An Aggie does not lie, cheat or steal or tolerate those who do.

<table>
<thead>
<tr>
<th>Useful Formulas:</th>
<th>Useless Conversion Factors</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z_{\text{eff}} = Z - \sigma$</td>
<td>2000 mockingbirds: 2 kilomockingbirds</td>
</tr>
<tr>
<td>I.E. $= - \frac{Z_{\text{eff}}^2}{n^2}$</td>
<td>10 cards: 1 decacards</td>
</tr>
<tr>
<td>$2\sqrt{s (s + 1)}$</td>
<td>1 kilogram of falling figs: 1 Fig Newton</td>
</tr>
<tr>
<td>$2s + 1_L$</td>
<td></td>
</tr>
</tbody>
</table>
I. A. The Bohr atom: The diagram at right represents the electronic transitions in the energy emission spectra for a hydrogen atom or a hydrogen-like ion (He⁺ or Li²⁺).

a) Label the electronic transition that leads to the first excited state of H.

b) Label the ionization energy transition.

c) From the "useful formula" above, what is the value of the ionization energy of H?

\[ 13.6 \text{ eV} \]

d) Calculate the energy emitted when an electron falls from an \( n = \infty \) to an \( n = 2 \) level of the H atom (which series is this?)

\[ \frac{1}{4} \times 13.6 \text{ eV} = 3.4 \text{ eV} \]

Balmer Series

e) What is the value of the third ionization energy of Li (i.e., Li²⁺ → Li³⁺)?

\[ \frac{3^2}{1} \times 13.6 \text{ eV} = 122.4 \text{ eV} \]

B. What was the major success and the major failure of Bohr's model of the atom?

**Success:** H-like (1s⁻⁻ system) energy calculation

**Failure:** For not H-like atoms, Bohr's model fails for without considering e⁻e⁻ repulsion.

C. Match the scientist to his or her contribution to the modern day atom:

- **d** de Broglie
  a) \( E \psi = H \psi \)

- **a** Schrödinger
  b) No identical quantum numbers

- **c** Hund
  c) Ground State Configuration

- **b** Pauli
  d) \( mv = h/\lambda \)
II.
A. A plot of the radial function for a 3s orbital is given below. Superimpose the radial function for a 3d orbital. Point out the radial nodes for each.

B. A plot of the radial distribution for a 1s orbital is given below. Superimpose the radial distribution for a 2s orbital on this plot. Point out radial nodes for each.

C. On the xyz coordinate axes below, sketch the contours (the shapes) of the orbitals indicated. Give signs on the lobes.

a) $p_y$ orbital

b) $d_{yz}$ orbital

c) $d_{x^2-y^2}$ orbital

d) 4s (indicating radial nodes)
III. A. Give ground state electronic configurations of the following, using core notation [inert gas]nsnp. Using Slater’s rules, calculate Z_{eff} on the outermost electron for each.

a. Br \[\text{Br}^{+} 4s^{2} 3d^{10} 4p^{5}\]
\[Z_{eff} = 3.5 - (0.35 \times 6 + 0.85 \times 18 + 10 \times 1) = 7.6\]

b. Ti \[\text{Ti}^{+} 4s^{2} 3d^{3}\]
\[Z_{eff} = 3.2 - (0.35 \times 1 + 10 \times 0.85 + 10 \times 1) = 3.15\]

c. O\[\text{O}^{2-}\]
\[\text{Z}_{\text{eff}} = 8 - (0.35 \times 7 + 2 \times 0.85) = 3.85\]

d. Sb \[\text{Sb}^{+} 5s^{2} 4d^{10} 5p^{3}\]
\[\text{Z}_{\text{eff}} = 51 - (0.35 \times 4 + 18 \times 0.85 + 28 \times 1) = 6.3\]

B. 1.) Give the electronic configuration for iron in the following species, using core notation [inert gas]nsnp?

i) Fe\[\text{Fe}^{0}(\text{g}) \text{[Ar]} 4s^{2} 3d^{6}\]

ii) Fe\[\text{Fe}^{0}(\text{CO})_{5} \text{[Ar]} 3d^{8}\]

iii) Fe\[\text{Fe}^{II} \text{as in Fe(H}_{2}\text{O})_{6}^{2+} \text{[Ar]} 3d^{6}\]

iv) Fe\[\text{Fe}^{III} \text{as in FeCl}_{4}^{+} \text{[Ar]} 3d^{5}\]

2.) Fe^{III} may exist in three spin states. They are described as high spin, low spin and intermediate spin, each with a different number of unpaired electrons. Represent d orbitals in the box diagram manner, give the maximum Σm for each state and derive ground state term symbols for each. Calculate the spin-only magnetic moment for each.

