Carbon Compounds

Chemical Bonding

Part 2

Introduction to Functional Groups: Alkanes

- **Alkanes**

  Compounds that contain only carbons and hydrogens, with no double or triple bonds.

- **Alkyl Groups**

  A part of a compound that contain only carbons and hydrogens, with no double or triple bonds.

ALKANE	ALKYL GROUP	ABBREVIATION
CH_4 **Methane**	CH_3— **Methyl group**	Me—
CH_3CH_3 **Ethane**	CH_3CH_2— or C_2H_5— **Ethyl group**	Et—
$CH_3CH_2CH_3$ **Propane**	$CH_3CH_2CH_2$— **Propyl group**	Pr—
$CH_3CH_2CH_3$ **Propane**	CH_3CHCH_3 (CH$_3$ on CH) or CH_3CH(CH$_3$)— **Isopropyl group**	*i*-Pr—

These and others can be designated by **–R**

Introduction to Functional Groups: Alkanes

- **Alkene**

  Carbon-based compound that contains at least one double bond.

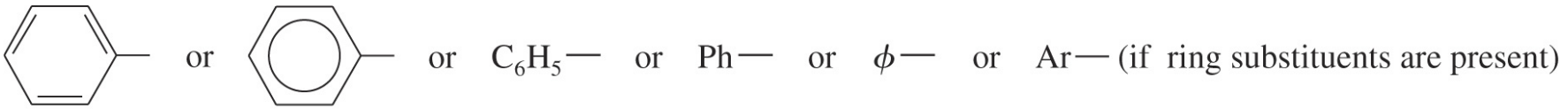
- **Alkyne**

  Carbon-based compound that contains at least one triple bond.

Aromatic Rings: Phenyl & Benzyl Groups

- **Phenyl group**

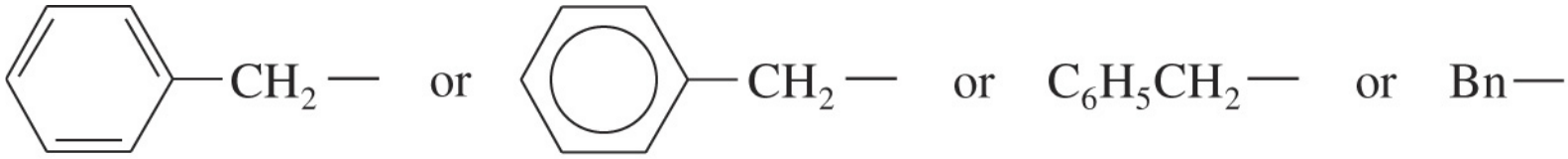
  benzene ring substituent



Ways of representing a phenyl group

- **Benzyl group**

  benzene ring with a -CH_2- bridge



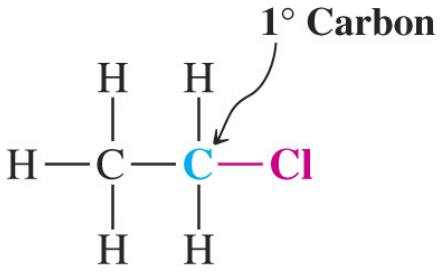
Ways of representing a benzyl group

Alkyl Halides and Degree of Substitution

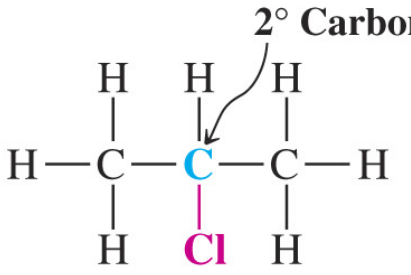
- Alkyl halide (Haloalkane)

  An alkane with a halide (Cl, F, Br, I) as a substituent.

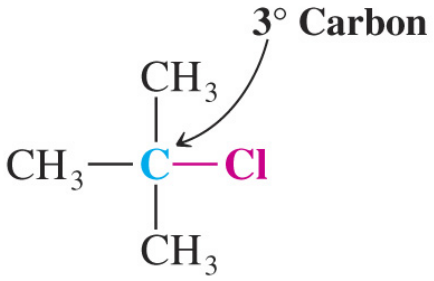
- Degrees of Substitution:
  - Primary (1°): carbon with the attached halide has only one other carbon attached to it.
  - Secondary (2°): carbon with the attached halide has only two other carbons attached to it.
  - Tertiary (3°): carbon with the attached halide has only three other carbons attached to it.



A 1° alkyl chloride



A 2° alkyl chloride

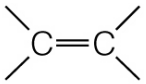
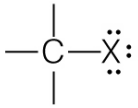
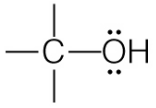
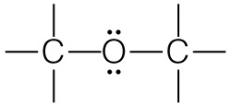
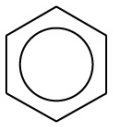


A 3° alkyl chloride

Other Functional Groups

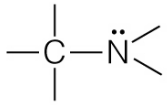
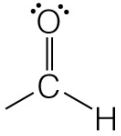
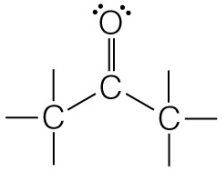
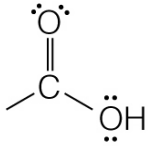
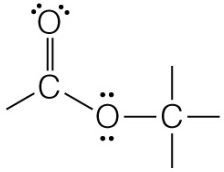
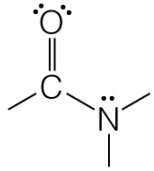
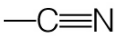
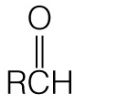
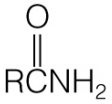
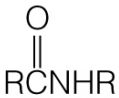
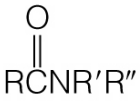
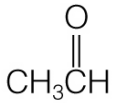
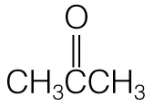
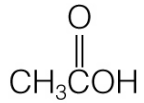
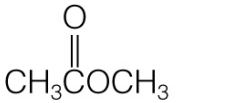
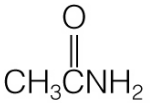
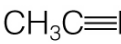
- Alcohols
- Ethers
- Amines
- Carbonyls:
  - Aldehydes
  - Carboxylic acids
  - Amides
  - Ketones
  - Esters
  - Acid chloride
- Nitriles
- Thiols
- Sulfides

Summary of Important Families of Organic Compounds

	Family						
	Alkane	**Alkene**	**Alkyne**	**Aromatic**	**Haloalkane**	**Alcohol**	**Ether**
Functional group	C—H and C—C bonds		—C≡C—	Aromatic ring			
General formula	RH	$RCH{=}CH_2$ RCH=CHR $R_2C{=}CHR$ $R_2C{=}CR_2$	RC≡CH RC≡CR	ArH	RX	ROH	ROR
Specific example	CH_3CH_3	$CH_2{=}CH_2$	HC≡CH		CH_3CH_2Cl	CH_3CH_2OH	CH_3OCH_3
IUPAC name	Ethane	Ethene	Ethyne	Benzene	Chloroethane	Ethanol	Methoxymethane
Common name[a]	Ethane	Ethylene	Acetylene	Benzene	Ethyl chloride	Ethyl alcohol	Dimethyl ether

[a]These names are also accepted by the IUPAC.

Summary of Important Families of Organic Compounds

Family						
Amine	**Aldehyde**	**Ketone**	**Carboxylic Acid**	**Ester**	**Amide**	**Nitrile**
						
RNH_2 R_2NH R_3N					  	RCN
CH_3NH_2						
Methanamine	Ethanal	Propanone	Ethanoic acid	Methyl ethanoate	Ethanamide	Ethanenitrile
Methylamine	Acetaldehyde	Acetone	Acetic acid	Methyl acetate	Acetamide	Acetonitrile

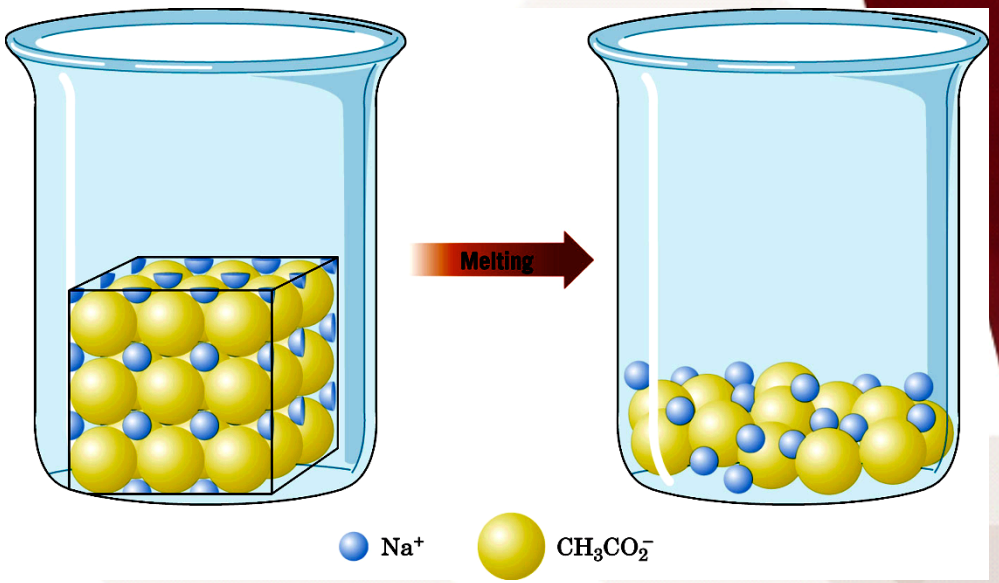
IM forces - Definition

- Intermolecular (IM) forces are the electrical attractions between atoms, molecules, and ions that hold solids and liquids together.

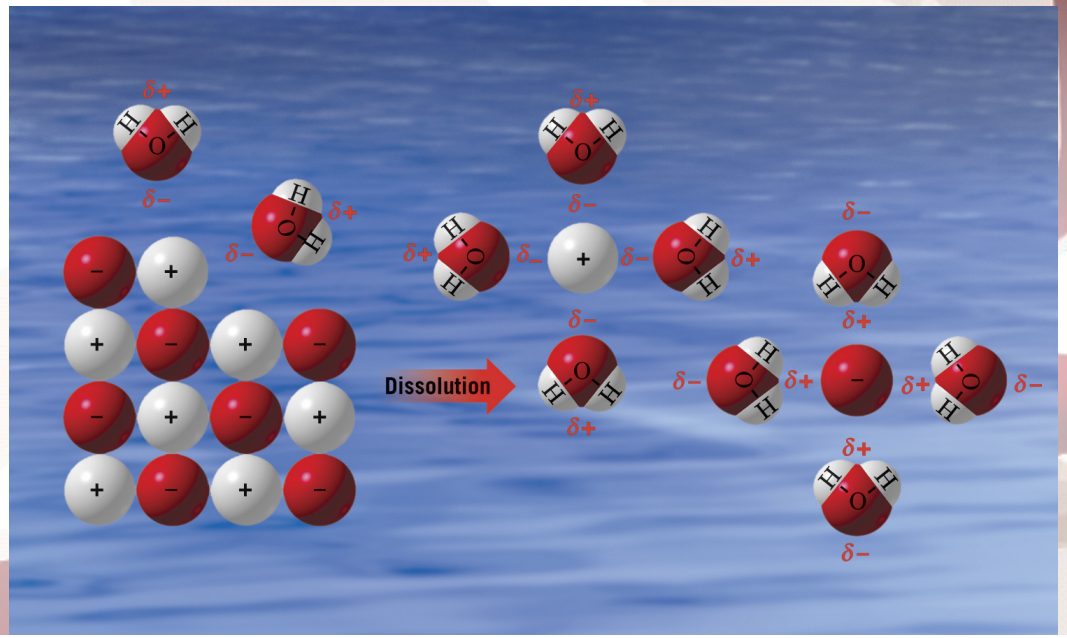
- Intermolecular forces also play a part in the solubilities of substances.

