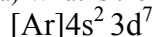


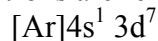
Solutions for Review Sheet for Final Exam

1) a) What is the electronic configuration of Cobalt, Co?



b) What is the electronic configuration of Cobalt, Co^{+1} ?

Electrons are removed from orbitals with the highest n , so we take one electron from the 4s orbital:

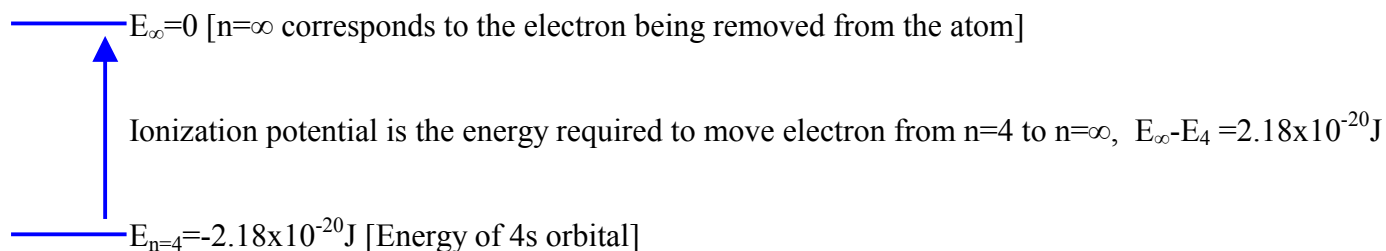


c) Using $Z_{\text{eff}}=0.4$, predict the ionization potential of Co.

The ionization potential is the energy required to remove an electron from the atom. As in part (b), we are taking the electron from the 4s orbital. We will use the Bohr model to determine the energy needed to remove the electron. In the Bohr model, the energy of the orbitals is given by

$$E_n = -[Z_{\text{eff}}^2/n^2] * R_h$$

where R_h is the Rydberg (2.18×10^{-18} J), n is the principle quantum number ($n=4$ for a 4s orbital), and $Z_{\text{eff}}=0.4$ from the problem statement. The ionization potential is the energy needed to take the electron from the 4s orbital [with energy $E_4 = -(0.4)^2/(4^2)(2.18 \times 10^{-18} \text{ J}) = -2.18 \times 10^{-20} \text{ J}$] to $n=\infty$ [with energy $E_\infty = -(0.4)^2/(\infty)^2 R_h = 0$].



Ionization potential is $2.18 \times 10^{-20} \text{ J}$

d) A photon with $\lambda=255 \text{ nm}$ ejects an electron from a Cobalt atom. What is the kinetic energy of the ejected electron?

The photon has an energy of $E = hc/\lambda = 7.79 \times 10^{-19} \text{ J}$. In part c, we found that it takes $2.18 \times 10^{-20} \text{ J}$ to eject an electron from the atom. This means that $7.79 \times 10^{-19} \text{ J} - 2.18 \times 10^{-20} \text{ J} = 7.57 \times 10^{-19} \text{ J}$ goes into the kinetic energy of the electron.

To be more explicit, we can use the relation

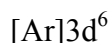
$$E_{\text{photon}} = E_{\text{bind}} + KE_{\text{electron}} \quad (\text{which says that the energy of the photon is used to eject the electron, } E_{\text{bind}}, \text{ with the remainder going into kinetic energy of the electron.})$$

The binding energy is the ionization potential of the atom ($2.18 \times 10^{-20} \text{ J}$), so

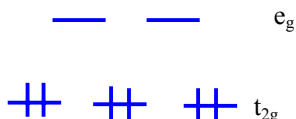
$$KE_{\text{electron}} = E_{\text{photon}} - E_{\text{bind}} = 7.79 \times 10^{-19} \text{ J} - 2.18 \times 10^{-20} \text{ J} = 7.57 \times 10^{-19} \text{ J}.$$

e) What is the electronic configuration of Co^{+3} ?

