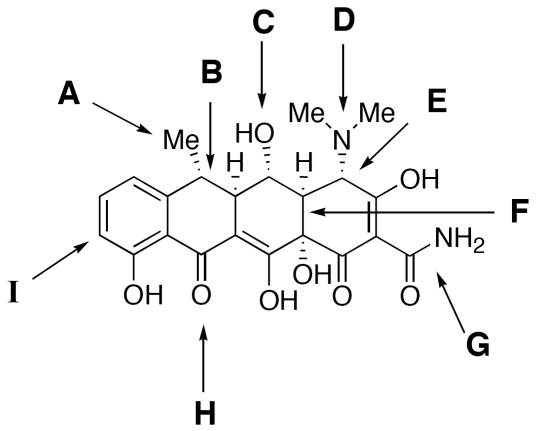
Name:_____ April 13, 2011

PEERS Workshop
Chemistry 30A
Worksheet 4

1. (9) Answer questions A-I below relative to the structure of Doxycycline (a common antibiotic agent). The lettered arrows in the structure refer to the questions.



A. (1) What orbitals does this carbon atom use for bonding? _____**sp3**_____

B. (1) What type of carbon (primary, etc) is this carbon atom? _____**Tertiary**_____

C. (1) What is the name of this functional group? _____**Alcohol**_____

D. (1) What is the name of this functional group? _____ **Amine** _____

E. (1) What is the chirality (R or S) at this position? _____**S**_____

F. (1) What is the geometric descriptor for this ring fusion? _____ **CIS** _____

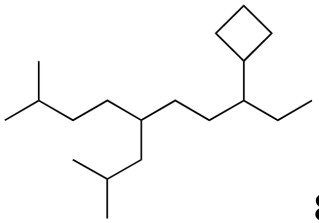
G. (1) What is the name of this functional group? _____ **Amide** _____

H. (1) What is the name of this functional group? _____ **Ketone** _____

I. (1) What orbitals does this carbon atom use for bonding? _____ **sp2 and p**_____

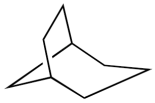
2. (28)

A. (4) Name the following compound using IUPAC rules.



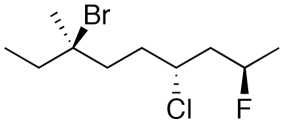
8-cyclobutyl-2-methyl-5-(2-methylpropyl)decane

B. (4) Name the following compound using IUPAC rules.



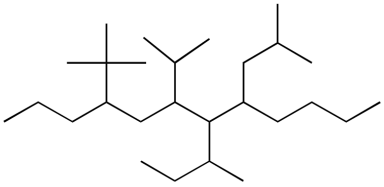
bicyclo[3.2.1]octane

C. (4) Name the following compound using IUPAC rules.

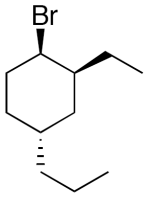


(2R, 4R, 7R)-7-bromo-4-chloro-2-fluoro-7-methylnonane

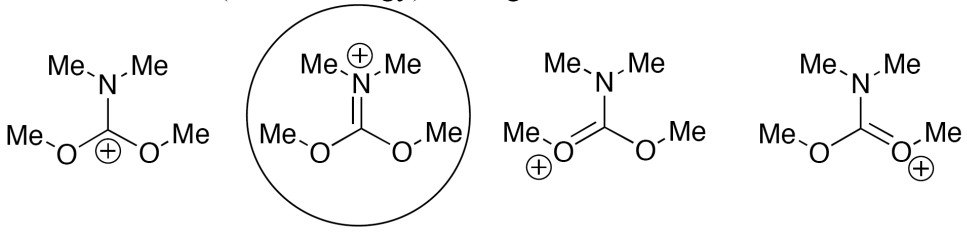
D. (4) Draw the structure of 4-tert-butyl-7-sec-butyl-8-isobutyl-6-isopropyldodecane.



