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MIDTERM 1: CHM 2311 – Introduction to Structure and Bonding

Professor: Jaclyn Brusso

Date: February 11, 2016

Duration: 70 minutes

Name:____

Student Number:____

Instructions:

- Be sure to print your name and ID number clearly on this test booklet.
- This is a closed book examination.
- Please write legibly and show your work to receive credit for your answers. Partial marks *in some cases* may be awarded for partially correct work.
- For remarking, the exam *must* be written in pen.
- There are 8 questions. You are expected to answer all 8 questions.
- There are 8 pages. Please make sure you have all 8 pages. NOTE: the last page is a DATA SHEET. You may tear it off.
- At the end of the exam, turn in this test booklet and the data sheet.

GOOD LUCK!

Question	**Grade**		**Question**	**Grade**
1	**/3**		**5**	**/9**
2	**/3**		**6**	**/6**
3	**/2**		**7**	**/6**
4	**/5**		**8**	**/14**
TOTAL				**/48**

1. (**3 marks**) A ground state hydrogen atom absorbs a single photon of radiation of wavelength 102.6 nm. What is the principal quantum number of the electron after the atom absorbs the photon?

Answer:

E = hc/lambda ✔
$E = (6.626 \times 10^{-34}\ Js)(2.99 \times 10^{8}\ m/s)/(102.6 \times 10^{-9}\ m)$
$E = 1.936 \times 10^{-18}\ J$

$E = R_H\,[(1/n_{lower}\text{^}2) - (1/n_{higher}\text{^}2)]$ ✔
$E/R_H = (1/n_{lower}\text{^}2) - (1/n_{higher}\text{^}2)$
$1 - (1/n_{higher}\text{^}2) = 0.8885$
n = 3 ✔

2. (**3 marks**) Calculate Z_{eff} for an electron in the 3d orbital of Se atom

Answer:

Electronic configuration of Se [Ar] $4s^2 3d^{10} 4p^4$ = [$1s^2 2s^2 2p^6 3s^2 3p^6$]$4s^2 3d^{10} 4p^4$

$(1s^2)(2s^2 2p^6)(3s^2 3p^6)(3d^{10})\ (4s^2 4p^4)$ ✔

Recall from Lecture Notes Part 2 that the electrons to the right of the group in question do not participate in shielding

$(1 \times 18) + (0.35 \times 9) = 21.15 = \sigma$ ✔

$Zeff = Z - \sigma = 34 - 21.15 = 12.85$ ✔

3. (**2 marks; 1 mark each**)
(a) One of the valence electrons in a ground state atom has the quantum numbers $n = 4$, $l = 1$, $m_l = 0$, $m_s = +½$. What element(s) could this be?

Answer: Any of the p-block elements of the fourth row

(b) What is the atomic orbital designation for an electron having the quantum numbers $n = 5$, $l = 3$, $m_l = -1$, $m_s = -½$.

Answer: 5f

4. (**5 marks**) The energy conservation principle that applies to the photoelectric effect is:

$$E_{photon} = KE_{electron} + W$$

where E_{photon} is the energy of the photon, KE is the kinetic energy of the ejected electron and W is the work function for the metal.

(a) If X-rays of frequency 30.3×10^{16} Hz are used to remove a 2s electron from neon and the kinetic energy of the ejected electron is 193.2×10^{-18} J, calculate the minimum energy required to remove a single 2s electron from neon (i.e., calculate the work function for neon). (**3 marks**)

Answer:

1 mark: $E_{photon} = h\nu = (6.626 \times 10^{-34}\text{ J s})(30.3 \times 10^{16}\text{ s}^{-1}) = 2.007678 \times 10^{-16}\text{ J}$

1 mark: $W = E_{photon} - KE_{ejected\ electron}$

1 mark: $W = (2.007678 \times 10^{-16}\text{ J}) - (193.2 \times 10^{-18}\text{ J}) = 7.5678 \times 10^{-18}\text{ J}$

(b) What are the speed and de Broglie wavelength of the ejected electron? (**2 marks**)

Answer: - this answer is wrong

$KE = 193.2 \times 10^{-18}$ J

1 mark: $KE = \frac{1}{2} m_e v^2 \rightarrow v = (2\ KE/m_e)^{1/2} = 2.06 \times 10^7$ m/s

I mark: de Broglie lambda = $h/m_e v = 0.03532$ nm

5. (**9 marks**) In class we worked through the solution to the particle in a one-dimensional box with infinite potential energy walls and length *a*.

