2025 SPRING Semester Mid-term Examination
For General Chemistry I

Date: April 16(Wed), Time Limit: 19:00 ~ 21:00

Write down your information neatly in the space provided below; print your Student ID in the upper right corner of every page.

Professor Name	Class	Student I.D. Number	Name

Problem	points	Problem	points	TOTAL pts
1	/7	**6**	/10	**/100**
2	/8	**7**	/15	
3	/10	**8**	/15	
4	/10	**9**	/10	
5	/15			

** This paper consists of 16 sheets and 9 problems (***pages 14 – 15:*** Equations, constants & periodic table, ***page 16***: claim form). Please check all page numbers before taking the exam. Write down your work and answers in the Answer sheet. Please supply units with the value of your answer where applicable. You will get 30% deduction for missing units per problem.

NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER.
(채점 답안지 분배 및 이의신청 일정)

1. Period, Location and Procedure

0 Return and Claim Period: **April 21 (Monday, 19:00 ~ 21:00, 2 hrs)**
The claim is in person and permitted only during this time period. Keep that in mind!
0 Location: Each designated room of Creative Learning Bldg. (E11)

Section	Room (E11)
A	201
B	202
C	301
D	302

0 Procedure
Rule 1: Students cannot bring their writing tools into the testing room (Use a pen only provided by TA).
Rule 2: Whether or not the student completes a "claim," they must submit the paper back to TA. (Do not go out of the room with it).

If you have any claims on it, write them on the claim form and attach it to the top of the exam paper with a stapler. Give the packet directly to your TA.

WARNING!!
If you deliberately alter any original answers or insert something on your marked paper to achieve a better grade, you will get an F grade for this course. Or if you don't keep the rules above, we will regard it as a kind of cheating and give you 0 points. So please don't cheat.

2. Final Confirmation

1) Period: ***April 24 (Thu.) ~ 25 (Fri.)***
2) Procedure: During this period, you can check the final score of the examination *on the website* again.
(No additional corrections. If no change in your score was made after reasoning, the claims were not accepted.)

***** For further information, please visit the KAIST General Chemistry website at www.gencheminkaist.pe.kr***

1. (7 points)

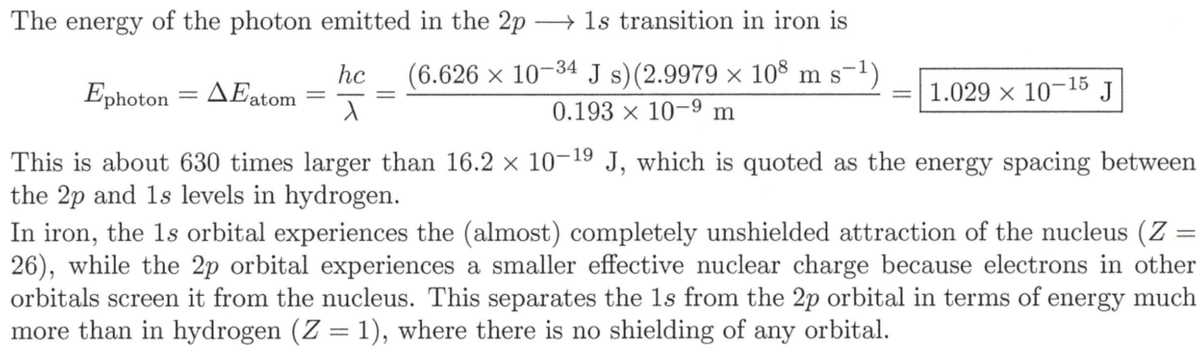
In the hydrogen atom, the electronic transition from the 2*p* state to the 1*s* state involves an emission of a photon with energy 16.2 $\times 10^{-19}$ J. In an iron atom, the same transition (from 2*p* to 1*s*) results in an emission of an X-ray of wavelength 0.193 nm.

(1) Calculate the energy difference between these two states in iron (3 pts).

(2) Explain the difference in the 2*p*-1*s* energy level spacing in these two atoms (4 pts).

(Answer)

(1) 3 Significant figures → 1.03×10^{-15} J
Deduct 1 point for incorrect significant figures.



The energy of the photon emitted in the $2p \longrightarrow 1s$ transition in iron is

$$E_{\text{photon}} = \Delta E_{\text{atom}} = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34}\ \text{J s})(2.9979 \times 10^{8}\ \text{m s}^{-1})}{0.193 \times 10^{-9}\ \text{m}} = \boxed{1.029 \times 10^{-15}\ \text{J}}$$

This is about 630 times larger than 16.2×10^{-19} J, which is quoted as the energy spacing between the $2p$ and $1s$ levels in hydrogen.
In iron, the $1s$ orbital experiences the (almost) completely unshielded attraction of the nucleus ($Z = 26$), while the $2p$ orbital experiences a smaller effective nuclear charge because electrons in other orbitals screen it from the nucleus. This separates the $1s$ from the $2p$ orbital in terms of energy much more than in hydrogen ($Z = 1$), where there is no shielding of any orbital.

(2) The explanation must include the keyword: ‘effective nuclear charge’ or ‘shielding (other electrons)’.

2. (8 points)

You have learned about the 2*p* and 3*d* orbitals both in terms of their energy levels and pictures of their overall shape (features including lobes, nodes, etc).

(1) State the number of nodes in the $3p_z$ and $4d_{z2}$ orbitals (2 pts).

(2) Compare the relative energies of the 3s, 3p, and 3d orbitals in the following cases: (6 pts)

(a) a hydrogen atom, and

(b) a multi-electron atom with an effective nuclear charge (Z_{eff}).

Briefly explain the differences.

(Answer)

(1) The student may explain in words simply, thus: the orbital 3pz will have 2 nodes; the orbital 4dz2 will have 3 nodes. The student is not expected to know but the common node type between these two orbitals is a radial node.

- **$3p_z$ orbital**:
  - Has **2 total nodes**:
    - **1 radial node** (a spherical region where the electron cannot be found)
    - **1 angular node** (a flat plane, the *xy*-plane, where the electron probability is zero)
- **$4dz^2$ orbital**:
  - Has **3 total nodes**:
    - **1 radial node** (spherical)
    - **2 angular node** (a cone-shaped region where electrons are not found)

(2) (a) In a hydrogen atom, all orbitals within the same principal quantum number (n = 3) — namely 3s, 3p, and 3d — have the same energy. This is because the energy depends only on the principal quantum number *n*, not on the orbital type (ℓ), due to the absence of electron–electron repulsion.

(b) In a multi-electron atom, the energy levels of the 3s, 3p, and 3d orbitals are no longer degenerate. The effective nuclear charge (*Z*eff) causes increased attraction between the nucleus and electrons, and orbitals with more electron penetration (such as 3s) experience a higher, thus are lower in energy. As a result, the relative energy ordering becomes:

3s < 3p < 3d.

