Macromolecules

Issues to Study:

Structure of Macromolecules
- different levels of structure
- random coils
- structure of proteins
- structure of nucleic acids

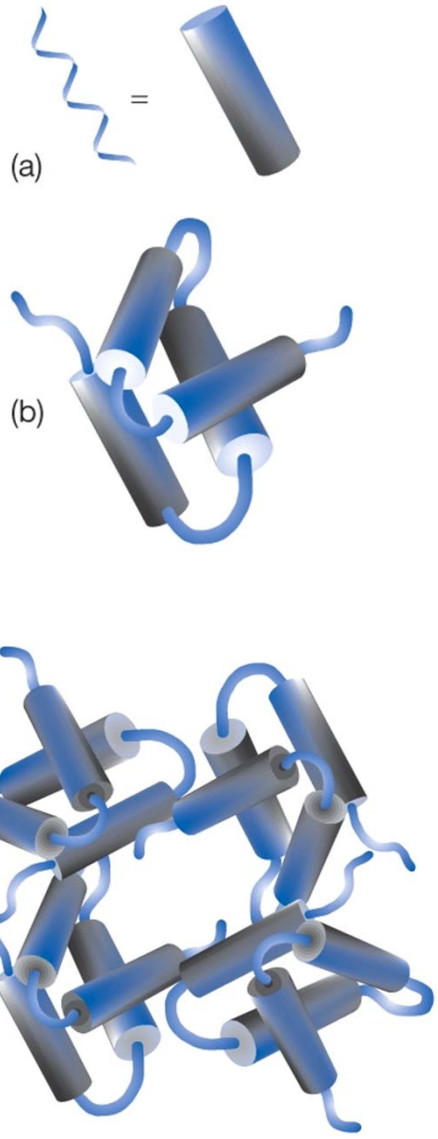
Determination Techniques of Size and Shape

Different Levels of Structure

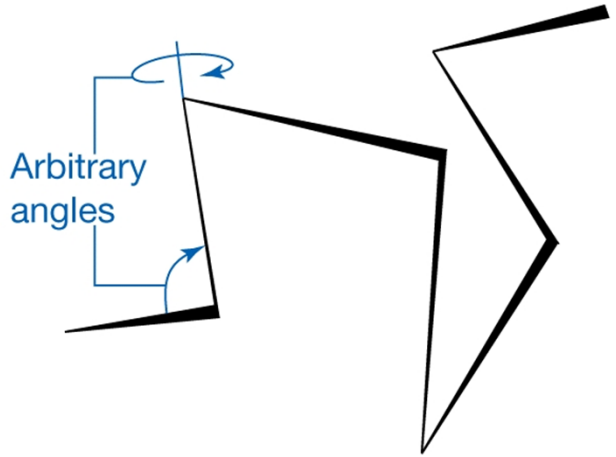
Configuration

Conformation

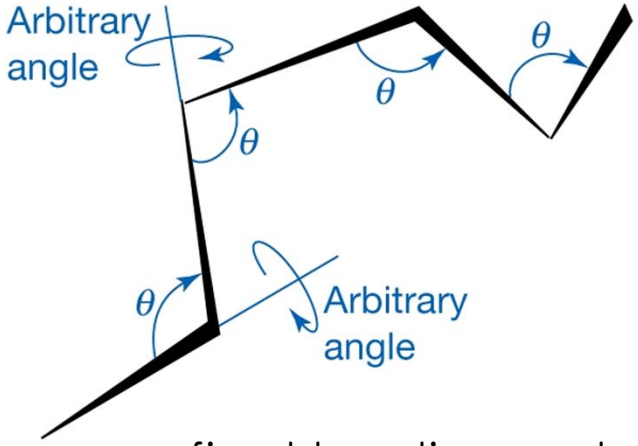
Primary structure
Secondary structure
Tertiary structure
Quaternary structure