Ions & IM forces

- **Ion – Ion Forces:**
  - Strong attraction of positive and negative ions.
  - Example: Sodium acetate

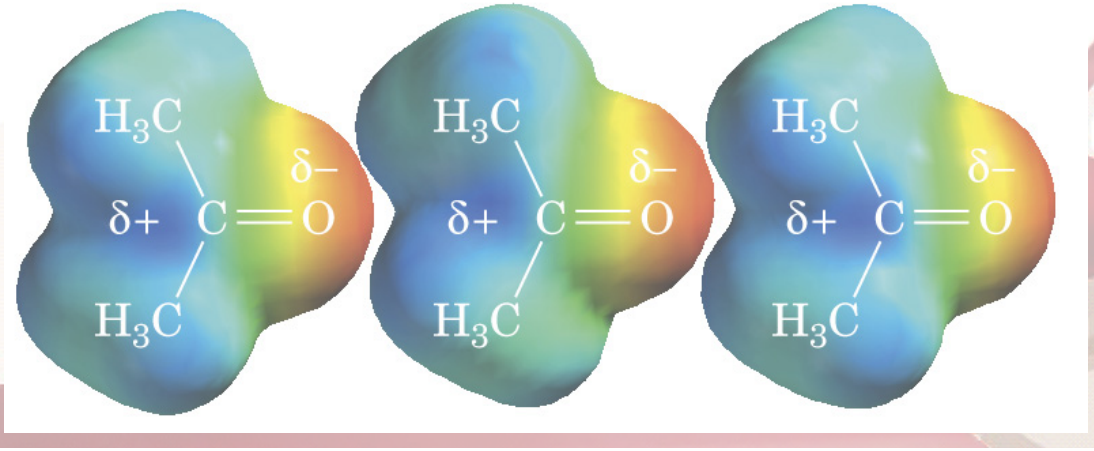


- **Ion-dipole forces:**
  - Attraction of an ion to one side of a polar molecule.
  - This interaction allows water to easily dissolve many ions.



Dipole-Dipole forces

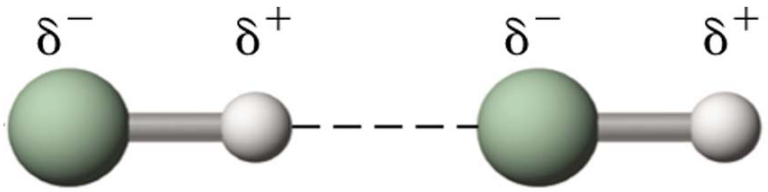
- Attraction of the oppositely charged sides of permanent dipoles.
- There is an interaction between δ+ and δ- areas in each molecule.
- These are much weaker than ion-ion forces.
- Molecules align to maximize attraction of δ+ and δ- parts of molecules
- May occur between molecules of the same or different compounds.
- *Example: acetone*



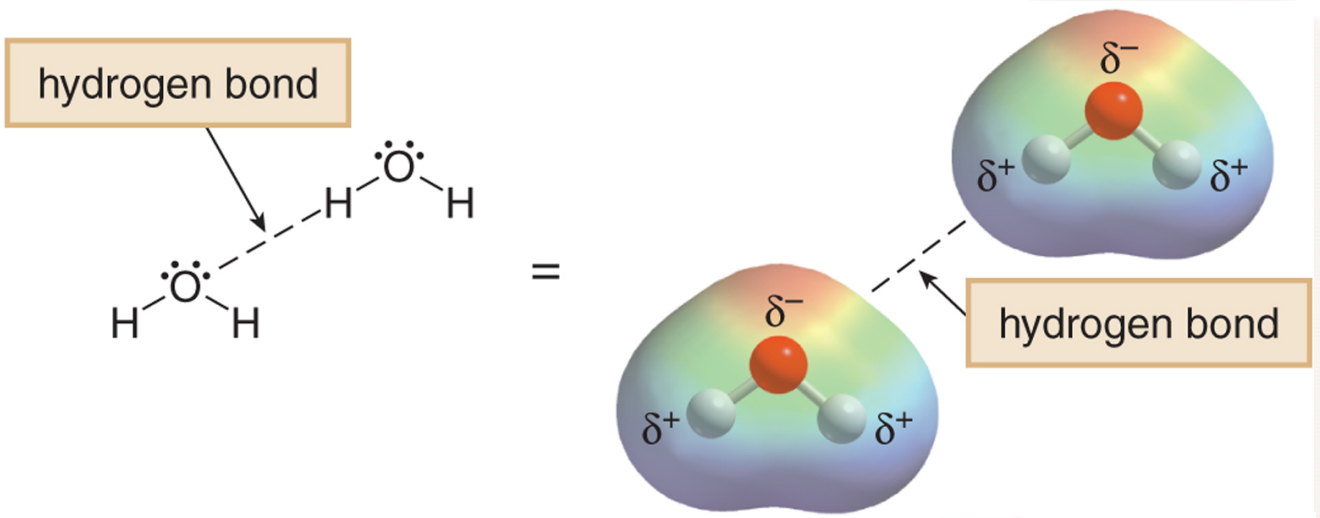
Dipole – dipole special case: Hydrogen bonding

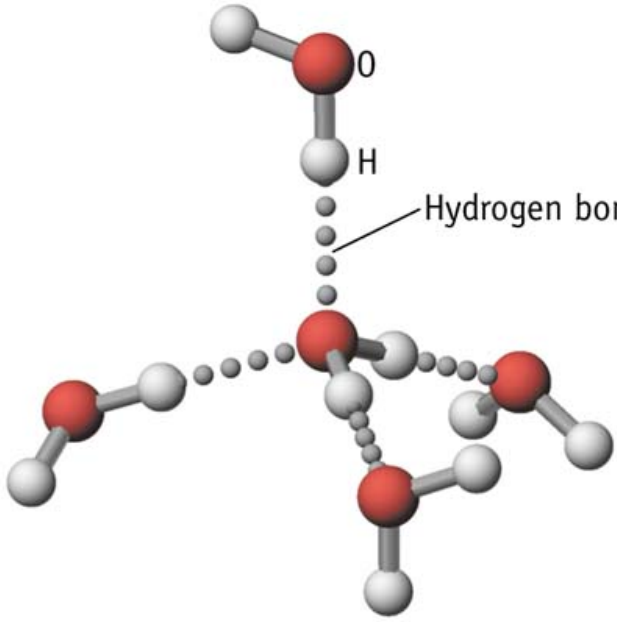
- A hydrogen bond is an especially strong dipole-dipole interaction. This is not a "bond" like a covalent bond.

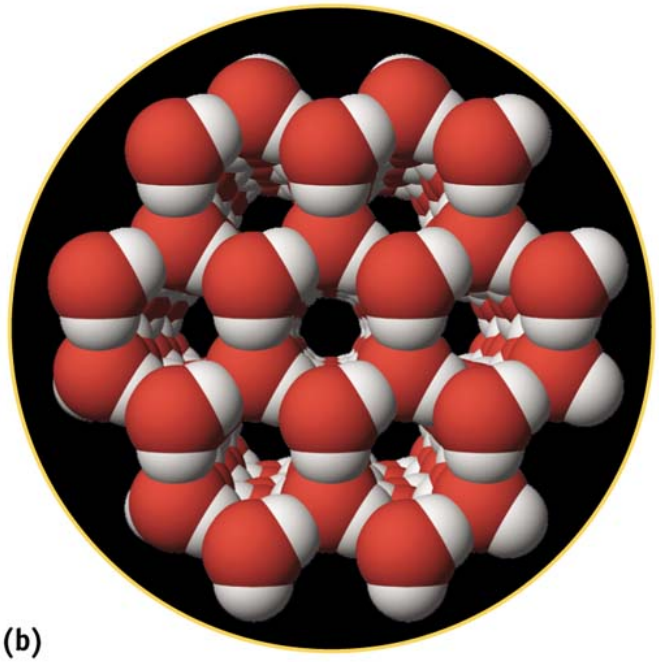
- Occurs when hydrogen is covalently bound to N, O, or F (all small, very electronegative atoms) and has a dipole-dipole interaction with a highly electronegative atom that has a lone pair. (usually another N, O, or F atom in a compound) .