This occurs because the 3s orbitals penetrate closer to the nucleus, while 3d orbitals are more shielded

3. (10 points)

(a) The ionization energies for the 1s electron for the second-row elements are as follows:

(Reminder: the 1s is a core orbital not outer orbital; Notes: IE of the first electron only; the atoms are neutral, not ion their ionic form; measurements are in gas phase):

Atom	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**
Li	4820	Be	10,600	B	18,300	C	27,000
N	38,600	O	51,000	F	66,600		

Now suppose that a certain substance is bombarded by X-rays of wavelength 0.989 nm. If photoelectrons with kinetic energies of 94,000 kJ/mol and 69,900 kJ/mol are ejected from the material, which of the elements listed above must be present in the sample? (6 pts)

(b) The energy needed to remove one electron from a gaseous potassium atom is only about two-thirds as much as that needed to remove one electron from a gaseous calcium atom, yet nearly three times as much energy as that needed to remove one electron from K^+ as from Ca^+. 1) What explanation can you give for this difference? 2) Next, compare the ionization energy of Ca^+ with that of neutral K (4 pts)

Answer

$E = h\upsilon = \frac{hc}{\lambda}$, part of which goes to satisfy for ionization(I) while the rest goes into the kinetic energy of the ejected photoelectron ($\frac{1}{2}mv^2$).

$$E = I + \frac{1}{2}mv^2$$

$$E = h\upsilon = \frac{(6.63 \times 10^{-34} Js)(3.00 \times 10^{8} s^{-1})}{0.989 \times 10^{-9} m} \times \frac{6.02 \times 10^{23}}{mol} = 1.21 \times 10^{5} kJ/mol$$

For 94,000 kJ/mol

$$E = I - \frac{1}{2}mv^2 = (1.21 - 0.94) \times 10^{5} kJ/mol = 2.7 \times 10^{4} kJ/mol$$

Attributed to the carbon (C) atom

3 pts

For 69,900 kJ/mol

$$E = I - \frac{1}{2}mv^2 = (1.21 - 0.699) \times 10^{5} kJ/mol = 5.11 \times 10^{4} kJ/mol$$

Attributed to the oxygen (O) atom

3 pts

(2 pts each)

1) For both K and Ca, the outer electrons are in the 4s shell, outside of the Ar core. K has the lower ionization energy because of its lower nuclear charge. The second 4s electron in Ca only partially

shields the first.

K^+ is isoelectronic with Ar; Ca^+ is isoelectronic with K. Thus, the comparison of the ionization energies of K^+ and Ca^+ echoes that of Ar and K. Since the electron in K^+ are in the inner core (have the Ar-like configuration), it requires much more energy to remove. Therefore, Ca^+ has an appreciably lower ionization energy.

2) In comparing K with Ca^+ (i.e., the first ionization energy of K with the second of Ca), one is comparing isoelectronic species (both in gas phase). The one with the higher nuclear charge (Ca^+) will be expected to have the higher ionization energy with everything else being the same.

4. (10 points)

Consider an electron confined in a box with infinite potential barriers (particle in a box). If the energy difference between the ground state (n=1) and the first excited state (n=2) corresponds to the absorption of light with a wavelength of either 800 nm or 400 nm (1 nm = 10^{-9} m), determine the length of the box in each case. Express your answers in angstroms (1 Å = 10^{-10} m).

(Answer)

$E_n = \frac{n^2h^2}{8mL^2}$, n = 1, 2, 3…

$m = 9.11 \times 10^{-31}$ kg, $h = 6.626 \times 10^{-34}$ J s, c = 3.00×10^{8} m s^{-1}

5 pts each answer, partial points apply

Since $E_n = \frac{n^2h^2}{8mL^2}$, ΔE = $E_2 - E_1 = 3 \times \frac{h^2}{8mL^2}$

$L = \sqrt{\frac{3h^2}{8mE}}$

For the wavelength of 800 nm)

$$E = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34}\text{ Js})(2.998 \times 10^{8}\text{ ms}^{-1})}{(800 \times 10^{-9}\text{m})} = 2.483..\times 10^{-19}\text{ J}$$

$L = 8.53 \times 10^{-10}$ m = 8.53 Å (3 significant figures. Deduct 1 pt for incorrect significant figures.)

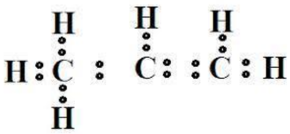
For the wavelength of 400 nm)

$$E = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34}\text{ Js})(2.998 \times 10^{8}\text{ ms}^{-1})}{(400 \times 10^{-9}\text{m})} = 4.966..\times 10^{-19}\text{ J}$$

$L = 6.03 \times 10^{-10}$ m = 6.03 Å (3 significant figures. Deduct 1 pt for incorrect significant figures.)

5. (15 points)

(1) Draw the Lewis dot structure of propene, CH_3CHCH_2, using dots only (2 pts). (note: do not draw bond lines).

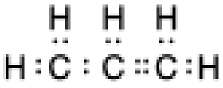


부분 점수 없음

(2) Assign the hybridization for each carbon atom in propene, based on the textbook notation (1 pt).
Each carbon center, from left to right, sp^3, sp^2, and sp^2.

부분 점수 없음

(3) The allylic cation can be formed by removing a hydride ion (H-) from the CH_3 group in propene. Draw the Lewis dot structure of the resulting allylic cation and assign the hybridization for each carbon atom (3 pts).

Resonance structures should be drawn. :  (2 pts)
from left, sp^2, sp^2, and sp^2.: 1 pt

총 3점

문제에 resonance structure에 대한 내용이 없어서 한 가지 구조만 그려도 (2점)

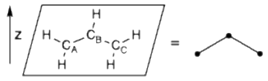
구조는 맞게 그렸으나 cation 표시가 없을 시 (1점)

Cation 표시 유무와 관계없이 구조가 틀렸으면 (0점)

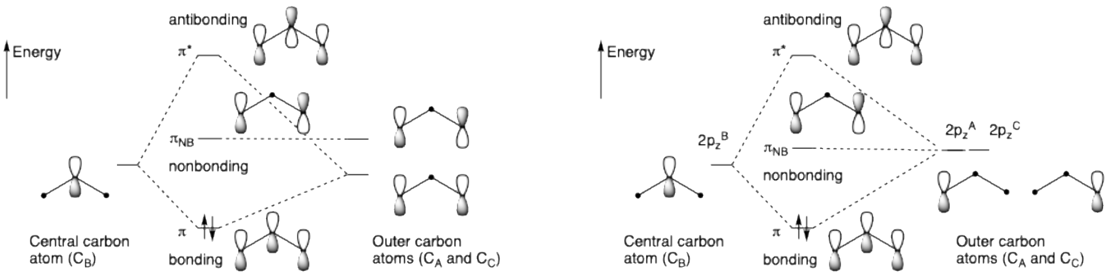
모든 탄소에 대해 Hybridization 옳게 적었으면 (1점)

(4) Construct the molecular orbital (MO) diagram for only the π electron system of the allylic cation, $CH_2CHCH_2^+$. Label each π MO with its relative energy level (bonding, nonbonding, or antibonding), and indicate how π electrons are distributed. Then, based on the delocalization of π electrons and the presence of σ bonds, predict the total bond order between each pair of carbon atoms in the cation (4 pts).