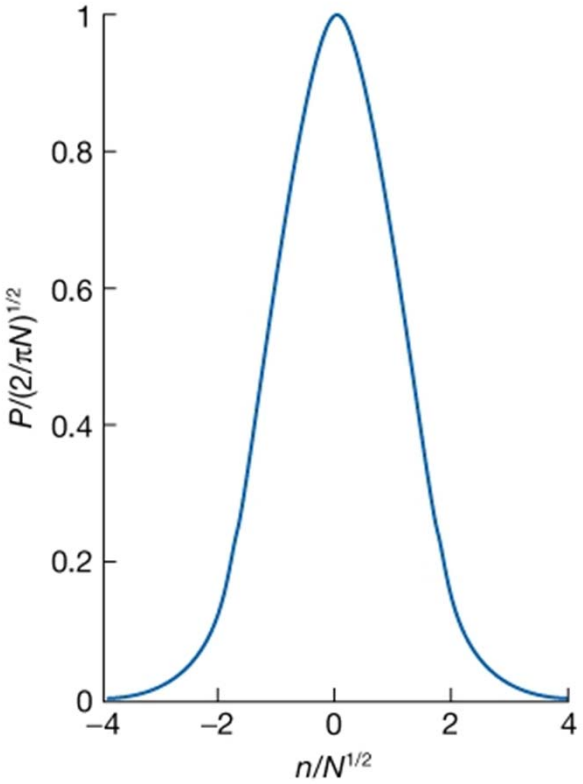
Random Coils



VS



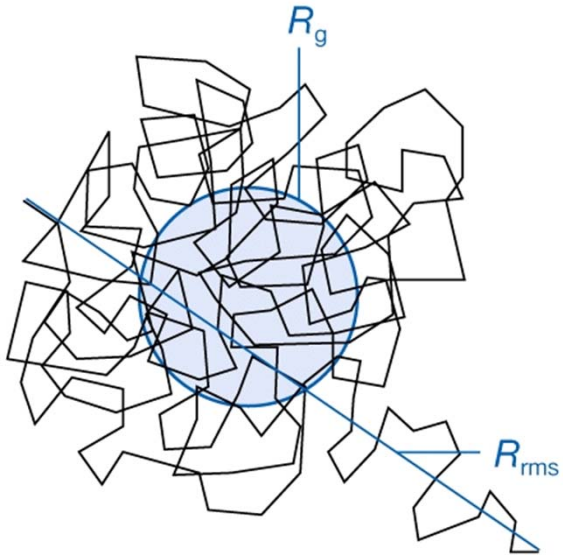
fixed bonding angle θ

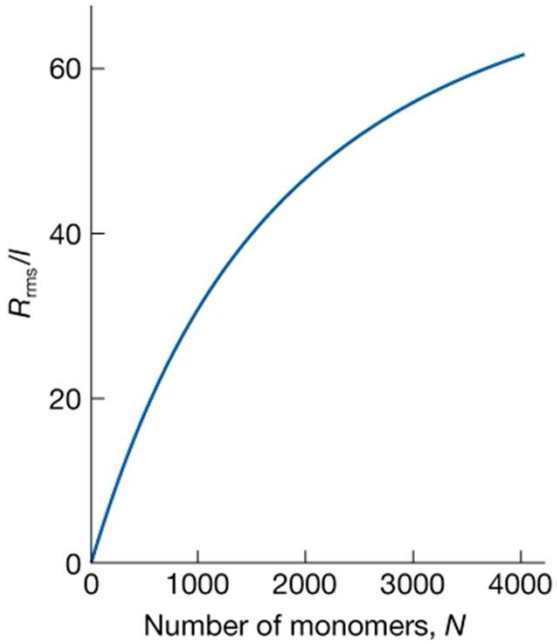


Probability distribution for separation of the ends of a 1-D random coil

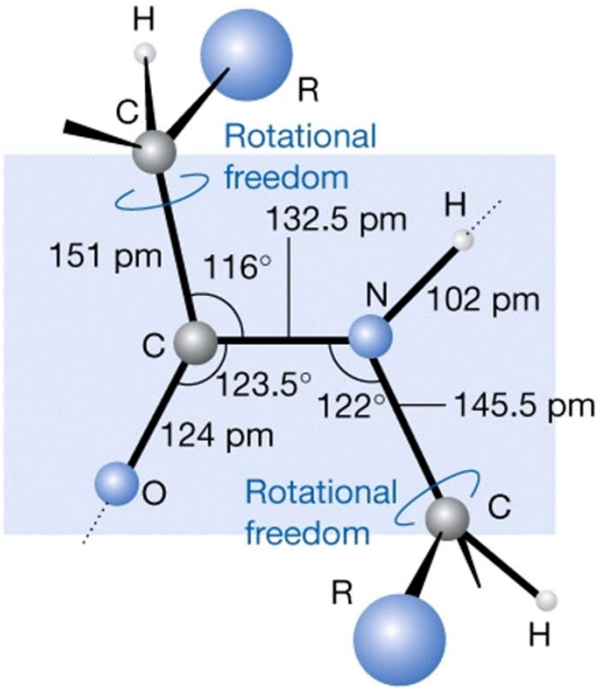
Measures of geometrical size of a random coil

Contour length $R_c = N*l$
Root mean square separation R_{rms}
Radius of gyration R_g