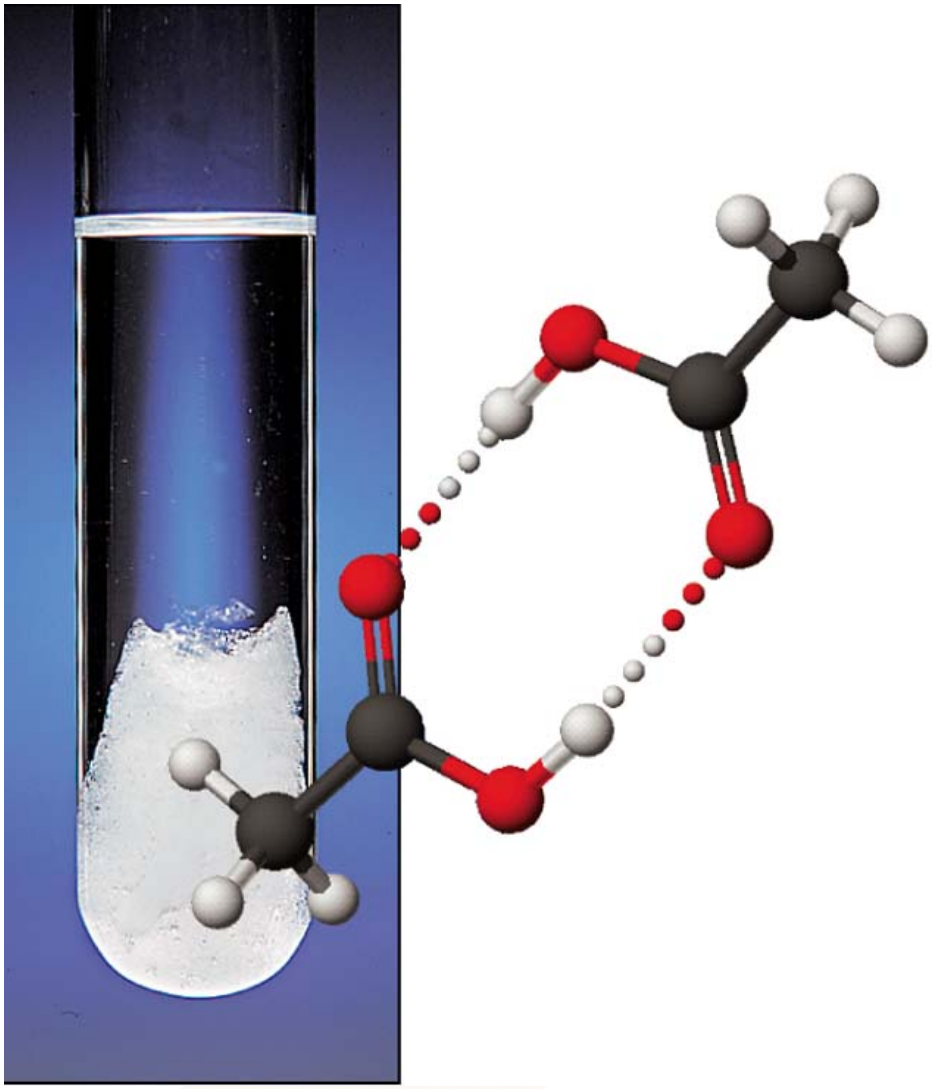
Hydrogen Bonding in Water





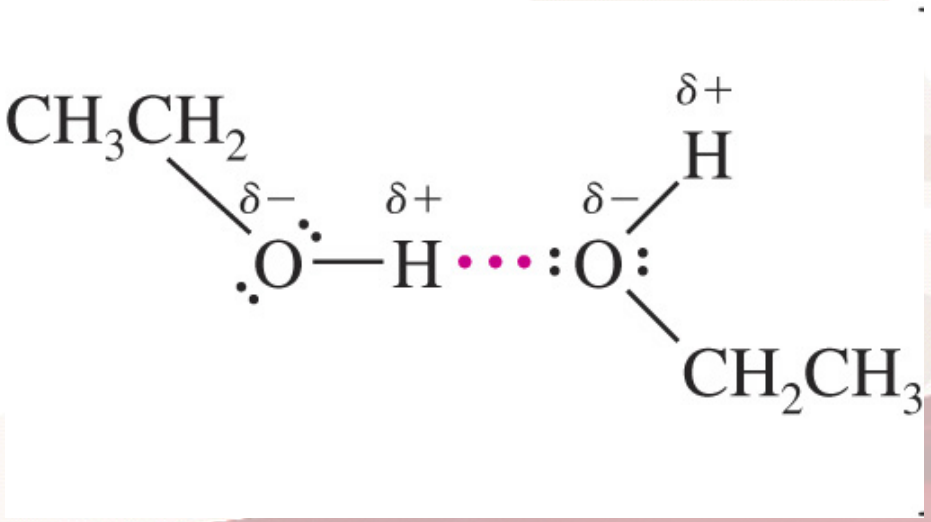


Hydrogen Bonding in Acetic Acid

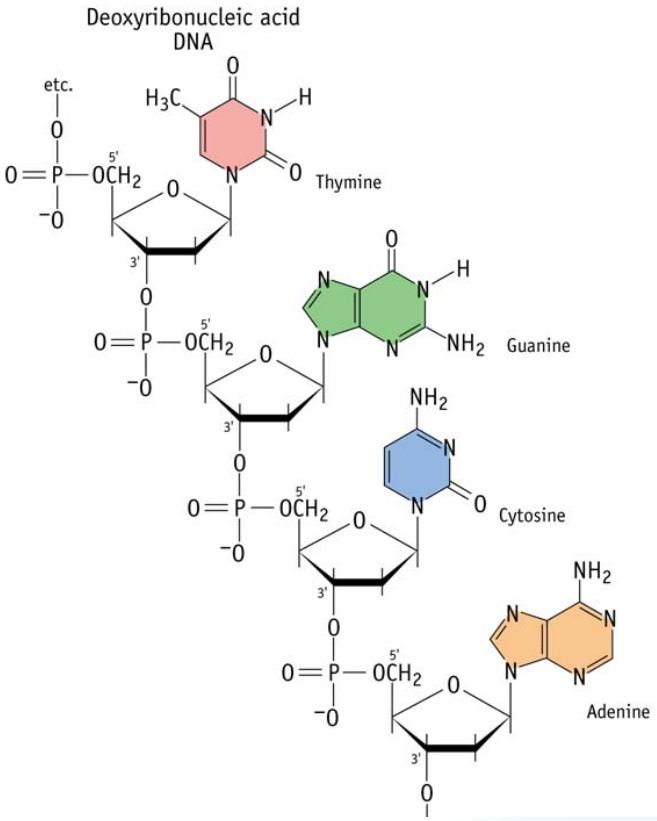


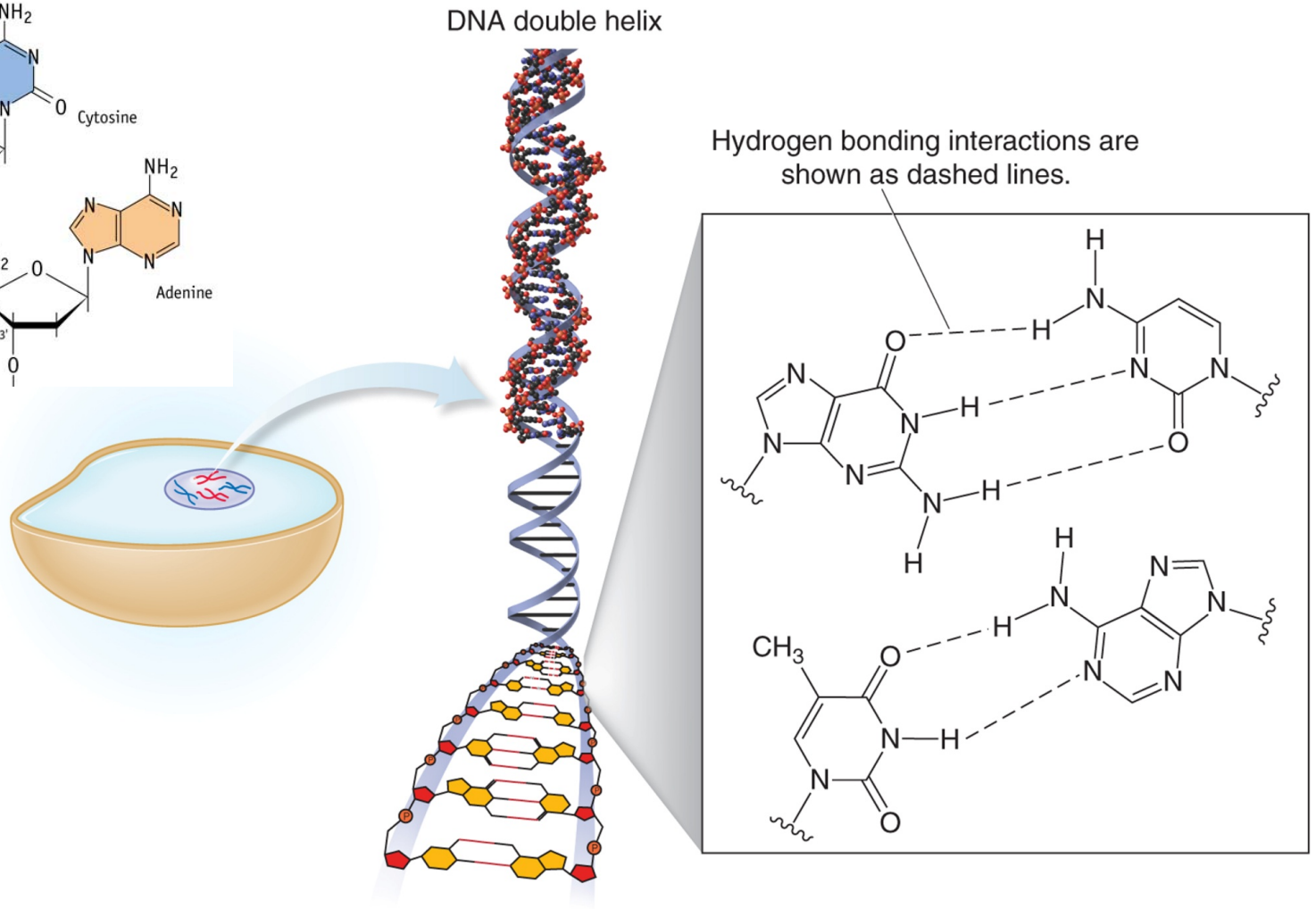
Consequences of H-bonding

- Ethanol (CH_3CH_2OH) has a boiling point of +78.5°C
- An isomer - methyl ether (CH_3OCH_3) - has a boiling point of -24.9°C
- Ethanol molecules are held together by hydrogen bonds.
- Methyl ether molecules are held together only by weaker dipole-dipole interactions



H-bonding in DNA





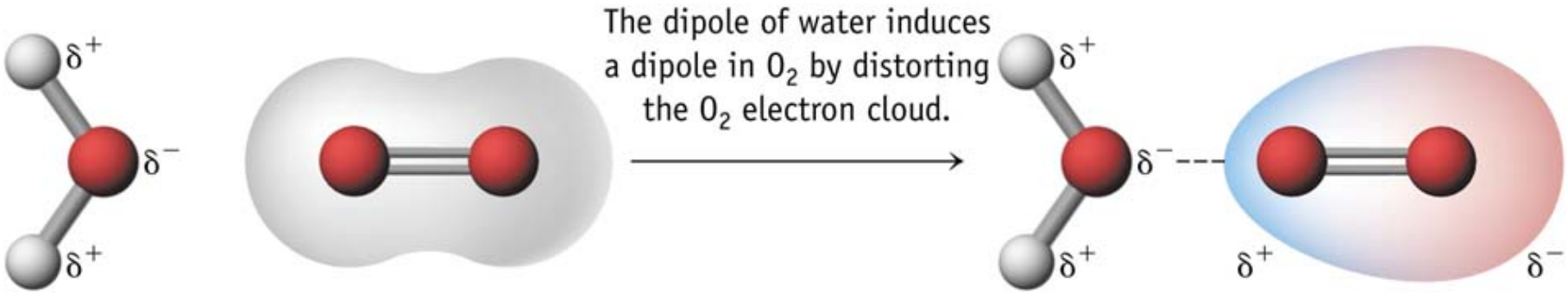
Induced dipoles

- Neutral, non-polar molecules can have a temporary, uneven distribution of their electrons. This is called an induced dipole.

- Forces between molecules that arise from these temporary dipoles are called ***van der Waal's forces***, **London forces**, or **dispersion forces**.