(3 pts for MO diagram)



(Two options, both are correct)



(Option 1: Pre-construct the fragment MOs of outer carbon atoms)

(Option 2 : Construct the MOs directly from the atomic orbitals)

Among the 16 valence electrons, 14 electrons form σ bonds and the remaining 2 electrons form π bonds. (Deduct 1 point for incorrect number of π electrons)

In each C-C bond, 2 electrons are involved in σ bond and 1 electron is involved in π bondindg orbtial. Because 3 electrons are in bonding orbtals and none are in nonbonding or antibonding orbitals, the bond order is 1.5.

Bond order: 1.5: 1 pts

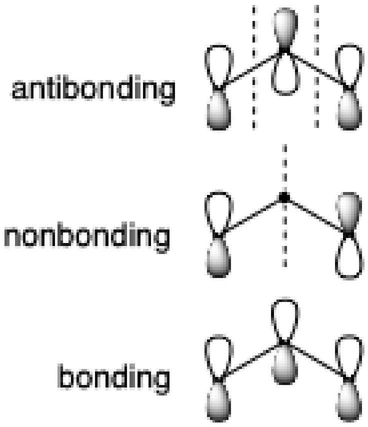
총 4점

Bonding, nonbonding, antibonding의 energy level 순서(1)와 전자 개수(2)가 맞으면 (3점)

(1) 혹은 (2) 둘 중 하나라도 틀렸으면 (1점)

Total Bond order 옳게 적었으면 (1점)

(5) Sketch the π MOs constructed in (4). Indicate phase relationships using shading or signs (+/−), and indicate where nodal planes are present, if applicable (3 pts).



각 Bonding, nonbonding, antibonding을 바르게 그리고 nodal plane까지 표현하였으면 각각 1점 (총 3점)

Bent 구조는 고려하지 않았음 (직선으로 그려도 정답)

(6) Predict whether the allylic radical ($CH_2CHCH_2^{\bullet}$) and the allylic anion ($CH_2CHCH_2^{-}$) can exist as stable species, based on the π MOs constructed in (4) (2 pts).

Both stable
(Should contain the explanation that the additional electron(s) occupy the nonbonding orbital in the MO diagram)

부분 점수 없음

추가 전자는 nonbonding orbital 을 차지하여 bond order 에 변화가 없기 때문에 둘 다 안정하다라고 작성하면 (2 점)

둘 중 하나라도 unstable 이라고 한 경우 (0 점)
Stable 하다고 작성하였으나 설명이 틀렸을 경우 (0 점)

6. (10 points)

(1) A wave function for a hydrogen atom is given below, where $\mathcal{N}$ is the normalization constant and a_0 is the Bohr radius. Predict the values for the quantum numbers n, ℓ, and m corresponding to this wave function, and give the orbital notation as described in the notes / textbook (2 pts).

$$\psi_{n\ell m}(r,\theta,\phi) = \mathcal{N}\left(\frac{r}{a_0}\right)^2 \exp\left(-\frac{r}{3a_0}\right)(3\cos^2\theta - 1)$$

3, 2, and 0; $3d_{z^2}$

(2) Based on the quantum numbers you identified in the previous question, predict the number of radial nodes and angular nodes for this orbital (2 pts).

0 and 2

(3) How many other orbitals have the same energy as the one described above? Justify your prediction (2 pts).

8 (For one-electron atoms, s, p, d orbitals are degenerated.)

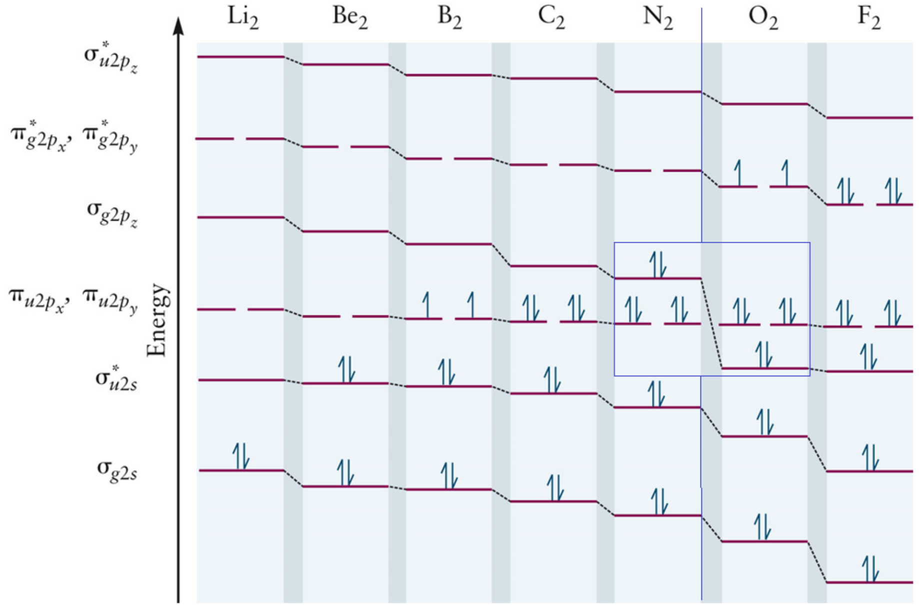
(4) Related to the question (3), how many other Hartree orbitals in fluorine (F) have the same energy as the Hartree orbital derived from the wave function described above? Justify your prediction (2 pts).

4 (For many-electron atoms, s, p, d orbitals are not degenerated.)

(5) Give the electronic configuration of fluorine in its first excited state, defined as the lowest-energy state above the ground state (2 pts).

$1s^2 2s^2 2p^4 3s^1$

7. (15 points)



Energy levels for the homonuclear diatomic molecules Li_2 through F_2

(1) As shown in the figure above, the energy levels of molecular orbitals decrease progressively from Li_2 to F_2. What is the main reason for this trend? (3 pts)

(2) Based on the molecular orbital energy levels provided in the figure, predict the third ionization energy (IE_3) of N_2 and O_2, and compare the two values. (3 pts).

(3) If the orbital energy level inversion discussed in question part (2) above did not occur in O_2, how would this affect the predicted IE_3 values of N_2 and O_2? Compare the two values under this assumption. (3 pts).