<table>
<thead>
<tr>
<th>High spin</th>
<th>Term Symbols</th>
<th>(\mu_{\text{B.M.}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>[\text{Box diagram} \quad \begin{array}{c</td>
<td>c</td>
<td>c</td>
</tr>
<tr>
<td>Low spin</td>
<td>[\begin{array}{c</td>
<td>c</td>
</tr>
<tr>
<td>Intermediate spin</td>
<td>[\begin{array}{c</td>
<td>c</td>
</tr>
</tbody>
</table>
IV. Periodic Table Trends

A. Labels for the Y axes on the following graphics are missing. One is "first ionization energy" and one is "atomic radius". Place these labels on the appropriate graphic.

B. The following values were obtained from Webelements for the radius of oxygen in various forms: 0.48Å, 0.57Å, 0.63Å, and 1.52Å. Match the value to the specific type:

- Van der Waals radius (non-bonded contacts): 1.52 Å
- Atomic O: 0.62 Å
- Covalent double bond (as in O₂): 0.48 Å
- Covalent single bond (as in H₂O₂): 0.57 Å

C. Select the best choice according to the description:

a) Smallest radius: Sc, Ti, V
b) Largest radius: Na⁺, Ne, F⁻
c) Greatest Volume: S²⁻, Ar, Ca²⁺
d) Lowest ionization energy: K, Rb, Cs
e) Highest electron affinity: O, F, Ne
V. A. Give the Lewis structures for the following molecules or molecular ions; use VSEPR to predict their molecular geometry and give a drawing of that structure.

<table>
<thead>
<tr>
<th>Molecule or molecular ion</th>
<th>Lewis structure</th>
<th>Sketch the VSEPR/Molecular geometry with principal rotation axis, ( C_n ), indicated</th>
<th>Number of ( \sigma_v )'s. Inversion center? (yes or no)</th>
<th>Symmetry Point group</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH(_3)</td>
<td></td>
<td><img src="image" alt="NH3 Lewis Structure" /></td>
<td>3( \sigma_v )'s. No i</td>
<td>C(_{3v})</td>
</tr>
<tr>
<td>(example)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PF(_2)Cl(_3)</td>
<td><img src="image" alt="PF2Cl3 Lewis Structure" /></td>
<td>3( \sigma_v )'s. No i</td>
<td>D(<em>{3h}) (If write C(</em>{2h}), D(<em>{3h}), similar to D(</em>{3h}), give 1 point)</td>
<td></td>
</tr>
<tr>
<td>CO(_2)</td>
<td>( \overset{\infty}{C} = \overset{\infty}{O} )</td>
<td>( \overset{\infty}{C} = \overset{\infty}{C} = \overset{\infty}{O} )</td>
<td>( \infty) ( \sigma_v )'s. Yes</td>
<td>D(<em>{4h}) (If write C(</em>{2v}), C(<em>{2h}), C(</em>{3v}), similar to C(_{2v}), give 1 point)</td>
</tr>
<tr>
<td>ICl(_3)</td>
<td></td>
<td><img src="image" alt="ICl3 Lewis Structure" /></td>
<td>2( \sigma_v )'s. No i</td>
<td>C(<em>{2v}) (If write D(</em>{2h}), C(<em>{2h}), C(</em>{3v}), similar to C(_{2v}), give 1 point)</td>
</tr>
</tbody>
</table>

B. Circle the correct answer with respect to the BrF\(_5\) molecule (shown alongside):

I. The number of lone pair(s) on Br in BrF\(_5\): \( 0 \) 1 2 4
II. The point group of square pyramidal BrF\(_5\): O\(_h\) D\(_{4h}\) T\(_d\) C\(_{4v}\)
III. The number of C\(_2\) rotation axes in BrF\(_5\): \( 0 \) 1 2 4
IV. The number of mirror planes in BrF\(_5\): \( 0 \) 1 2 4
V. The highest order rotation axis in BrF\(_5\): \( 1 \) 2 4 5