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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.

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

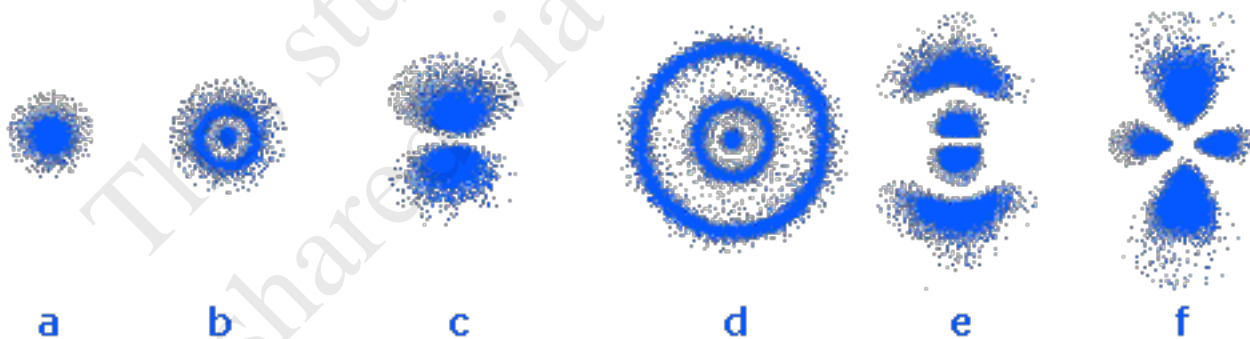
Longest wavelength: $n_1 = 6$; $n_2 = 5$

$$\begin{aligned} \lambda &= hc / \{ R_H [(1/n_2^2) - (1/n_1^2)] \} \\ &= hc / \{ R_H [(1/25) - (1/36)] \} \\ &= 7.46 \times 10^{-6} \text{ m} \end{aligned}$$

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

$$\begin{aligned} E &= hc/\lambda = R_H [(1/n_{\text{lower}}^2) - (1/n_{\text{higher}}^2)] \\ \lambda &= hc / \{ R_H [(1/n_2^2) - (1/n_1^2)] \} \\ &= hc / \{ R_H [(1) - (1/36)] \} \\ &= 93.8 \text{ nm} \end{aligned}$$

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

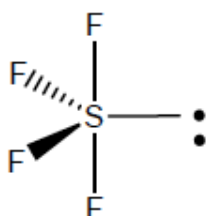
3. (a) Provide a detailed valence electronic configuration including the number of unpaired electrons for a sulphur atom. Is this atom paramagnetic or diamagnetic? (2 marks)
 (b) SF₄ is a stable compound. Using the valence electron configuration, provide a valence bond description (including hybridization) for the bonding in this compound. (3 marks)

Answer:

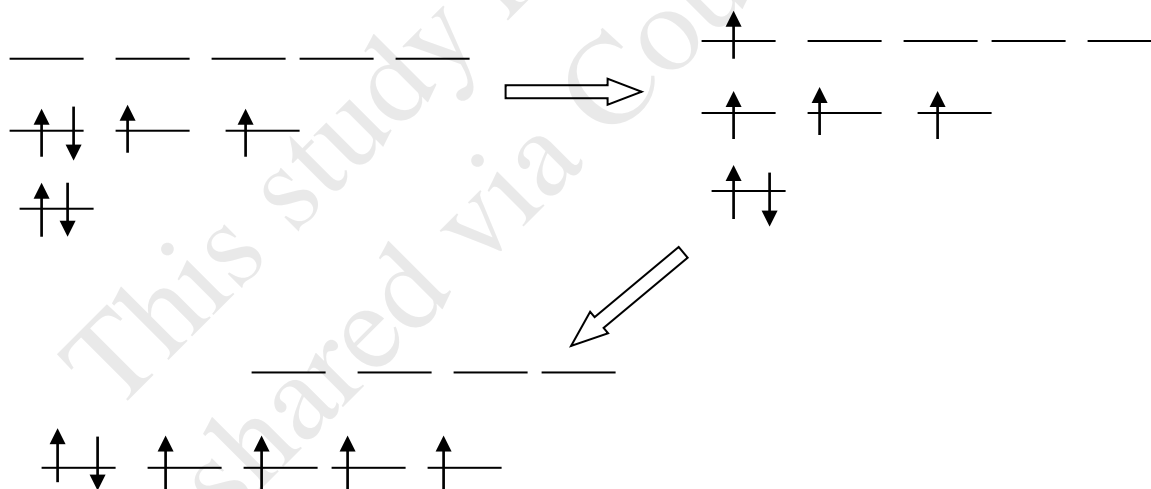
(a) [Ne] 3s²3p⁴ or 1s²2s²2p⁶3s²3p⁴

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 × sp³d 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:

