Hogeschool van Arnhem en Nijmegen
HAN University of Applied Sciences

Course bi5b chemistry: proteomics



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Eigen werk auteur (c) Dr. Ing. P.J. de Groot

Reference

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Fundamentals of General, Organic, and Biological

Chemistry

Seventh Edition

John McMurry
Cornell University

David S. Ballantine
Northern Illinois University

Carl A. Hoeger
University of California, San Diego

Virginia E. Peterson
University of Missouri, Columbia

PEARSON

Boston Columbus Indianapolis New York San Francisco Upper Saddle River
Amsterdam Cape Town Dubai London Madrid Milan Munich Paris Montréal Toronto
Delhi Mexico City São Paulo Sydney Hong Kong Seoul Singapore Taipei Tokyo

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(Reference: First page in McMurry et al.)

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Refresh your knowledge

10.12 Some Common Acid–Base Reactions

10.7 Measuring Acidity in Aqueous Solution: pH

10.8 Working with pH

17.3 Acidity of Carboxylic Acids

8.2 Intermolecular Forces

13.7 Alkene Polymers

17.7 Polyamides and Polyesters

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 (Reference: Chapter captions from McMurry et al.)

Acid-base properties #1

10.12 Some Common Acid–Base Reactions

When acids and bases are mixed in the correct proportion, both acidic and basic properties disappear because of a **neutralization reaction**. The most common kind of

A neutralization reaction: $\underset{\text{Acid}}{HA(aq)} + \underset{\text{Base}}{MOH(aq)} \longrightarrow \underset{\text{Water}}{H_2O(l)} + \underset{\text{A salt}}{MA(aq)}$

$$HCl(aq) + KOH(aq) \longrightarrow H_2O(l) + KCl(aq)$$

$$2\,HCl(aq) + K_2CO_3(aq) \longrightarrow H_2O(l) + 2\,KCl(aq) + CO_2(g)$$

(Reference: Chapter 10.12 from McMurry et al.)

Acid-base properties #2

10.7 Measuring Acidity in Aqueous Solution: pH

$$pH = -\log[H^+] \quad (\text{or}[H_3O^+]) \qquad\qquad [H_3O^+] = 10^{-pH}$$

Remember that the equilibrium between H_3O^+ and OH^- in aqueous solutions is expressed by K_w, where

$$K_w = [H_3O^+][OH^-] = 1 \times 10^{-14} \quad (\text{at } 25\,°C)$$

If we convert this equation to its negative logarithmic form, we obtain

$$-\log(K_w) = -\log(H_3O^+) - \log(OH^-)$$

$$-\log(1 \times 10^{-14}) = -\log(H_3O^+) - \log(OH^-)$$

$$or \quad 14.00 = pH + pOH$$

(Reference: Chapter 10.7 from McMurry et al.)

Acid-base properties #3

10.8 Working with pH

The H_3O^+ concentration in blood with pH = 7.4 is

$$[H_3O^+] = \text{antilog}(-7.4) = 4 \times 10^{-8}\ M$$

The pH of a solution with $[H_3O^+] = 4.6 \times 10^{-3}$ M is

$$pH = -\log(4.6 \times 10^{-3}) = -(-2.34) = 2.34$$

$$\text{antilog}(-7.\underbrace{4}_{\text{1 digit after decimal point}}) = \underbrace{4}_{\text{1 digit}} \times 10^{-8}$$

$$\log(\underbrace{4.6}_{\text{2 digits}} \times 10^{-3}) = -2.\underbrace{34}_{\text{2 digits after decimal point}}$$

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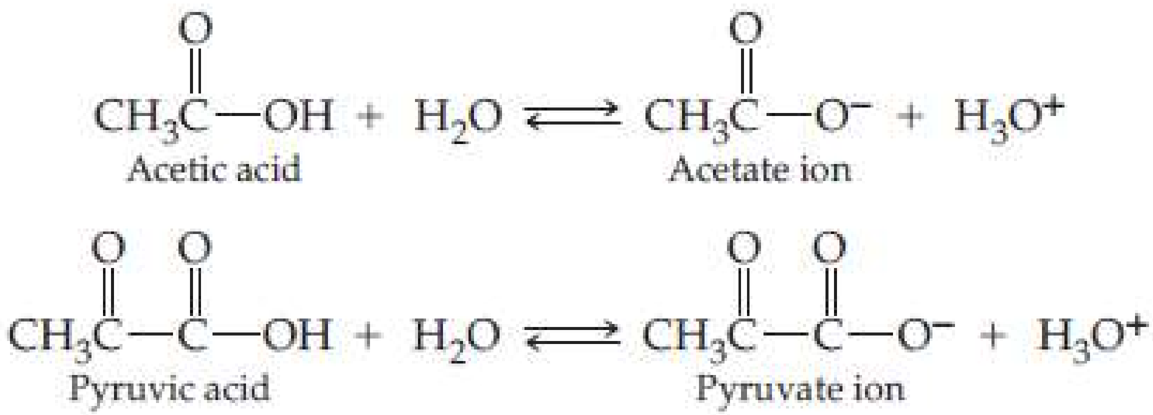
(Reference: Chapter 10.8 from McMurry et al.)