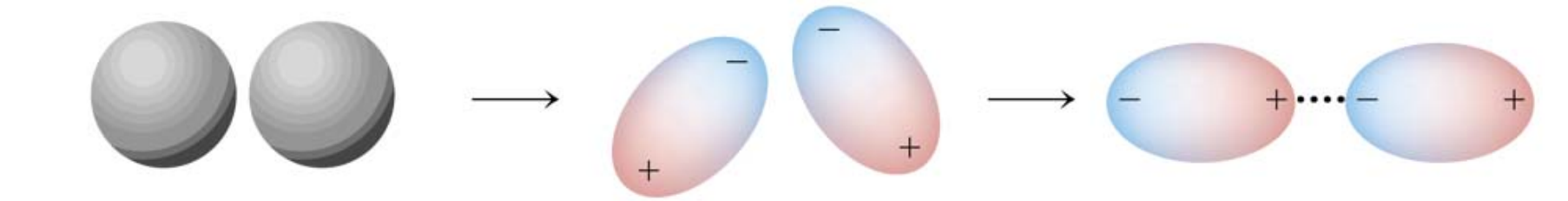
Dipole – induced dipole

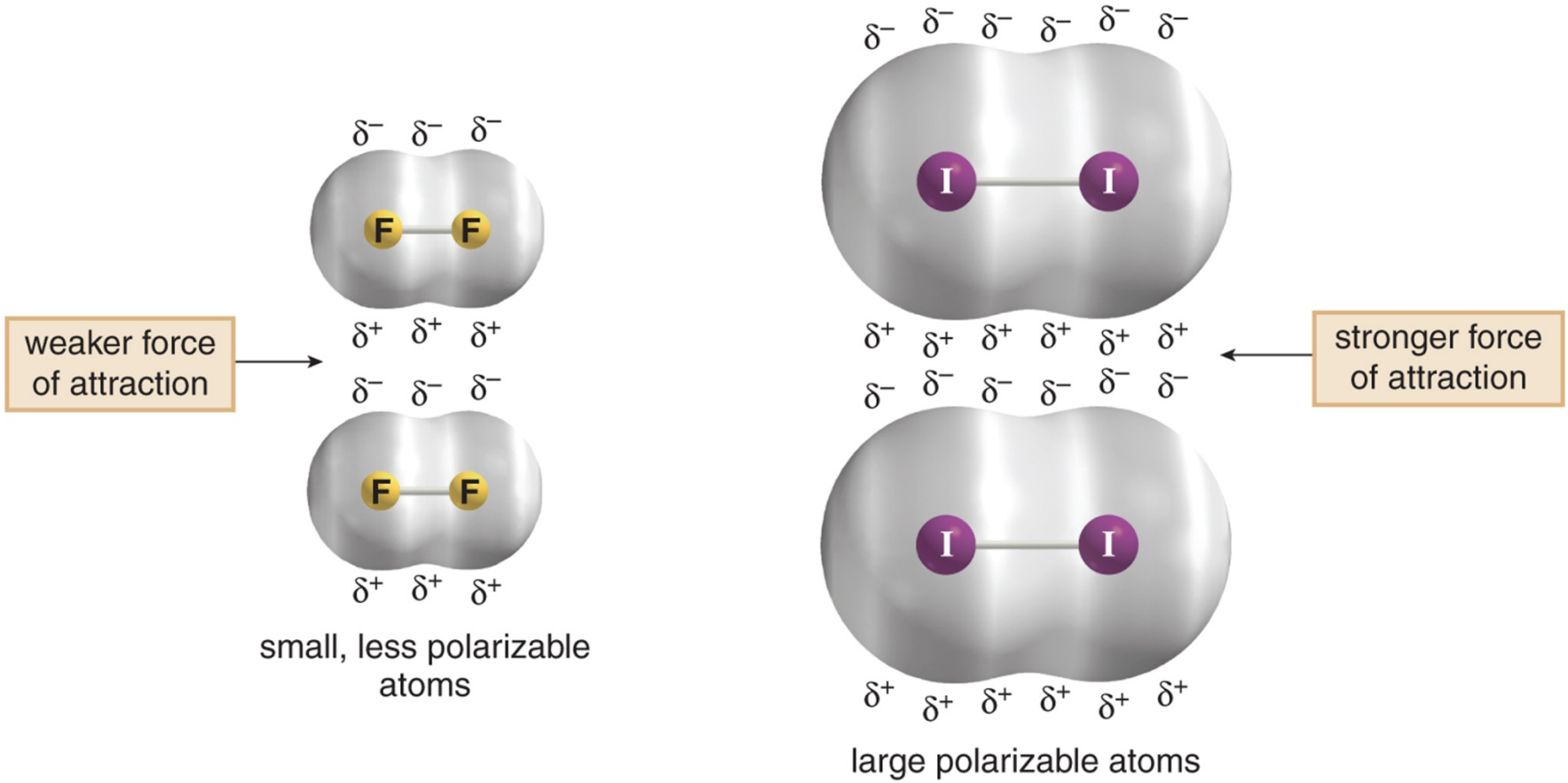
- Occurs when a permanent dipole causes a non-polar species to polarize, forming a temporary dipole.
- This is a weak interaction.
- This phenomenon allows non-polar molecular to dissolve slightly in polar solvents (and vice-versa).



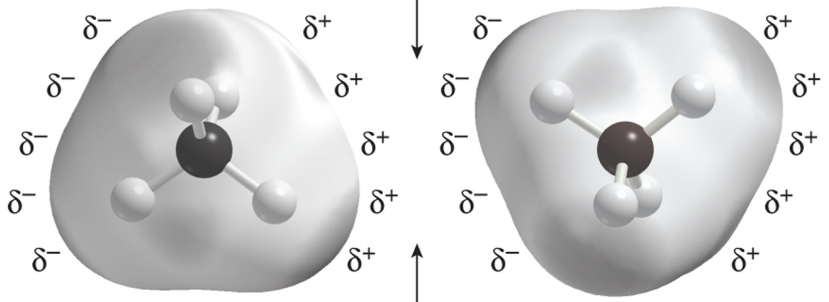
Induced dipole – induced dipole

- Also called London or Dispersion forces.
- These forces occur when a temporary dipole forms by chance in one molecule and induces a dipole in a second.
- This is a weak interaction.




weaker force of attraction
δ− δ− δ−
F F
δ+ δ+ δ+
δ− δ− δ−
F F
δ+ δ+ δ+
small, less polarizable atoms
δ− δ− δ− δ− δ− δ−
I I
δ+ δ+ δ+ δ+ δ+ δ+
δ− δ− δ− δ− δ− δ−
I I
δ+ δ+ δ+ δ+ δ+ δ+
large polarizable atoms
stronger force of attraction

van der Waals interaction between two CH_4 molecules



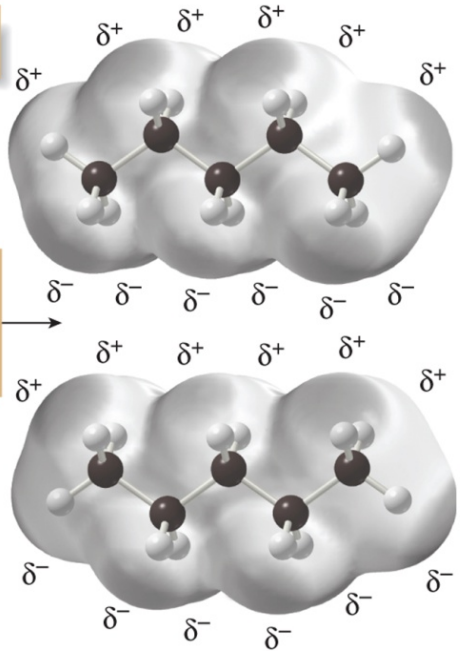
Unsymmetrical electron density creates a temporary dipole.

A long, cylindrical molecule

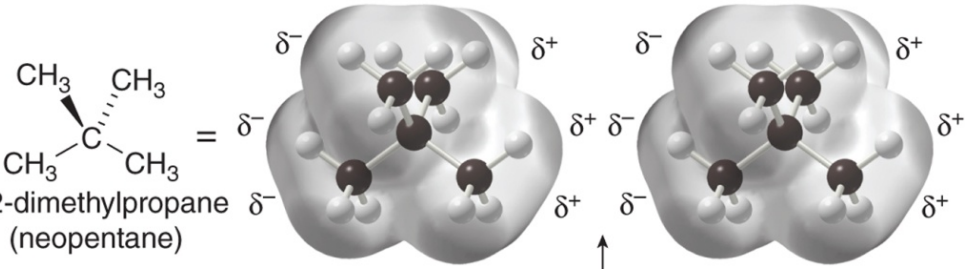
$CH_3CH_2CH_2CH_2CH_3$ = pentane

larger surface area

stronger van der Waals interactions



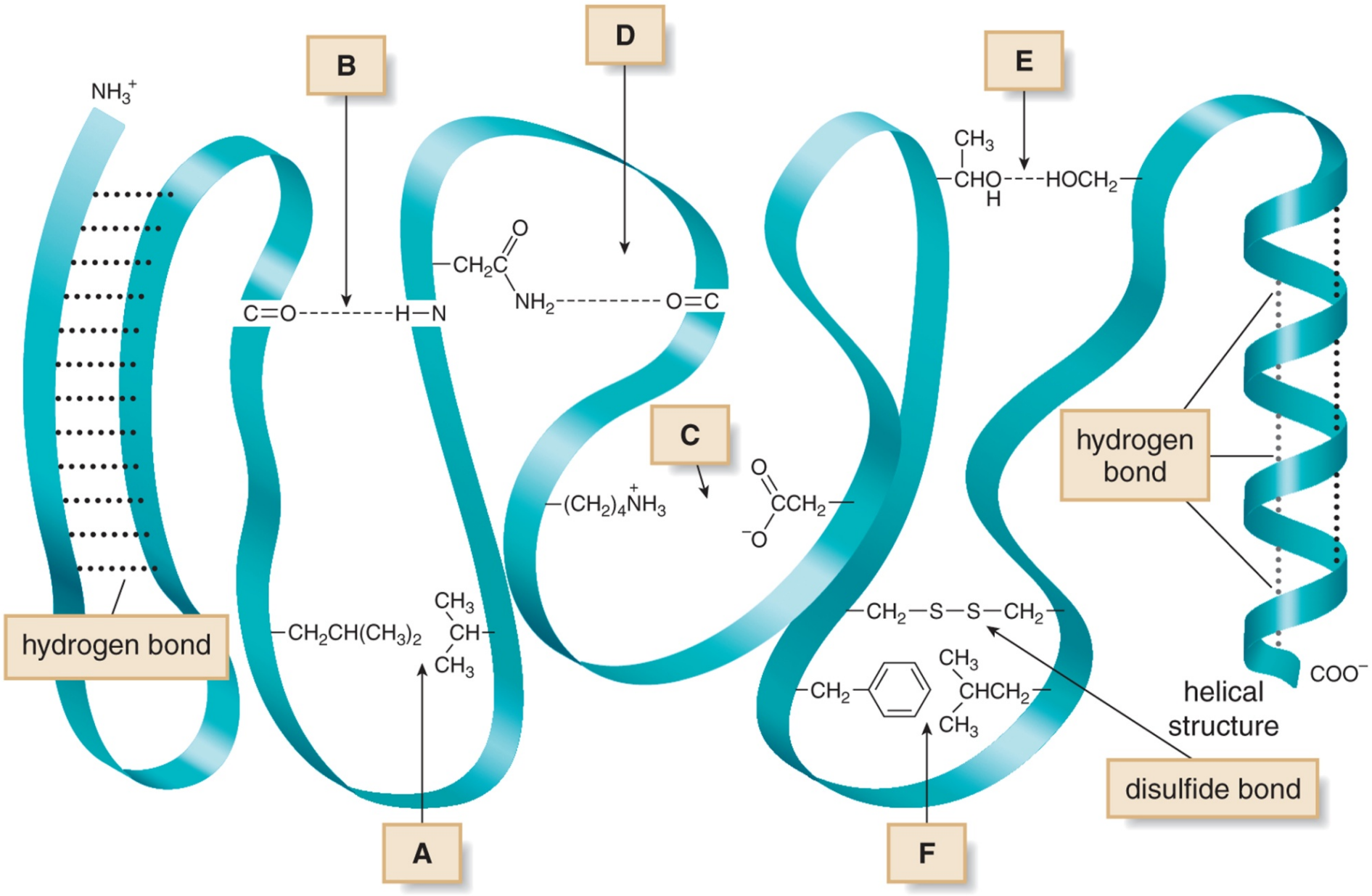
A compact, spherical molecule



2,2-dimethylpropane (neopentane)

