Properties of Organic Molecules

(Which organic molecules are soluble in water?)

Model: Polarity and properties of organic molecules

Bond polarities are determined by the electronegativity difference between the bonded atoms. Recall that C-H bonds are nonpolar, but C-N and C-O bonds are polar. Since water is a polar solvent, the more polar an organic molecule, the more soluble it will be in water.

Table 1: Polarity, solubility and boiling points of selected compounds*

Alkane	Structure	Molar mass, g/mol	Dipole moment, Debyes	Boiling point, °C	Water solubility, grams per 100 mL H_2O
propane	$CH_3CH_2CH_3$	44	0	-42	0.007
butane	$CH_3CH_2CH_2CH_3$	58	0	0	0.006
pentane	$CH_3CH_2CH_2CH_2CH_3$	72	0	36	0.04
hexane	$CH_3(CH_2)_4CH_3$	86	0	69	0.001
heptane	$CH_3(CH_2)_5CH_3$	100	0	98	0.01

Alcohol	Structure	Molar mass, g/mol	Dipole moment, Debyes	Boiling point, °C	Water solubility, grams per 100 mL H_2O
ethanol	CH_3CH_2OH	46	1.7	78	∞
1-propanol	$CH_3CH_2CH_2OH$	60	1.7	82	∞
1-butanol	$CH_3CH_2CH_2CH_2OH$	74	1.67	118	6.3
1-pentanol	$CH_3(CH_2)_4OH$	88	1.7	137	2.7
1-hexanol	$CH_3(CH_2)_5OH$	102	1.8	157	0.6
1-heptanol	$CH_3(CH_2)_6OH$	116	1.7	176	0.1

Ether	Structure	Molar mass, g/mol	Dipole moment, Debyes	Boiling point, °C	Water solubility, grams per 100 mL H_2O
dimethyl ether	CH_3OCH_3	46	1.3	-23	∞
diethyl ether	$CH_3CH_2OCH_2CH_3$	74	1.15	35	6.9
dipropyl ether	$CH_3(CH_2)_2O(CH_2)_2CH_3$	102	1.2	89	0.25

Amine	Structure	Molar mass, g/mol	Dipole moment, Debyes	Boiling point, °C	Water solubility, grams per 100 mL H_2O
propyl amine	$CH_3CH_2CH_2NH_2$	59	1.3	48	∞
butyl amine	$CH_3CH_2CH_2CH_2NH_2$	73	1.3	77	∞
hexyl amine	$CH_3(CH_2)_5NH_2$	101	–	131	1.2
octyl amine	$CH_3(CH_2)_7NH_2$	129	–	180	0.02

* Sources: CRC Handbook of Chemistry and Physics, 47th ed., 1967; ChemFinder.com; IPCS INCHEM, www.inchem.org; Korea thermophysical properties Data Bank, www.cheric.org/kdb/ [accessed June 2006]

Notes: The dipole moment is a measure of the polarity of a molecule; ∞ means infinitely soluble (*i. e.*, the liquids are miscible); a dash means the data were unavailable.

Critical Thinking Questions:

1. Considering the dipole moments of the molecules in Table 1, which functional group is most **nonpolar**?

2. In general, do polar compounds have **higher** or **lower** boiling points than nonpolar compounds (circle one)?

3. For each functional group listed below, indicate how the boiling point changes as the molar mass increases.

   a. alkane

   b. alcohol

   c. amine

4. The boiling point of a liquid increases as the attractions between molecules increase. These attractions are called intermolecular forces. Based on your answers to CTQ 3, how do the intermolecular forces between molecules change as the molar mass increases?

5. Find one molecule from each functional group (alkane, alcohol, ether, amine) with roughly the same molar mass (within 5 g/mol), and write their names below. Rank these compounds from the highest to lowest boiling point.

6. Repeat CTQ 5 with another set of four compounds.

7. Based on relative boiling points, write the numbers from 1 to 4 under the functional group names below, with the number 1 being the group with the most intermolecular attractions, and 5 being the least.

   alkane alcohol ether amine

8. For each functional group below, circle <u>each</u> type of bond contained in the molecule. You may refer to Table 1.

functional group	Type of bond			
alkane	C-H	C-O	O-H	N-H
alcohol	C-H	C-O	O-H	N-H
ether	C-H	C-O	O-H	N-H
amine	C-H	C-O	O-H	N-H

9. Based on your answer to CTQ 8, which two types of bonds are present in the molecules with the strongest intermolecular attractions?