Acid-base properties #4

17.3 Acidity of Carboxylic Acids

At pH 7.4 in body fluids, carboxylic acids exist mainly as their carboxylate anions:



acid dissociation constant K_a

$$RCOOH + H_2O \rightleftharpoons RCOO^- + H_3O^+ \qquad K_a = \frac{[RCOO^-][H_3O^+]}{[RCOOH]}$$

 (Reference: Chapter 17.3 from McMurry et al.)

Acid-base properties #5

17.3 Acidity of Carboxylic Acids

TABLE 17.2 Carboxylic Acid Dissociation Constants*

NAME	STRUCTURE	ACID DISSOCIATION CONSTANT (K_a)
Trichloroacetic acid	Cl_3CCOOH	2.3×10^{-1}
Chloroacetic acid	$ClCH_2COOH$	1.4×10^{-3}
Formic acid	$HCOOH$	1.8×10^{-4}
Acetic acid	CH_3COOH	1.8×10^{-5}
Propanoic acid	CH_3CH_2COOH	1.3×10^{-5}
Hexanoic acid	$CH_3(CH_2)_4COOH$	1.3×10^{-5}
Benzoic acid	C_6H_5COOH	6.5×10^{-5}
Acrylic acid	$H_2C{=}CHCOOH$	5.6×10^{-5}
Oxalic acid	$HOOCCOOH$	5.4×10^{-2}
	$^{-}OOCCOOH$	5.2×10^{-5}
Glutaric acid	$HOOC(CH_2)_3COOH$	4.5×10^{-5}
	$^{-}OOC(CH_2)_3COOH$	3.8×10^{-6}

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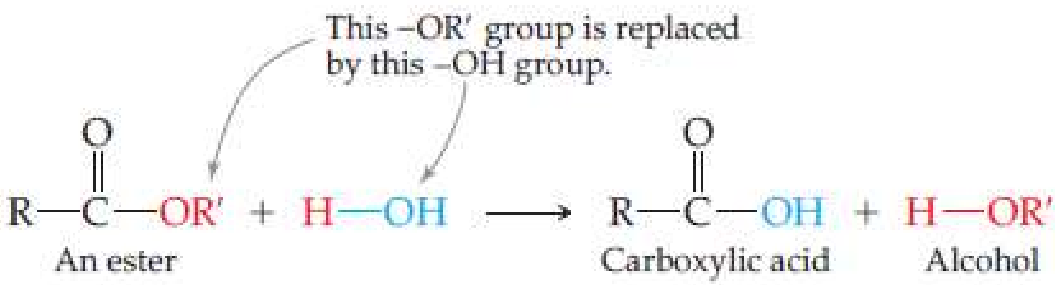
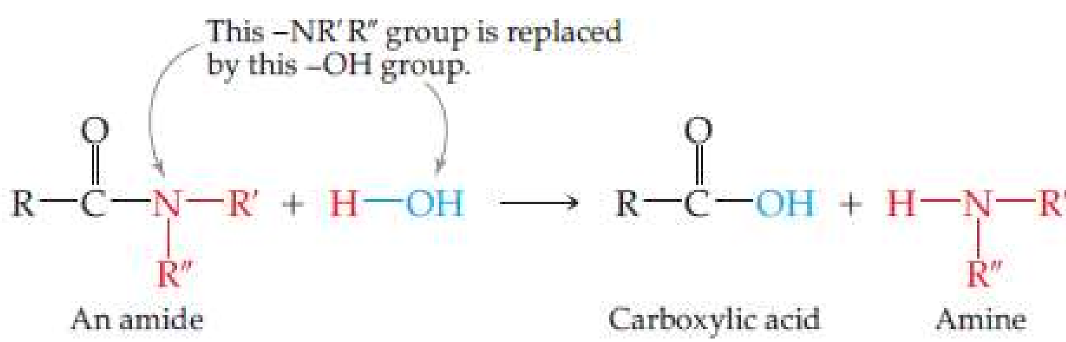
 (Reference: Table 17.2 (Chapter 17.3) from McMurry et al.)

17.6 Hydrolysis of Esters and Amides

For esters, the net effect of hydrolysis is substitution of —OH for —OR′:



For amides, the net effect of hydrolysis is substitution of —OH for —NH_2 or the substituted amide nitrogen:

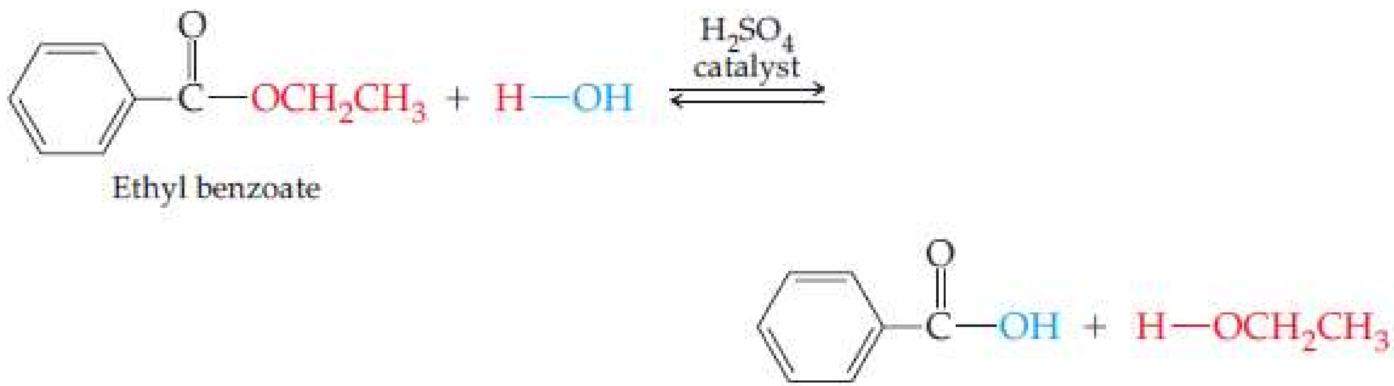


 (Reference: Chapter 17.6 from McMurry et al.)

