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MIDTERM 1: CHM 2311 – Introduction to Structure and Bonding

Professor: Jaclyn Brusso

Date: February 12, 2015

Duration: 75 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	**/5**		**5**	**/5**
2	**/3**		**6**	**/8**
3	**/5**		**7**	**/7**
4	**/8**		**8**	**/14**
TOTAL				**/55**

1. (**5 marks**) Calculate the shortest and longest wavelengths you would expect in the emission spectrum of an "excited" hydrogen atom whose initially in the n = 6 state.

$E = hc/\lambda = R_H [(1/n_{lower}^2) - (1/n_{higher}^2)]$

Longest wavelength: $n_1 = 6$; $n_2 = 5$

$\lambda = hc/\{R_H [(1/n_2^2) - (1/n_1^2)]\}$

$= hc/\{ R_H [(1/25) - (1/36)]\}$

$= 7.46 \times 10^{-6}$ m

Shortest wavelength: $n_1 = 6$; $n_2 = 1$

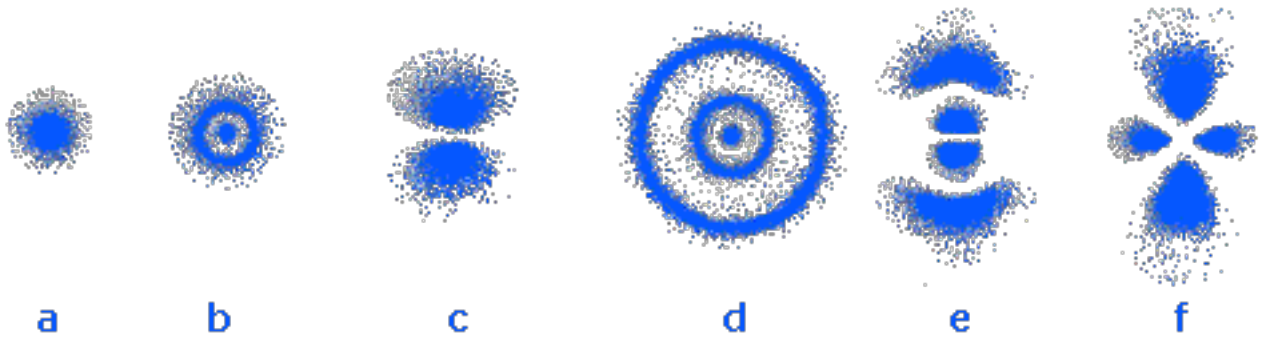
$E = hc/\lambda = R_H [(1/n_{lower}^2) - (1/n_{higher}^2)]$

$\lambda = hc/\{R_H [(1/n_2^2) - (1/n_1^2)]\}$

$= hc/\{ R_H [(1) - (1/36)]\}$

$= 93.8$ nm

2. (**3 marks**) What do each of the following figures represent? Provide the name for each.



Answer:

a) 1s
b) 2s
c) 2p
d) 3s
e) 3p
f) 3d

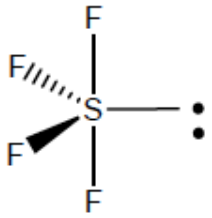
3. (a) Provide a detailed valence electronic configuration including the number of unpaired electrons for a sulphur atom. Is this atom paramagnetic or diamagnetic? (**2 marks**)
(b) SF_4 is a stable compound. Using the valence electron configuration, provide a valence bond description (including hybridization) for the bonding in this compound. (**3 marks**)

Answer:

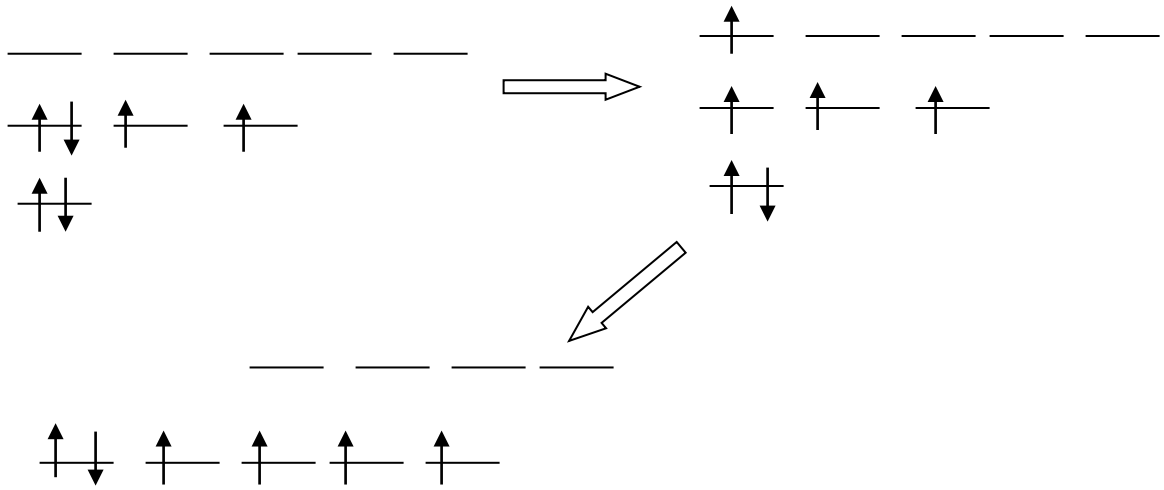
(a) [Ne] $3s^2 3p^4$ or $1s^2 2s^2 2p^6 3s^2 3p^4$

Two of the electrons in the 3p level are unpaired, therefore sulphur is paramagnetic.

(b) Lewis and VSEPR can help but are not necessary.



Using unhybridized orbitals, sulphur can only form two bonds to fluorine atoms. In order to make four bonds, four unpaired electrons are needed. This can be achieved by promoting one of the 3p electrons to the 3d level. Hybridization of the 1 × 3s + 3 × 3p + 1 × 3d orbitals leads to 5 × sp^3d orbitals, which have the correct geometry to make the four S—F bonds with one of the hybridized orbitals containing a lone pair.



4. (**8 marks**) In class we looked at radial and angular wave functions of hydrogen orbitals.

(a) Under what conditions do orbitals have nodes? (**1 mark**)

Nodes occur when the wave function changes sign *or* when the probability is equal to zero.

(b) The angular wave function for an orbital is given by:

$$Y = \frac{1}{4}\sqrt{\frac{15}{\pi}}\frac{(x^2 - y^2)}{r^2}$$

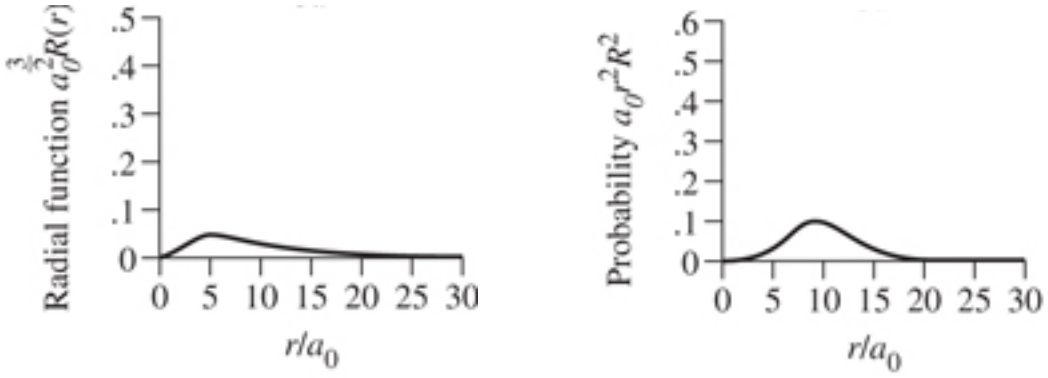
Where r is the radial distance. Under what condition does this wave function have an angular node? Describe the nodal surface for this orbital (i.e., which plane or planes correspond to nodes for this orbital). (**4 marks**)

Nodes occur when Y = 0 ✔
Therefore for this wave function nodes occur when:
$x^2 - y^2 = 0$ ✔
$x^2 = y^2$
$x = \pm y$ ✔
The nodal surfaces for this wave function are planes at x = y and x = -y ✔

(c) What is the value of the quantum number *l* for this orbital? (**1 mark**)

Since there are two angular nodes this corresponds to an *l* value of 2

(d) Below is the radial wave function and radial probability function plots. Taken with the angular wave function from part (b), what orbital does this describe? (**1 mark**)



Answer: 3d

(e) How many nodes does this orbital have? (**1 mark**)

Radial nodes = 0
Angular nodes = 2
Total nodes = 2

5. (**5 marks**) The first ionization potential and electron affinities of the atoms C, Ca, Cl, Cr and Cs are:

IP: 3.89, 6.11, 6.76, 11.26, 13.01 (eV)
EA: +1.62, -0.47, -0.66, -1.27, -3.61 (eV)

Although not necessarily in that order. Assign an IP and EA to each element. Explain your reasoning.