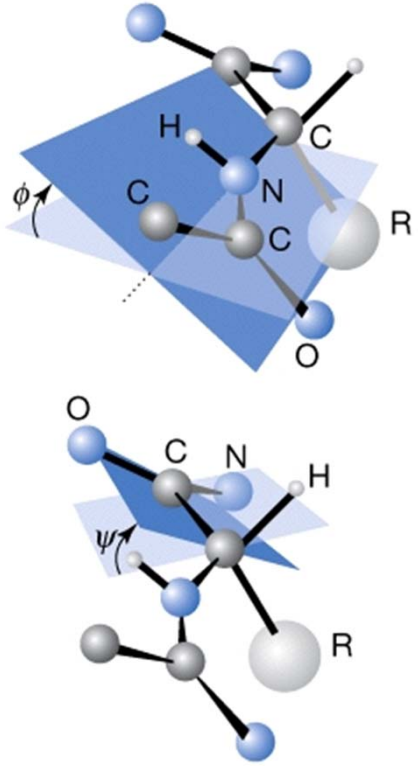




Structure of Proteins

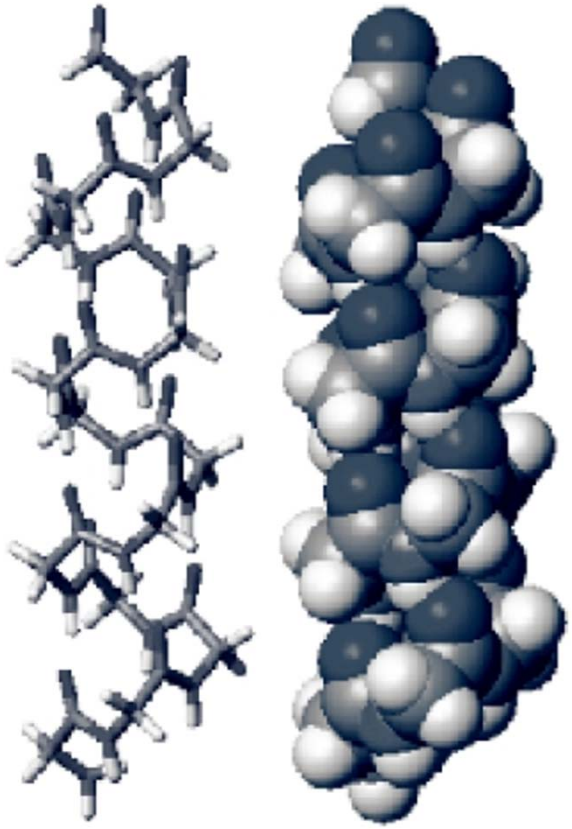


Corey–Pauling rule

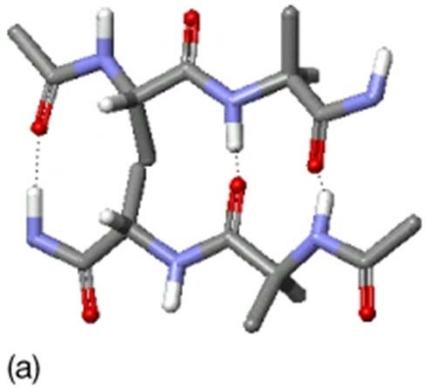


torsional angles ϕ and ψ
between 2 peptide units

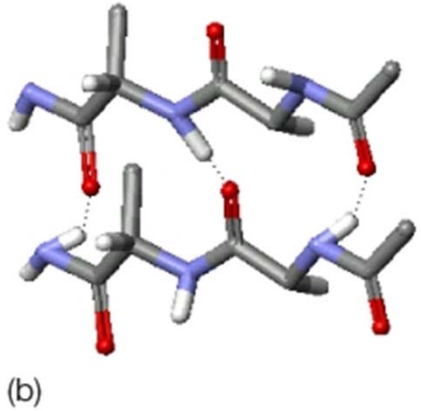
α-helix



β-sheets



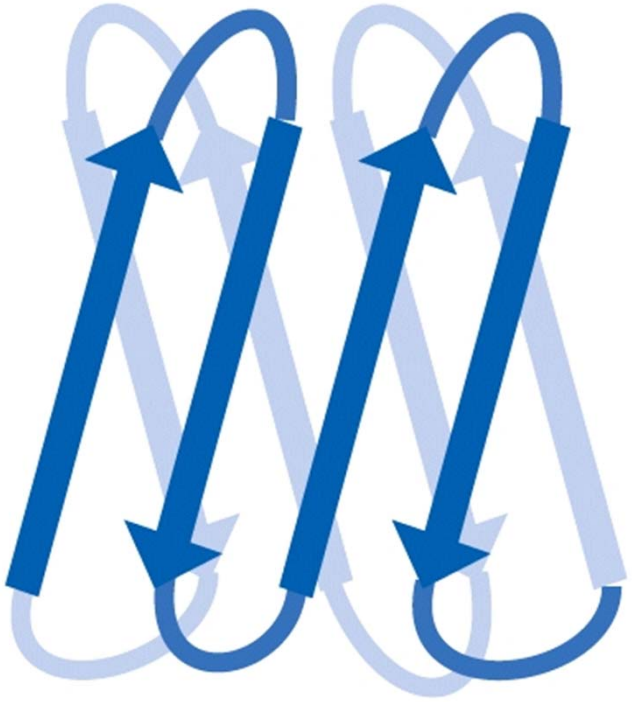