17.6 Hydrolysis of Esters and Amides

Ester Hydrolysis

Both acids and bases can cause ester hydrolysis. Acid-catalyzed hydrolysis is simply the reverse of the esterification. An ester is treated with water in the presence of a strong acid catalyst such as sulfuric acid, and hydrolysis takes place:



Ethyl benzoate

Benzoic acid

Ethanol

An excess of water pushes the equilibrium to the right.

(Reference: Chapter 17.6 from McMurry et al.)

8.2 Intermolecular Forces

Intermolecular forces: the forces that act between different molecules rather than within an individual molecule.

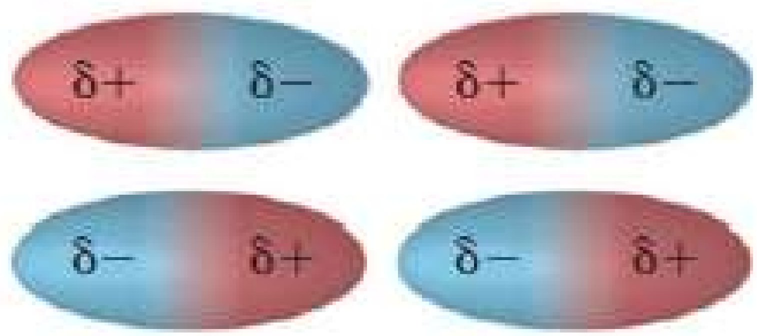
TABLE 8.2 A Comparison of Intermolecular Forces

Force	Strength	Characteristics
Dipole–dipole	Weak (1 kcal/mol, 4 kJ/mol))	Occurs between polar molecules
London dispersion	Weak (0.5–2.5 kcal/mol, 2–10 kJ/mol)	Occurs between all molecules; strength depends on size
Hydrogen bond	Moderate (2–10 kcal/mol, 8–40 kJ/mol)	Occurs between molecules with O—H, N—H, and F—H bonds

(Reference: Chapter 8.2 from McMurry et al.)

8.2 Intermolecular Forces

Dipole–Dipole Forces

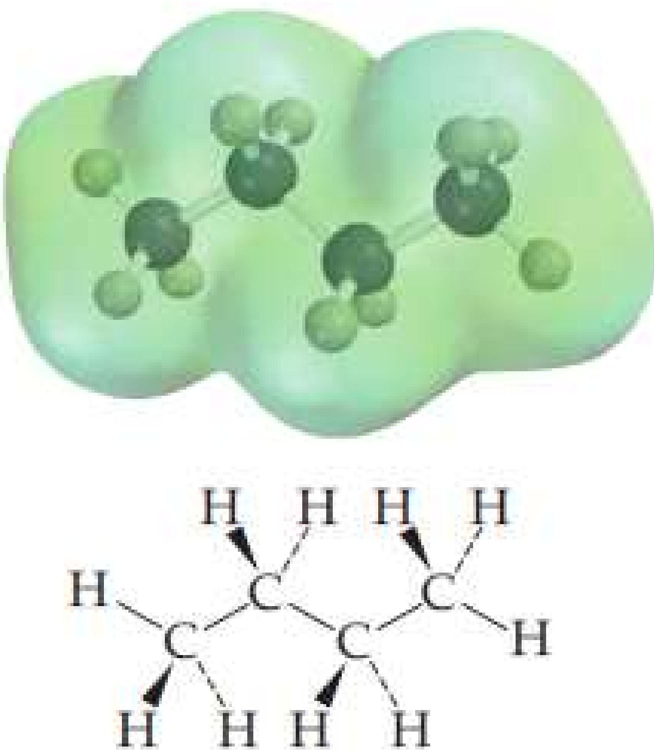


▲**Figure 8.3**
Dipole–dipole forces.
The positive and negative ends of polar molecules are attracted to one another by dipole–dipole forces. As a result, polar molecules have higher boiling points than nonpolar molecules of similar size.

 (Reference: Chapter 8.2 from McMurry et al.)

