

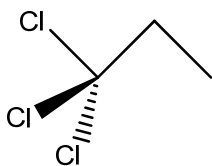
1 – Assigning IUPAC Names for Organic Structures

16 pts total: 2 pts each, –1 if answer is not the correct IUPAC name, but would result in the correct structure. Do not deduct points for extra “e”s (such as –yn-1-ol vs. –yne-1-ol)

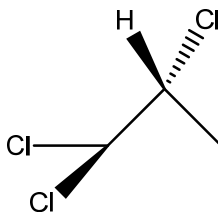
- 2-pentyn-1-ol (or pent-2-yn-1-ol)
- 2-methoxy-2-methylpropane (also accept *tert*-butyl methyl ether, although this is worse)
- ethane-1,2-diol (or 1,2-ethanediol)
- 3-ethyl-4-methyloctane
- 3-heptyn-2-one (or hept-3-yn-2-one)
- 3,3,3-trifluoropropanal
- 2-hydroxybenzoic acid, or ortho-hydroxybenzoic acid (IUPAC names)
OR 2-hydroxybenzenecarboxylic acid, or ortho-hydroxybenzenecarboxylic acid
(RC uses the third and fourth names)
- 3-butyl-2-methyl-2-heptene (or 3-butyl-2-methylhept-2-ene)

2 – Constitutional Isomers

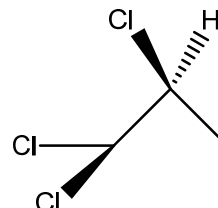
(12 pts total: 1 pt per structure, 1 pt per name. Students do not need to draw both the (R)-1,1,2 and (S)-1,1,2 structures, in which case these structures and names are worth 2 pts each)



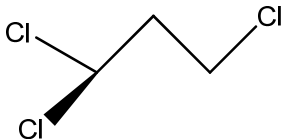
1,1,1-trichloropropane



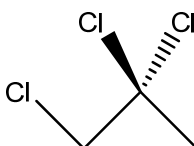
(R)-1,1,2-trichloropropane



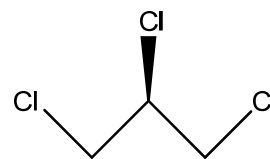
(S)-1,1,2-trichloropropane



1,1,3-trichloropropane



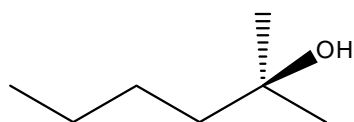
1,2,2-trichloropropane



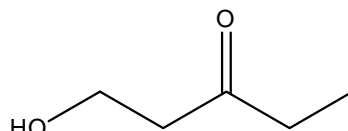
1,2,3-trichloropropane

3 – Drawing More Structures

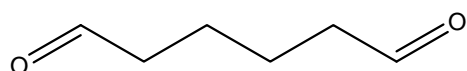
12 pts: 3 pts each, -1 for one mistake (wrong number of carbons, incorrect branching, mistake in position or structure of functional group), -3 for two or more mistakes. No deduction for not using wedges or dashes. No deduction for not drawing the cyclohexane ring as a chair.