We need to remove 3 electrons from Cobalt. We first remove two electrons from the 4s orbital and then one from the 3d orbitals. This leads to:

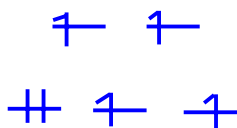


f) Sketch the d-orbitals and electron occupations for $\text{Co}^{+3}(\text{NH}_3)_6$.



This is an octahedral complex, so the orbitals are as shown. Since Co is in the 3d row of the transition metals, we need to look at the spectrochemical series to see if it will go high spin or low spin. Since NH_3 is on the low spin side of the series, the electrons fill as shown.

g) Sketch the d-orbitals and electron occupations for $\text{Co}^{+3}(\text{OH}_2)_6$. If $\text{Co}^{+3}(\text{OH}_2)_6$ is red, what is the splitting (in kJ/mol) between the d-orbitals (Δ_o)?



Just as in part f, this is an octahedral complex. But here, OH_2 is on the high spin side of the spectrochemical series, so the electrons fill as shown.

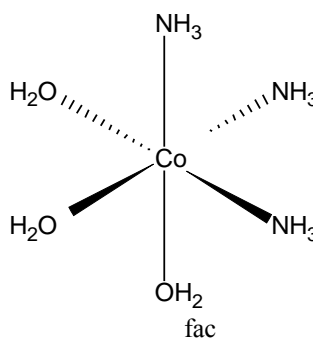
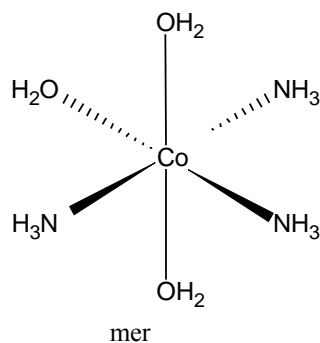
If the molecule is red, then it absorbs green photons, which have $\lambda=520\text{nm}$. The splitting then corresponds to the energy of a green photon, which is $E=hc/\lambda = (6.626076 \times 10^{-34} \text{ J s})(2.99792458 \times 10^8 \text{ m s}^{-1})/(520 \times 10^{-9} \text{ m}) = 3.82 \times 10^{-19} \text{ J}$. To convert to kJ/mol:

$$3.82 \times 10^{-19} \text{ J} (1 \text{ kJ}/1000 \text{ J}) (6.022 \times 10^{23} / \text{mol}) = 230 \text{ kJ/mol}$$

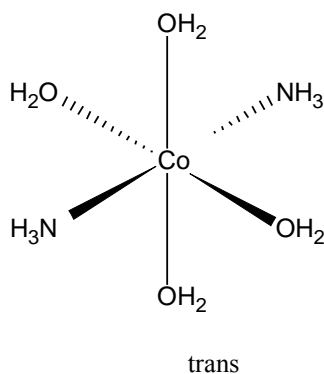
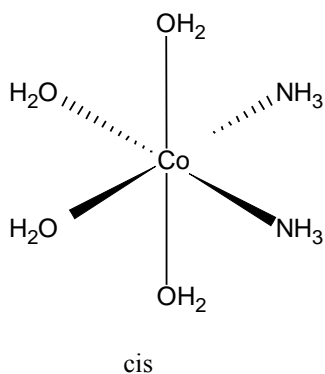
h) Are either $\text{Co}^{+3}(\text{NH}_3)_6$ or $\text{Co}^{+3}(\text{OH}_2)_6$ paramagnetic?

Since $\text{Co}^{+3}(\text{OH}_2)_6$ has unpaired electrons, it is paramagnetic.

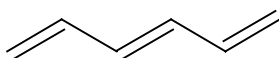
i) Draw all isomers of $\text{Co}^{+3}(\text{NH}_3)_3(\text{OH}_2)_3$.



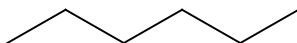
j) Draw all isomers of $\text{Co}^{+3}(\text{NH}_3)_2(\text{OH}_2)_4$.



