Chapter 2: Molecular Representations

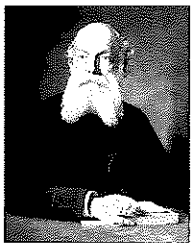
[Sections 2.1, 2.2, 2.4-2.12]

"burning methane leads to the formation of carbon dioxide and water"

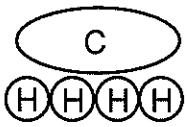
$$CH_4 + O_2 \longrightarrow H_2O + CO_2$$

Drawing Organic Molecules

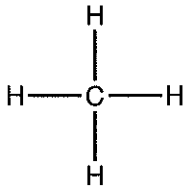
older methods



Friedrich Kekule
1829-1896



sausage
(really old)
~1850's

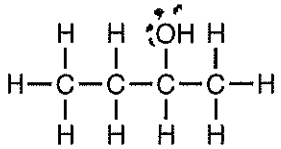


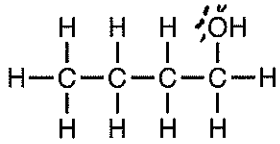
Lewis dot
structures
~1916

CH_4

condensed
structure

Lewis dot:





- *a "functional group" is defined as the reactive portion of a molecule*

Condensed: $CH_3CH_2CHOHCH_3$ $CH_3CH_2CH_2CH_2OH$

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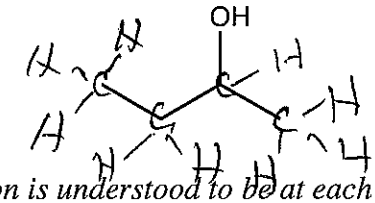
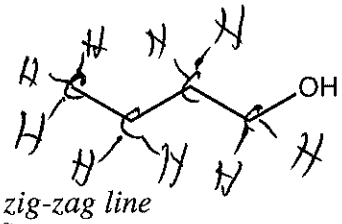
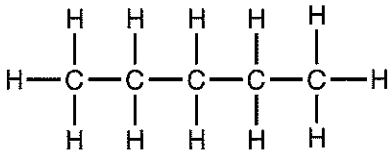
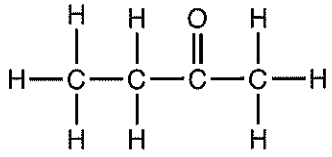
newer method: bond-line structures (skeletal structures)

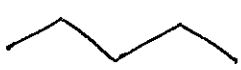


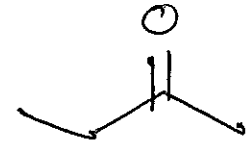


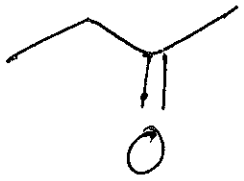
- *a carbon is understood to be at each end of a zig-zag line*
- *generally, the longest carbon chain is drawn first*
- *the proper number of hydrogens are understood to be connected to the carbons*
- *heteroatoms (non-carbon atoms) are always drawn with attached hydrogens (e.g., OH, NH, SH, PH)*
- *lone pairs may or may not be drawn explicitly*

