Lecture 1: Molecular Structure
Discussion Section Problems Solutions

1. Structure Flaw Corrected Structure

(a) 

\[ \text{Implies C-N-H-C bonding} \]

\[ \text{Ten electrons on oxygen} \]

This structure is not a good answer. While it does not have ten electrons on oxygen, it has very high ring strain because of the C=O=C moiety. In addition, oxygen (and other elements in the northeast corner of the periodic table) almost never have a +2 or −2 formal charge.

(b) 

\[ \text{When carbon is shown as "C" all other attachments must be specified.} \]

\[ \text{"Stick" = CH}_3, \text{ Not an error but not very clear either, if a methyl is really here.} \]

\[ \text{Appears to be floating above ring; not attached} \]

Other correct representations may be possible in each case.

2. C_{47}H_{51}NO_{14} When writing the formula of an organic compound, list carbons, then hydrogens, then all other elements in alphabetical order.

3. (a) 29 lone pairs (see top of next page).
(b) 51 atoms that do not have eight valence shell electrons (i.e., the hydrogens)

(c) 30 (ignoring conjugation) or 25 (including conjugation, so this is a better answer). We'll discuss conjugation in lectures 3 and 4.
(d) 32 (ignoring ester and amide conjugation) or 37 (including ester and amide conjugation).

(e) 0 (no triple bonds in this molecule).

(f) 51 (only the hydrogen atoms are not hybridized).

(g) 16 (three in each of three benzene rings, one alkene and six carbonyls).

4. Benzene ring (three), amide (one), ester (four), alcohol (three), alkene (one), ketone (one) and ether (one).

**Does One Functional Group Contain Another Functional Group?**

We do not say that one functional group contains a simpler functional group. For example we do not say that a benzene ring contains three alkenes, and we do not say that a carboxylic acid contains an alcohol. However, because a benzene ring and an alkene both have carbon-carbon pi bond electrons, we do expect some similarity in the properties of these functional groups. Likewise, because carboxylic acids and alcohols both contain a hydroxyl group (OH) these functional groups will share some properties as well.

5. The most polar bond has the atoms with the largest electronegativity difference. Of the atoms in paclitaxel, oxygen (EN = 3.5) and hydrogen (EN = 2.1) meet this requirement. Thus the O–H bond is predicted to be the most polar.

6. (a) The carbons of a benzene ring are trigonal planar, and all the C–C–C bond angles are very close to 120°.
(b) An oxygen atom with four electron groups (one hydrogen atom, one R, and two lone pairs) is approximately tetrahedral, so our first guess at the bond angle is approximately 109.5°. In this case it is not obvious which should have greater repulsion: two lone pairs (which gives a C–O–H bond angle a bit less than 109.5°) or the H/R repulsion (which gives a C–O–H bond angles of a bit more than 109.5°). Your exact answer, therefore, depends upon which repulsion you assume to be larger. Computer models give a C–O–H bond angle of about 107°, suggesting that the R/H repulsion is weaker than lone pair/lone pair repulsion in this case.

(c) The analysis for this bond angle is very much like part (b) of this question. The carbon bearing the two methyl groups has four electron groups: the two methyl groups and the two sides of the ring. If we make the reasonable assumption that the methyl groups are smaller than the other groups, then the methyl–C–methyl bond is predicted to be less than 109.5°. Computer modeling gives the bond angle as about 108°, suggesting that our assumption is accurate.

7. (a) Only the staggered conformations can be the most stable. There are three of these, as shown below. Ph = phenyl = benzene ring with a single substituent (i.e., a single attachment that is not a hydrogen).

(b) This is the most stable conformation of this molecule because it has the least number of significant gauche repulsions.

8. First we need to draw 2–isopropyl–5–methylecyclohexanol. An alcohol has more priority than an alkyl group (such as methyl or isopropyl), so the cyclohexane ring numbering starts at the carbon bearing the OH group.

A cyclohexyl substituent experiences less torsional strain in the equatorial position than in the axial position. Therefore the most stable isomer of this molecule has all three substituents in the equatorial position.
The enantiomer of this structure can also be shown. (Enantiomers will be covered when we discuss stereochemistry in a week or two.)