Solutions to Individual Round #1: Chemical Structures & Properties

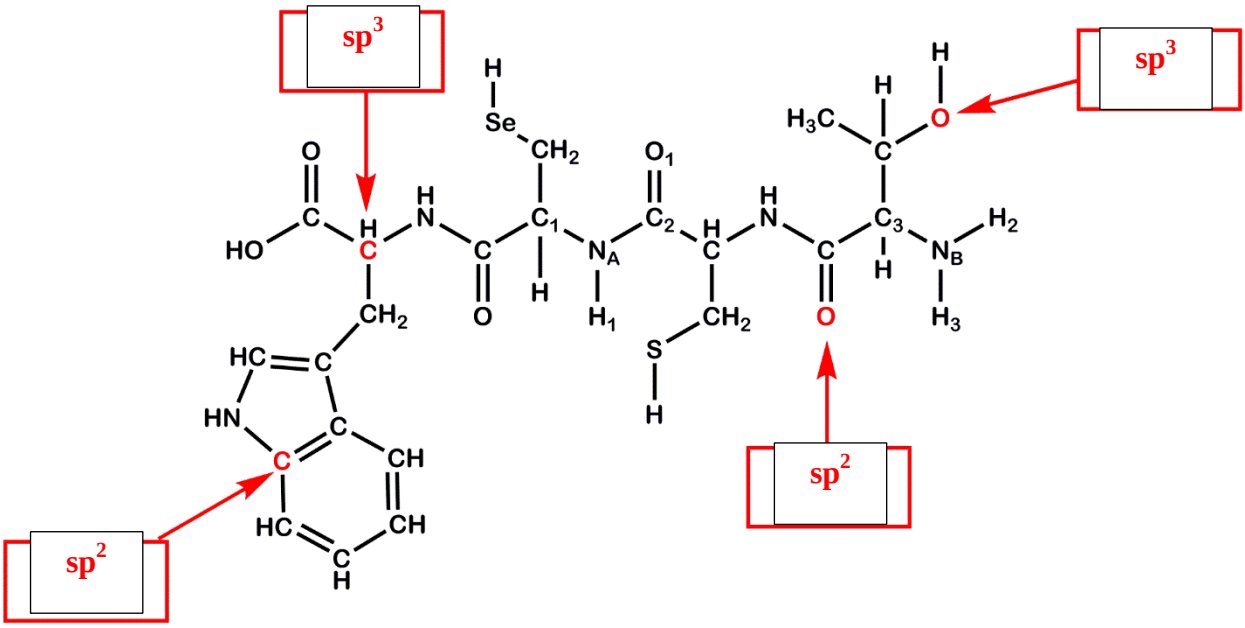
1) Compound X consists solely of carbon, hydrogen, and oxygen atoms. The composition of compound X is 40.92 % C, 54.50 % O, and 4.58 % H. Suppose we prepared a solution with 36.33 g of the solute and 1 kg of phenol, an organic solvent. We measured the freezing point of the solution to be 41.5^{o}C. What are the molar mass (in g/mol) and molecular formula of compound X, given the freezing point of phenol is 43^{o}C and $k_f = 7.27\ \frac{K*kg}{mol}$, where k_f is the molal freezing point depression constant? Assume that compound X does not dissociate in phenol.

Assume a 100 g sample of Compound X. This molecular formula would be $C_{3.41}H_{4.54}O_{3.41}$. This simplifies to an empirical formula $C_3H_4O_3$.

$\Delta T_f = k_f$ * molality
1.5 K = 7.27 (K*kg/mol) * molality
Molality = 0.2063 = (moles solute) / 1 kg phenol
There are 0.2063 moles of solute.
36.33 g solute / 0.2063 moles of solute = 176.10 g/mol

Molecular Formula: $C_6H_8O_6$

2) For the following series of questions, consider the following peptide. Note: both alpha and numeric subscripts are used for particular atoms to distinguish atoms of the same element.



a) 4 of the atoms shown in red in the molecule above have arrows pointing at them. In the red boxes connected to the arrow, write the hybridization of that atom (*e.g.*, sp).