(a) What is the energy of the particle in the ground state? (**3 marks**)

Answer: The ground state of the particle is $n = 1$ ✔

$$E = \frac{n^2 h^2}{8ma^2} = \frac{1^2(6.626\times10^{-34}\,J\bullet s)^2}{(8)(9.11\times10^{-31}\,kg)a^2} = (6.02 \text{ x } 10^{-38}/\,a^2)\text{ J}$$ ✔ ✔

(b) How much energy is required to excite this particle to its *second excited* state? (**3 marks**)

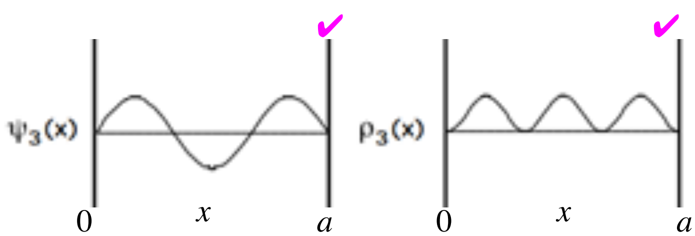
Answer: The first excited state of the particle is $n = 2$; the second excited state is $n = 3$. ✔ Calculate the energy of the particle in the second excited state and determine the difference between the ground state.

$$E = \frac{n^2 h^2}{8ma^2} = \frac{3^2(6.626\times10^{-34}\,J\bullet s)^2}{(8)(9.11\times10^{-31}\,kg)a^2} = 9(6.02 \text{ x } 10^{-38}/\,a^2)\text{ J} = (5.42 \text{ x } 10^{-37}/\,a^2)\text{ J}$$ ✔

The difference in energy is $(4.82 \text{ x } 10^{-37}/\,a^2)$ J ✔

(c) Sketch ψ and ψ^2 for the second excited state. (**2 marks**)

Answer:



(d) What is(are) the value(s) of *a* for the maximum probability of finding the particle in the second excited state? (**1 mark**)

Answer: Maximum probabilities for the second excited state occur at (1/6)*a*, (3/6)*a* and (5/6)*a*

6. (**6 marks; 2 marks each**) Predict and explain whether:

(a) The boiling point of SO_2 is higher or lower than CO_2.

Answer:
Sulphur dioxide is a polar molecule (bent) while carbon dioxide is nonpolar (linear). The dipole-dipole forces between SO_2 molecules are stronger than the induced dipole-induced dipole forces between CO_2 molecules. Therefore, SO_2 has a higher boiling point.

(b) The first electron affinity of Si is higher or lower than P.

Answer:
Adding an electron to electron to Si ($3s^2$ $3p^2$) is more favourable than adding to phosphorus ($3s^2$ $3p^3$), therefore the electron affinity will be more negative.

(c) The bond angle in H_2S should be bigger or smaller than that found in H_2O.

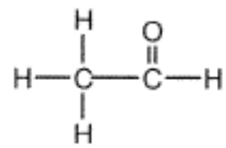
Answer:
The H-S-H bond should be smaller. Sulphur is more electropositive than oxygen, more electronegative atoms draw electron density towards the central atom, causing an increase in the electron-electron repulsion and hence, larger bond angle

7. **(8 marks)** Draw the valence bond representation of acetaldehyde ($CH_3\underline{C}HO$). Be sure to classify each bond as σ or π, identifying the orbitals involved. Predict the bond angles associated with the underlined carbon atom. Which of the two bonds C-C or C-O is likely to be weaker? Explain your reasoning.

Answer:
1 mark: correct shape and bonding
3.5 marks: bond types and labels (½ mark each)
$3 \times \sigma\ (Csp^3 – Hs)$; $1 \times \sigma\ (Csp^2 – Hs)$; $1 \times \sigma\ (Csp^3 – Csp^2)$; $1 \times \sigma\ (Csp^2 – Osp^2)$; $1 \times \pi\ (Cp – Op)$

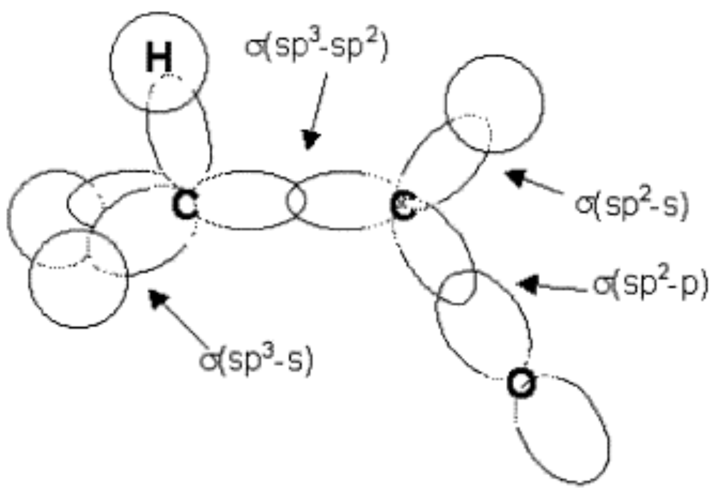
1.5 mark: bond angles for sp^2 carbon (½ mark each)
one <120; two >120

