Explain why.

The ground state electron configuration of CO is $(\sigma_{2s})^2(\sigma_{2s}^*)(\pi_{2p_x}, \pi_{2p_y})^4(\pi_{2p_z})^2$ and the ground state electron configuration of NO is $(\sigma_{2s})^2(\sigma_{2s}^*)(\pi_{2p_x}, \pi_{2p_y})^4(\pi_{2p_z})^2(\pi_{2p_{x,y}}^*)^1$. The highest energy occupied orbital in NO is $(\pi_{2p_{x,y}}^*)$ which is much higher in energy than the highest energy occupied orbital in CO, (π_{2p_z}) thus accounting for the greater ionization energy of CO.

You do not have to write the full electron configurations for both molecules; it's enough to explain that the highest occupied molecular orbitals (HOMOs) for two molecules are different. (+2 pts)

Simply showing bond order difference will not get any credit. Bond order is not necessarily proportional to the energy required to remove the HOMO electron. Any mentioning of "no electron in the antibonding orbital of CO" will get the full credit, however.

Even if the answer is right (CO), points will NOT be given if explanation is incorrect.

(c) (3 pts) 2s orbitals of N and O combine into bonding and antibonding orbitals, but the 1s orbital of H and the 2s orbital of F do not form any MOs in a HF molecule. Explain why.

Potential energy difference between H 1s orbital and F 2s orbital is much larger than that between 2s orbitals of N and O.

There must be a mention of great energy difference to get ANY credit.

Correct explanation +3 pts

4. (5 pts) The molecular orbital of the ground state of a heteronuclear diatomic molecule AB is

$$\Psi_{\text{mol}} = C_A \varphi^A + C_B \varphi^B$$

If a bonding electron spends 90% of its time in an orbital φ^A on atom A and 10% of its time in φ^B on atom B, what are the values of C_A and C_B ? (Note: Assume $\varphi^A \varphi^B = 0$).

The molecular orbital and the square of the molecular orbital for the ground state of the heteronuclear molecule are

$$\psi = C_A\psi_A + C_B\psi_B \quad \text{and} \quad \psi^2 = C_A^2\psi_A^2 + 2C_AC_B\psi_A\psi_B + C_B^2\psi_B^2$$

where the C 's are constants. The *square* of the wave-function is given because its value in any small region of space is proportional to the probability of finding the electron within that region. Neglecting the overlap of the two orbitals means neglecting the cross-term in the squared wave-function

$$\psi^2 \approx C_A^2\psi_A^2 + C_B^2\psi_B^2$$

If the electron spends 90 percent of its time in orbital ψ_A , then $C_A^2 = 9C_B^2$. Also, the electron must be either on atom A or atom B so $C_A^2 + C_B^2 = 1$. Solution of the two simultaneous equations gives

$$C_A = 0.949 \quad \text{and} \quad C_B = 0.316$$

For the ratio of two coefficients, please refer to p. 248 of your textbook for more explanation.

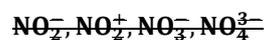
+5 pts for the correct C_A and C_B values

Showing derivation is not necessary, but it is included here to help your understanding.

If the values are wrong, +1 pt for each equation in the red rectangle

5. (Total 4 pts) Answer the following questions.

(a) (4 pts) Give the steric number of each ion. What hybridization is expected for the central nitrogen atom in each ion?



	NO_2^-	NO_2^+	NO_3^-	NO_4^{3-}
Steric number	3	2	3	4
Hybridization	sp^2	sp	sp^2	sp^3

If BOTH steric number and hybridization of each molecule is correct, +1 pt each

We found out that one of the classes did NOT go over this concept before taking the quiz.

As a result, ALL STUDENTS who took the quiz get the credit (+4 pts)