2) a) Consider the molecules

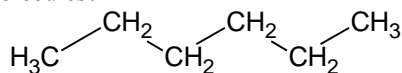
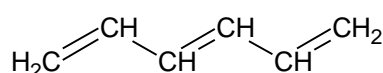


hexatriene



hexane

a) What is the molecular formula of each of these molecules?





b) What is the hybridization of each of the carbon atoms?

hexatriene: all carbons are sp^2 hybridized

hexane: all carbons are sp^3 hybridized

c) Does hexatriene have a dipole moment? Does hexane have a dipole moment?

Neither has a dipole moment.

d) When placed next to a Sodium ion (Na^+), which would have a larger induced dipole moment, hexatriene or hexane?

The pi molecular orbitals in the hexatriene make it more polarizable than hexane. So the charge on the Na^+ will induce a larger dipole moment in hexatriene than in hexane.

e) Which would have larger dispersion interactions, two hexatriene molecules or two hexane molecules?

Dispersion interactions are larger between molecules with larger polarizability, so dispersion will be larger for two hexatriene molecules.

f) Is hexatriene hydrophobic or hydrophilic? Which would be more hydrophobic hexatriene or hexane?

Both of the molecules are hydrophobic, but hexane is more hydrophobic than hexatriene. [Since hexatriene is more polarizable, it will have a larger (dipole)-(induced dipole) interaction with water and so like water more than hexane.]

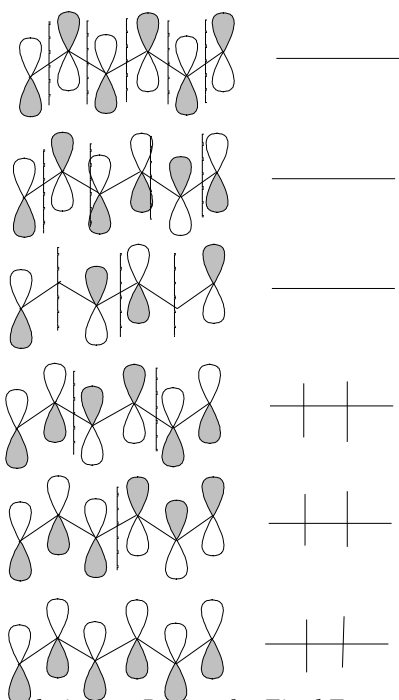
g) Which of the following would be a better solvent for hexane: water, acetone ($(CH_3)_2C=O$) or ethyl ether ($CH_3CH_2OCH_2CH_3$)?

Both water and acetone are polar (i.e. have dipole moments). Ethyl ether doesn't have dipole, so it is non-polar. Since hexane is hydrophobic, it likes non-polar solvents, so ethyl ether is a good solvent for hexane.

h) How many pi molecular orbitals are there for hexatriene? How many of these orbitals are filled?

Each of the 6 sp^2 hybridized carbon atoms contributes one p_z orbital to the pi orbitals. These 6 p_z orbitals lead to 6 pi molecular orbitals. Each of the six carbon atoms contributes one electron to the pi orbitals, so there are 6 electrons. This is enough to fill 3 of the orbitals. So there are 6 pi molecular orbitals, and 3 are filled.

i) Sketch the highest occupied molecular orbital and lowest unoccupied molecular orbitals for this molecule.



The number of nodes increases from zero to five as we go from the lowest to the highest pi molecular orbital. These nodes are roughly evenly spaced. The highest filled orbital has two nodes and the lowest unfilled orbital has three nodes (to make three evenly spaced nodes, two of the nodes have to nearly pass through carbon atoms, as drawn on the left).

j) A photon with $\lambda=350\text{nm}$ can promote an electron from the high occupied molecular orbital to the lowest unoccupied molecular orbital. What is the different in energy between these orbitals (in kJ/mol)?