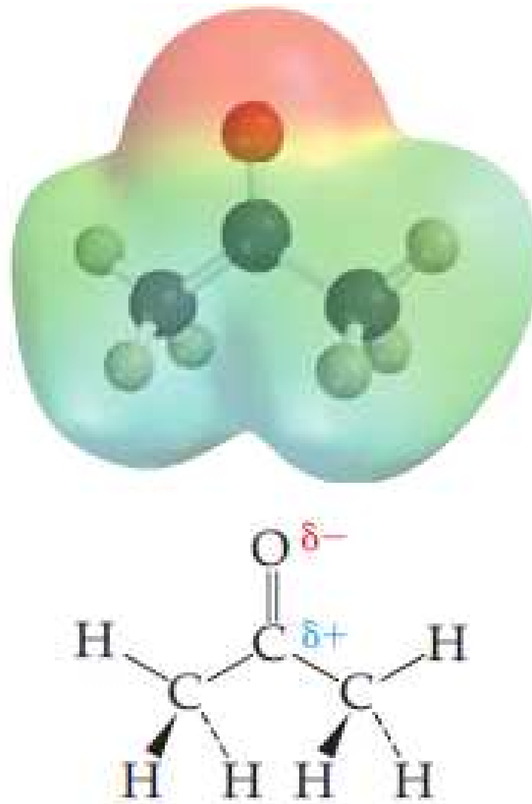
8.2 Intermolecular Forces

Dipole–Dipole Forces



Butane (C_4H_{10})

Mol wt = 58 amu
bp = −0.5 °C



Acetone (C_3H_6O)

Mol wt = 58 amu
bp = 56.2 °C

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(Reference: Chapter 8.2 from McMurry et al.)

8.2 Intermolecular Forces

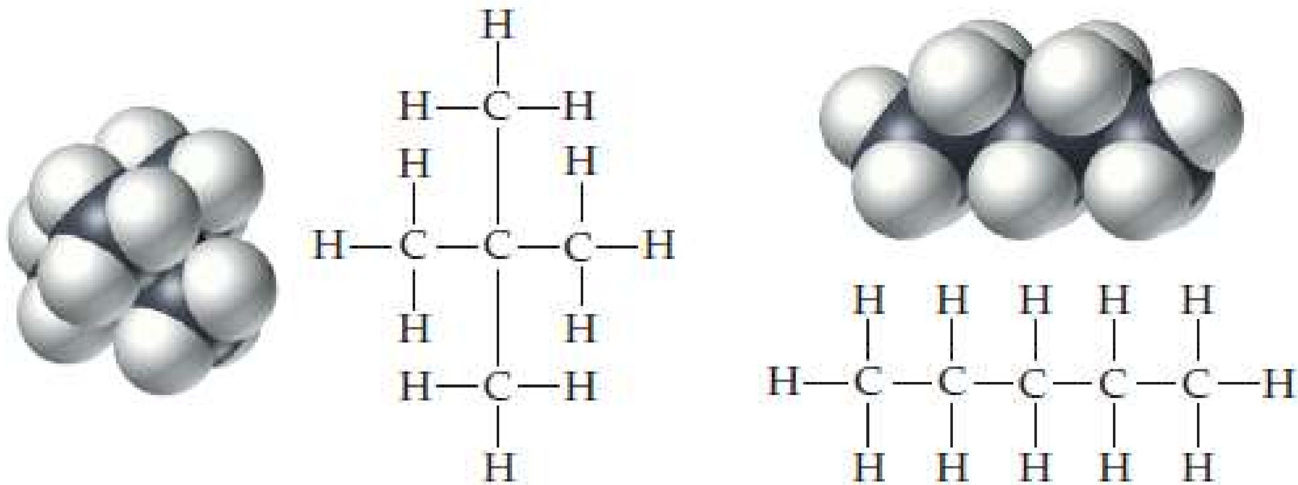
London Dispersion Forces

Figure 8.4
(a) Averaged over time, the electron distribution in a Br_2 molecule is symmetrical. (b) At any given instant, however, the electron distribution may be unsymmetrical, resulting in a temporary polarity that induces a complementary polarity in neighboring molecules.

(Reference: Chapter 8.2 from McMurry et al.)

8.2 Intermolecular Forces

London Dispersion Forces



(a) 2,2-Dimethylpropane (bp = 9.5 °C)

(b) Pentane (bp = 36 °C)

Figure 8.5

London dispersion forces.
More compact molecules like 2,2-dimethylpropane have smaller surface areas, weaker London dispersion forces, and lower boiling points. By comparison, flatter, less compact molecules like pentane have larger surface areas, stronger London dispersion forces, and higher boiling points.

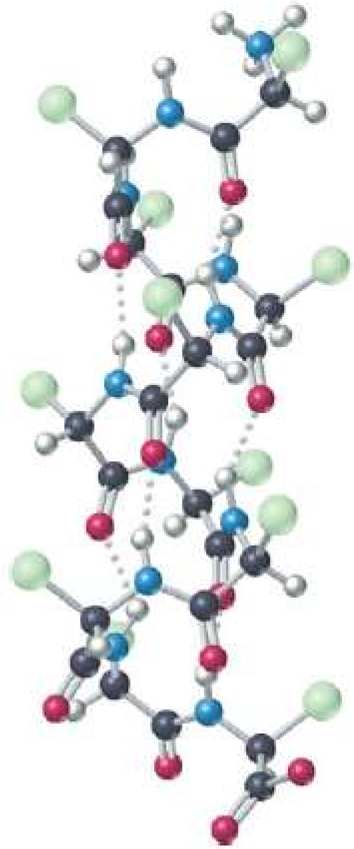
(Reference: Chapter 8.2 from McMurry et al.)