(4) What notable and distinctive property is observed in O_2 (and B_2), which experimental method was used to confirm this property in the case of O_2? (3 pts)

(5) The parallel spin configuration of unpaired electrons is consistent with which fundamental rule? (3 pts)

(answers)

Koopmans' theorem is typically employed to approximate the first ionization energy (IE_1), but it may not be suitable for higher ionization energies. For the purpose of these questions, assume that Koopmans' theorem is also applicable to the third ionization energy (IE_3). An additional 2 points will be awarded for any relevant discussion on Koopmans' theorem.

(1) As Z (nuclear charge) increases, all MOs are stabilized by increased nucleus charge Columbic attraction.

(2) IE3 (N_2) ~ 0 – Energy level of (N_2's π_{u2px} or π_{u2py} orbital), IE3 (O_2) ~ 0 – Energy level of (O_2's π_{u2px} or π_{u2py} orbital). Therefore, IE3 (N_2) < IE3 (O_2), very slightly larger or nearly same.

(3) IE3 (N_2) ~ 0 – Energy level of (N_2's π_{u2px} or π_{u2py} orbital) same above, IE3 (O_2) ~ 0 – Energy level of (σ_{g2pz} orbital). Therefore, IE3 (N_2) > IE3 (O_2).

(4) Dioxygen (and diboron) is paramagnetic; liquid oxygen ($O_2(l)$) poured between the two poles of a magnet is attracted and held there.

(5) Hunt's rule is obeyed when there is a maximum of parallel spins (maximum multiplicity)

8. (15 points)

Answer the following questions below:

(1) Employing Bohr's assumptions, derive the de Broglie wavelength equation for an electron engaged in circular standing wave oscillations around the atomic nucleus (4 pts).

(2) What is the problem with Rutherford's hydrogen model from the point of view of classical mechanics? Which assumption of Bohr's model helps to solve this problem? (2 pts)

(3) What is the Hartree approximation for multi-electron atomic systems? (2 pts)

(4) Explain the Born–Oppenheimer approximation. Then, describe the self-consistent field (SCF) method used to solve the Schrödinger equation under this approximation. (3 pts)

(5) (a) What is the Linear Combination of Atomic Orbitals (LCAO)? (b) What is valence bond (VB) theory? (c) Compare LCAO-MO and VB theory and discuss their strengths and weaknesses for explaining the nature of bonds or properties of molecules. (4 pts).

(answer)

(1) In classical mechanics, if an electron rotates around the nucleus (proton), it will emit light while losing kinetic energy. Therefore, an electron will collide with the nucleus, so no stable hydrogen atom can exist. With Bohr's angular momentum quantization assumption (different descriptions are possible: that the angular momentum of an electron in a hydrogen atom is quantized / that only certain discrete orbits are allowed / that the electron "jumps" from one stable orbit to another as the light is emitted or absorbed), an electron can rotate without losing kinetic energy.

(2) The electron with a circular standing wave oscillating about the nucleus of the atom.

$n\lambda = 2\pi r \qquad n = 1, 2, 3, \ldots$ (1pts)

From Bohr's assumption, $m_e vr = n\frac{h}{2\pi}$ $\quad 2\pi r = n\frac{h}{m_e v}$, $\quad \lambda = \frac{h}{m_e v} = \frac{h}{p}$ (3 pts)

(3) It assumes that the wavefunction can be approximated by a product of single-electron wavefunctions. The Hartree approximation is based on the idea that each electron experiences an

effective potential from the nucleus and the other electrons by using Zeff.

(4) (a) A nucleus is much more massive than an electron is; the nuclei in the molecules will move much more slowly than the electrons. **Consider the nuclei to be fixed at a specific set of positions. Then solve Schrödinger's equation for the electrons which are in motion; obtain the energy levels and wave functions. Next, move the nuclei a bit, and repeat the calculation. Continue this procedure in steps.** (key idea: bold face section above, 3pts)

(5) (a) LCAO method: selecting sums and differences (linear combinations) of atomic orbitals to generate the best approximation to each type of molecular orbital (1 pt) (b) Valence Bond Theory begins with the concept that **a covalent bond forms when an electron pair is shared between two atoms.** This theory treats a molecule as a collection of atoms that are held together by localized bonds between specific pairs of atoms. The fundamental principle is that atomic orbitals from different atoms overlap, allowing electrons to be shared between the nuclei. (1 pt)
(c) 2 pts (the student doesn't have to describe all of them, 1 pt for each correct answer)
Advantages of LCAO-MO theory: can describe the configuration of electrons delocalized (spread) over the entire molecule (spread beyond between two atoms), can explain the observed magnetism of a molecule
Disadvantages of LCAO-MO theory: less intuitive
Advantages of VB theory: intuitive for explaining bonds and shapes of a molecule
Disadvantages of VB theory: cannot explain the delocalization of electrons, cannot explain magnetic behavior

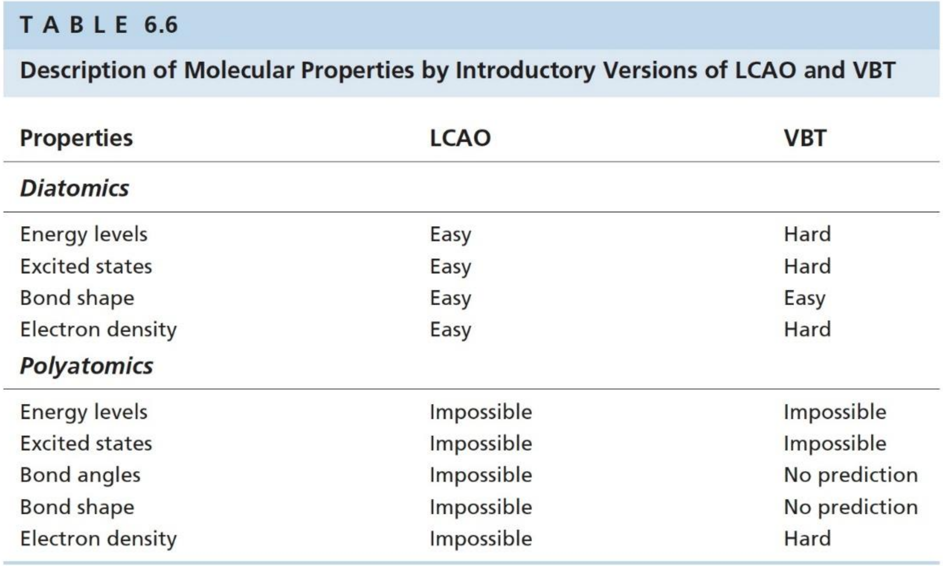


TABLE 6.6

Description of Molecular Properties by Introductory Versions of LCAO and VBT

Properties	**LCAO**	**VBT**
Diatomics		
Energy levels	Easy	Hard
Excited states	Easy	Hard
Bond shape	Easy	Easy
Electron density	Easy	Hard
Polyatomics		
Energy levels	Impossible	Impossible
Excited states	Impossible	Impossible
Bond angles	Impossible	No prediction
Bond shape	Impossible	No prediction
Electron density	Impossible	Hard

9. (10 points)

Answer the following questions regarding the Reactive Oxygen Species (ROS), which are generated through the addition of one electron to dioxygen (O_2) resulting in O_2^- (superoxide) or through the addition of two electrons to dioxygen generating O_2^{2-} (peroxide). ROS can be harmful, prompting organisms to develop mechanisms to eliminate them; on the other hand, they are necessary species in health as well at low concentrations in biological systems.

