

**Chem 1A, Fall 2015, Midterm Exam 2. Version A**  
**October 20, 2015**  
**(Prof. Head-Gordon)<sup>2</sup>**

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Student ID: \_\_\_\_\_ TA: \_\_\_\_\_

**Contents: 7 pages**

- A. Multiple choice (7 points)
- B. Big Molecules (9 points)
- C. Molecular orbitals of diatomic molecules (9 points)
- D. Molecular orbitals of polyatomic molecules (12 points)
- E. Gas laws and kinetic theory (7 points)

**Total Points: 44 points**

**Instructions:** Closed book exam. Basic scientific calculators are OK. Best wishes to all for success!

**Some possibly useful facts and figures:**

$$\begin{array}{ll}
 R = 8.3145 \text{ J mol}^{-1} \text{ K}^{-1} & \text{molar volume at STP} = 22.4 \text{ L} \\
 h = 6.6261 \times 10^{-34} \text{ J s} & \hbar = h / 2\pi \\
 c = 2.9979 \times 10^8 \text{ m s}^{-1} & 1 \text{ eV} = 1.60 \times 10^{-19} \text{ J} \\
 m_e = 9.1094 \times 10^{-31} \text{ kg} & \\
 N_0 = 6.0221 \times 10^{23} \text{ mol}^{-1} & 
 \end{array}$$

**Some possibly relevant equations:**

$$\begin{array}{l}
 \Delta E_{\text{vib}} = E_{n+1} - E_n = h\nu \quad E_{\text{rot}} = hBJ(J+1) \quad J = 0, 1, 2, \dots \\
 V(x) = \frac{1}{2}kx^2; \quad \nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \\
 P = \frac{F}{A} = \frac{mg}{A} = \frac{mgh}{V} = \rho gh \quad \bar{\epsilon} = \frac{1}{2}m\bar{v}^2 = \frac{3}{2}kT \quad \frac{\text{rate}_A}{\text{rate}_B} = \frac{n_A}{n_B} \sqrt{\frac{M_B}{M_A}} \\
 PV = \frac{1}{3}Nm\bar{v}^2 \quad \bar{v}^2 = \frac{3RT}{M} \quad f(v) = \left(\frac{2\pi kT}{m}\right)^{-3/2} 4\pi v^2 \exp(-mv^2/2kT) \\
 P_{\text{ideal}} V_{\text{ideal}} = nRT \quad V_{\text{ideal}} = V - nb \quad P_{\text{ideal}} = P + a\left(\frac{n}{V}\right)^2 \quad Z = \frac{PV}{nRT}
 \end{array}$$

**Multiple choice (10 points):** *there may be one or more correct solutions, so circle all that apply*

**1. The strength of intermolecular interactions increase in the following order**

- (a) London < Dipole-Dipole < Ion-Ion                      (b) London < Hydrogen-bonding < Dipole-Dipole  
(c) London < Hydrogen-bonding < Ion-Ion                      (d) Dipole-Dipole < Hydrogen-bonding < Ion-Ion

**2. Which spectroscopies describe the interaction of photons with electrons and not nuclei?**

- (a) Photoelectron spectroscopy                      (b) Infrared spectroscopy  
(c) Microwave spectroscopy                      (d) UV/vis spectroscopy

**3. The deviations from ideal gas behavior**

- (a) occurs at high pressures                      (b) show decreased volume with respect to  $V_{\text{ideal}}$   
(c) since real gases undergo phase transitions                      (d) occurs at low temperatures

**4. Colloids differ from solutions in what ways?**

- (a) Colloids scatter light better                      (b) Colloids are more stable than solutions  
(c) are more miscible                      (d) Composed of two phases

**5. Which molecule(s) would be expected to have an allowed transition in microwave spectroscopy?**

- (a)  $\text{N}_2$                       (b)  $\text{HC}=\text{CH}$   
(c)  $\text{HF}$                       (d)  $\text{O}_3$

**6. From a molecular orbital perspective, a metallic solid is conductive because**

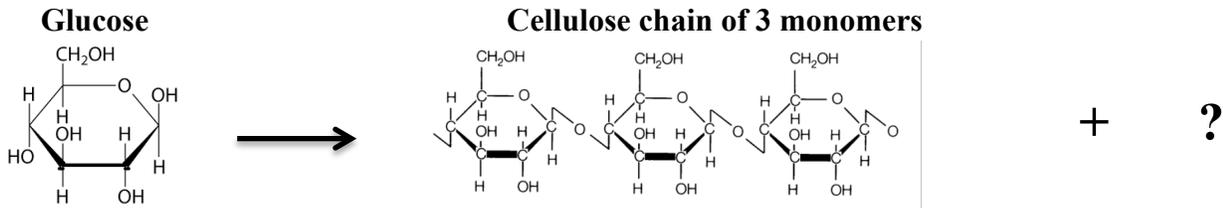
- (a) it has delocalized molecular orbitals                      (b) energy spacing between bonding orbitals increases  
(c) band gap is small                      (d) band gap is large