Information:

The types of bonds you identified in CTQ 8 can exhibit what is known as **hydrogen bonding**. A "hydrogen bond" is simply a particularly strong attraction between the bonded hydrogen atom and a lone pair on another atom. This attraction causes molecules to stick together, but is much weaker than a covalent bond (up to one-tenth as strong), and so can be broken and reformed continually at room temperature.

Water has O-H bonds, and the O has two lone pairs, meaning that water meets the requirements for hydrogen bonding. Therefore, water is particularly suitable for dissolving organic molecules that can exhibit hydrogen bonding, since the water and organic molecule can "hydrogen-bond" together.

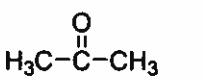
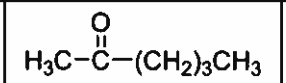
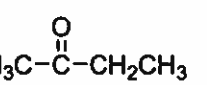
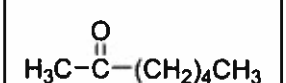
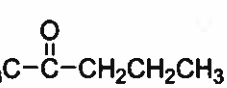
Consider the molecule ethanol, CH_3CH_2OH. It has one polar functional group (the –OH) and a two-carbon nonpolar alkyl group (CH_3CH_2-). Since the nonpolar group is not attracted to the water, it is reasonable to say that the –OH is the reason that ethanol is miscible with water.

Critical Thinking Question:

10. Suppose that we consider anything over about <u>1 gram per 100 mL water</u> to be "soluble." Then, considering the water solubilities of the alcohols, ethers, and amines in Table 1, the presence of <u>one polar functional group</u> is sufficient to dissolve a molecule containing about how many nonpolar carbons? Circle one of the following choices:

1-2 3-4 5-6 7-8

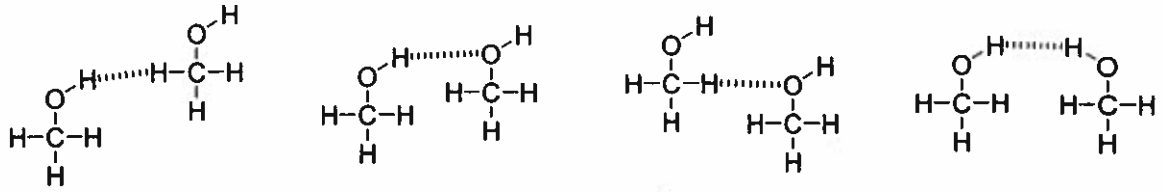
Table 2: Water solubility of selected ketones

Ketone	Structure	Water solubility, grams per 100 mL H_2O	Ketone	Structure	Water solubility, grams per 100 mL H_2O
acetone		∞	2-hexanone		1.4
2-butanone		25.6	2-heptanone		0.4
2-pentanone		4.3			

Exercises:

1. Consider the water solubilities of the ketones shown in Table 2. Are they consistent with your answer to CTQ 10? Write a sentence that generalizes how many nonpolar carbons can be dissolved by one polar functional group.

2. A hydrogen bond is usually depicted by a dashed or dotted line. Circle the picture that correctly represents a hydrogen bonding interaction.



3. Describe what is wrong with each of the other three pictures in Exercise 1.

4. Draw a representation of one water molecule participating in a hydrogen bond with another water molecule. Then place the symbols δ+ and δ− near each atom to indicate the polarity of the bonds.

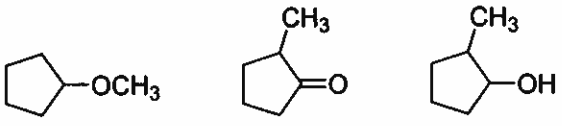
5. Without looking up any information in a table, identify the molecule in each group that would have the highest boiling point, and explain your answer.

   a. CH_3CH_2OH $CH_3CH_2CH_2OH$ $HOCH_2CH_2OH$

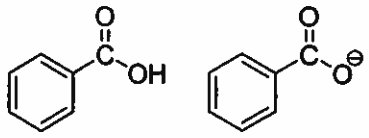
   b. $H_3C-\overset{\overset{O}{\|}}{C}-CH_3$ CH_3CH_2OH $CH_3CH_2NH_2$

   c. $H_3C-\overset{\overset{OH}{|}}{C}HCH_3$ $H_3C-\overset{\overset{OH}{|}}{C}HCH_2CH_2CH_3$ $CH_3CH_2-\overset{\overset{OH}{|}}{C}HCH_3$

   d. $CH_3CH_2NHCH_2CH_3$ $CH_3CH_2CH_2CH_2CH_3$ 

   e. 

6. Benzoate ion is very soluble in water, but benzoic acid is not. Based on this information which species do you think has a larger dipole moment—benzoic acid or benzoate? Explain.



benzoic acid benzoate

7. Read the assigned pages in your text, and work the assigned problems.