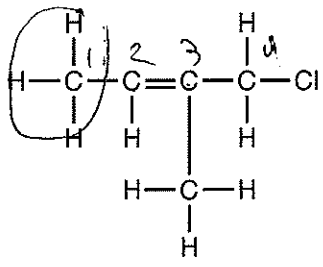


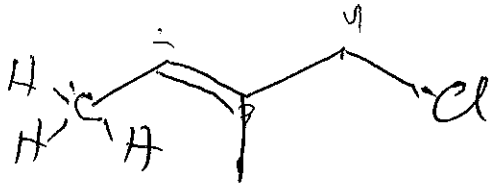


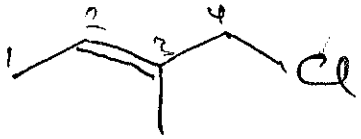




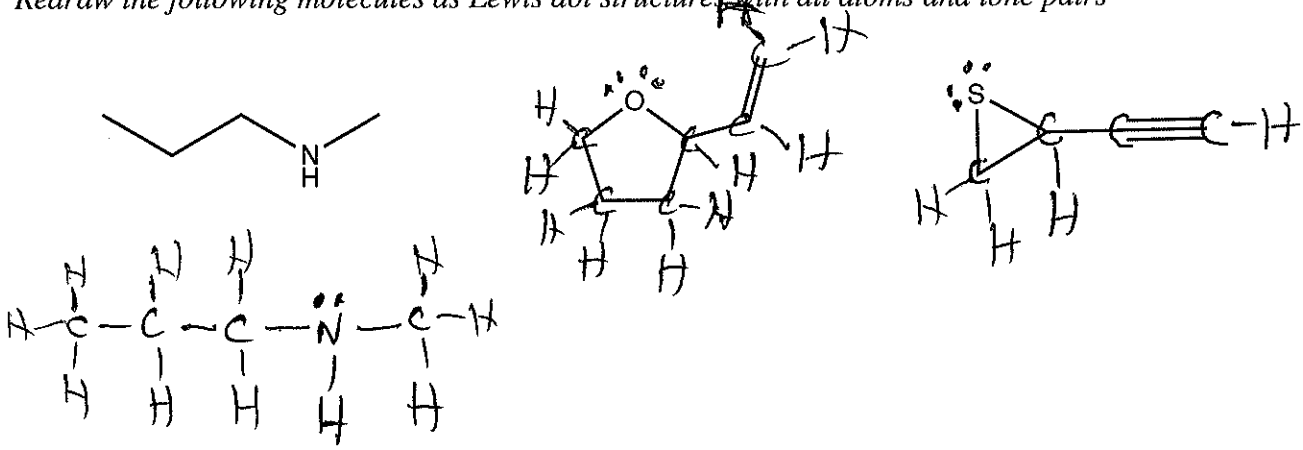








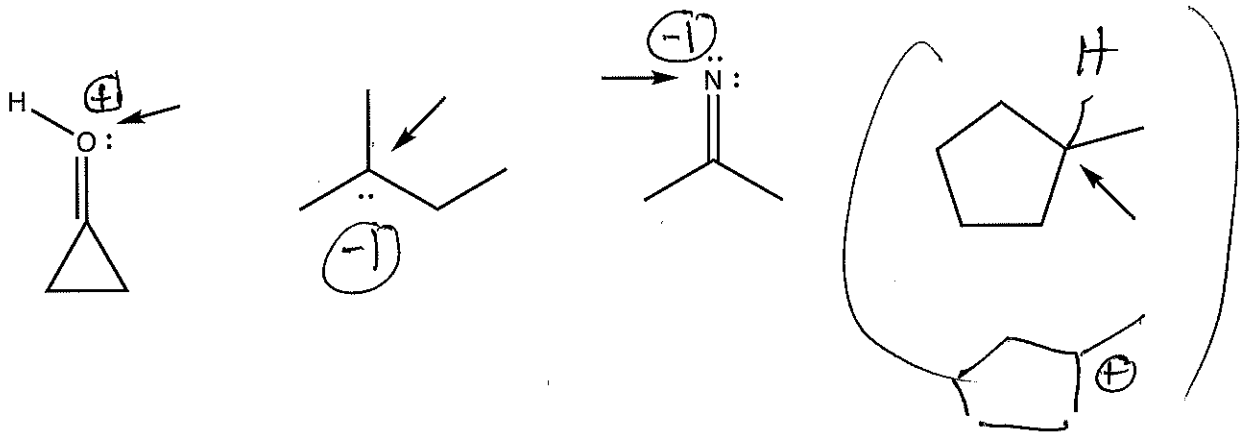
Redraw the following molecules as Lewis dot structures with all atoms and lone pairs



