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Name

CHEMISTRY 3311, Fall 1997
Professor Walba
First Hour Exam
September 25, 1997

scores:

1)

2)

3)

4)

5)

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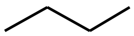
This is a closed-book "open model" exam. You <u>may</u> use models, but no notes or books. Please put all your answers on the test. Use the backs of the pages for scratch. There are additional scratch sheets at the end of the exam.

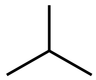
PLEASE read the questions carefully!

Partial Periodic Table

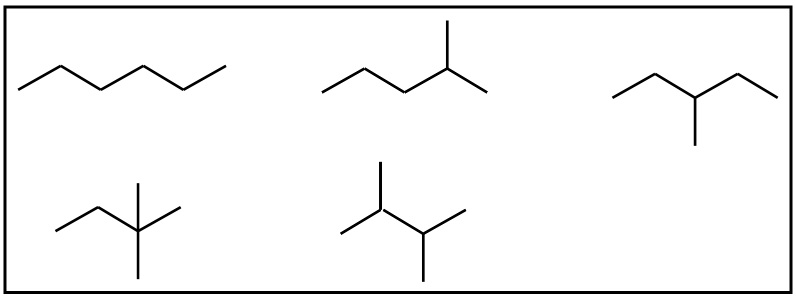
							8A
		1 H					2 He
1A	2A	3A	4A	5A	6A	7A	
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
						35 Br	
						53 I	

1) (20 pts) All of the possible isomers (that is, different compounds at room temperature) with formula C_4H_{10} are shown below. There are two C_4H_{10} isomers, and each isomer is drawn only once, using molecular graphs.

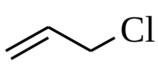


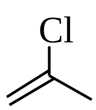


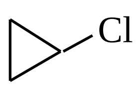
(a) Draw all of the possible isomers with the formula C_6H_{14}. Draw each isomer only once, using molecular graphs to show the structures.

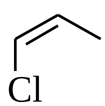


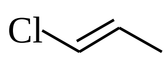
(b) Draw all of the possible isomers with formula C_3H_5Cl. . Draw each isomer only once, using molecular graphs to show the structures (you have to show the chlorine atoms explicitly in these molecules, but not the H atoms). PLEASE be sure that your structures have the correct molecular formula!











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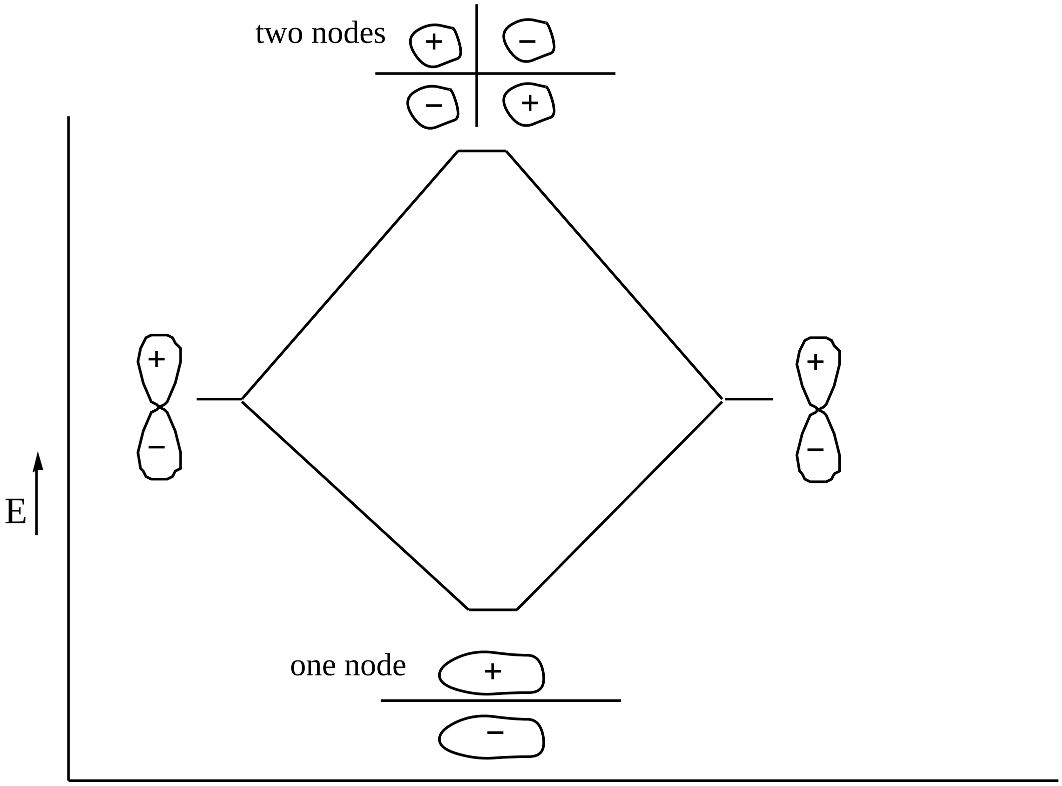
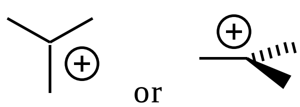
2) (20 pts) (a) Indicate the relative energy, shape, and phase (i.e. plus and minus signs) of the molecular orbitals obtained by sideways overlap of two carbon p atomic orbitals on the diagram below. Indicate the location and number of nodes in the molecular orbitals.