Hybridizations are labelled on diagram.

b) **i)** What is the hybridization of N_B if the surrounding atoms are not in the same plane?

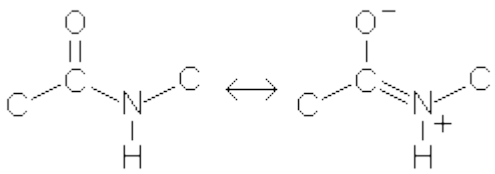
ii) Despite the fact that N_A is also surrounded by 3 atoms, it is known that C1, C2, N_A, and H1 reside in the same plane. Given this, what is the hybridization of N_A?

N_A is sp^2 hybridized, and N_B is sp^3 hybridized.

c) Given the connectivity of N_A to its surrounding atoms, give a resonance structure to explain the hybridization.

N_A is situated adjacent to a double bond (C=O). In this circumstance, the nitrogen atom does not adopt a sp3 configuration as one may first expect, but instead adopts a sp2 configuration with trigonal planar geometry. The result is that the lone pair of electrons exists in a p-orbital that is parallel to the adjacent bond. The pi bond is delocalized (one can see this in the resonance structure shown below), resulting in added stability.

Washington University in St. Louis Chemistry Tournament
Sample Problem Solutions for Individual Round #1: Chemical Structures & Properties



3) In a multi-electron atom, no electron ever experiences the full positive charge from its nucleus, due to a phenomenon known as "shielding." The effective nuclear charge (Z*) experienced by a particular electron is defined as Z* = Z – S, where S is equal to the shielding coefficient (S), and Z is equal to the atomic number.

Slater's rules for determining the value of the shielding coefficient, S, for any electron are as follows (adapted from Introductory Chemistry website of Oklahoma State University, http://intro.chem.okstate.edu/WorkshopFolder/SlaterRule.html):

1) Write the electron configuration for the atom and group the electrons using the following design:
   (1s)(2s, 2p)(3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p)
2) Any electrons in groups to the right of the electron of interest contribute essentially no shielding.
3) All other electrons in the same group as the electron of interest shield to an extent of 0.35 nuclear charge units.
4) If the electron of interest is an s or p electron: All electrons with one less value of the principal quantum number shield to an extent of 0.85 units of nuclear charge. All electrons with two less values of the principal quantum number shield to an extent of 1.00 units.
5) If the electron of interest is a d or f electron: All electrons in groups to the left shield to an extent of 1.00 units of nuclear charge.
6) Sum the shielding amounts from steps 2 through 5 and subtract from the nuclear charge value to obtain the effective nuclear charge.

Use these given rules to answer the following questions.

a) Calculate Z* for an outermost electron of a ground-state chlorine atom.

Electronic configuration of chlorine: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

S = (6 * 0.35) + (8 * 0.85) + (2 * 1.00) = 10.9

Z* = 17 – 10.9 = 6.10

b) Calculate Z* for an outermost electron of a ground-state phosphorus atom.

Electronic configuration of phosphorus: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

S = (4 * 0.35) + (8 * 0.85) + (2 * 1.00) = 10.2

Z* = 15 – 10.2 = 4.80

c) Answer the following questions and provide justification.

i. Using periodic trends, predict the difference in ionization energy between these two atoms and provide justification.

Chlorine has higher ionization energy than phosphorus, because it lies to the right of chlorine, and within a period, ionization increases with increasing atomic number.

ii. Do these values from parts (a) and (b) explain the difference in ionization energy between chlorine and phosphorus atoms? If you did not obtain answers to parts (a) or (b), you can use the values 30.5 and 20.4, respectively, for partial credit.

Yes. The outermost electron of a chlorine atom experiences a larger Z* than that of a phosphorus atom. Because they are in the same orbital, they are at similar distances from the nucleus. This means that the electrostatic attractive force on the chlorine electron will be greater, so it will be harder to ionize it.

d) An orbital is particularly stable if the number of electrons in the orbital is half of the maximum that can be in that orbital. Given this information, calculate the shielding coefficient, S, for a 3d electron in a ground-state chromium atom.

Electronic configuration of chromium: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$

$S = (4 * 0.35) + (18 * 1.00) = 19.40$