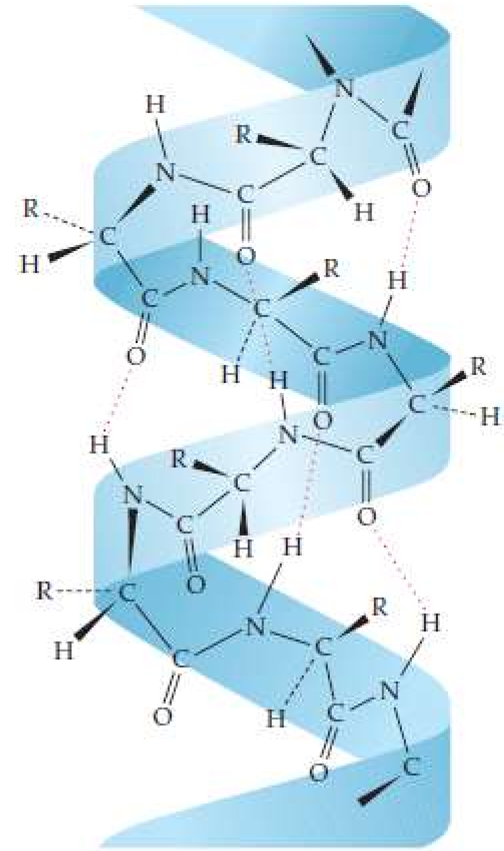
8.2 Intermolecular Forces

Hydrogen Bonds

▸ **Figure 8.6**

The α-helical structure of keratin results from hydrogen bonding along the amino acid backbone of the molecule. Hydrogen bonding is represented by gray dots in the ball and stick model on the left and red dots in the molecular structure on the right.

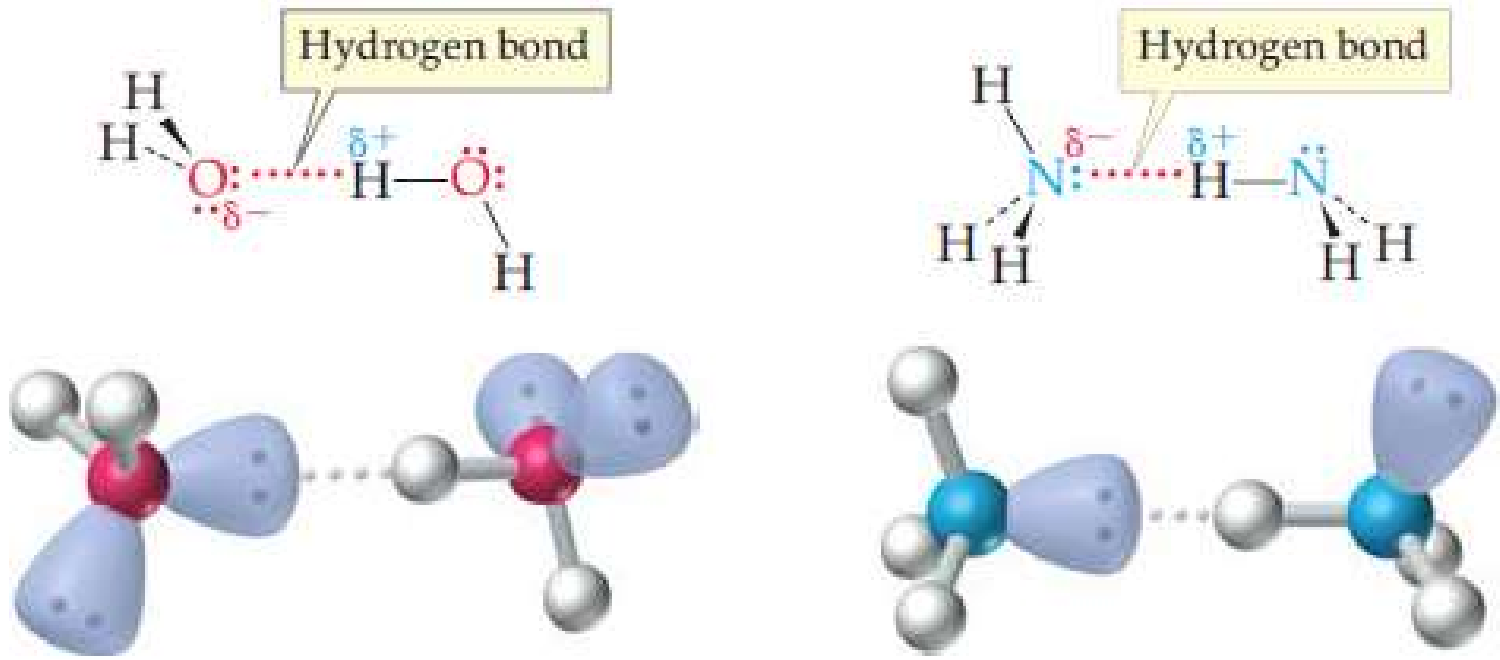




(Reference: Chapter 8.2 from McMurry et al.)

8.2 Intermolecular Forces

Hydrogen Bonds



Hydrogen bonding is really just a special kind of dipole–dipole interaction. The O—H, N—H, and F—H bonds are highly polar, with a partial positive charge on the hydrogen and a partial negative charge on the electronegative atom. In addition, the hydrogen atom has no inner-shell electrons to act as a shield around its nucleus, and it is small so it can be approached closely.