(a) Using only the 2s and 2p orbitals and with the z-axis aligned parallel to the O-O bond, draw correlation diagrams for O_2, O_2^-, O_2^{2-}(3 pts).

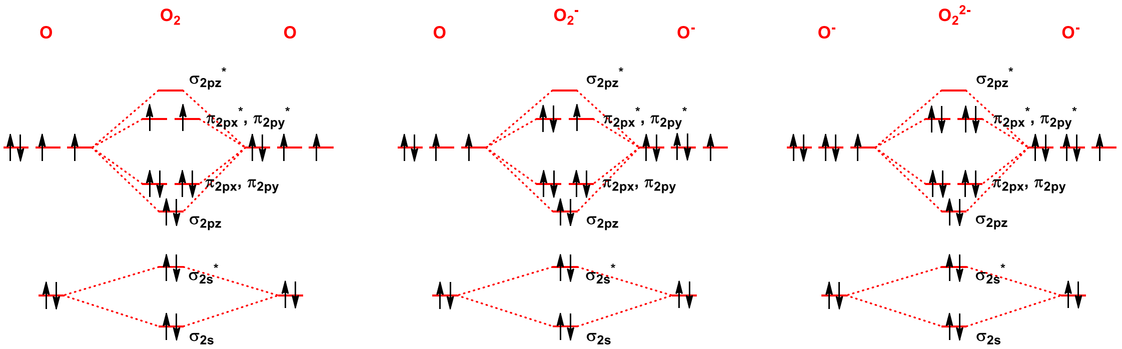
(b) Are these three species paramagnetic or diamagnetic? (2 pts)

(c) Can you explain why certain enzymes in biological systems would be designed to introduce two electrons to O_2, causing the cleavage of the double bond in O=O? (3 pts)

(d) Do the first ionization energies of these ROS increase or decrease compared to that found in an oxygen atom? Support your answer with the correlation diagrams (2 pts).

(answer)

(a) 3 points (each 1 point)



(b) **2 points (each 1 point)** O_2 and O_2^- are paramagnetic, whereas O_2^{2-} is diamagnetic

(c) **3 points (no discussion of bond orders, 1 point)** The bond orders of O_2, O_2^- and O_2^{2-} are 2, 3/2 and 1, respectively. In terms of bond order, O_2^{2-} has the weakest O-O bond strength. So, it can readily be dissociated.

(d) **2 points.** Those species have electrons in the antibonding orbital originated from the oxygen p-orbital (π_{2px}^* and π_{2py}^*). And, this antibonding orbital has higher energy than that of the original p-orbital. So, they have lower ionization energies.

Physical Constants

Avogadro's number	$N_A = 6.02214179 \times 10^{23}$ mol^{-1}
Bohr radius	$a_0 = 0.52917720859$ Å $= 5.2917720859 \times 10^{-11}$ m
Boltzmann's constant	$K_B = 1.3806504 \times 10^{-23}$ J K^{-1}
Electronic charge	$e = 1.602176487 \times 10^{-19}$ C
Faraday constant	$F = 96485.3399$ C mol^{-1}
Masses of fundamental particles:	
Electron	$m_e = 9.10938215 \times 10^{-31}$ kg
Proton	$m_P = 1.672621637 \times 10^{-27}$ kg
Neutron	$m_n = 1.674927211 \times 10^{-27}$ kg
Permittivity of vacuum	$\varepsilon_o = 8.854187817 \times 10^{-12}$ C^{-2} J^{-1} m^{-1}
Planck's constant	$h = 6.62606896 \times 10^{-34}$ J s
Ratio of proton mass to electron mass	$m_P / m_e = 1836.15267247$
Speed of light in a vacuum	$c = 2.99792458 \times 10^{8}$ m s^{-1} (exactly)
Standard acceleration of terrestrial gravity	$g = 9.80665$ m s^{-2} (exactly)
Universal gas constant	$R = 8.314472$ J mol^{-1} K^{-1} $= 0.0820574$ L atm mol^{-1} K^{-1}

Values are taken from the 2006 CODATA recommended values,
as listed by the National Institute of Standards and Technology.

Conversion factors

Ångström	1 Å $= 10^{-10}$ m
Atomic mass unit	1 u $= 1.660538782 \times 10^{-27}$ kg
	1 u $= 1.492417830 \times 10^{-10}$ J $= 931.494028$ MeV (energy equivalent form $E = mc^2$)
Calorie	1 cal = 4.184 J (exactly)
Electron volt	1 eV $= 1.602177 \times 10^{-19}$ J $= 96.485335$ kJ mol^{-1}
Foot	1 ft = 12 in = 0.3048 m (exactly)
Gallon (U. S.)	1 gallon = 4 quarts = 3.785412 L (exactly)
Liter	1 L $= 10^{-3}$ m^3 $= 10^3$ cm^3 (exactly)
Liter-atmosphere	1 L atm = 101.325 J (exactly)
Metric ton	1 t = 1000 kg (exactly)
Pound	1 lb = 16 oz = 0.4539237 kg (exactly)
Rydberg	1 Ry $= 2.17987197 \times 10^{-18}$J $= 1312.7136$ kJ mol^{-1} $= 13.60569193$ eV
Standard atmosphere	1 atm $= 1.01325 \times 10^5$ Pa $= 1.01325 \times 10^5$ kg m^{-1} s^{-2} (exactly)
Torr	1 torr = 133.3224 Pa

PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/

GROUP NUMBERS IUPAC RECOMMENDATION (1985) — 13
GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986) — IIIA
ATOMIC NUMBER — 5
RELATIVE ATOMIC MASS (1) — 10.811
SYMBOL — **B**
ELEMENT NAME — BORON