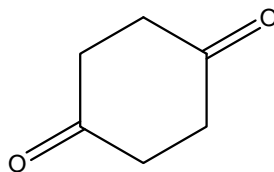
2-methyl-2-hexanol



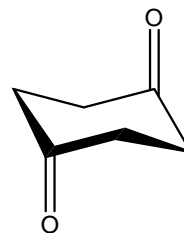
1-hydroxy-3-pentanone



hexanedial



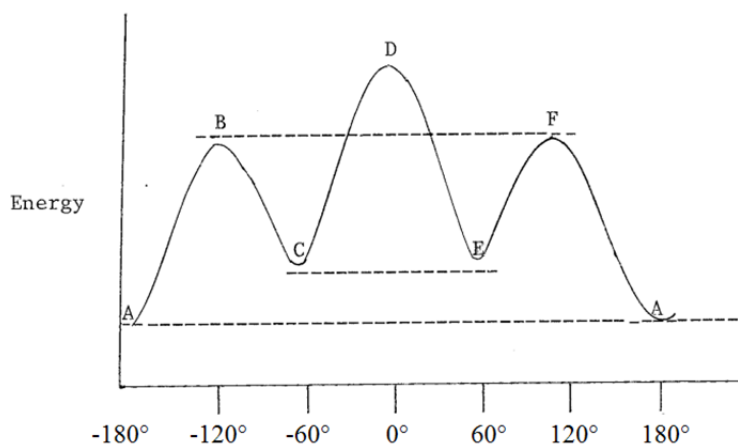
OR



1,4-cyclohexanedione

4 – Drawing Structures and Energy Diagrams

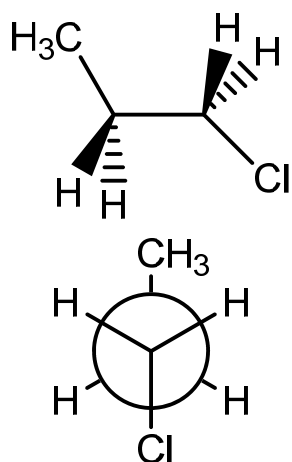
(18 pts: 6 pts for diagram, 1 pt per each wedge/dash structure, 1 pt for each Newman projection)



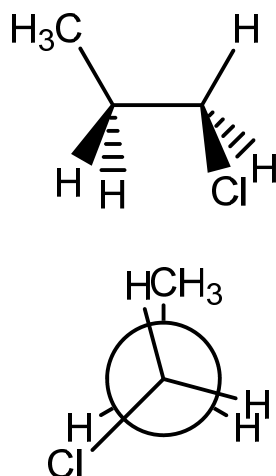
6 points, divided as follows:

- 1 pt for three peaks
- 1 pt for correct peak positions (0° , 120° , -120° or similar)
- 1 pt for correct dip positions (60° , 180° , -60° or similar)
- 0.5 pts for C and E being equal energy
- 0.5 pts for B and F being equal energy
- 1 pt for Conformer A being lower than C and E
- 1 pt for Conformer D being higher than B and F
- Do not deduct if 0° is labeled differently, as long as the diagram is consistent
- OK to label E as C and F as B, since they are technically equivalent