antiparallel



parallel

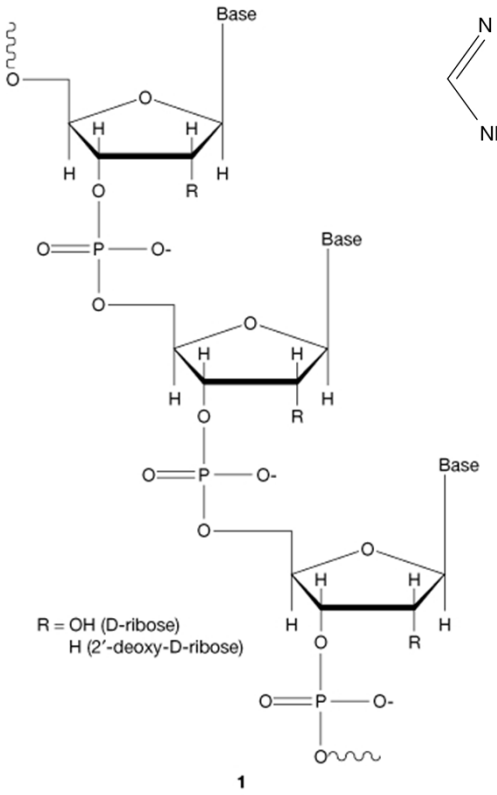
Higher-order structures

4-helix bundle

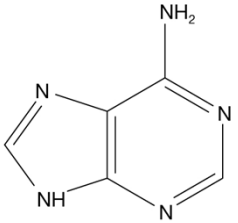


8 antiparallel β-sheets

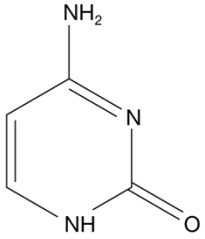
Structure of Nucleic Acids



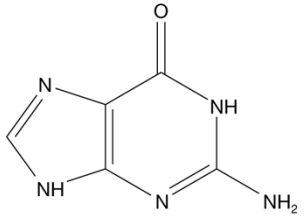
1