PERIOD	GROUP 1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 1.0079 **H** HYDROGEN																	2 4.0026 **He** HELIUM
2	3 6.941 **Li** LITHIUM	4 9.0122 **Be** BERYLLIUM											5 10.811 **B** BORON	6 12.011 **C** CARBON	7 14.007 **N** NITROGEN	8 15.999 **O** OXYGEN	9 18.998 **F** FLUORINE	10 20.180 **Ne** NEON
3	11 22.990 **Na** SODIUM	12 24.305 **Mg** MAGNESIUM											13 26.982 **Al** ALUMINIUM	14 28.086 **Si** SILICON	15 30.974 **P** PHOSPHORUS	16 32.065 **S** SULPHUR	17 35.453 **Cl** CHLORINE	18 39.948 **Ar** ARGON
4	19 39.098 **K** POTASSIUM	20 40.078 **Ca** CALCIUM	21 44.956 **Sc** SCANDIUM	22 47.867 **Ti** TITANIUM	23 50.942 **V** VANADIUM	24 51.996 **Cr** CHROMIUM	25 54.938 **Mn** MANGANESE	26 55.845 **Fe** IRON	27 58.933 **Co** COBALT	28 58.693 **Ni** NICKEL	29 63.546 **Cu** COPPER	30 65.39 **Zn** ZINC	31 69.723 **Ga** GALLIUM	32 72.64 **Ge** GERMANIUM	33 74.922 **As** ARSENIC	34 78.96 **Se** SELENIUM	35 79.904 **Br** BROMINE	36 83.80 **Kr** KRYPTON
5	37 85.468 **Rb** RUBIDIUM	38 87.62 **Sr** STRONTIUM	39 88.906 **Y** YTTRIUM	40 91.224 **Zr** ZIRCONIUM	41 92.906 **Nb** NIOBIUM	42 95.94 **Mo** MOLYBDENUM	43 (98) **Tc** TECHNETIUM	44 101.07 **Ru** RUTHENIUM	45 102.91 **Rh** RHODIUM	46 106.42 **Pd** PALLADIUM	47 107.87 **Ag** SILVER	48 112.41 **Cd** CADMIUM	49 114.82 **In** INDIUM	50 118.71 **Sn** TIN	51 121.76 **Sb** ANTIMONY	52 127.60 **Te** TELLURIUM	53 126.90 **I** IODINE	54 131.29 **Xe** XENON
6	55 132.91 **Cs** CAESIUM	56 137.33 **Ba** BARIUM	57-71 **La-Lu** **Lanthanide**	72 178.49 **Hf** HAFNIUM	73 180.95 **Ta** TANTALUM	74 183.84 **W** TUNGSTEN	75 186.21 **Re** RHENIUM	76 190.23 **Os** OSMIUM	77 192.22 **Ir** IRIDIUM	78 195.08 **Pt** PLATINUM	79 196.97 **Au** GOLD	80 200.59 **Hg** MERCURY	81 204.38 **Tl** THALLIUM	82 207.2 **Pb** LEAD	83 208.98 **Bi** BISMUTH	84 (209) **Po** POLONIUM	85 (210) **At** ASTATINE	86 (222) **Rn** RADON
7	87 (223) **Fr** FRANCIUM	88 (226) **Ra** RADIUM	89-103 **Ac-Lr** **Actinide**	104 (261) **Rf** RUTHERFORDIUM	105 (262) **Db** DUBNIUM	106 (266) **Sg** SEABORGIUM	107 (264) **Bh** BOHRIUM	108 (277) **Hs** HASSIUM	109 (268) **Mt** MEITNERIUM	110 (281) **Uun** UNUNNILIUM	111 (272) **Uuu** UNUNUNIUM	112 (285) **Uub** UNUNBIUM		114 (289) **Uuq** UNUNQUADIUM				

LANTHANIDE

6	57 138.91 **La** LANTHANUM	58 140.12 **Ce** CERIUM	59 140.91 **Pr** PRASEODYMIUM	60 144.24 **Nd** NEODYMIUM	61 (145) **Pm** PROMETHIUM	62 150.36 **Sm** SAMARIUM	63 151.96 **Eu** EUROPIUM	64 157.25 **Gd** GADOLINIUM	65 158.93 **Tb** TERBIUM	66 162.50 **Dy** DYSPROSIUM	67 164.93 **Ho** HOLMIUM	68 167.26 **Er** ERBIUM	69 168.93 **Tm** THULIUM	70 173.04 **Yb** YTTERBIUM	71 174.97 **Lu** LUTETIUM

ACTINIDE

7	89 (227) **Ac** ACTINIUM	90 232.04 **Th** THORIUM	91 231.04 **Pa** PROTACTINIUM	92 238.03 **U** URANIUM	93 (237) **Np** NEPTUNIUM	94 (244) **Pu** PLUTONIUM	95 (243) **Am** AMERICIUM	96 (247) **Cm** CURIUM	97 (247) **Bk** BERKELIUM	98 (251) **Cf** CALIFORNIUM	99 (252) **Es** EINSTEINIUM	100 (257) **Fm** FERMIUM	101 (258) **Md** MENDELEVIUM	102 (259) **No** NOBELIUM	103 (262) **Lr** LAWRENCIUM

(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)
Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.
However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@nettlinx.com)

2025 SPRING Semester Mid-term Examination
For General Chemistry I

Date: April 16(Wed), ***Time Limit: 19:00 ~ 21:00***

Write down your information neatly in the space provided below; print your Student ID in the upper right corner of every page.

Professor Name	Class	Student I.D. Number	Name

Problem	points	Problem	points	TOTAL pts
1	/7	**6**	/10	**/100**
2	/8	**7**	/15	
3	/10	**8**	/15	
4	/10	**9**	/10	
5	/15			

** This paper consists of 16 sheets and 9 problems (***pages 14 - 15***: Equations, constants & periodic table, ***page 16***: claim form). Please check all page numbers before taking the exam. Write down your work and answers in the Answer sheet. Please supply units with the value of your answer where applicable. You will get 30% deduction for missing units per problem.

NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER.
(채점 답안지 분배 및 이의신청 일정)

1. Period, Location and Procedure

0 Return and Claim Period: **April 21 (Monday, 19:00 ~ 21:00, 2 hrs)**

The claim is in person and permitted only during this time period. Keep that in mind!

0 Location: Each designated room of Creative Learning Bldg. (E11)

Section	Room (E11)
A	201
B	202
C	301
D	302

0 Procedure

Rule 1: Students cannot bring their writing tools into the testing room (Use a pen only provided by TA).

Rule 2: Whether or not the student completes a "claim," they must submit the paper back to TA. (Do not go out of the room with it).

If you have any claims on it, write them on the claim form and attach it to the top of the exam paper with a stapler. Give the packet directly to your TA.

WARNING!!

If you deliberately alter any original answers or insert something on your marked paper to achieve a better grade, you will get an F grade for this course. Or if you don't keep the rules above, we will regard it as a kind of cheating and give you 0 points. So please don't cheat.