(b) Draw the structure, indicating geometry, of methyl cation (CH_3^+).



(c) Give the hybridization (the name of the hybridization, i.e. sp^3, sp^2, or sp) of the carbon atom of methyl cation.

sp^2

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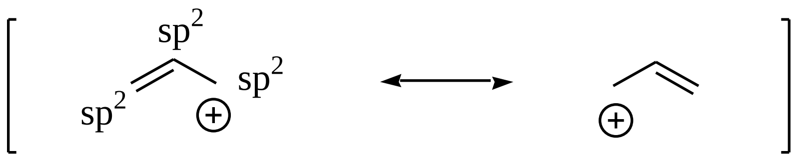
-2-continued

(d) Draw the two major resonance contributors to the structure of the allyl cation ($C_3H_5^+$) (you don't need to show geometry or H atoms, but be SURE to carefully indicate formal charges and lone pairs if necessary). The connectivity of allyl cation is H_2C—CH—CH_2. Give the name of the hybridization of each carbon atom on one of your structures.



(e) Are the two C—C bonds the same length, or different lengths in allyl cation?

Same

(e) How many p orbitals are overlapping to make molecular orbitals in the allyl cation?

Three

(f) Are there electrons in nonbonding orbitals in allyl cation?

No [There are two electrons in the pi orbitals of allyl cation. Overlap of three p orbitals affords three new pi orbitals, one bonding, one nonbonding, and one antibonding. The two electrons can both go into the bonding orbital.]

(f) Are there electrons in nonbonding orbitals in the allyl anion ($C_3H_5^-$)?

Yes [The allyl anion has four electrons in the pi orbitals, so two of them have to go into the nonbonding pi orbital.]