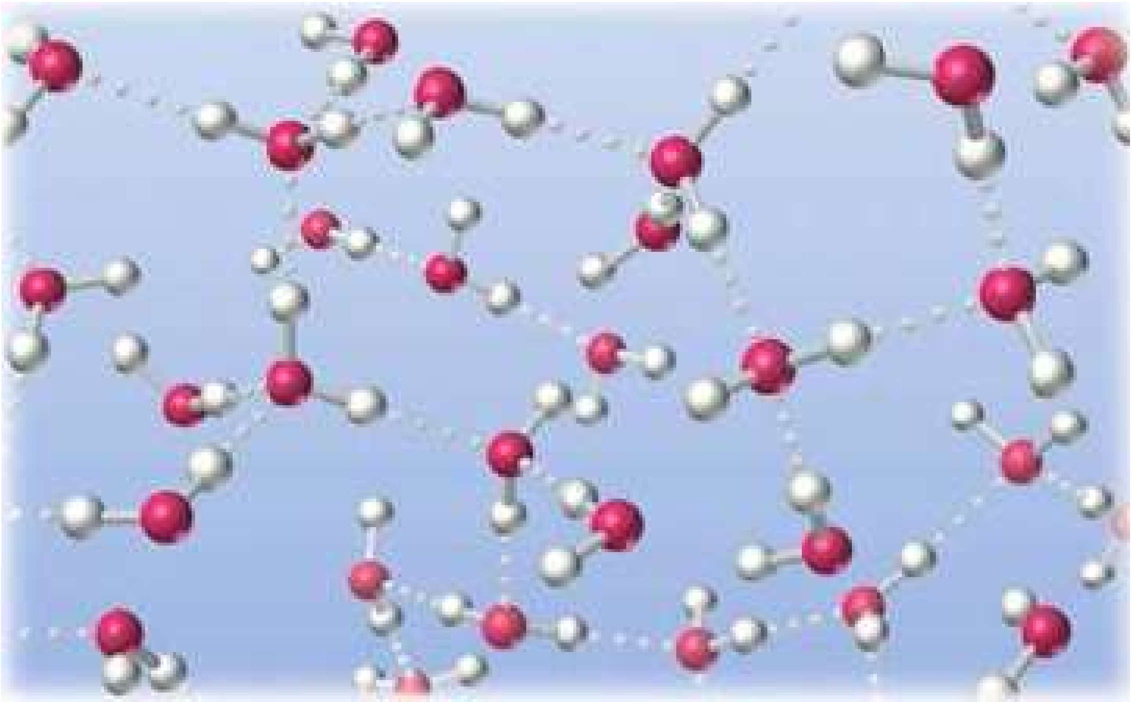
 (Reference: Chapter 8.2 from McMurry et al.)