2. Final Confirmation

1) Period: ***April 24 (Thu.) ~ 25 (Fri.)***
2) Procedure: During this period, you can check the final score of the examination *on the website* again.
(No additional corrections. If no change in your score was made after reasoning, the claims were not accepted.)

***** For further information, please visit the KAIST General Chemistry website at www.gencheminkaist.pe.kr***

1. (7 points)

In the hydrogen atom, the electronic transition from the 2*p* state to the 1*s* state involves an emission of a photon with energy 16.2×10^{-19} J. In an iron atom, the same transition (from 2*p* to 1*s*) results in an emission of an X-ray of wavelength 0.193 nm.

(1) Calculate the energy difference between these two states in iron (3 pts).
(2) Explain the difference in the 2*p*-1*s* energy level spacing in these two atoms (4 pts).

2. (8 points)

You have learned about the 2*p* and 3*d* orbitals both in terms of their energy levels and pictures of their overall shape (features including lobes, nodes, etc).

(1) State the number of nodes in the $3p_z$ and $4d_{z2}$ orbitals (2 pts).
(2) Compare the relative energies of the 3s, 3p, and 3d orbitals in the following cases: (6 pts)
    (a) a hydrogen atom, and
    (b) a multi-electron atom with an effective nuclear charge (Z_{eff}).
  Briefly explain the differences.

3. (10 points)

(1) The ionization energies for the 1s electron for the second-row elements are as follows:

(Reminder: the 1s is a core orbital not outer orbital; Notes: IE of the first electron only; the atoms are neutral, not ion their ionic form; measurements are in gas phase):

Atom	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**	**Atom**	**Energy (kJ/mol)**
Li	4820	Be	10,600	B	18,300	C	27,000
N	38,600	O	51,000	F	66,600		

Now suppose that a certain substance is bombarded by X-rays of wavelength 0.989 nm. If photoelectrons with kinetic energies of 94,000 kJ/mol and 69,900 kJ/mol are ejected from the material, which of the elements listed above must be present in the sample? (6 pts)

(2) The energy needed to remove one electron from a gaseous potassium atom is only about two-thirds as much as that needed to remove one electron from a gaseous calcium atom, yet nearly three times as much energy as that needed to remove one electron from K^+ as from Ca^+. (a) What explanation can you give for this difference? (b) Next, compare the ionization energy of Ca^+ with that of neutral K (4 pts)

4. (10 points)
Consider an electron confined in a box with infinite potential barriers (particle in a box). If the energy difference between the ground state (n=1) and the first excited state (n=2) corresponds to the absorption of light with a wavelength of either 800 nm or 400 nm (1 nm = 10^{-9} m), determine the length of the box in each case. Express your answers in angstroms (1 Å = 10^{-10} m).

5. (15 points)

(1) Draw the Lewis dot structure of propene, CH_3CHCH_2, using dots only (2 pts). (note: do not draw bond lines).

(2) Assign the hybridization for each carbon atom in propene, based on the textbook notation (1 pt).

(3) The allylic cation can be formed by removing a hydride ion (H-) from the CH_3 group in propene. Draw the Lewis dot structure of the resulting allylic cation and assign the hybridization for each carbon atom (3 pts).

(4) Construct the molecular orbital (MO) diagram for only the π electron system of the allylic cation, $CH_2CHCH_2^+$. Label each π MO with its relative energy level (bonding, nonbonding, or antibonding), and indicate how π electrons are distributed. Then, based on the delocalization of π electrons and the presence of σ bonds, predict the total bond order between each pair of carbon atoms in the cation (4 pts).

(5) Sketch the π MOs constructed in (4). Indicate phase relationships using shading or signs (+/−), and indicate where nodal planes are present, if applicable (3 pts).

(6) Predict whether the allylic radical ($CH_2CHCH_2^{\bullet}$) and the allylic anion ($CH_2CHCH_2^{-}$) can exist as stable species, based on the π MOs constructed in (4) (2 pts).

6. (10 points)

(1) A wave function for a hydrogen atom is given below, where $\mathcal{N}$ is the normalization constant and a_0 is the Bohr radius. Predict the values for the quantum numbers n, ℓ, and m corresponding to this wave function, and give the orbital notation as described in the notes / textbook (2 pts).

$$\psi_{n\ell m}(r,\theta,\phi) = \mathcal{N}\left(\frac{r}{a_0}\right)^2 \exp\left(-\frac{r}{3a_0}\right)(3\cos^2\theta - 1)$$

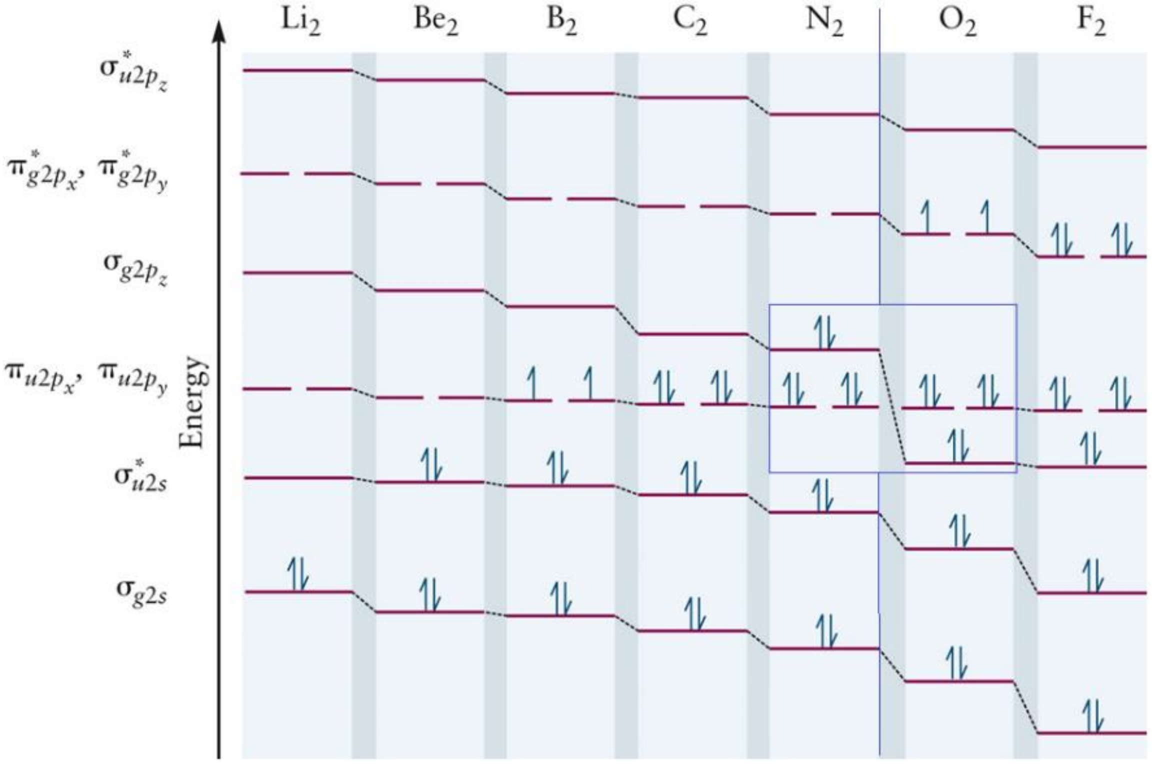
(2) Based on the quantum numbers you identified in the previous question, predict the number of radial nodes and angular nodes for this orbital (2 pts).