This photon is able to promote an electron between these orbitals, so the energy of the photon is equal to the energy difference between these orbitals. The energy of the photon is:

$$E=hc/\lambda = (6.626076 \times 10^{-34} \text{ J s})(2.99792458 \times 10^8 \text{ m s}^{-1}) / (350 \times 10^{-9} \text{ m}) = 5.67 \times 10^{-19} \text{ J}$$

to convert to kJ/mol:

$$5.67 \times 10^{-19} \text{ J} (1 \text{ kJ}/1000 \text{ J}) (6.022 \times 10^{23} / \text{mol}) = 342 \text{ kJ/mol}$$

k) Suppose we wanted to model this system as a particle in a box. In this model, a photon with $\lambda=350\text{nm}$ promotes the particle from the $n=3$ to $n=4$ level. What must the energy difference be between the $n=3$ and $n=4$ levels ($E_{n=4}-E_{n=3}$) for a transition between these levels to arise from a photon with $\lambda=350\text{nm}$? Lets assume the particle is in a 12Angstrom box. What must the mass of the particle be to obtain this value for ($E_{n=4}-E_{n=3}$)?

From part j, we have that the energy of a photon with $\lambda=350\text{nm}$ is $5.67 \times 10^{-19} \text{ J}$. For a particle in a box, the energy levels are given by:

$$E_n = h^2 n^2 / (8 m L^2)$$

The box length is $L=12\text{Angstroms}$ or $12 \times 10^{-10} \text{ m}$. We want to know the mass the particle must have for

$$E_4 - E_3 = 5.67 \times 10^{-19} \text{ J}$$

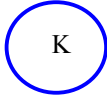

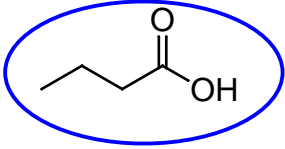
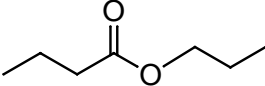
or

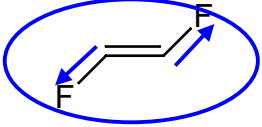
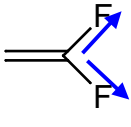
$$E_4 - E_3 = h^2 4^2 / (8 m L^2) - h^2 3^2 / (8 m L^2) = h^2 (4^2 - 3^2) / (8 m L^2) = 5.67 \times 10^{-19} \text{ J}$$

or

$$\begin{aligned} m &= h^2 (16-9) / [(5.67 \times 10^{-19} \text{ J})(8 L^2)] \\ &= (6.626076 \times 10^{-34} \text{ J s})^2 (16-9) / [(5.67 \times 10^{-19} \text{ J})(8 (12 \times 10^{-10} \text{ m})^2)] \\ &= 4.70 \times 10^{-31} \text{ kg} \quad (\text{or } 0.516 \text{ times the mass of an electron}) \end{aligned}$$

3) Circle the best answer to the following statements.

Lower Ionization Energy		Ca	K and Ca are in the same row of the periodic table with Ca to the right of K. Ionization energies increase as you go across the periodic table. (Electron sees larger effective nuclear charge Z_{eff})
Greater solubility in acetone, 			The oxygen of acetone is a hydrogen bond acceptor, and the OH on the first molecule can donate a hydrogen bond; so it will interact better with acetone than the second molecule.

Higher Electron Affinity	Br	Cl	Electron affinity gets smaller as you go down the periodic table.
Higher boiling point	CH ₃ NH ₂	CH ₃ CH ₂ CH ₂ CH ₂ NH ₂	larger molecule will have higher boiling point.
Smaller atomic radius	S	Te	Atomic radius increases as you go down the periodic table
Larger bond dipole	CO	NO	There is a larger difference in electronegativity between C and O than between N and O.
Oxidation state of Mn in MnO ₂	+II	+IV	Each of the oxygens has a -2 oxidation number, so Mn will have +4 for the oxidation numbers to add to zero.
Hybridization of N in NH ₃	sp ²	sp ³	In the lewis dot structure, the nitrogen has a lone pair. This lone pair plus the three hydrogen atoms leads to a coordinate number of 4, or sp ³ hybridization.
Nonpolar molecule			The bond dipoles cancel in the first molecule, making it a nonpolar molecule.