**7. On a phase diagram, the critical temperature is**

- (a) the temperature required to melt a solid                      (b) temperature at which all 3 states coexist  
(c) when liquid and gas appear indistinguishable                      (d) none of the above

## B. (10 points) Big Molecules

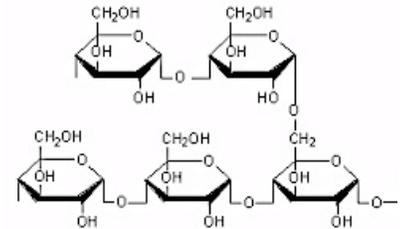
Cellulose is a big molecule known as a “polysaccharide” that is used to create structural support for plants. Cellulose is derived from a polymerization reaction using glucose monomers.



(a) (2 points) What kind of polymerization reaction is this? What is the missing product?

(b) (3 points) What is the strongest intermolecular force between cellulose chains? Draw how 2 monomers in different chains might interact through this force.

(c) (2 points) Starch is also a polysaccharide and it is used in plants to store energy. However it forms branched linkages (as shown here) rather than the linear chains of cellulose. Discuss why the mechanical strength of starch is so much less than the strength of cellulose.



(d) (2 points) Human digestion of plant starches is catalyzed by the amylase enzyme which attaches to starch and breaks the linkages to recover glucose for energy. However amylase does not work on cellulose, and thus we can't digest the cellulose components of plants. Suggest why amylase can't break down cellulose.

**C. (9 points) Molecular orbitals of diatomic molecules.** The CH molecule has been detected in the interstellar medium and may be involved in reactions that form larger organic molecules in space.

(a)(1 point) Draw a Lewis structure for the CH molecule, showing all electrons.

(b) (4 points) Use the 2s and 2p atomic orbitals on C, and the 1s atomic orbital on H to make a molecular orbital (MO) energy diagram for the CH molecule. (i) Show which AO's mix to give which MOs. (ii) Give each MO a symmetry label (i.e.  $\sigma$  or  $\pi$ ) and indicate whether it is antibonding (\*) or not. (iii) Show which are occupied.

C atom (AO)	CH molecule (MO)	H atom (AO)

(c)(2 points) Will the CH molecule show an infrared spectrum? Explain concisely why or why not.

(d) (2 points) Absorbing 266 nm radiation causes the CH radical to photodissociate. State what kind of excitation is involved (e.g. from which MO to which MO does absorption occur?), and give a reason (with a diagram) about why this electronic transition is allowed.

What type of excitation?	Why is it allowed?

**D. (12 points) Molecular orbitals of polyatomic molecules.** The formate anion,  $\text{OCHO}^-$  is formed from formic acid (i.e. methanoic acid,  $\text{O=CHOH}$ ) by proton loss and is an intermediate species in  $\text{CO}_2$  reduction.

(a) (2 points) Draw resonance structures for formate anion showing all electrons.

(b) (1 point) Evaluate the steric number of C in formate anion.

(c) (1 point) Use your answer to state what type of hybrid orbitals (on C & O) should be used to form MOs.

(d) (1 point) Indicate how many p orbitals are available to make delocalized  $\pi$  MOs

(e) (1 point) Indicate how many hybrid orbitals and 1s orbitals of H are available to make localized  $\sigma$  MOs.

(b)	(c)	(d)	(e)

(f) (3 points) Draw an MO energy level diagram showing all  $\sigma$  MOs (i.e. bonding, lone pair (LP), and antibonding (\*)) in the formate anion. Label them appropriately and show which are occupied. Make sure that you distinguish big energy differences clearly.

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(g)(3 points) Draw an MO diagram showing all  $\pi$  MOs for the formate anion, showing their relative energies, whether or not they are occupied, and sketching their rough form corresponds to each level.

Energy level diagram	Sketch of orbitals

**E. (7 points) Gas laws and kinetic theory.** A gas mixture of  $\text{H}_2$  and  $\text{N}_2$  occupies a balloon of volume of 15L with 2 atm pressure, and a temperature of 300K. It is known that the mixture contains 0.25 mol of  $\text{H}_2$

(a) (2 points) What is the partial pressure of  $\text{N}_2$  in the mixture?

(b) (2 points) Calculate the root mean square (RMS) velocity of the  $\text{H}_2$  molecules, in  $\text{m s}^{-1}$

(c) (3 points) Calculate the relative rates of escape (effusion) of the  $\text{H}_2$  and  $\text{N}_2$  molecules if a small hole was poked in the balloon.