

Full Name: _____

Seat Number: _____

Student Number: _____

CHM 2311
Midterm 1
February 16, 2012
Professor Darrin Richeson

You have 80 minutes to complete this exam.

Please read the questions carefully.

There some useful equations and a periodic table on the last 2 pages of the exam.

Please write legibly and show your work to receive credit for your answers.

Partial marks may in some cases be awarded for partially correct work.

Question	Mark		Question	Mark
1	/ 10		6	/ 5
2	/ 8		7	/ 12
3	/ 5		8	/ 10
4	/ 3		9	/ 8
5	/ 5			
Total				/66

1. (10 points) In class, we worked on the one-dimensional particle in a box with infinite potential energy walls and length of a . In this problem our particle is an electron.

- What is the energy of the particle in the ground state?
- How much energy is required to excite this particle to its *second excited* state?
- Sketch ψ and ψ^2 for the second excited state (use the space provided below)
- What are the values of a for the maximum probability of finding the particle in the excited state?
- As this excited particle falls to the ground state, light with wavelength of 715 nm is emitted. What is the size of the box?

ψ



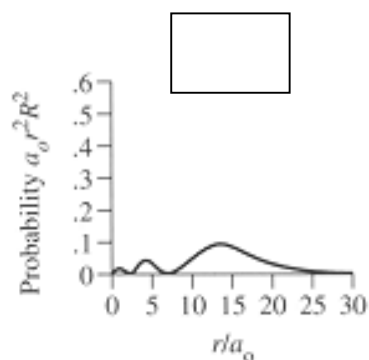
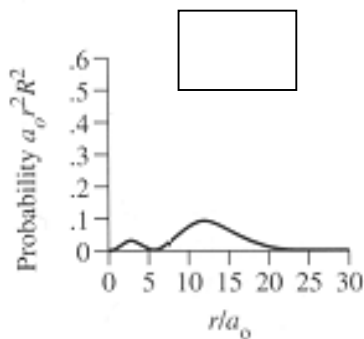
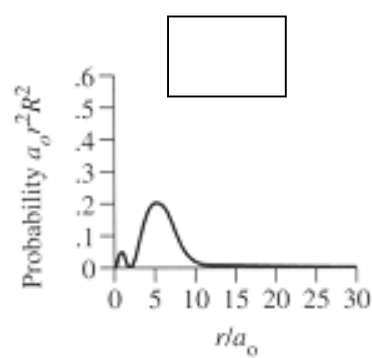
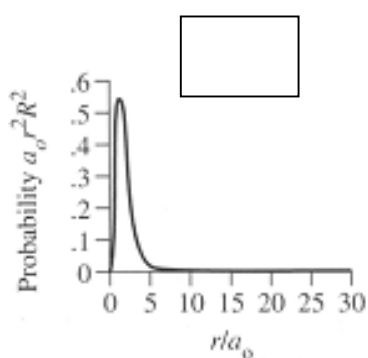
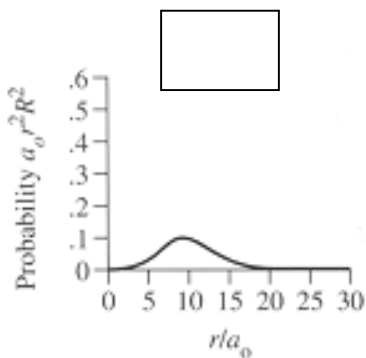
ψ^2



2. **(8 points)** When the Schrödinger equation is solved for a hydrogen atom, three quantum numbers are obtained. What are their symbols and possible values? What is the symbol and what are the allowed values for the fourth quantum number?

Quantum number	Possible Values

3. (5 points, no partial marks) The graphs show the radial probability for some selected orbitals. In the boxes provided next to each graph indicate which of the radial probability functions matches with the orbitals **1s**, **2s**, **3s**, **3p**, and **3d**.



4. (3 points) Calculate Z_{eff} for an electron in the 3d orbital of the Se atom.

5. **(5 points)** We learned in class and from the text that we can only distinguish between areas of high-probability and low-probability for the electron density. We can be sure of the location of zero-probability features of the orbitals.

(a) **(1 point)** Sketch the $4d(xy)$ orbital with clearly labeled axes and phases of each lobe.

(b) **(1 point)** How many angular nodes does the $4d(xy)$ have?

(c) **(1 point)** How many radial nodes does the $4d(xy)$ orbital have?

d) **(2 points)** Suggest very simple mathematical formulas for all of the angular nodes in the $4d(xy)$ orbital and describe the physical appearance (shape) of each node (e.g. planar or conical).

6. **(5 points)** (a) Provide a detailed valence electronic configuration including the number of unpaired electrons for a sulfur atom? Is this atom paramagnetic or diamagnetic?