$$x^2 - y^2 = 0 \quad ✓$$

$$x^2 = y^2 \quad ✓$$

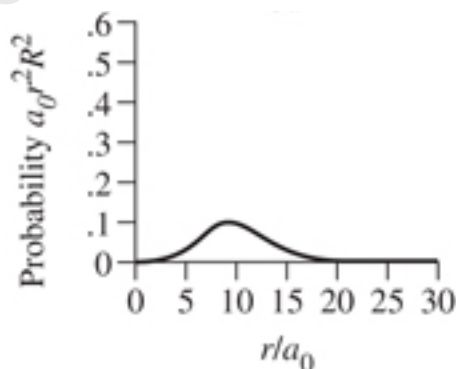
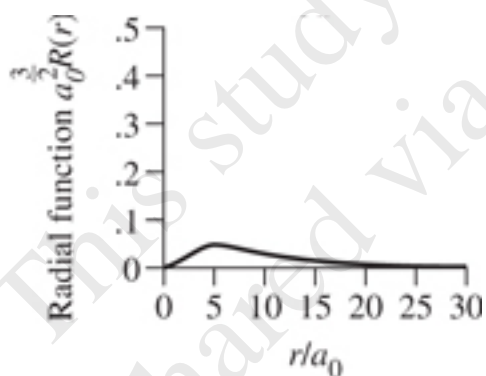
$$x = \pm y \quad ✓$$

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 Z_{eff}) order → Cs, -0.47; Cr, -0.66; C, -1.27 eV.

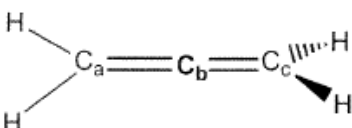
6. (8 marks) When the Schrödinger equation is solved for a hydrogen atom, three quantum numbers are obtained. What are the symbols and possible values for those quantum numbers? What is the symbol for the fourth quantum number and what are the allowed values?

Answer:

Quantum Number	Possible Values
n	Integers beginning at 1
l	0, 1, 2, ... $n - 1$
m_l	- l ... 0 ... $+l$
m_s	$-\frac{1}{2}, +\frac{1}{2}$

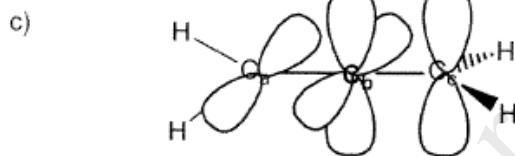
7. (7 marks) Consider the allene molecule, $\text{H}_2\text{C}=\text{C}=\text{CH}_2$. Draw the Lewis structure and answer the following questions:
- Classify each bond as σ or π and identify the orbitals involved. (5 marks)
 - What is the H-C-C bond angle? What is the C-C-C bond angle? (1 mark)
 - Explain why the four H atoms cannot all lie in the same plane. (1 mark)

Answer:

a)	bond	classification?	orbitals involved?
	H-C	σ ✓	$\text{C}(\text{sp}^2) - \text{H}(1\text{s})$ ✓
	$\text{C}_a=\text{C}_b$	$\sigma + \pi$ ✓ ✓	σ : $\text{C}_a(\text{sp}^2) - \text{C}_b(\text{sp})$ ✓ π : $\text{C}_a(2\text{p}_x) - \text{C}_b(2\text{p}_x)$ ✓
	$\text{C}_b=\text{C}_c$	$\sigma + \pi$ ✓ ✓	σ : $\text{C}_b(\text{sp}) - \text{C}_c(\text{sp}^2)$ ✓ π : $\text{C}_b(2\text{p}_y) - \text{C}_c(2\text{p}_y)$ ✓

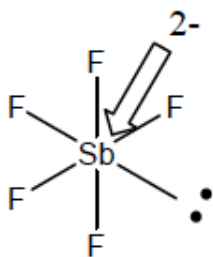
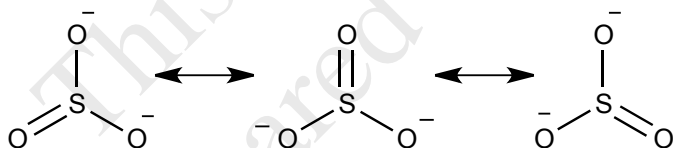
The important point here is that C_b makes two π bonds using two different p orbitals that are perpendicular.

- 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.



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

(a) SbF_5^{2-} **Lewis Structure:**Lewis: $7 \times 5 + 5 + 2 = 42$ valence electrons**3D Drawing:**Geometry: Octahedron Shape: square pyramidPolarity: Polar Hybridization: sp^3d^2 (b) SO_3^{2-} **Lewis Structure:**Lewis: $6 \times 3 + 6 + 2 = 26$ valence electrons**3D Drawing:**Geometry: Tetrahedral Shape: Trigonal pyramidalPolarity: Polar Hybridization: sp^3

DATASHEET

Key																																																																							
11	Atomic number	Na	Element symbol	Sodium	Element name	22.99	Average atomic mass*																																																																
1	1A	1	H	Hydrogen	1.01	2	2A	3	3B	4	4B	5	5B	6	6B	7	7B	8	8B	9	10	11	11B	12	12B	13	3A	14	4A	15	5A	16	6A	17	7A	18	8A	2	He	Helium	4.00																														
3	Li	Lithium	6.94	4	Be	Beryllium	9.01	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																																
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
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
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)
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	Mittherium	(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)				

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

Constants:

$$N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$$

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

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

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

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

$$\text{Bohr radius} (a_0) = 52.9 \text{ pm}$$

Conversion Factors:

$$1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2}$$

$$1 \text{ J} = 6.241 \times 10^8 \text{ eV}$$

Useful Equations:

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

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

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

The volume element is $r^2 \sin\theta d\theta d\phi dr$

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

$$h = mv\lambda$$

$$h = \lambda p$$