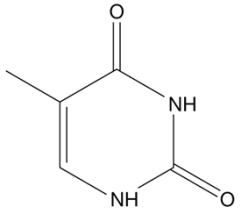
2 Adenine, A



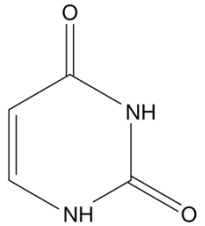
3 Cytosine, C



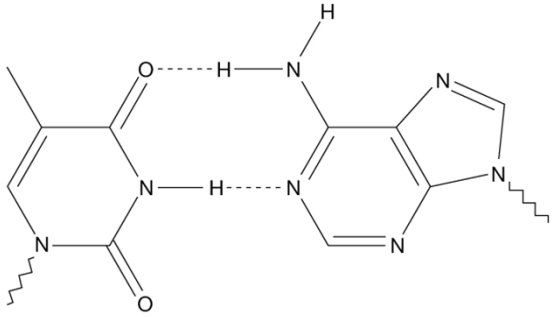
4 Guanine, G



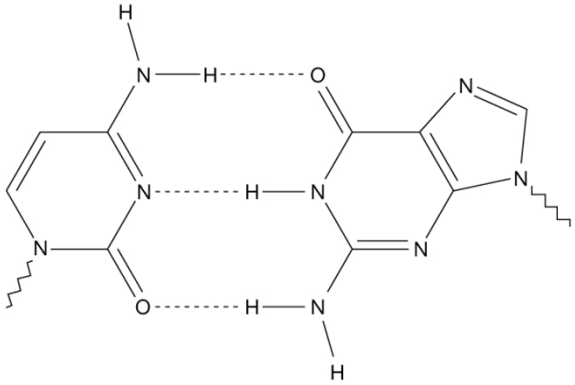
5 Thymine, T



6 Uracil, U



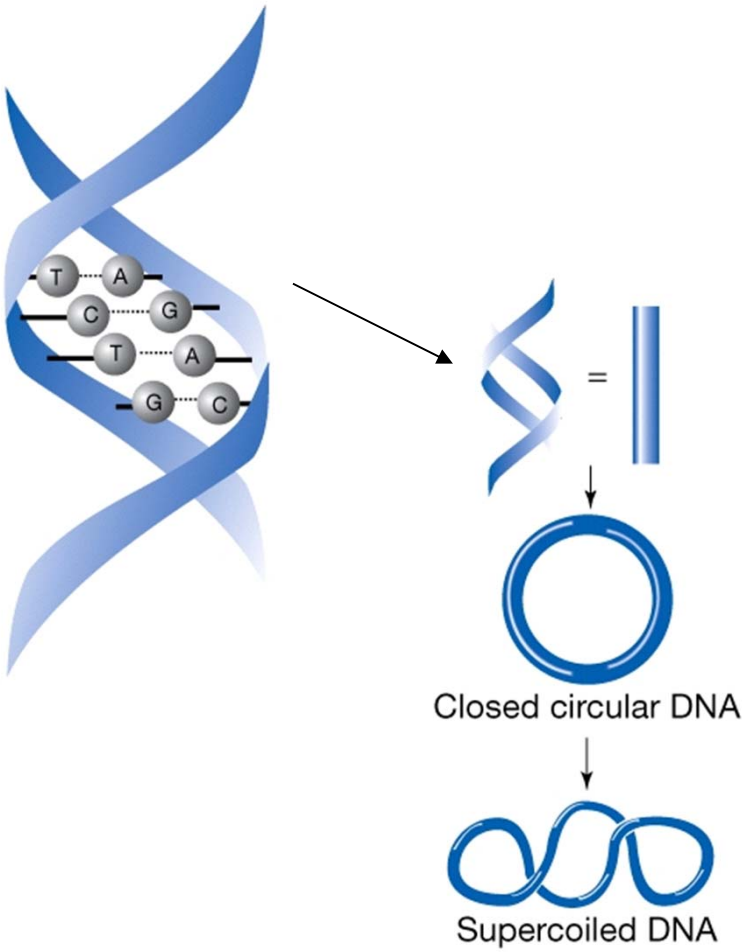
7 A—T base pair



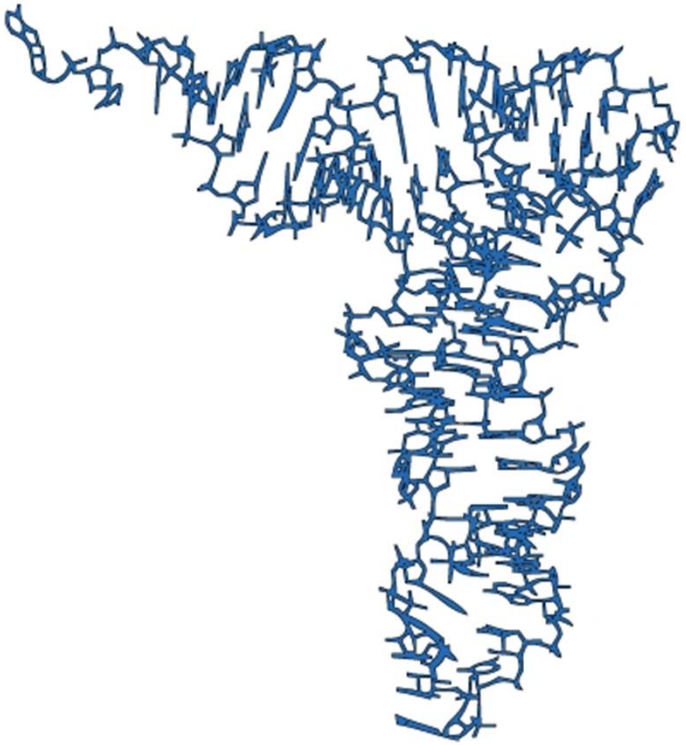