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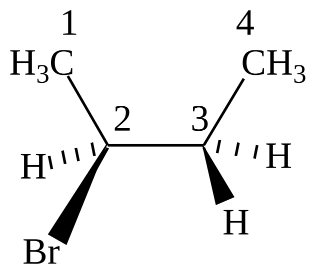
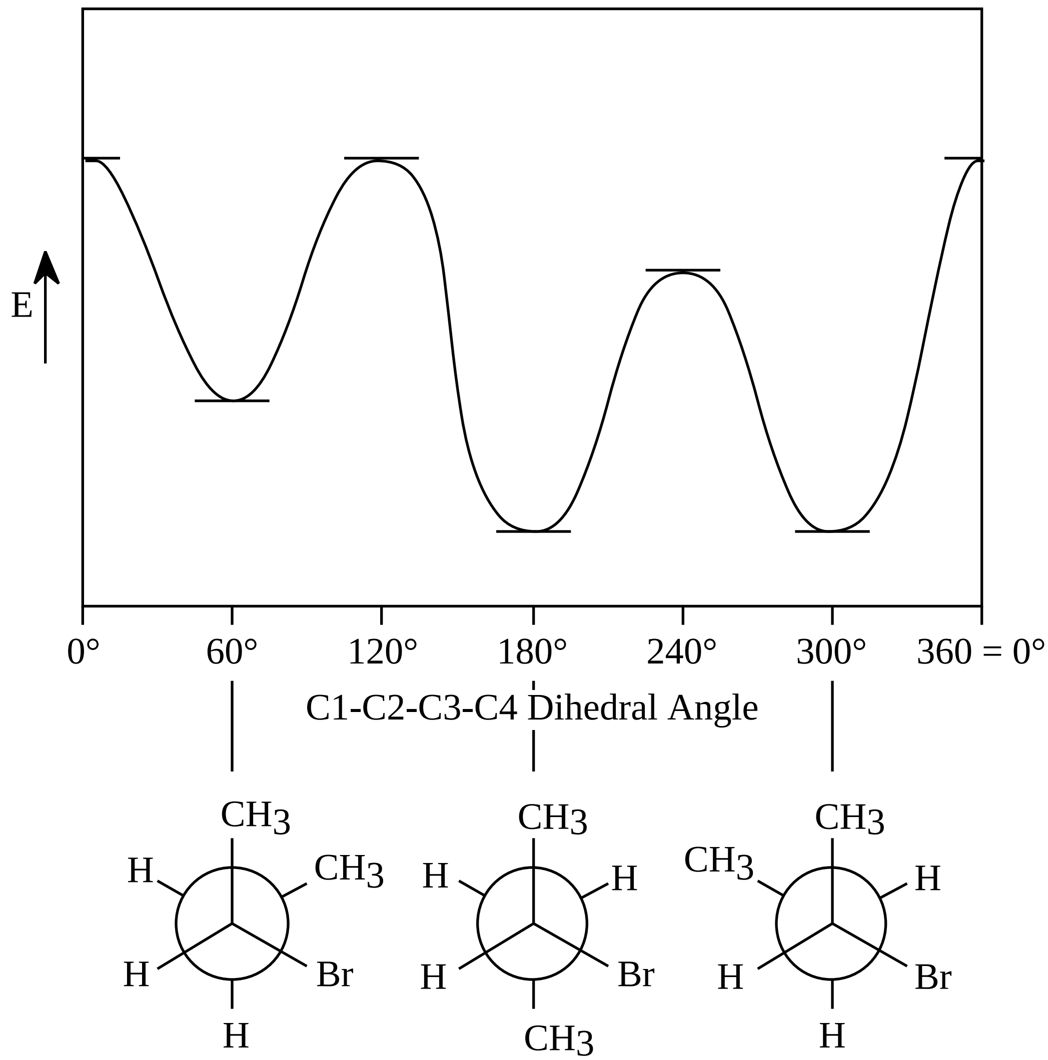
3) (20 pts) An eclipsed conformation of 2-bromobutane is given below. The C1-C2-C3-C4 dihedral angle for this conformation is 0°. Complete the energy diagram showing relative energies of all the conformations generated by rotating C3 clockwise about the C2-C3 bond, and complete the Newman projections for the three staggered conformations. NOTE!!! Bromine is the same size as a methyl group.