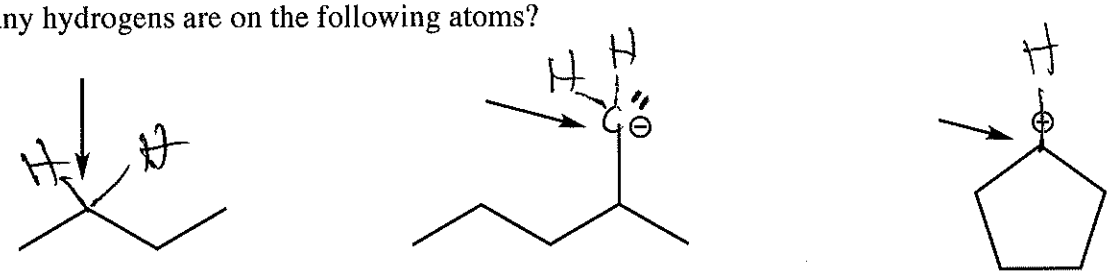
Drawing Structures With Formal Charges and Non-Standard Lone Pairs

- *formal charges are ALWAYS drawn explicitly*
- *the formal charge dictates the number of bonds and/or lone pairs present on an atom*

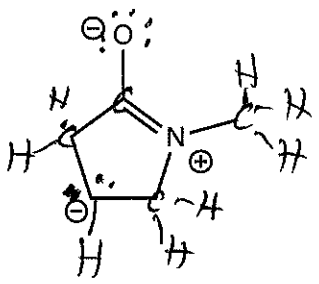
What are the formal charges on the following atoms?



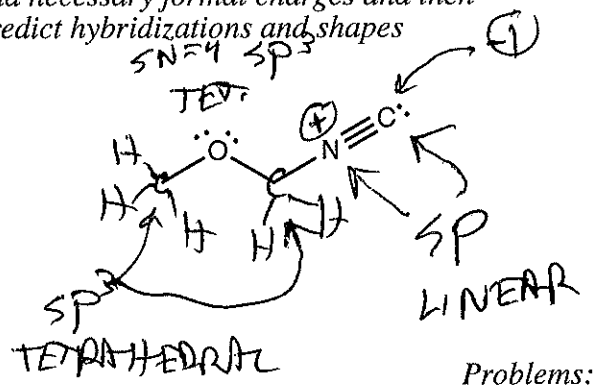
How many hydrogens are on the following atoms?