8 C—G base pair

polynucleotides

DNA



tRNA



Determination of Size and Shape

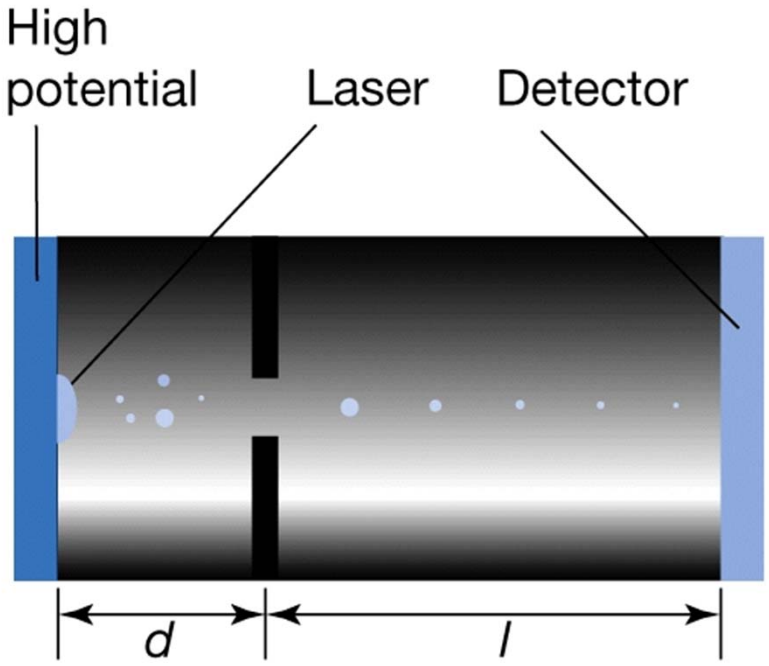
Mean Molar Masses

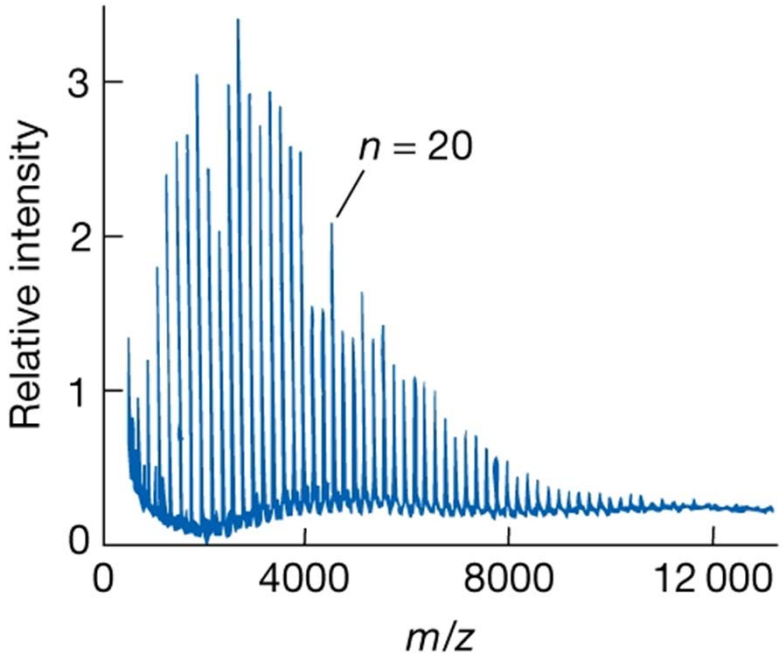
number-average molar mass M_n
weight-average molar mass M_w
Z-average molar mass M_z
viscosity-average molar mass M_v