8.2 Intermolecular Forces

Hydrogen Bonds

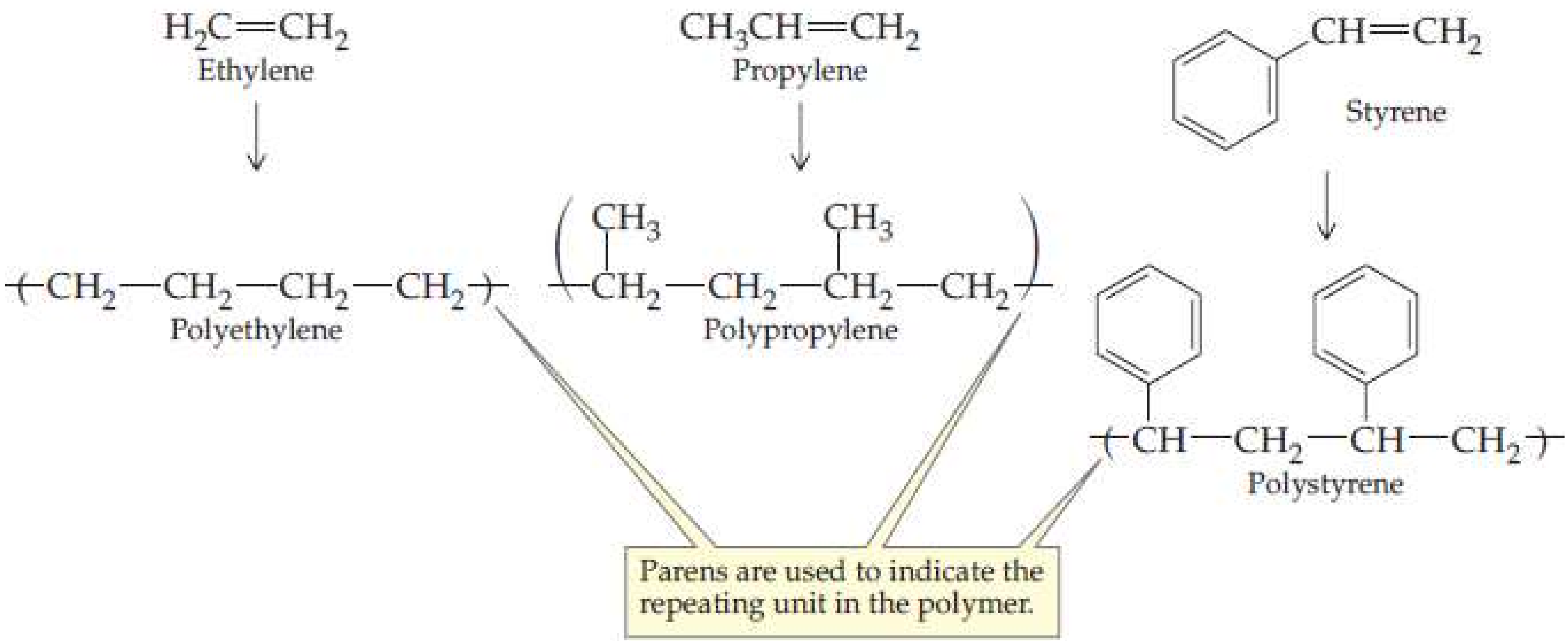
▸ **Figure 8.7**

Hydrogen bonding in water.
The intermolecular attraction in water is especially strong because each oxygen atom has two lone pairs and two hydrogen atoms, allowing the formation of as many as four hydrogen bonds per molecule. Individual hydrogen bonds are constantly being formed and broken.



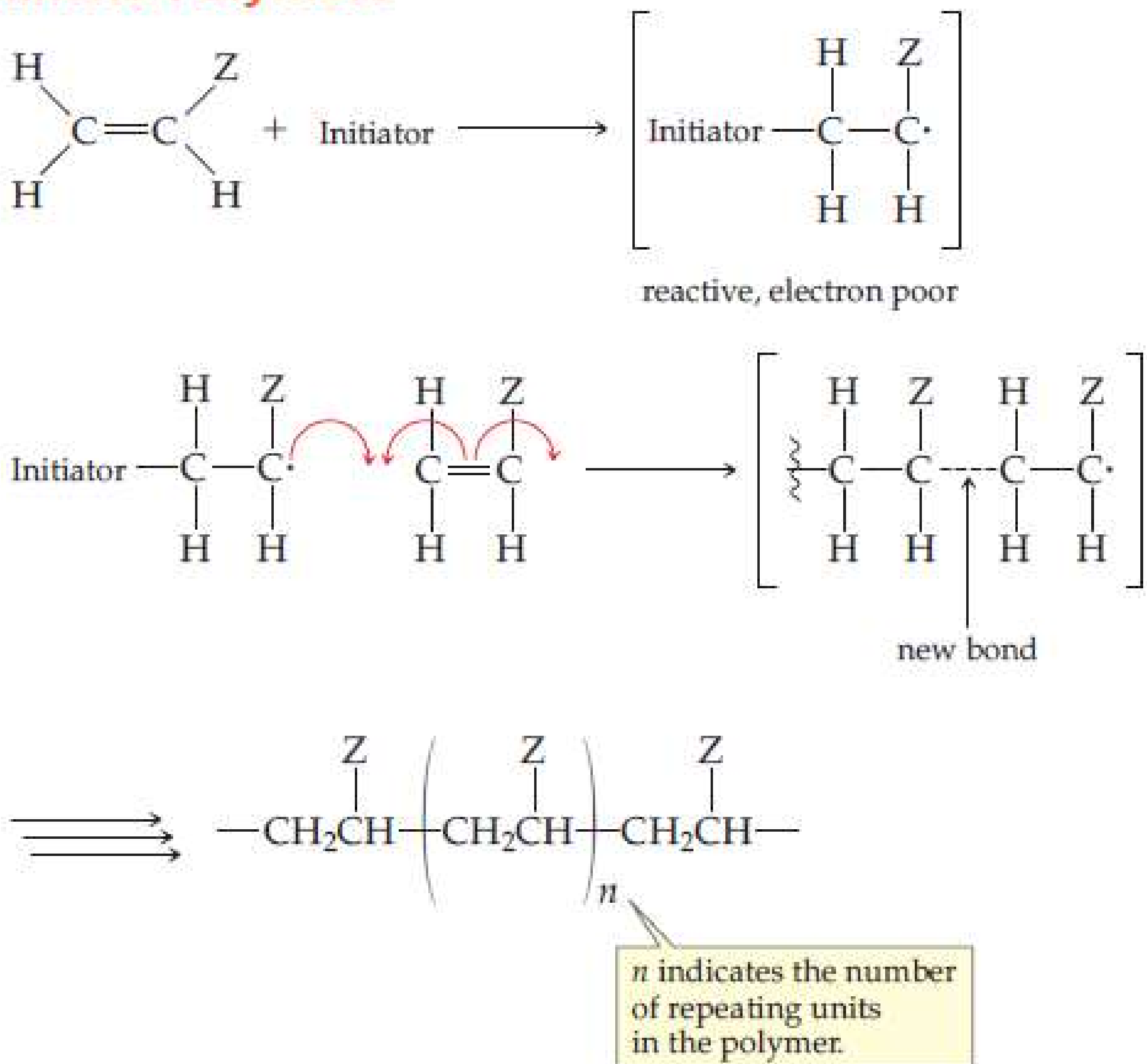
(Reference: Chapter 8.2 from McMurry et al.)