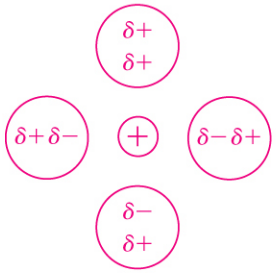
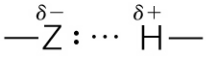
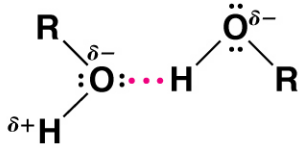
smaller surface area

weaker van der Waals interactions


B
D
E
C
A
F
hydrogen bond
hydrogen bond
disulfide bond
helical structure
NH_3^+
$C{=}O\cdots\cdots H{-}N$
$-CH_2C(=O)NH_2\cdots\cdots O{=}C$
$-(CH_2)_4\overset{+}{N}H_3$
$-CH_2CH(CH_3)_2$
$-CH(CH_3)_2$
$-CH_2{-}S{-}S{-}CH_2-$
$-CH_2C_6H_5$
$-CH_2CH(CH_3)_2$
$-CH(CH_3)CH_2O\cdots\cdots HOCH_2-$
$-CH_2CO_2^-$
COO^-

Inter- and Intra-molecular forces

- **Order of Strength:** Ionic bonds > Covalent bonds > Ion-dipole > Hydrogen Bonds > Dipole-Dipole > van der Waal's forces

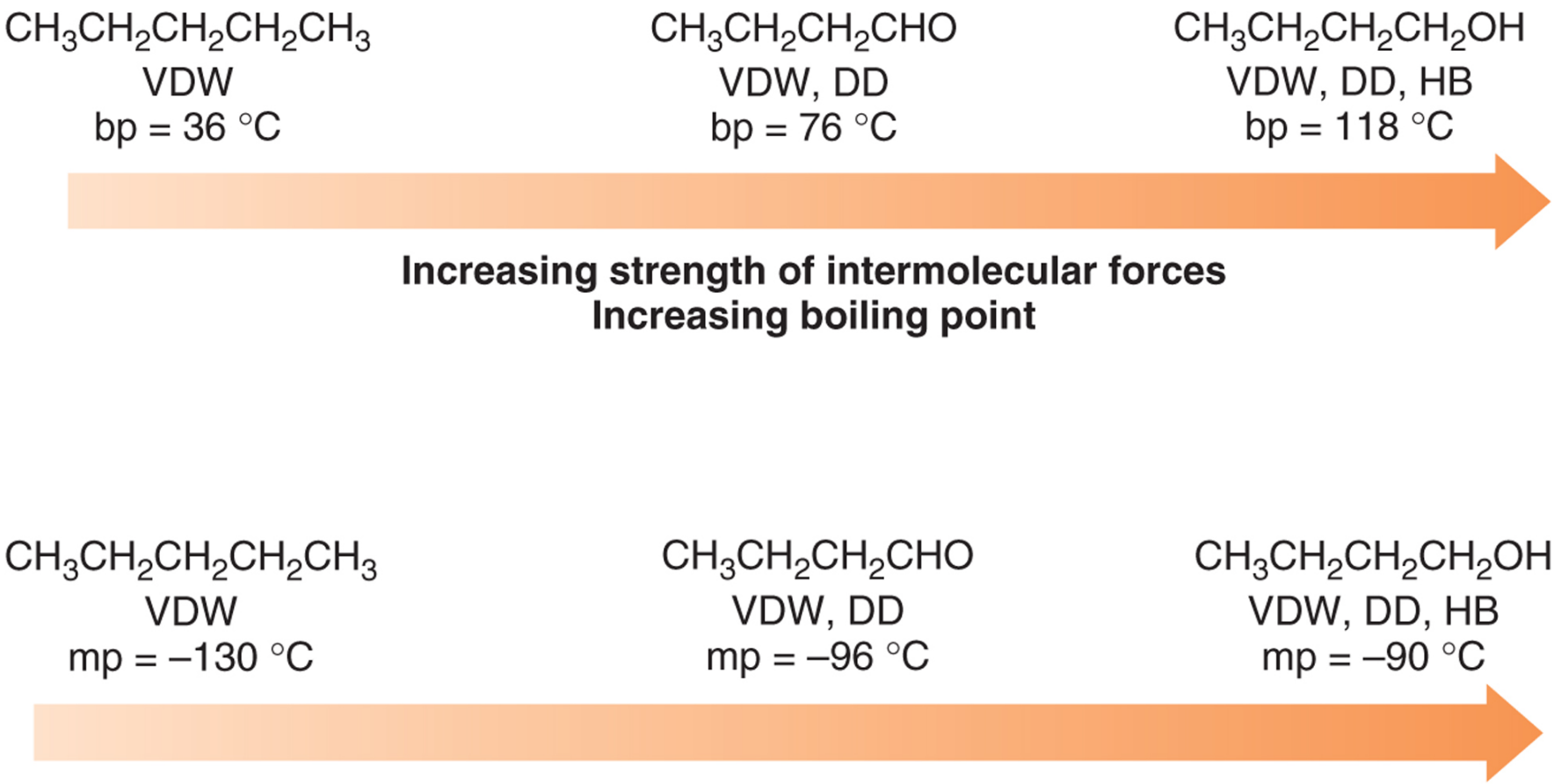
Electric Force	Relative Strength	Type	Example
Cation–anion (in a crystal)	Very strong		Lithium fluoride crystal lattice
Covalent bonds	Strong (140–523 kJ mol^{-1})	Shared electron pairs	H—H (436 kJ mol^{-1}) CH_3—CH_3 (378 kJ mol^{-1}) I—I (151 kJ mol^{-1})
Ion–dipole	Moderate		Na^+ in water (see Fig. 2.9)
Dipole–dipole (including hydrogen bonds)	Moderate to weak (4–38 kJ mol^{-1})		 and
van der Waals	Variable	Transient dipole	Interactions between methane molecules

Intermolecular interactions and physical properties

- **Consider Boiling Point – there are 2 major influences on the BP of compounds:**
  - Molar mass effects
  - Intermolecular interactions

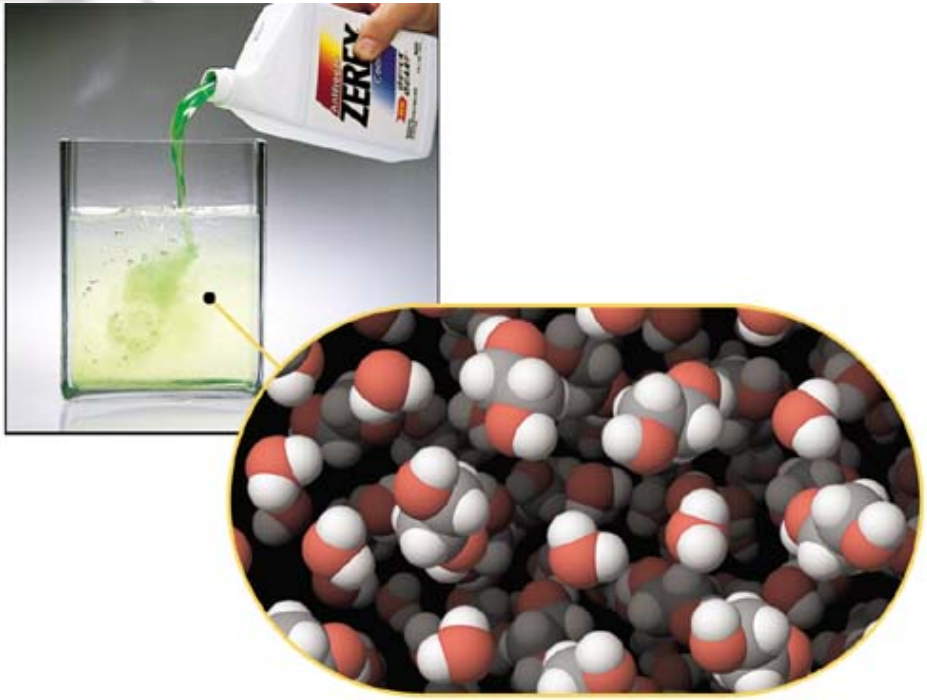
- All things being equal larger and heavier molecules have higher boiling points.
  - Larger molecules need more energy to escape the surface of the liquid.
  - Larger organic molecules tend to have more surface area in contact with each other and so have stronger van der Waals interactions.
  - Branching decreases van der Waal's interactions.

Compound	Molar Mass (g/mol)	ΔH°_{vap} (kJ/mol)†	Boiling Point (°C) (Vapor pressure = 760 mm Hg)
Nonpolar Compounds			
CH_4 (methane)	16.0	8.2	−161.5
C_2H_6 (ethane)	30.1	14.7	−88.6
C_3H_8 (propane)	44.1	19.0	−42.1
C_4H_{10} (butane)	58.1	22.4	−0.5

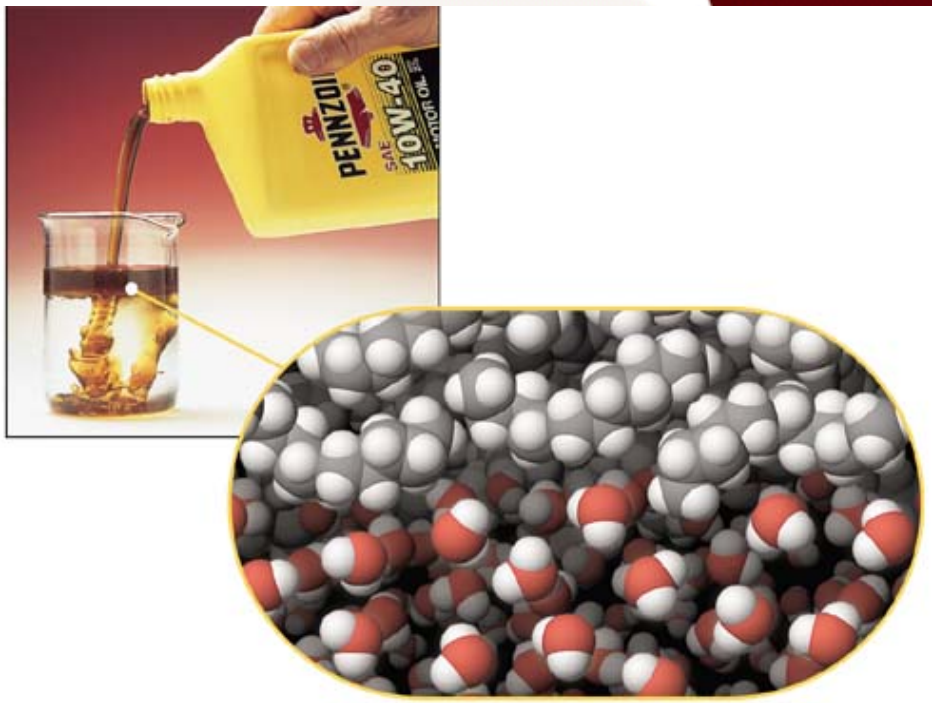

$CH_3CH_2CH_2CH_2CH_3$
VDW
bp = 36 °C
$CH_3CH_2CH_2CHO$
VDW, DD
bp = 76 °C
$CH_3CH_2CH_2CH_2OH$
VDW, DD, HB
bp = 118 °C
Increasing strength of intermolecular forces
Increasing boiling point

$CH_3CH_2CH_2CH_2CH_3$
VDW
mp = –130 °C
$CH_3CH_2CH_2CHO$
VDW, DD
mp = –96 °C
$CH_3CH_2CH_2CH_2OH$
VDW, DD, HB
mp = –90 °C
Increasing strength of intermolecular forces
Increasing melting point