* Heterogeneity index: M_w/M_n

$M_w/M_n < 1.1$: monodisperse

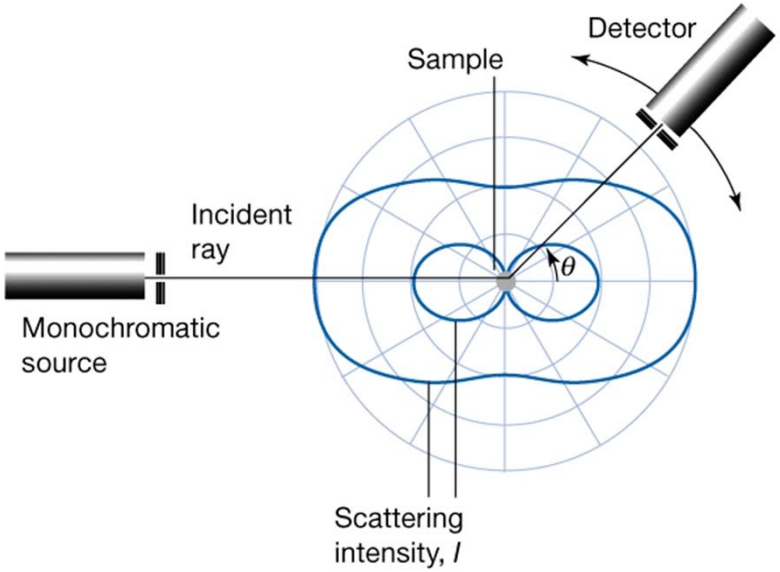
Mass Spectrometry

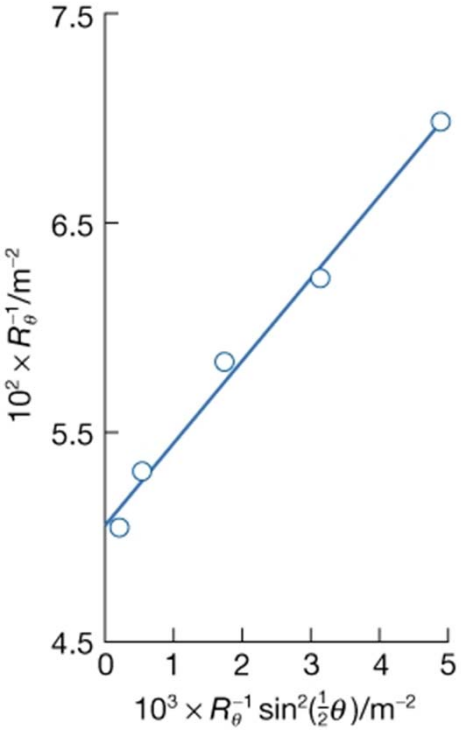