Answer:

½ mark for each correct assignment:

Cs at the bottom left of the PT should have the lowest IP (3.89 eV). In the left to right the others should be Ca, 6.11 eV; Cr, 6.76, C 11.26 eV; Cl, 13.01 eV.

For EA values, Cl with a p^5 configuration should have the highest value (-3.61 eV). The only positive (1.62 eV) value should apply to Ca (4s2), which must add a 4p or 3d electron. The other three values should lie in a left to right (increasing Zeff) order → Cs, -0.47; Cr, -0.66; C, -1.27 eV.

6. (**8 marks**) When the Schrödinger equation is solved for a hydrogen atom, three quantum numbers are obtained. What are the symbols and possible values for those quantum numbers? What is the symbol for the fourth quantum number and what are the allowed values?

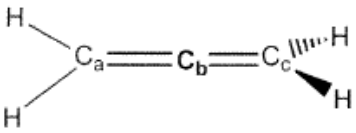
Answer:

Quantum Number	Possible Values
n	Integers beginning at 1
l	0, 1, 2,... n - 1
m_l	$-l$ ... 0 ... $+l$
m_s	_½ , +½

7. **(7 marks)** Consider the allene molecule, $H_2C=C=CH_2$. Draw the Lewis structure and answer the following questions:
   (a) Classify each bond as σ or π and identify the orbitals involved. (**5 marks**)
   (b) What is the H-C-C bond angle? What is the C-C-C bond angle? (**1 mark**)
   (c) Explain why the four H atoms cannot all lie in the same plane. (**1 mark**)

Answer:

a)

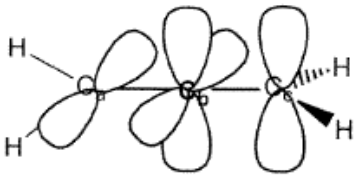


bond	classifcation?	orbitals involved?
H-C	σ ✔	$C(sp^2)$ – H(1s) ✔
$C_a=C_b$	σ ✔ + π ✔	σ: $C_a(sp^2)$-$C_c(sp)$ ✔ π: $C_a(2p_x)$-$C_c(2p_x)$ ✔
$C_b=C_c$	σ ✔ + π ✔	σ: $C_b(sp)$-$C_c(sp^2)$ ✔ π: $C_b(2p_y)$-$C_c(2p_y)$ ✔

The important point here is that C_b makes two π bonds using two different p orbitals that are perpendicular.

b) The H-C_a-C_b bond angle is 120° ✔ because C_a is sp^2-hybridized. The C_a-C_b-C_c bond angle is 180° ✔ because C_b is sp-hybridized.

c)



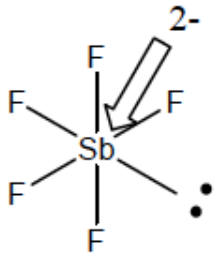
The diagram above shows the unhybridized 2p orbitals involved in forming the π bonds. In order for C_b to make two π bonds, the 2p orbitals of C_a and C_c must be at right angles. This forces the hybrid orbitals of C_a and C_c to lie in different planes and therefore the H's bonded to C_a lie in a different plane than those bonded to C_c.