E. (4) Draw the structure of (1R, 2S, 4R)-1-bromo-2-ethyl-4-propylcyclohexane.

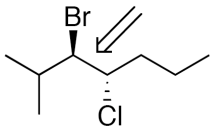


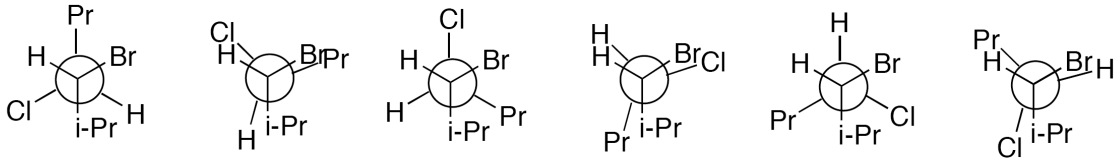
G. (8) Draw THREE more resonance structures for the following cation and CIRCLE the "best resonance contributor" (lowest energy) among the four structures.



3. (22)

A. (12) Draw **SIX** Newman Projections for rotation looking down the 3-4 bond indicated in the following molecule. **LABEL** the staggered conformations A, B, and C. **LABEL** the eclipsed conformations X, Y, and Z.



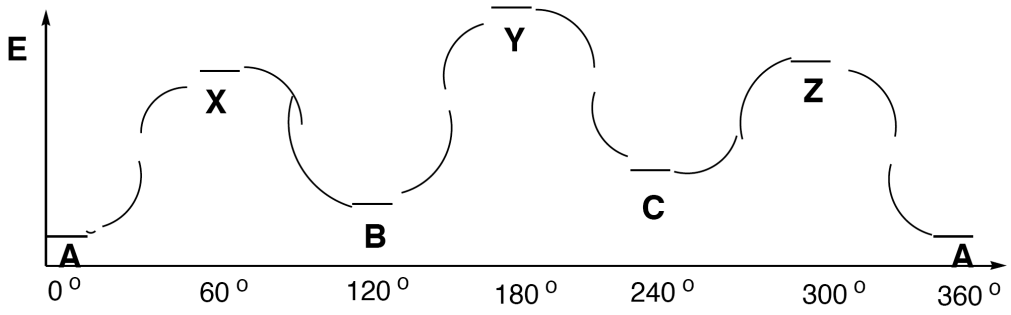


A **X** **B** **Y** **C** **Z**

B. (2) Which staggered conformation (A, B, or C) is expected to have the lowest energy? **A**

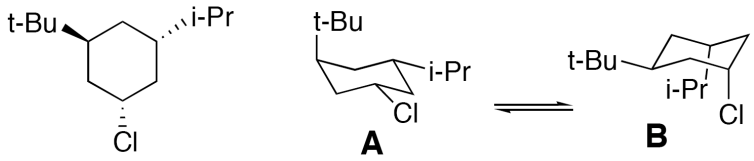
C. (2) Which eclipsed conformation (X, Y, or Z) is expected to have the highest energy? **Y**

D. (6) Draw the Potential Energy Diagram for rotation about the bond indicated in part 3A. Clearly label where A, B, C, X, Y, and Z occur.



4. (18)

A. (6) Draw two chair conformations for the following molecule and label them A and B.



B. (6) Calculate the equilibrium ratio of conformers for this compound and list the %A and %B.

Group	A-value	$\Delta G = -RT(LnK)$
t-Bu	5.00 kcal/mol	$K = e(-\Delta G/RT)$
i-Pr	2.15 kcal/mol	T = 298 deg
Cl	0.53 kcal/mol	$R = 1.987 \times 10^{-3}$ kcal/mol deg

$\Delta G = (-5.00) + (+2.15) + (+0.53) = -2.32$

$K = e(-\Delta G/RT) = 50.3 = [B] / [A]$

%A = 2% %B = 98%

C. (2) The specific rotation for (-)-Atorvastatin (Lipitor™) is $[\alpha] = -32$.
What is the specific rotation for (+)-Atorvastatin?

$[\alpha] = +32$

D. (2) What would be the observed rotation for a 70% ee sample of (-)-Atorvastatin?

$[\alpha] = 0.7 \times (-32) = -22.4$

E. (2) The observed rotation for an unknown sample of Atorvastatin is +25.6.
What is the composition (% - and + enantiomers) of this sample?

+25.6/+32 x 100 = 80% ee of (+)-Atorvastatin

80% ee = 90% of (+)-Atorvastatin + 10% of (-)-Atorvastatin