add necessary lone pairs



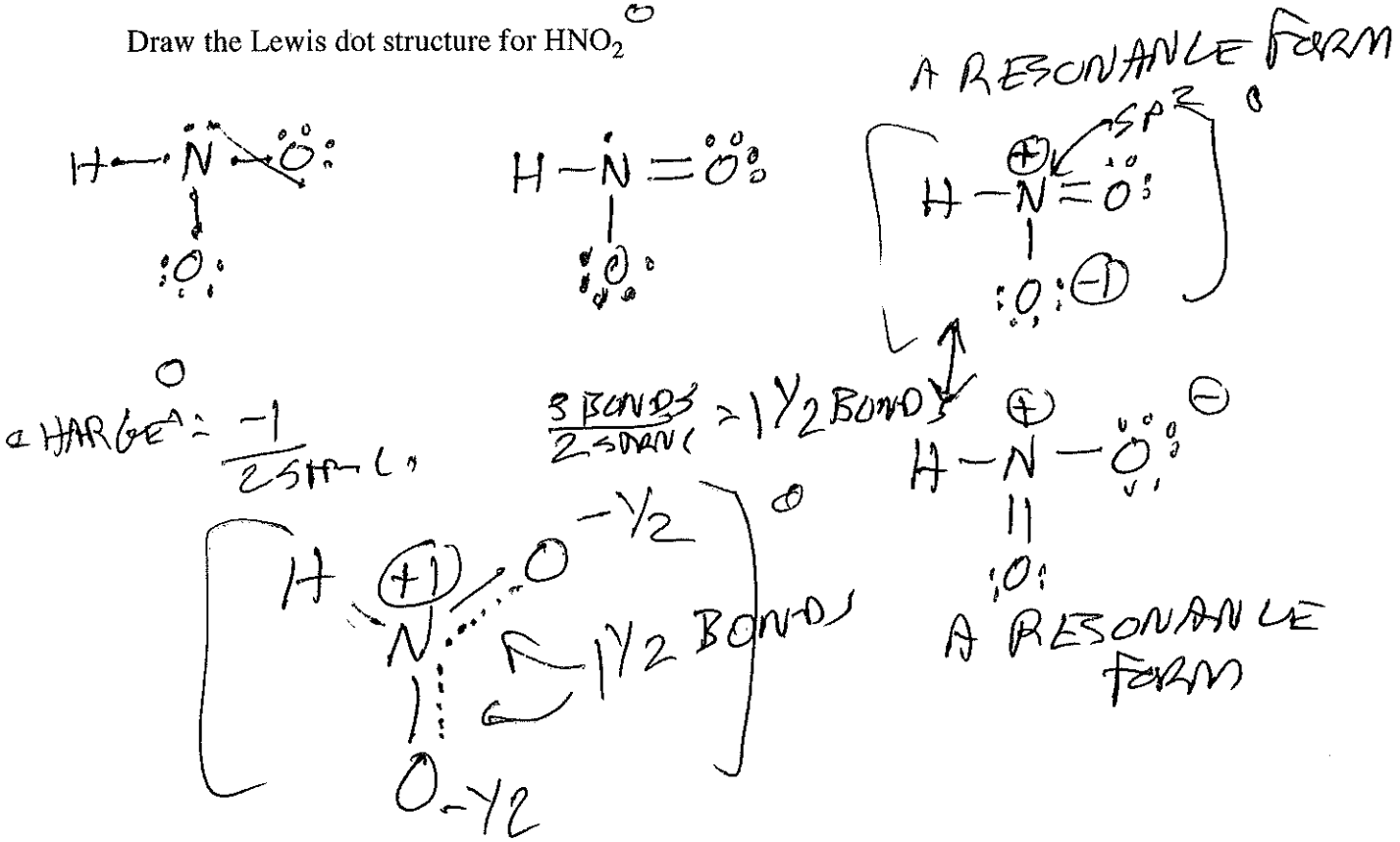
add necessary formal charges and then predict hybridizations and shapes



Problems: 1-6

Resonance Forms

Draw the Lewis dot structure for HNO_2



hybrid structure

- *sometimes more than one Lewis dot structure can be drawn for the same compound*
- *the only difference between the structures is the arrangement of electrons (i.e. atoms cannot be moved)*
- *the two stuctures are said to be* ***resonance forms***
- *the actual structure, the* ***hybrid structure****, is a superposition (mixture) of all of the contributing resonance forms*
- *the bond order between any two specific atoms = [sum of total bonds between those two specific atoms across ALL of the contributing resonance forms] / [total number of contributing resonance forms]*
- *the charge on any specific atom = [sum of charges on that specific atom for ALL of the contributing resonance forms]* ***divided by*** *[total number of contributing resonance forms]*

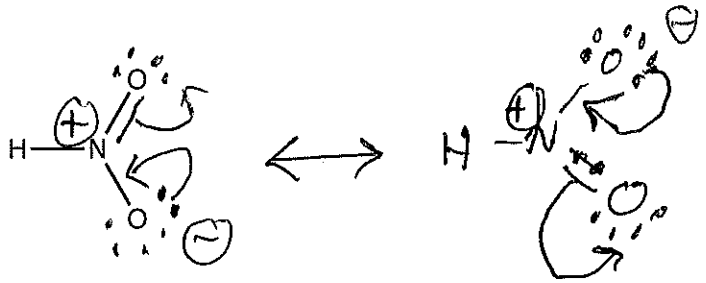
shortcut to interconverting between resonance forms

curved arrow notation

electrons coming ***from*** → *electrons going* ***to***

NOTE: always follow the ***electrons*** *and not the* ***atoms***

"atoms don't form bonds, electrons do"