(b) SF_4 is a stable compound. Using your answer in part (a), provide a valence bond description (including hybridization) for the bonding in this compound.

7. (12 points, 1/2 point per blank; *no partial credit*) For the following molecules:
Draw the Lewis structure
Determine the VSEPR shape and geometry of the molecule
Draw the three-dimensional representation of the molecule in the box provided
Determine whether the molecule is polar or non-polar
Give the hybridization of the central atom
Indicate any *non-zero formal charges* on every element where they occur.

(a). SbF_5^{2-}

3-D Drawing:



Geometry: _____

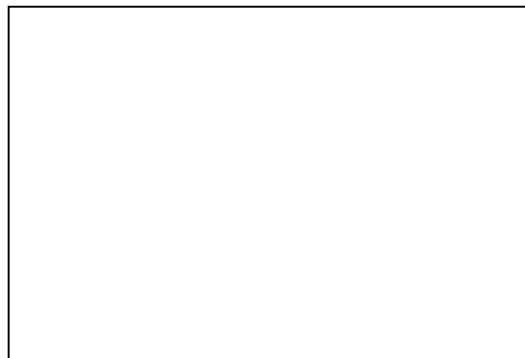
Shape: _____

Polarity: _____

Hybridization: _____

(b) SO_3^{2-}

3-D Drawing:



Geometry: _____

Shape: _____

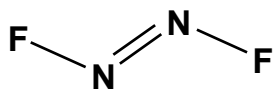
Polarity: _____

Hybridization: _____

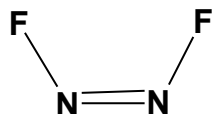
8. (10 points, 2 points each; *no partial credit*) For the following molecules or ions, indicate highest rotation axis and if there is a plane of reflection.

Example: BF_3 C_3, σ_h

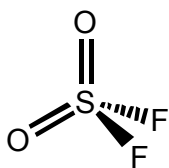
(a) *trans* - N_2F_2 (a) _____



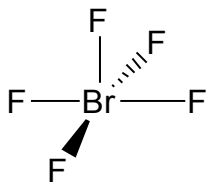
(b) *cis* - N_2F_2 (b) _____



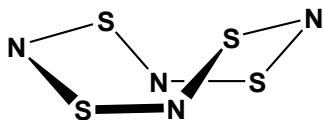
(c) (c) _____



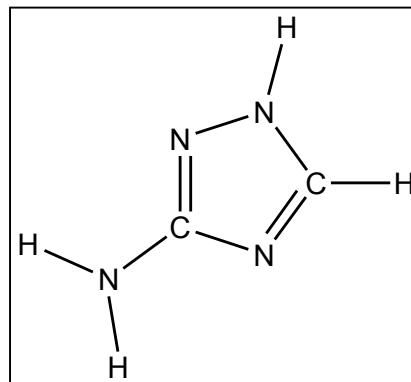
(d) (d) _____



(e) S_4N_4 (e) _____



9. **(8 points)** The diagram provides one representation of the Lewis structure of AtzH = 3-amino-1,2,4-triazole. The lone electron pairs are missing. Indicate the location of all of the lone electron pairs **(4 points)**.



(1 point) What are the hybridizations of the carbon atoms in this depiction?

(1 point) Based on this drawing, how many σ -bonds and the π -bonds on the molecule?

(2 points) Triazole is a stronger acid than phenol (C_6H_5OH) but weaker than acetic acid (CH_3COOH). A key rationale for these observations is given by the resonance structures for the anion of the deprotonated triazole. Draw a possible resonance structure of deprotonated triazole with appropriate formal charges.

Useful equations, constants, and conversion factors:

$$E = hc/\lambda \quad E = R_H \left(\frac{1}{n_l^2} - \frac{1}{n_h^2} \right) \quad E_{PIB} = \frac{n^2 h^2}{8ma^2} \quad \psi_{PIB} = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

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

$\psi(r, \theta, \phi) = R(r)Y(\Theta, \Phi)$ The volume element is $r^2 \sin\Theta d\Theta d\Phi dr$

Angular wave functions: $Y(\Theta, \Phi) = (1/4\pi)^{1/2} y(\Theta, \Phi)$

orbital	$y(\Theta, \Phi)$
S	1
Pz	$3\cos\Theta$
px, py	$(2/3)^{1/2} \sin\Theta e^{\pm i\phi}$
dz^2	$(5/4)^{1/2} (3\cos 2\Theta - 1)$
dyz, dxz	$(15/4)^{1/2} \sin\Theta \cos\Theta e^{\pm i\phi}$
$dx^2 - y^2, dxy$	$(15/8)^{1/2} \sin 2\Theta e^{\pm 2i\phi}$

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

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

$1 \text{ m} = 10^9 \text{ nm} = 10^{12} \text{ pm}$

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

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

Bohr radius (a_0) = 52.9 pm

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

