



Chem 220a - Organic Chemistry

Problem Set 1

Chapters 1 and 2

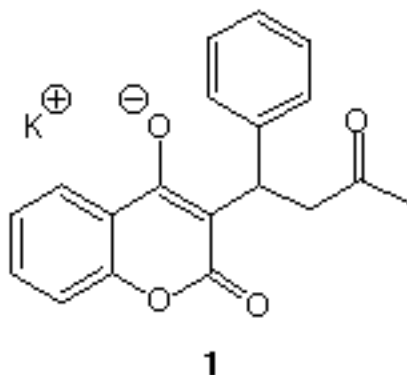
Due: Monday, September 17, 2001

	<p><u>John Dalton (1766-1844)</u></p> <p>Made important contributions to early atomic theory [Law of Multiple Proportions]. Unfortunately, his 'rule of greatest simplicity' led to the idea that water was a binary compound (two atoms) caused confusion in the ensuing years.</p>		<p><u>G. N. Lewis (1875-1946)</u></p> <p>Developed the concept of the covalent bond and the octet rule. An early version of the octet rule had the electrons located at the corners of a cube.</p>
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1. Draw Lewis structures for methyl acetylene (CH_3CCH) and allene (1,2-propadiene, CH_2CCH_2), the tautomeric components of **MAPP** gas. Illustrate and explain the tautomeric relationship.

2. Illustrate resonance in diazomethane (CH_2N_2 ; this formula not only indicates composition but also atom connectivity) and in acetate ion.

3. Draw two other resonance structures of the anion of the anti-coagulant drug, coumadin **1** (warfarin). Draw the three possible tautomeric forms of the conjugate acid of coumadin. Can the anion of coumadin be converted to its conjugate acid with acetic acid? [To assist you in this part of the question, assume that the conjugate acid of **1** is protonated on carbon. Name and circle the two proximate functional groups. Use the [pKa table](#) to find an appropriate model for the conjugate acid.]



[**Historical Note:** The development of coumadin (warfarin) as an anticoagulant follows from the isolation of [dicoumarol](#) from rotting sweet clover after a Wisconsin farmer noted that his cattle were [bleeding and dying](#). The research that led to the development of [warfarin](#) was sponsored by the Wisconsin Alumni Research Foundation (WARF), hence its [name](#). (see WARF History at this site)].

4.

In a historical paper in 1852, Williamson reported the preparation of an [unsymmetrical ether](#). This new ether had a vapor density approximately twice that of air. A combustion analysis was conducted.

"... the ether being burnt by oxide of copper, the following results were obtained:

0.2215 gm. of liquid gave:

0.482 " " carbonic acid [CO₂], and

0.2685 " " water ..."

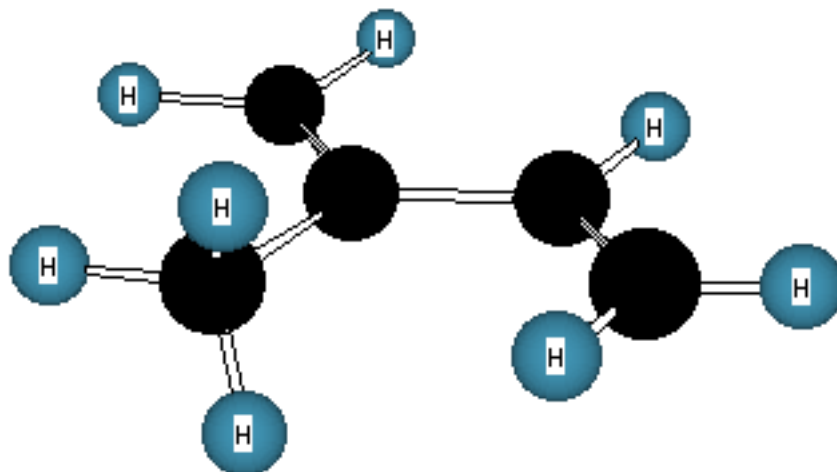
From these data, determine the molecular formula of this ether and draw its structure. Show your work. [Remember: Oxygen is not determined directly in a combustion analysis but rather by difference. The ideal gas law relates molecular weight and gas density at the same temperature and pressure.]