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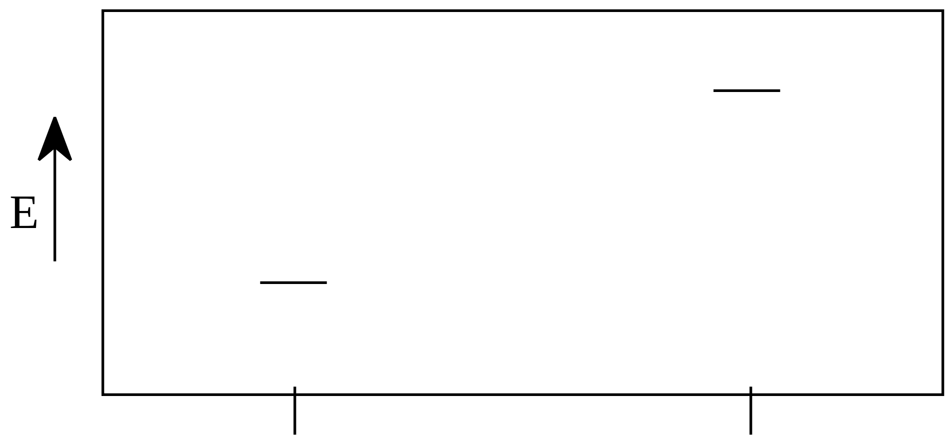
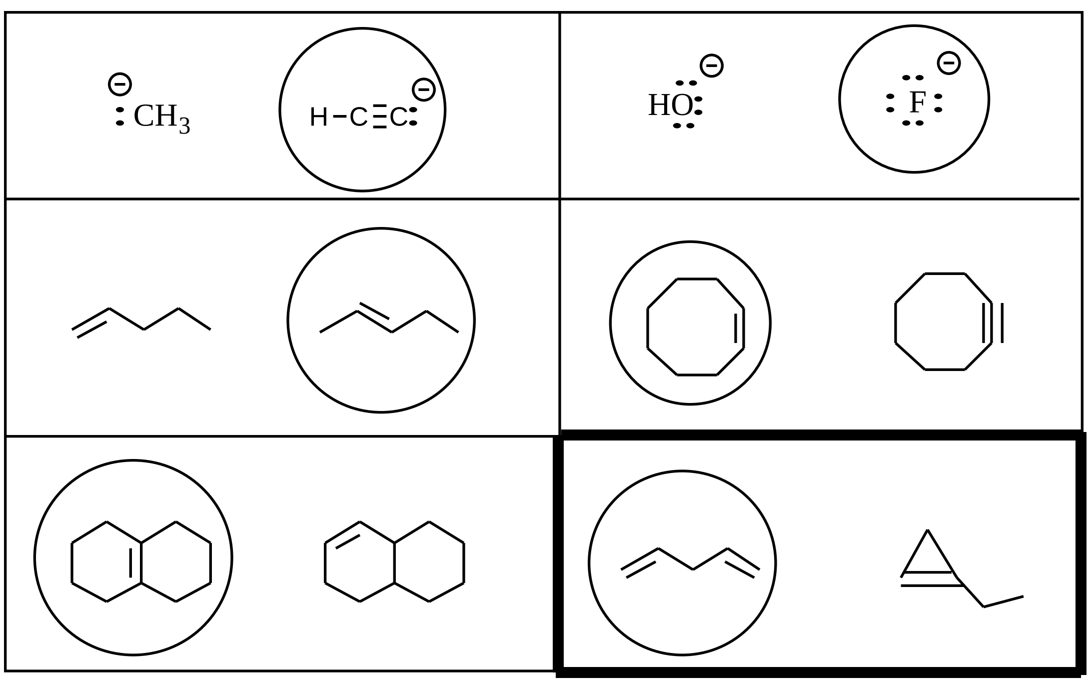
4) (20 pts) (a) The heat of formation of ethylene is +12.5 Kcal / mole. Indicate on this energy diagram the relative energies of (two graphite carbons plus two H_2 molecules) and ethylene ($CH_2=CH_2$)