(3) How many other orbitals have the same energy as the one described above? Justify your prediction (2 pts).

(4) Related to the question (3), how many other Hartree orbitals in fluorine (F) have the same energy as the Hartree orbital derived from the wave function described above? Justify your prediction (2 pts).

(5) Give the electronic configuration of fluorine in its first excited state, defined as the lowest-energy state above the ground state (2 pts).

7. (15 points)



Energy levels for the homonuclear diatomic molecules Li_2 through F_2

(1) As shown in the figure above, the energy levels of molecular orbitals decrease progressively from Li_2 to F_2. What is the main reason for this trend? (3 pts)

(2) Based on the molecular orbital energy levels provided in the figure, predict the third ionization energy (IE_3) of N_2 and O_2, and compare the two values. (3 pts).

(3) If the orbital energy level inversion discussed in question part (2) above did not occur in O_2, how would this affect the predicted IE_3 values of N_2 and O_2? Compare the two values under this assumption. (3 pts).

(4) What notable and distinctive property is observed in O_2 (and B_2), which experimental method was used to confirm this property in the case of O_2? (3 pts)

(5) The parallel spin configuration of unpaired electrons is consistent with which fundamental rule? (3 pts)

8. (15 points)

Answer the following questions below:

(1) Employing Bohr's assumptions, derive the de Broglie wavelength equation for an electron engaged in circular standing wave oscillations around the atomic nucleus (4 pts).

(2) What is the problem with Rutherford's hydrogen model from the point of view of classical mechanics? Which assumption of Bohr's model helps to solve this problem? (2 pts)

(3) What is the Hartree approximation for multi-electron atomic systems? (2 pts)

(4) Explain the Born–Oppenheimer approximation. Then, describe the self-consistent field (SCF) method used to solve the Schrödinger equation under this approximation. (3 pts)

(5) (a) What is the Linear Combination of Atomic Orbitals (LCAO)? (b) What is valence bond (VB) theory? (c) Compare LCAO-MO and VB theory and discuss their strengths and weaknesses for explaining the nature of bonds or properties of molecules. (4 pts).

9. (10 points)

Answer the following questions regarding the Reactive Oxygen Species (ROS), which are generated through the addition of one electron to dioxygen (O_2) resulting in O_2^- (superoxide) or through the addition of two electrons to dioxygen generating O_2^{2-} (peroxide). ROS can be harmful, prompting organisms to develop mechanisms to eliminate them; on the other hand, they are necessary species in health as well at low concentrations in biological systems.

(1) Using only the 2s and 2p orbitals and with the z-axis aligned parallel to the O-O bond, draw correlation diagrams for O_2, O_2^-, O_2^{2-}(3 pts).

(2) Are these three species paramagnetic or diamagnetic? (2 pts)

(3) Can you explain why certain enzymes in biological systems would be designed to introduce two electrons to O_2, causing the cleavage of the double bond in O=O? (3 pts)

(4) Do the first ionization energies of these ROS increase or decrease compared to that found in an oxygen atom? Support your answer with the correlation diagrams (2 pts).

Physical Constants

Avogadro's number	N_A = 6.02214179 x 10^{23} mol^{-1}
Bohr radius	a_0 = 0.52917720859 Å = 5.2917720859 x 10^{-11} m
Boltzmann's constant	K_B = 1.3806504 x 10^{-23} J K^{-1}
Electronic charge	e = 1.602176487 x 10^{-19} C
Faraday constant	F = 96485.3399 C mol^{-1}
Masses of fundamental particles:	
Electron	m_e = 9.10938215 x 10^{-31} kg
Proton	m_P = 1.672621637 x 10^{-27} kg
Neutron	m_n= 1.674927211 x 10^{-27} kg
Permittivity of vacuum	ε_o = 8.854187817 x 10^{-12} C^{-2} J^{-1} m^{-1}
Planck's constant	h = 6.62606896 x 10^{-34} J s
Ratio of proton mass to electron mass	m_P / m_e = 1836.15267247
Speed of light in a vacuum	c = 2.99792458 x 10^8 m s^{-1} (exactly)
Standard acceleration of terrestrial gravity	g = 9.80665 m s^{-2} (exactly)
Universal gas constant	R = 8.314472 J mol^{-1} K^{-1} = 0.0820574 L atm mol^{-1} K^{-1}

Values are taken from the 2006 CODATA recommended values,
as listed by the National Institute of Standards and Technology.

Conversion factors

Ångström	1 Å= 10^{-10} m
Atomic mass unit	1 u = 1.660538782 x 10^{-27} kg
	1 u = 1.492417830 x 10^{-10} J = 931.494028 MeV (energy equivalent form $E = mc^2$)
Calorie	1 cal = 4.184 J (exactly)
Electron volt	1 eV = 1.602177 x 10^{-19} J = 96.485335 kJ mol^{-1}
Foot	1 ft = 12 in = 0.3048 m (exactly)
Gallon (U. S.)	1 gallon = 4 quarts = 3.785412 L (exactly)
Liter	1 L = 10^{-3} m^3 = 10^3 cm^3 (exactly)
Liter-atmosphere	1 L atm = 101.325 J (exactly)
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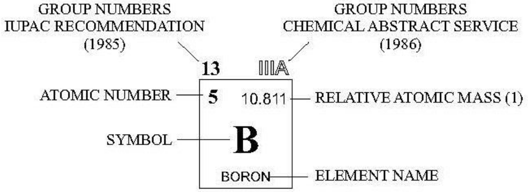

PERIOD	GROUP 1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
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Editor: Aditya Vardhan (adivar@nettlinx.com)

Claim Form for General Chemistry Examination

Page (/)

Class:____________, Professor Name:_____________, I.D.# :_______________, Name:__________________________

If you have any claims on the marked paper, please write down them on this form and ***submit this with your paper in the assigned place***. (And this form should be attached ***on the top of the marked paper with a stapler***.) Please, ***copy this sheet if you need more bef***

By Student		By TA	
Question #	Claims	Accepted? Yes(√) or No(√)	
		Yes: ☐	No: ☐
		Pts (+/-)	Reasons