Solubility: *like dissolves like*

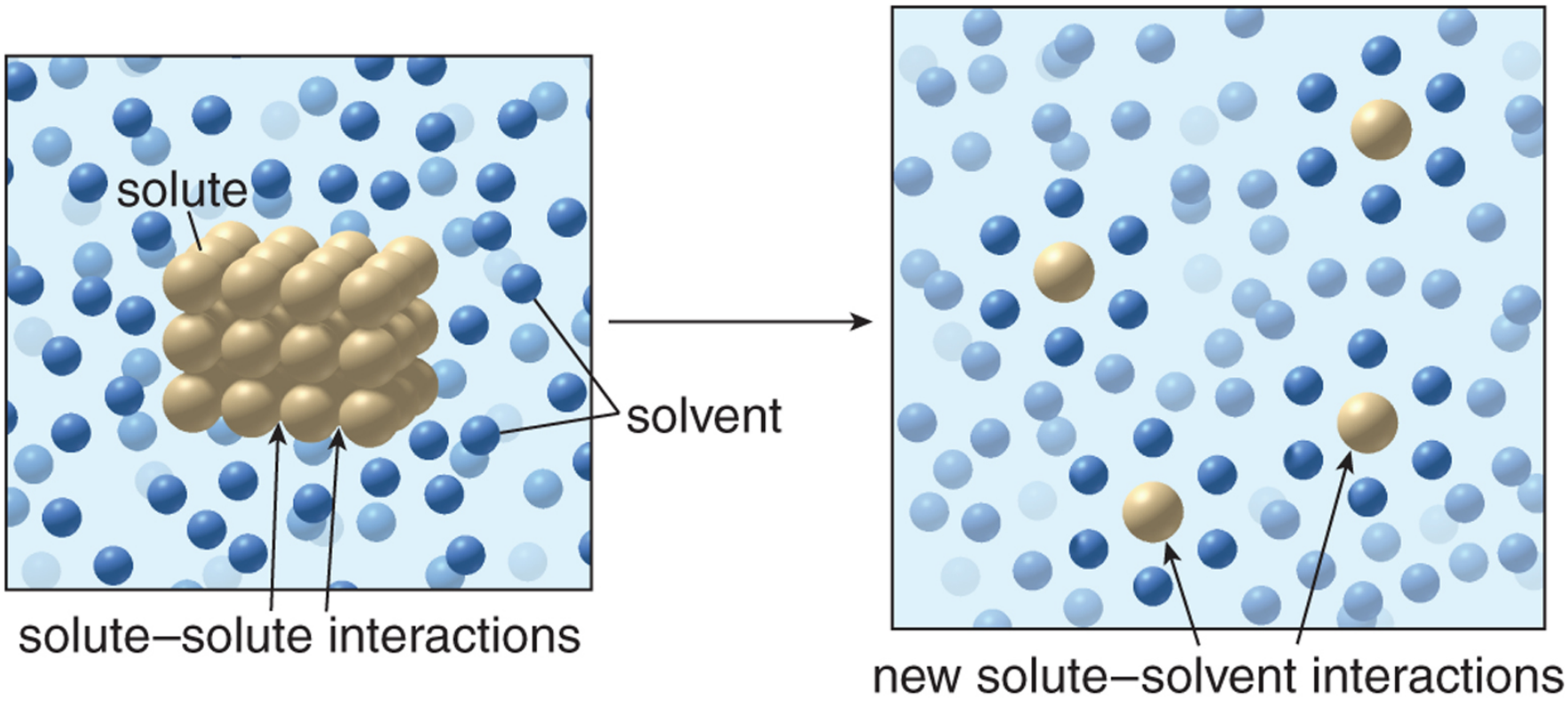


(a) Ethylene glycol ($HOCH_2CH_2OH$), a polar compound used as antifreeze in automobiles, dissolves in water.

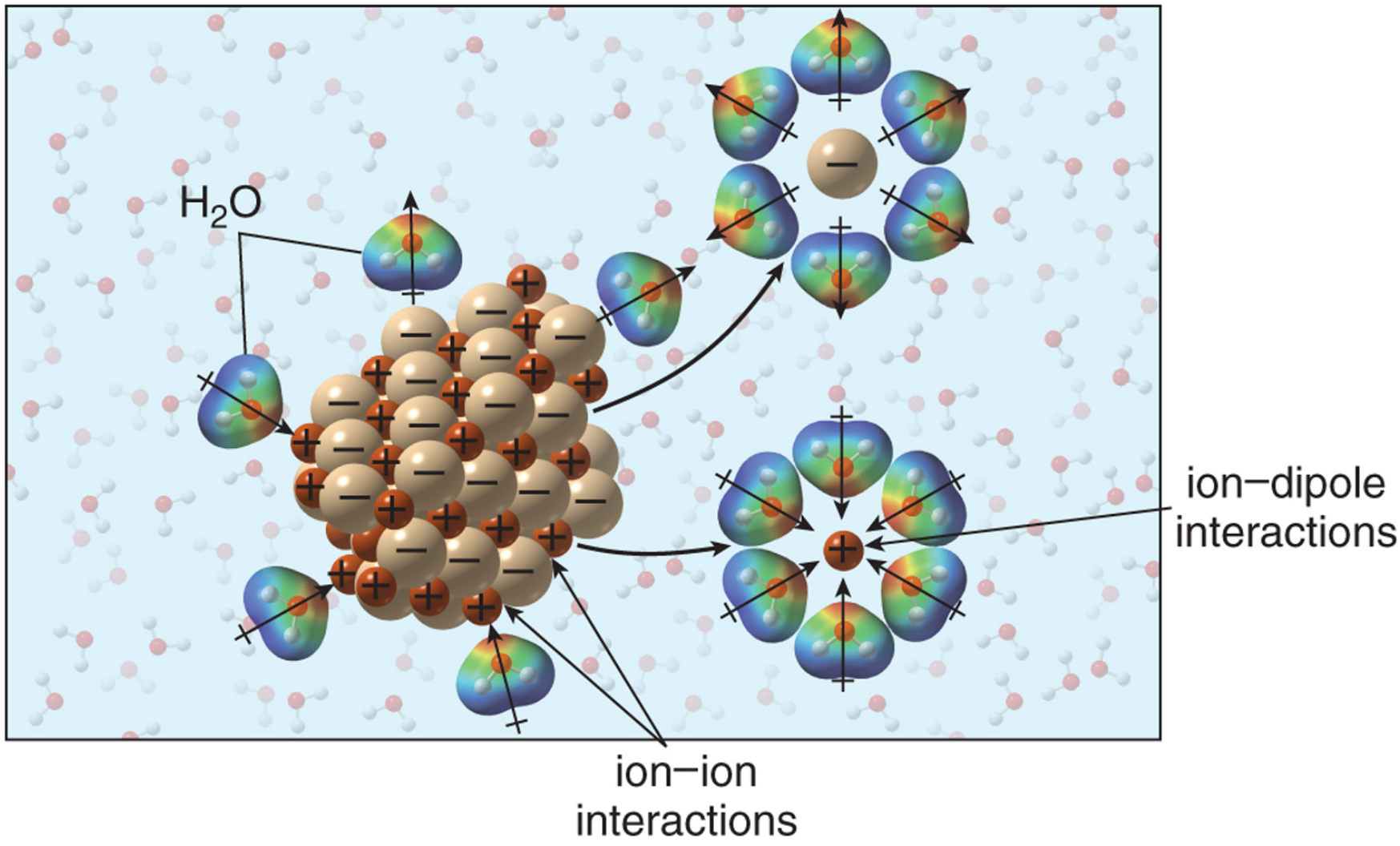


(b) Nonpolar motor oil (a hydrocarbon) dissolves in nonpolar solvents such as gasoline or CCl_4. It will not dissolve in a polar solvent such as water, however. Commercial spot removers use nonpolar solvents to dissolve oil and grease from fabrics.

- Hydrophilic – water loving
- Hydrophobic – water fearing

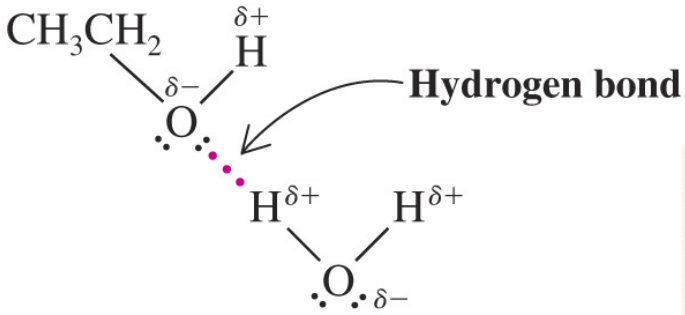


Energy comes from the new interactions of the solute with the solvent.

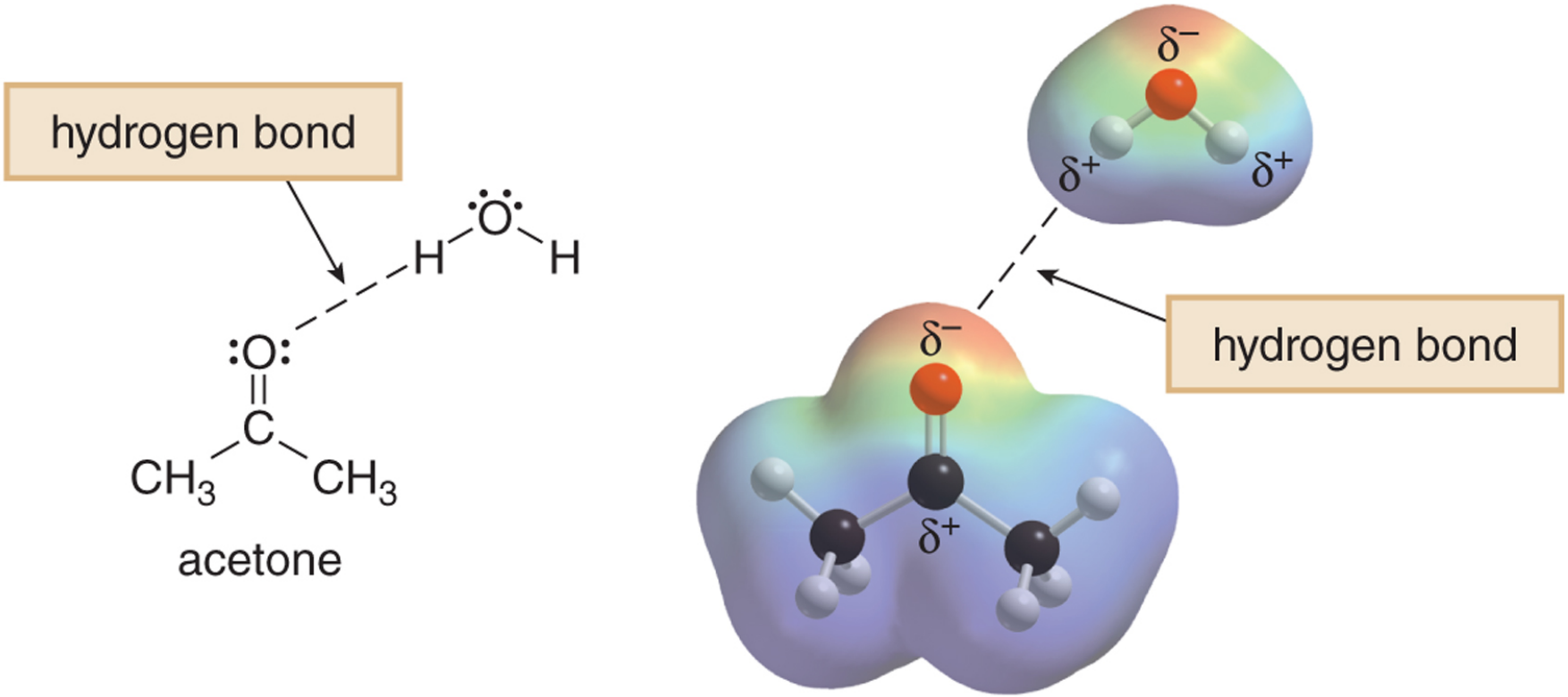

H_2O
ion–dipole
interactions
ion–ion
interactions

Solubility of organic molecules in water

- Generally like dissolves like:
  - Polar solvents tend to dissolve polar solids or polar liquids
- Ethanol dissolves in water in all proportions.