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) SbF_5^{2-}

Lewis Structure:

Lewis: 7 × 5 + 5 + 2 = 42 valence electrons



3D Drawing:

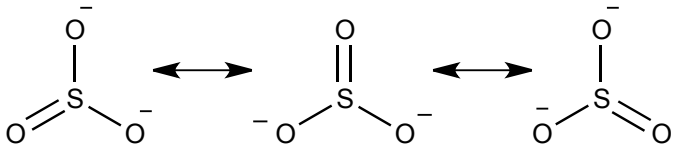
Geometry: _Octahedron _____ **Shape:** __square pyramid_____

Polarity: __Polar _____ **Hybridization**:____sp^3d^2_____

(b) SO_3^{2-}

Lewis Structure:

Lewis: 6 × 3 + 6 + 2 = 26 valence electrons

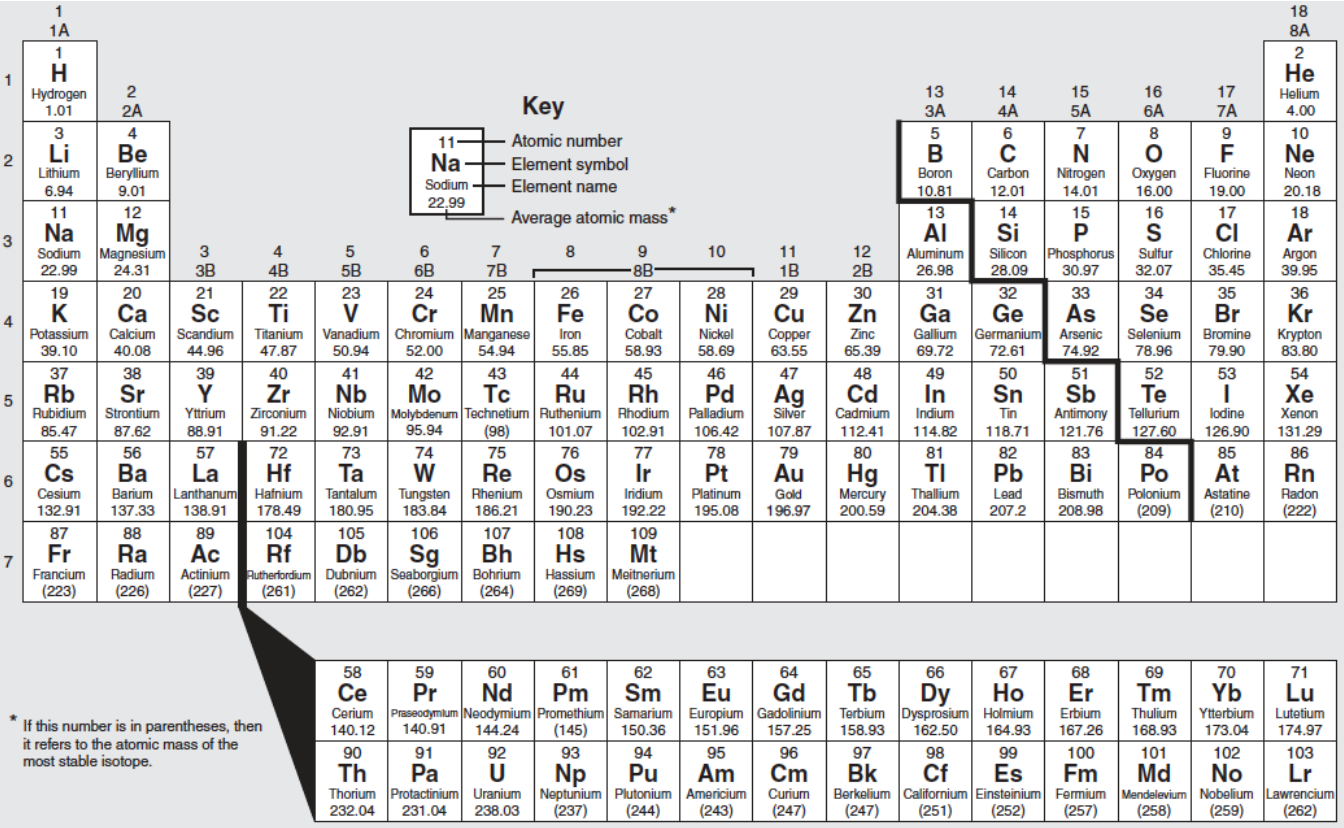


3D Drawing:

Geometry: ____Tetrahedral _____ **Shape:** _____Trigonal pyramidal_____

Polarity: ____Polar _____ **Hybridization**:__sp^3_____

DATASHEET



1 1A												13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1	1 H Hydrogen 1.01	2 2A															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	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	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)									

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)

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:

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

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

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

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

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

$h = m\nu\lambda$

$h = \lambda\rho$