[Alexander Williamson](#)

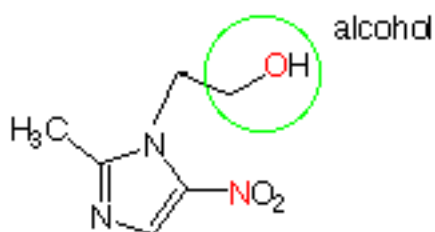
(1824-1904)

5. Isoprene (2-methyl-1,3-butadiene, **1**) is an important monomer in the formation of essential oils (terpenes: camphor, β -carotene, etc.) and rubber. Draw a molecular orbital representation of isoprene in the conformation shown below. Label the hybridization (sp , sp^2 , sp^3) of all carbons and label σ - and π -bonds.

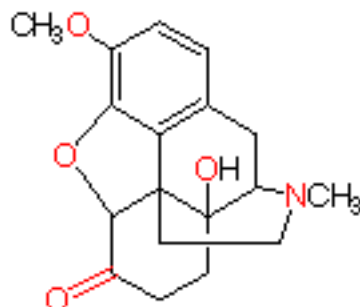


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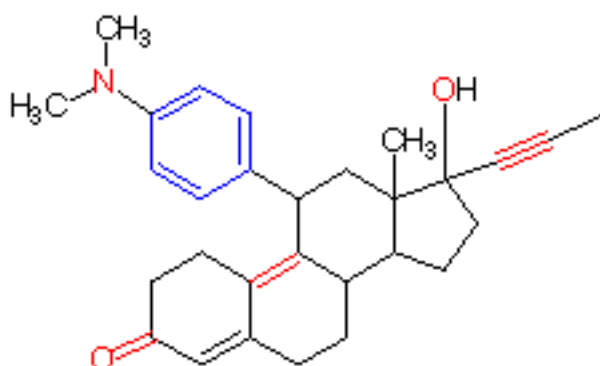
6. In each of the following structures certain atoms, or groups of atoms, are highlighted in red or blue. Either print out the structures, or better yet, draw them, and circle each of the functional groups in which each atom, or group of atoms, is contained. Write the name of the functional group next to each circle. For example, the red oxygen in metronidazole is part of an alcohol, $-\text{CH}_2\text{OH}$. Note that the lefthand side of the structures of capsaicin and vanillin are the same, but what a difference your taste buds discern!



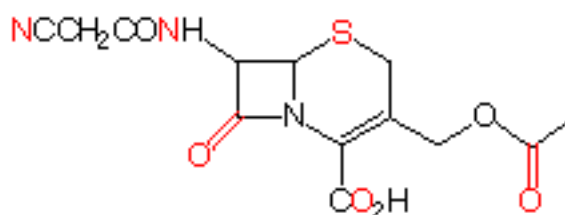
metronidazole
(treatment for rosacea)



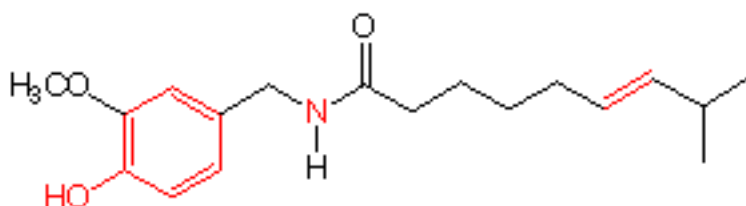
oxycodone
(a.k.a OxyContin)



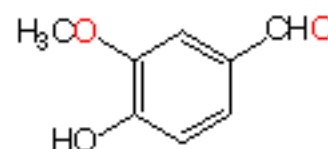
mifepristone (RU-486)
(abortifacient)



cephacetrile
(cephalosporin antibiotic)



capsaicin
(active ingredient in hot chili peppers)



vanillin
(flavor of vanilla)

SKYLAR: Well, have you studied organic chemistry?

WILL: A little bit.

SKYLAR: Oh, just for fun.

WILL: Yeah, for kicks.

SKYLAR: Yeah, it's SO much fun studying organic chemistry. Are you mad? Have you completely lost your

mind? Nobody studies it for fun. It's not a necessity, especially for someone like you.Good Will Hunting,
Miramax Films