- Many small organic molecules with polar groups are water soluble. The following guidelines for these compounds may be helpful.
  - 1-3 carbons – soluble in water
  - 4-5 carbons – borderline
  - 6 or more carbons – not soluble in water.
- Multiple polar functionality can make larger organic molecules soluble in water.

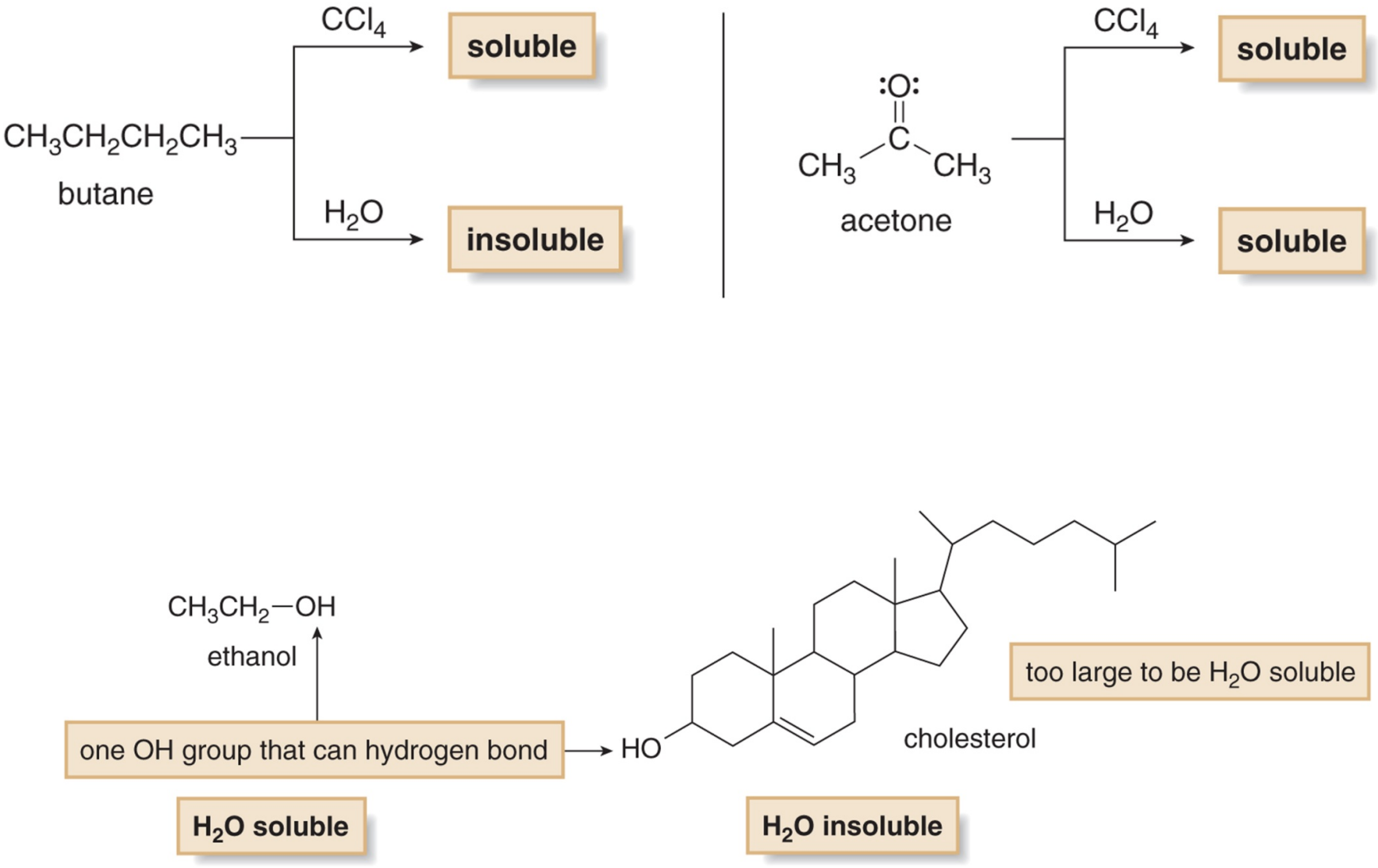


Hydrogen bonding makes the small polar molecule acetone H_2O soluble.

Solubility of organic molecules in water

- A large alkyl group can overwhelm the ability of the polar group to solubilize a molecule in water.

- Decyl alcohol is only slightly soluble in water.
  - The large alkyl portion is hydrophobic and overwhelms the capacity of the hydrophilic hydroxyl group.

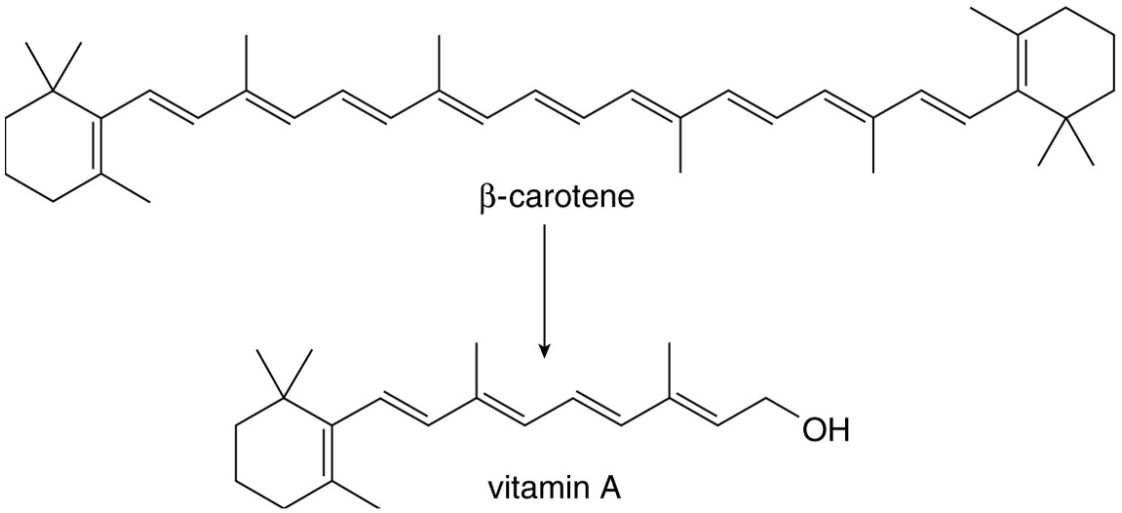

CCl4
soluble
CH3CH2CH2CH3
butane
H2O
insoluble
:O:
C
CH3
CH3
acetone
CCl4
soluble
H2O
soluble
CH3CH2—OH
ethanol
one OH group that can hydrogen bond
H2O soluble
HO
too large to be H2O soluble
cholesterol
H2O insoluble

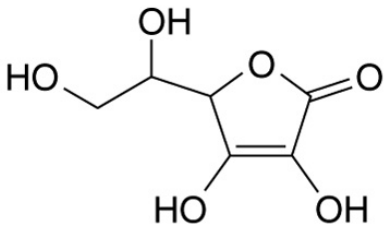
Solubility of organic compounds

- Organic molecules with no polar groups do not dissolve readily in water.
- Non-polar organic molecules dissolve very well in other non-polar organic compounds used as solvents.
- Polar organic molecules and non-polar organic molecules have varying solubilities in one another based on the polarity of functional groups and size of hydrophobic groups.

Application—Vitamins

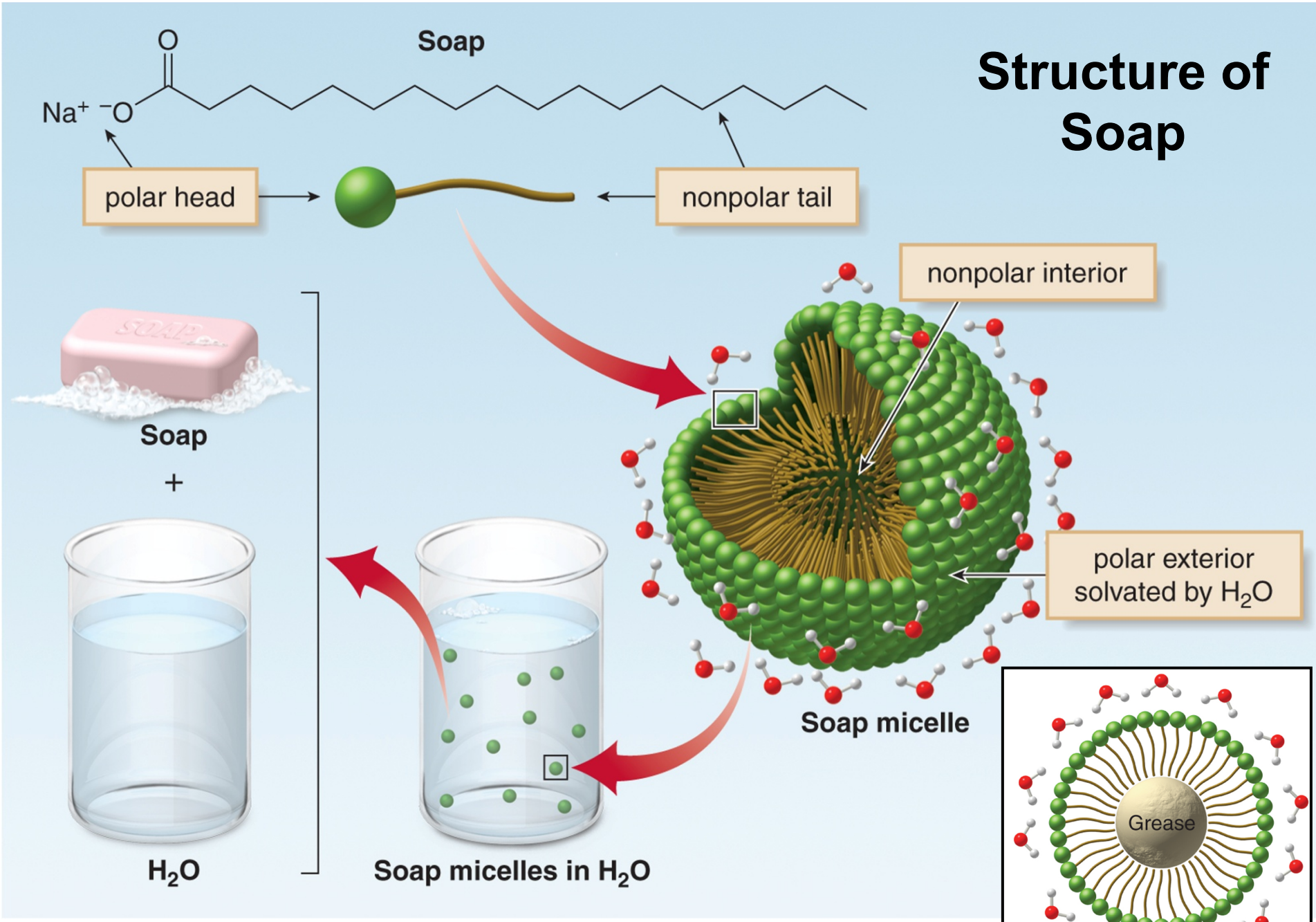
- Vitamins are organic compounds needed in small amounts for normal cell function.
- Most cannot be synthesized in our bodies, and must be obtained from the diet.
- Most are identified by a letter, such as A, C, D, E, and K.
- Vitamins can be fat soluble or water soluble depending on their structure.