Acetaldehyde is CH_3CHO. The Lewis structure is



One of the carbons is sp^3 hybridized (having 4 VSEPR pairs) and the other is sp^2 hybridized (having 3 VSEPR pairs). The orbitals involved with the sigma bonds in this molecule are shown below.

sigma bonds:



One carbon is sp^3 hyrbrized and the other is sp^2. The double bond between C and O consists of a σ and π bond. The π bond is formed by the unhybridized p-orbital on the sp^2-hybridized carbon and p-orbital on O. The p orbitals on C and O are perpendicular to the plane of the page. The C-C bond is expected to be weaker than C=O as it consists only of one σ bond (no π bond). The bond energies are 348 kJ/mol and 802 kJ/mol, respectively. (**2 marks**)

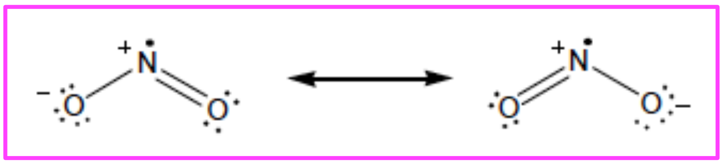
8. **(14 marks; 1 mark per blank; *no partial credit*)** For the following molecules:

i) Draw the Lewis structure. If more than one non-equivalent resonance structure is possible, only draw the most stable structure.
ii) Indicate any non-zero formal charges in the Lewis structure
iii) Determine the VSEPR geometry and shape of the molecule
iv) Draw the three-dimensional representation of the molecule
v) Determine whether the molecule is polar or non-polar
vi) Give the hybridization of the central atom

(a) NO_2

Lewis Structure:

Lewis: 2 × 6 + 5 = 17 valence electrons



3D Drawing:

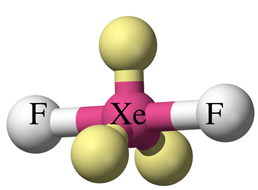
Geometry: __**Trigonal Planar**____________ **Shape:** __**bent or V-shaped**______

Polarity: __Polar ____________ **Hybridization**:____sp^2______________

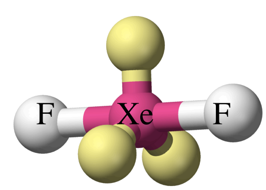
(b) XeF_2

Lewis Structure:

Lewis: 7 × 2 + 8 = 22 valence electrons



3D Drawing:



Geometry: ____Trigonal Bipyramidal______ **Shape:** _____Linear_________

Polarity: ____Nonpolar ____________ **Hybridization**:__sp^3d^3_____________

DATASHEET

	1 (1A)	2 (2A)	3 (3B)	4 (4B)	5 (5B)	6 (6B)	7 (7B)	8 (8B)	9 (8B)	10 (8B)	11 (1B)	12 (2B)	13 (3A)	14 (4A)	15 (5A)	16 (6A)	17 (7A)	18 (8A)
1	1 H Hydrogen 1.01																	2 He Helium 4.00
2	3 Li Lithium 6.94	4 Be Beryllium 9.01											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
3	11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Al Aluminum 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.07	17 Cl Chlorine 35.45	18 Ar Argon 39.95
4	19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.87	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.39	31 Ga Gallium 69.72	32 Ge Germanium 72.61	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
5	37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.60	53 I Iodine 126.90	54 Xe Xenon 131.29
6	55 Cs Cesium 132.91	56 Ba Barium 137.33	57 La Lanthanum 138.91	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (269)	109 Mt Meitnerium (268)									

Key

11 – Atomic number
Na – Element symbol
Sodium – Element name
22.99 – Average atomic mass*

58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.97
90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

* If this number is in parentheses, then it refers to the atomic mass of the most stable isotope.

Constants:

$N_A = 6.022\times10^{23}$ mol^{-1}

Rydberg constant = $R_H = 2.179 \times 10^{-18}$ J

Planck's constant = $h = 6.626 \times 10^{-34}$ J s

Speed of light = $c = 2.998 \times 10^{8}$ m s^{-1}

Electron mass = $m_e = 9.11 \times 10^{-31}$ kg

Bohr radius (a_o) = 52.9 pm

Conversion Factors:

1 J = 1 kg m^2 s^{-2}

1 J = 6.241×10^{8} eV

Useful Equations:

$$E_{PIB} = \frac{n^2h^2}{8ma^2} \qquad \psi_{PIB} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

$$\left[-\left(\frac{h^2}{8\pi^2 m}\right)\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right) + V\right]\Psi = E\Psi$$

$\psi(r,\theta,\phi) = R(r)Y(\Theta, \Phi)$

The volume element is $r^2\sin\Theta d\Theta d\Phi dr$

$E = ½\, mv^2$

$h = mv\lambda$

$h = \lambda\rho$