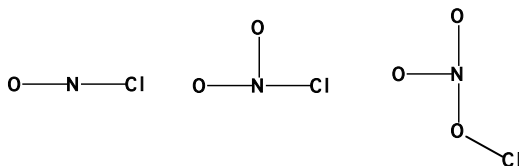


CHEM 101: PROBLEM SET #8

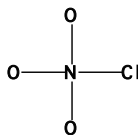
Due: Wednesday, November 14, 2007 by 11 AM.

Turn in to the Chem 101 box at the beginning of lecture or if you want to turn it in early, the box will be in Kathy Kennedy's office, the Chemistry Department secretary (Chem 303).

- The 20 amino acids can be identified with either a 3-letter code or a 1-letter code. These codes can be used to designate the primary structure or amino acid sequence of a peptide, typically written in order from the N-terminus (the end containing the $-\text{NH}_3^+$ group) to the C-terminus (the end containing the $-\text{CO}_2^-$ group). Consider the tetrapeptide constructed from condensation reactions of the following four amino acids (in order): arginine—glutamate—glutamate—aspartate. Using the 3-letter codes, this peptide would be abbreviated: Arg-Glu-Glu-Asp. With the 1-letter codes however, the abbreviation is REED.
 - Draw the *Lewis structures* (show all atoms and draw complete octets) for each of the 3 amino acids arginine, glutamate, and aspartate in their zwitterionic form including any resonance structures. Be sure to indicate any nonzero formal charges. If you are missing the handout from Maggie's lecture on the structures of the 20 amino acids, it can be found on the Chem 101 website (look under News). Also note that glutamate is not the same as glutamine.
 - Now consider the formation of the tetrapeptide REED. Three water molecules are lost when these amino acids undergo a condensation reaction to form the tetrapeptide. Draw the structure of the resulting tetrapeptide.
- The structures of NOCl , NO_2Cl and NO_3Cl were determined in 1995 and may play a role in atmospheric chemistry. Given the skeleton structures below, complete the Lewis structures for these molecules, including nonzero formal charges and resonance structures, if appropriate.



Explain why NO_3Cl does not have the skeleton structure shown below.



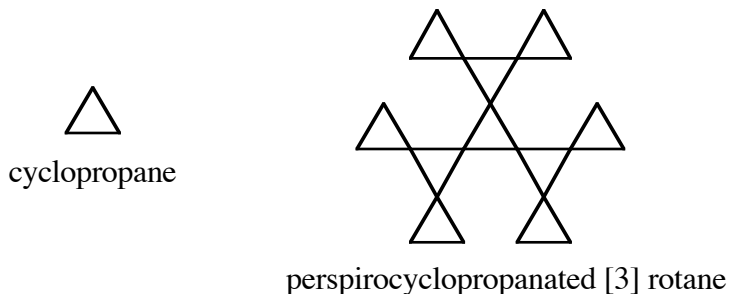
- Consider valence bond pictures for the following hydrocarbons:



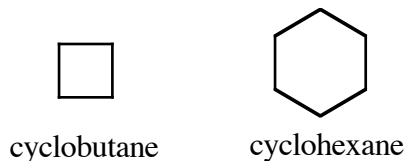
- Are these molecules isomers or resonance structures? Explain.
- For each structure, identify the hybridization scheme at each carbon atom.
- How many total σ -bonds are there in each of these molecules? How many π -bonds are there?
- Can either of these structures exhibit cis- and trans- isomers? Explain and draw the two isomers if they can exist.
- According to considerations of maximum orbital overlap, how many atoms must lie in the same plane for each of these structures? Explain. *Note:* Please include orbital overlap pictures in your explanation and be sure these convey three-dimensional perspectives of the molecules.

MORE ON THE BACK

4. Three-membered rings of atoms generally do not form due to excessive amounts of *strain energy*. One book defines the concept of strain energy in the following way: “If the ideal bond angle about a carbon atom in a particular hybridization state is deformed, a *strain* is produced that significantly raises the energy content of the molecule.”
- (a) Cyclopropane is a classic example of an organic molecule with considerable strain energy, and the molecule shown on the right (this bond line structure does not do justice to the real 3-dimensional structure) should have an enormous amount of strain energy. Yet, surprisingly, the molecule on the right has a melting point of over 200°C (go figure!). Explain why the strain energy should be so high in these molecules.



- (b) Consider the cyclobutane molecule. Would you expect all four carbon atoms to lie in the same plane? Would you expect the strain energy per carbon atom in cyclobutane to be greater than or less than the strain energy per carbon atom in cyclopropane? Explain.



- (c) The ring in cyclohexane is not considered to be strained. Give a possible reason why. Suggestion: you might invest in some gumdrops and toothpicks and build some test models.
5. (a) Draw a Lewis structure for the urea molecule $\text{CO}(\text{NH}_2)_2$ with no formal charges on any of the atoms.
- (b) Based on your Lewis structure from part (a), predict the electronic geometry around each of the central atoms and draw the valence bond picture for urea showing well-labeled and overlapping orbitals. I would suggest using a different color for drawing hybrid orbitals vs. leftover *p* orbitals.
- (c) Now draw a valid Lewis structure for urea that places nonzero formal charges on some of the atoms.
- (d) Revise your valence bond picture to agree with the Lewis structure you drew in part (c).
- (e) Experimentally, the urea molecule is found to be planar (*all atoms lie in a single plane*) and all the bond angles are 120° . Draw a single valence bond picture that agrees with this experimental information.