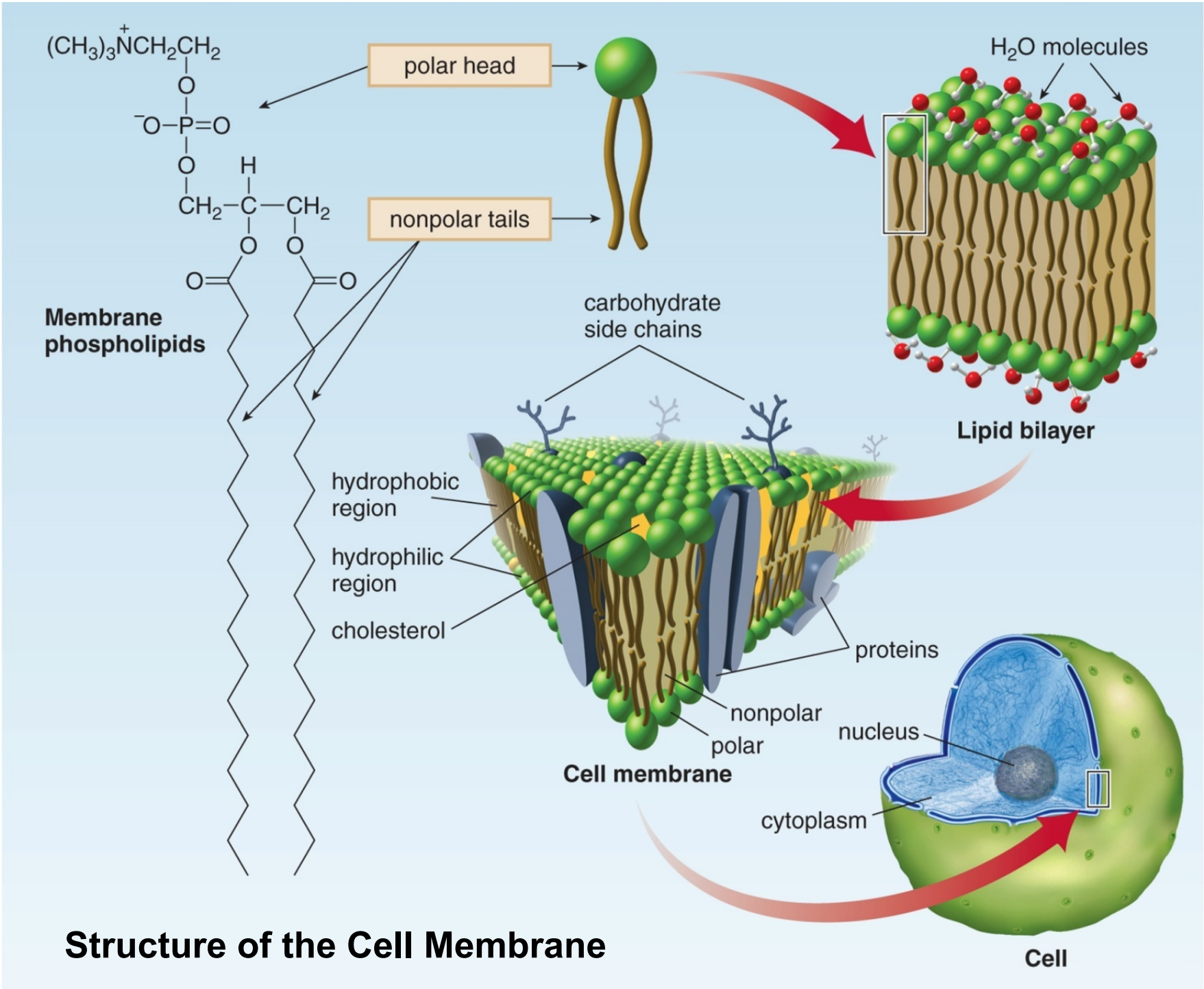




vitamin C
(ascorbic acid)

Structure of Soap

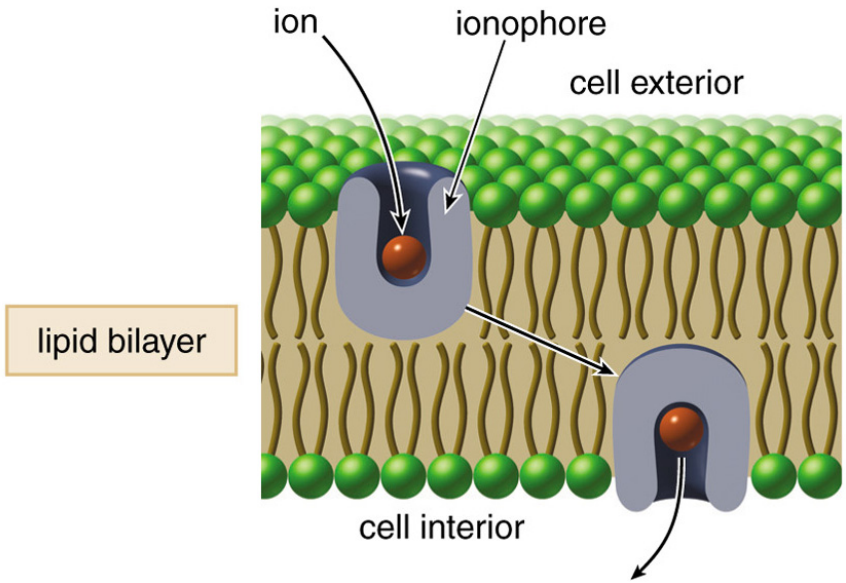




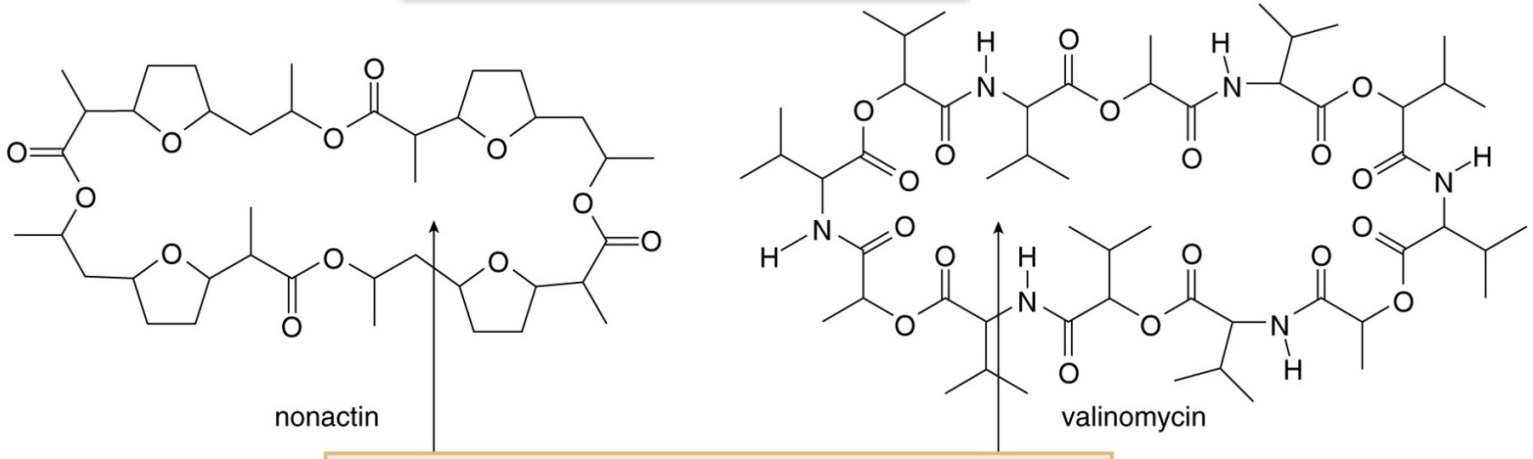
Structure of the Cell Membrane

Transport Across The Cell Membrane

- An ionophore transports an ion across a cell membrane (from the side of higher concentration of the ion to a side of lower ion concentration).



Naturally occurring antibiotic ionophores

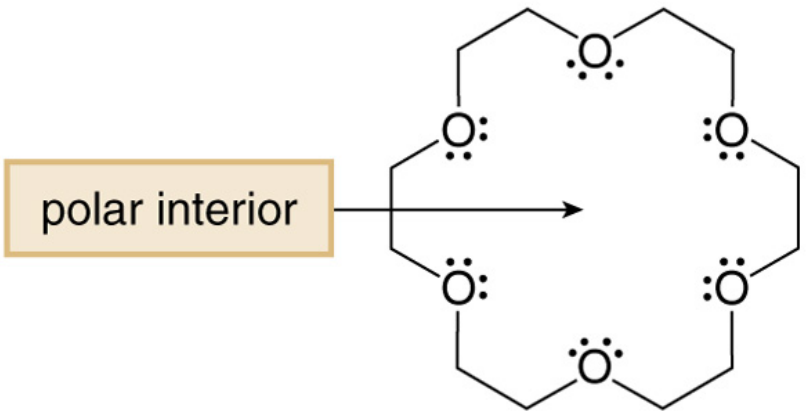


Each molecule contains a large central cavity to hold a cation.

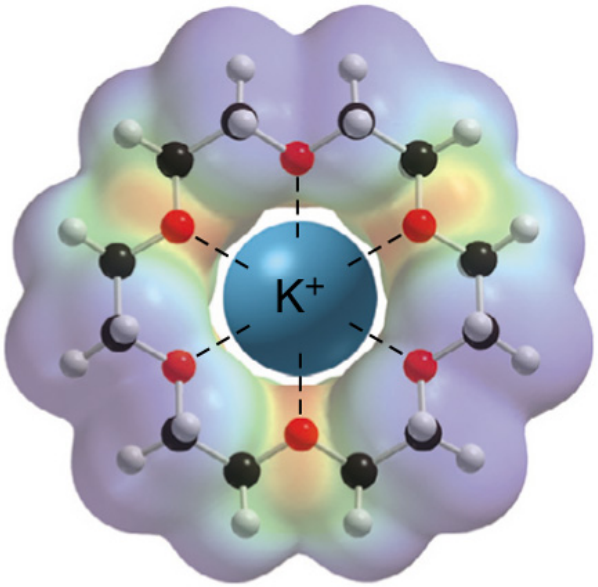
Crown Ethers

- **Several synthetic ionophores have also been prepared, including one group called crown ethers.**

- **Crown ethers are cyclic ethers containing several oxygen atoms that bind specific cations depending on the size of their cavity.**



18-crown-6



complex with K^+