2C(graphite) plus 2 H_2 $CH_2=CH_2$

(b) For each pair of structures below, circle the MORE STABLE structure. **Give a short explaination of your answer to the question outlined in bold.**



Points come from the explaination in this question; a reasonable case can be made for circling either molecule. The actual correct answer is that the diene is more stable because the cyclopropene has enormous angle strain, which stongly overwhelms the fact that the double bond is trisubsituted. One can make the argument that the cyclopropene should be more stable because it has more sp^2—sp^3 bonds and more sigma bonds than the diene. Just stating that the cyclopropene is more stable because is has a trisubstituted double bond will not get full credit.

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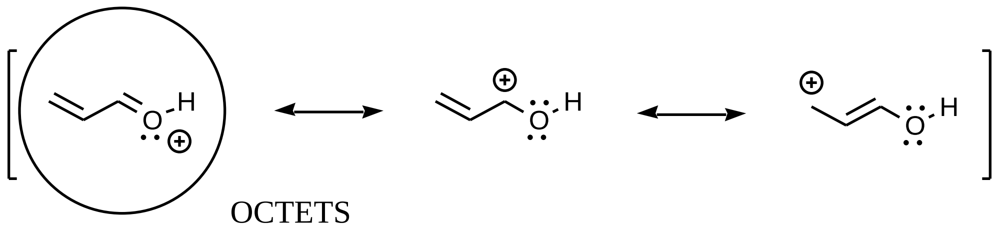
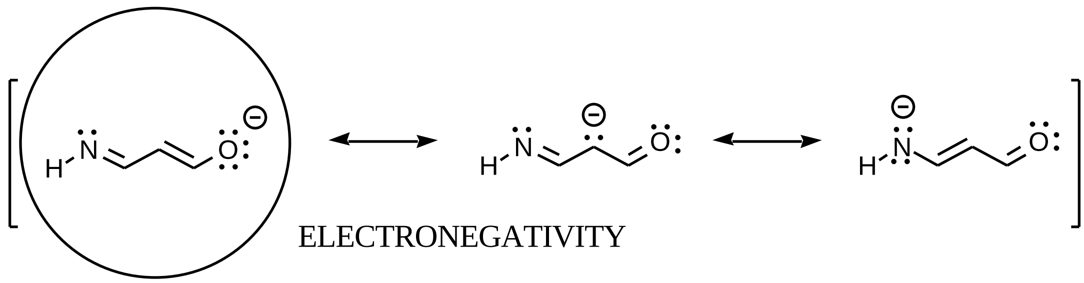
5) (20 pts) (a) Circle the major resonance contributor to the structure of each of the following molecules AND give a ONE-WORD explaination for your answer.

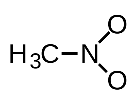


OCTETS

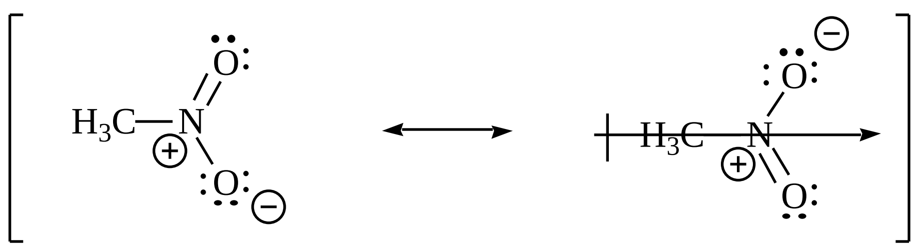


ELECTRONEGATIVITY

(b) Give the two major resonance contributors to the structure of nitromethane (CH_3NO_2). The connectivity of nitromethane is shown. Show all lone pairs and formal charges in your resonance contributors.



Connectivity of nitromethane



(c) Nitromethane has a large dipole moment. Show on one of your structures which direction the dipole points.

As shown, the dipole moment of nitromethane is right along the carbon-nitrogen bond.