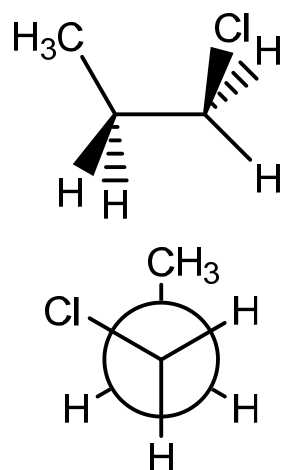
Conformer A



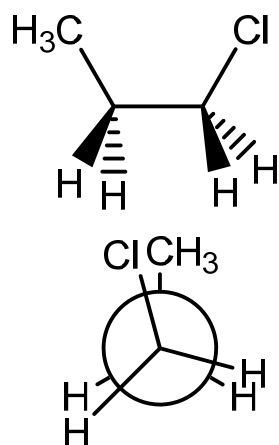
Conformer B



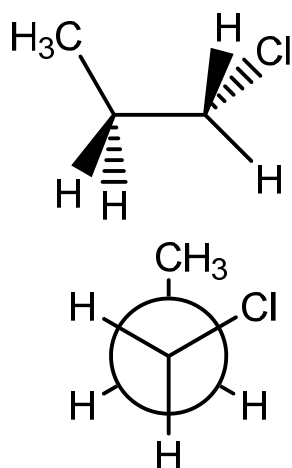
Conformer C



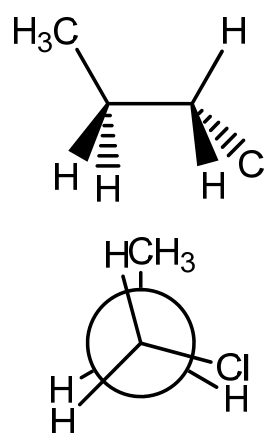
Conformer D



Conformer E



Conformer F

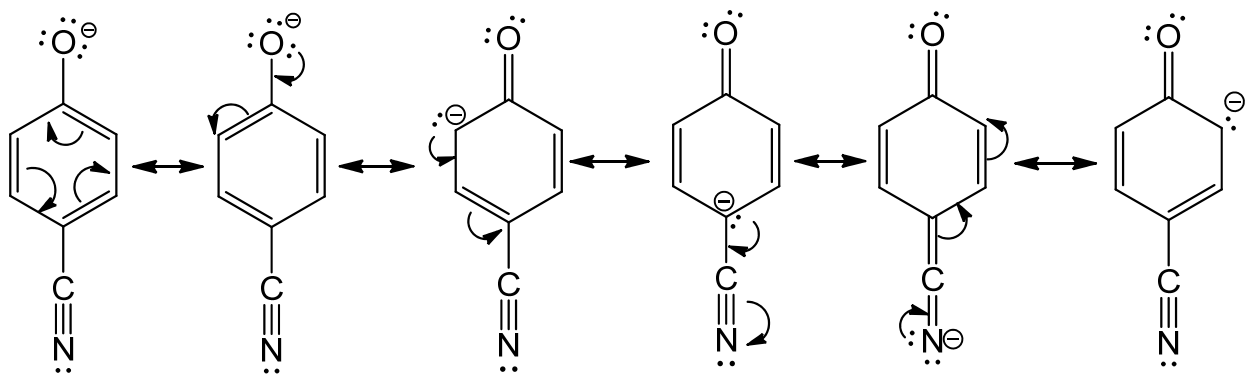


1 pt per structure. Half credit for any structures that are unlabeled (compared to the energy diagram). Half credit for a structure that is valid, but does not match the appropriate position on the energy plot.

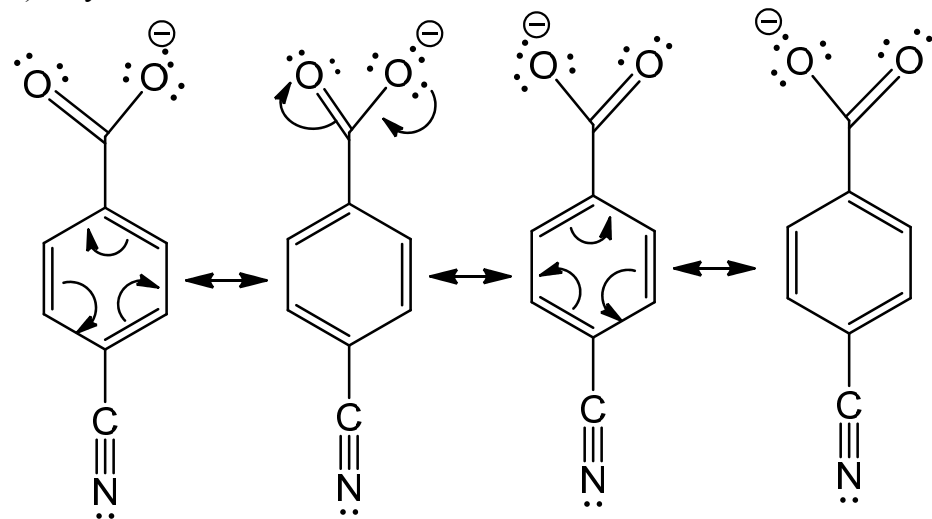
5 – Drawing Structures and Energy Diagrams

(20 pts, 4 pts per molecule. -1 per missing resonance structure, incorrect resonance structure, or correct resonance structure without lone pairs or curved arrows. Max deduction 4 pts per molecule. Names are not required; they are here to tell the student what the molecule is) Although this was not our intention, no deduction if “and x equivalent structures” is used properly, because we forgot to specify not to do this.