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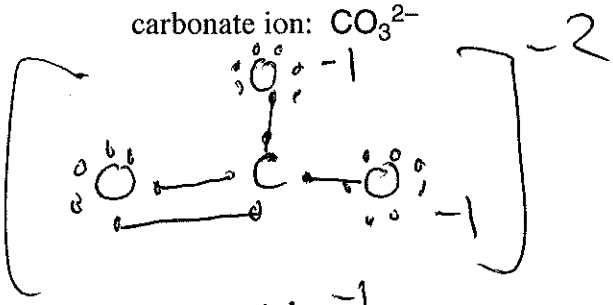
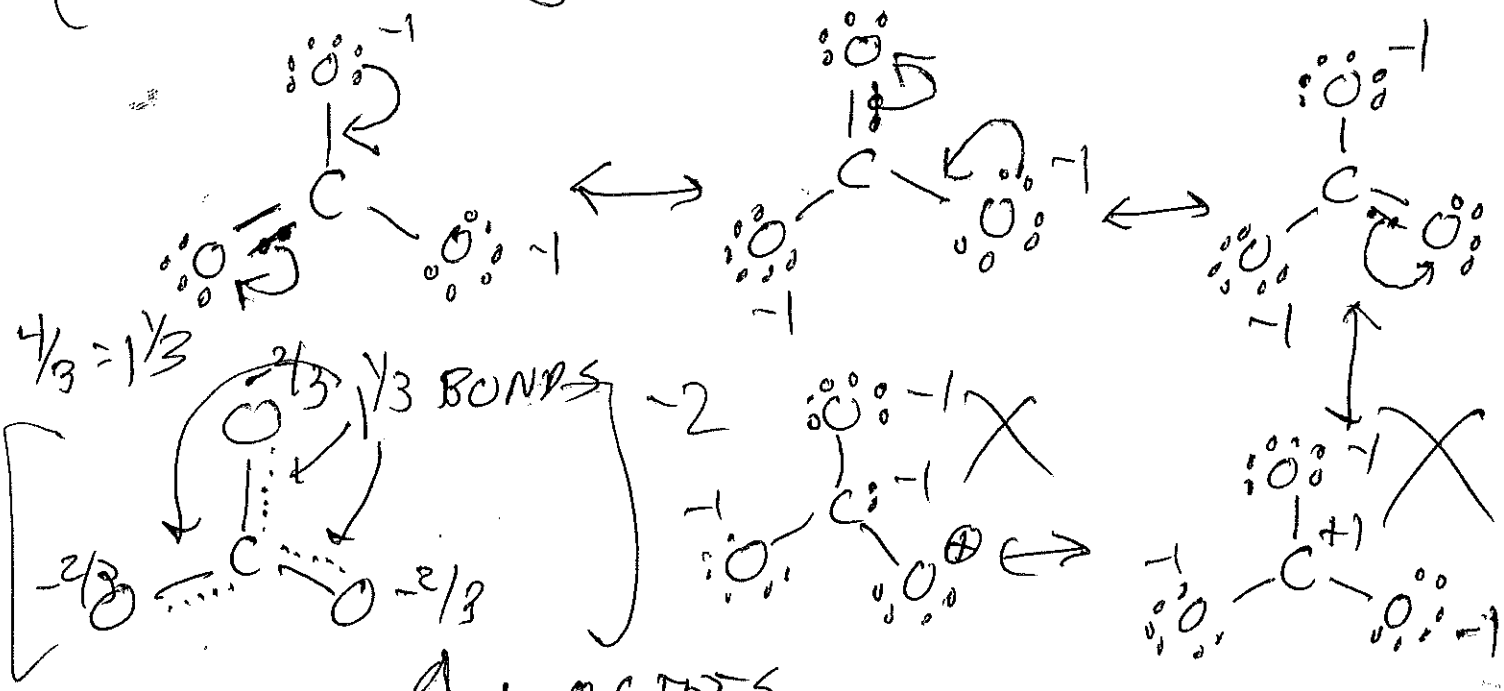
carbonate ion: CO_3^{2-}





HYBRID

1. OCTETS
2. MAXIMIZE BONDS
3. ~~CH~~ MINIMIZE CHARGE
4. CHARGE APPROPRIATE

Problems: 7–11