13.7 Alkene Polymers



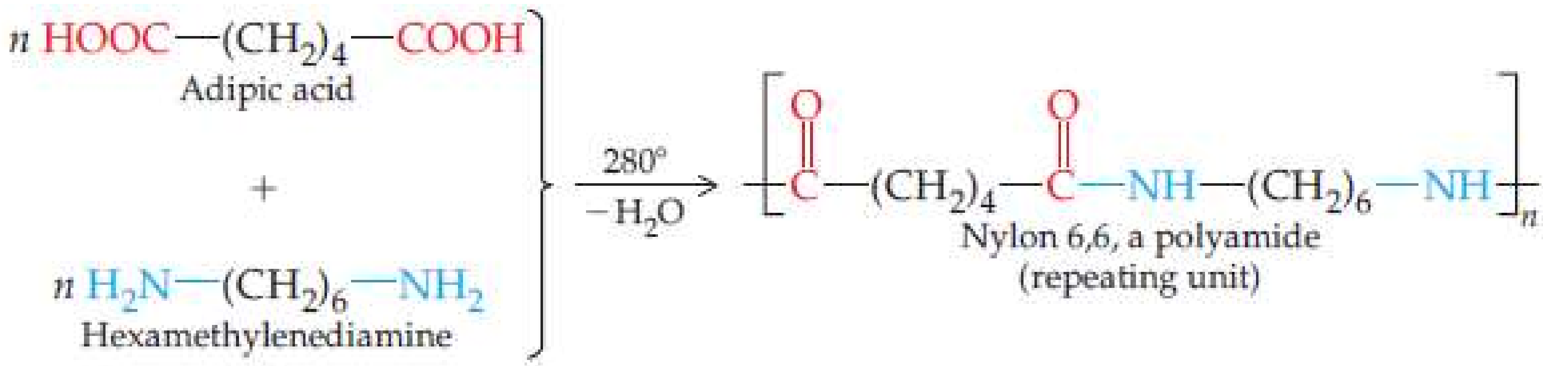
 (Reference: Chapter 13.7 from McMurry et al.)

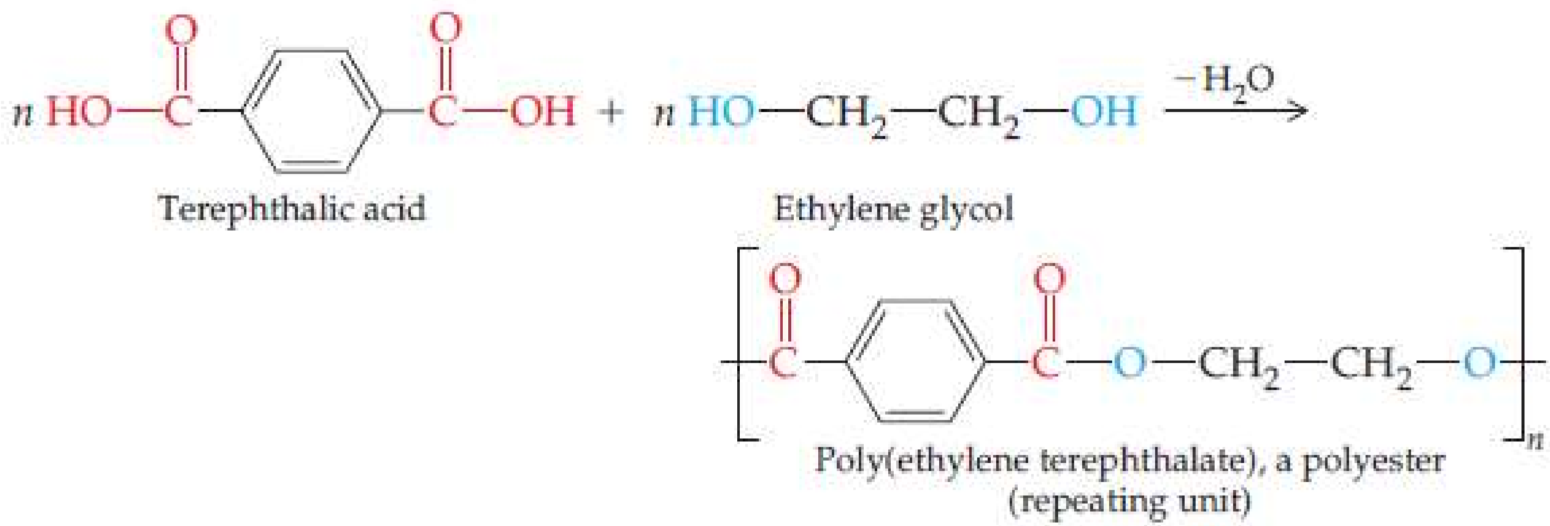
13.7 Alkene Polymers



(Reference: Chapter 13.7 from McMurry et al.)

17.7 Polyamides and Polyesters





(Reference: Chapter 17.7 from McMurry et al.)

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Résumé

Acids and bases

- Neutralization reactions
- pH, K_w, K_a

Hydrolysis reactions

- Ester hydrolysis

Intermolecular forces

- Dipole-dipole forces
- London dispersion forces
- Hydrogen bonds

Polymers

- Alkene polymers
- Polyamides and polyesters

Required for a better understanding of amino acids and proteins!

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