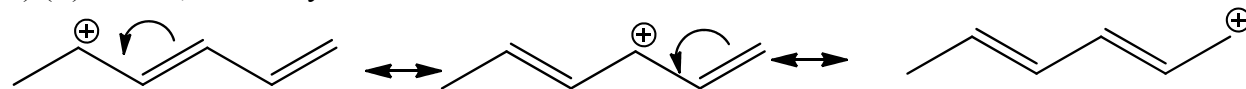
a) 4-cyanophenolate



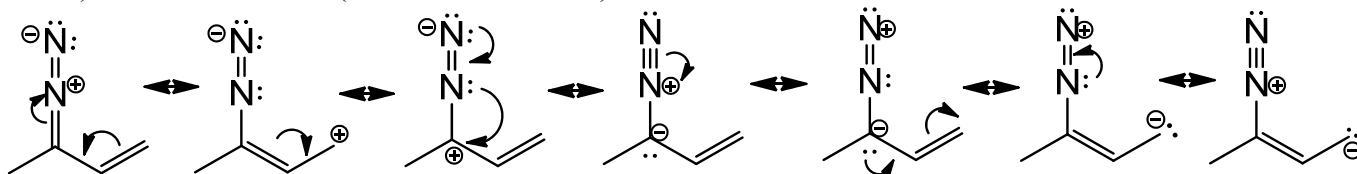
b) 4-cyanobenzoate



c) (E)-hexa-3,5-dien-2-ylum

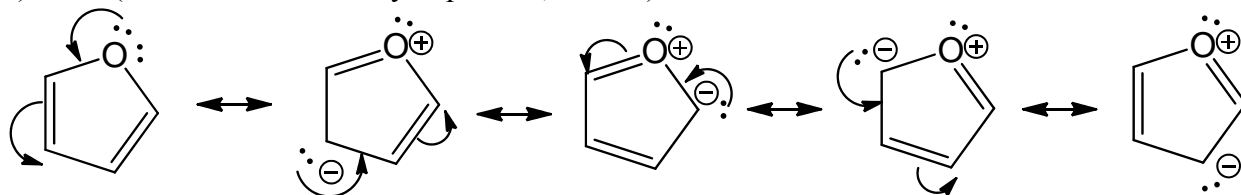


d) 3-diazo-but-1-ene (or 3-diazo-1-butene)



(No deduction for missing the structures that lack an octet on the N, but you should be aware that they exist)

e) furan (IUPAC name 5-oxacyclopenta-1,3-diene)



6 – Dipole Moments of Methyl Halides (12 points, divided as shown below)

- The carbon atoms for all molecules have a positive partial charge. (2 points) The F, Cl, Br, and I atoms are all more electronegative than the carbon atom and electrons are drawn away from the carbon atom toward the more electronegative atom. (2 points)
- Largest magnitude charge on carbon: CH_3F ; Smallest: CH_3I (2 points each)
- The dipole moment (μ) is the product of the magnitude of the partial charge (δ) and the distance (a) between charge centers, $\mu = a\delta$. (2 points for statement or equation; both are not required. –1 if student states that they depend on each other, but does not call it a product). If the partial charge varies and the dipole moment stays the same, then the distance between charge centers must vary. (2 points)

7 –More Dipole Moments (10 pts, divided as shown below)

a) Order of molecular dipole moment: $\text{CCl}_4 < \text{CHCl}_3 < \text{CH}_2\text{Cl}_2 < \text{CH}_3\text{Cl}$ (6 points)

Only 3 pts for $\text{CCl}_4 < (\text{CH}_3\text{Cl} = \text{CHCl}_3) < \text{CH}_2\text{Cl}_2$, see note 2 below
(no credit otherwise)

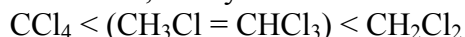
b) Major effect: The Cl are not independent: each draws a different amount of electron density away, resulting in different partial charges on each Cl, changing the magnitude of the dipole.
Minor effect: Even though we are adding polar bonds to the molecules (going from CH_3Cl , CH_2Cl_2 , CHCl_3 to CCl_4), the effects of the individual bonds cancel because of vector math. C-H bond does not have equal length as C-Cl bond)

(4 points for any reasonable answer that mentions electron density or vector math)
(Full credit for “vector math” if the student responded with the 3 pt answer to part a)

SIDE NOTE #1: “We want proof!” Here is the experimental data (CRC Handbook):



SIDE NOTE #2: If you work out the vector math and use 109.4° for all H-C-H, H-C-Cl and Cl-C-Cl bond angles by placing the atoms at alternating corners of a cube and assuming Cl has the same partial charge for all four molecules, then you will find that:



There are two problems with this analysis. The most significant one is that the Cl atoms are not independent of each other, and the individual partial charges change as Cl atoms are added. This clearly will affect calculation of the dipole.

The second, and less significant problem, is that the model assumes a perfect tetrahedron for all four molecules. The model doesn't account for differences in C-H and C-Cl bond lengths. (In this case, the bond angles do not change too much when replacing H with Cl) Both bond length and bond angle are critical when estimating molecular dipole moment. Even though we didn't assign many points to the correct order versus the vector math order, this aspect of molecular dipole moments and molecular structure was important enough to highlight.