* Number and weight-average molar masses cand be calculated.

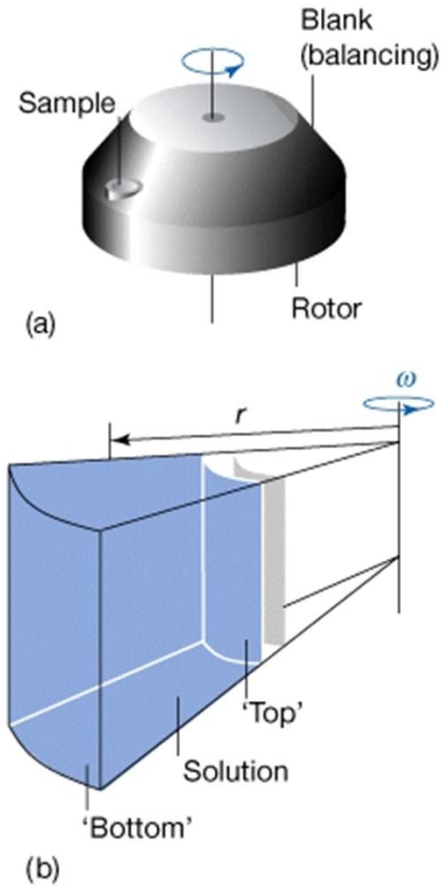
Laser Light Scattering



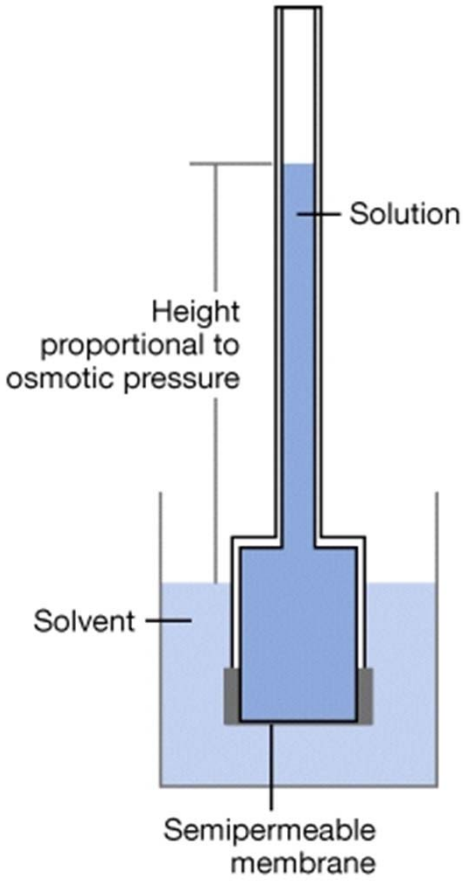


* weight-average molar mass

Ultracentrifugation

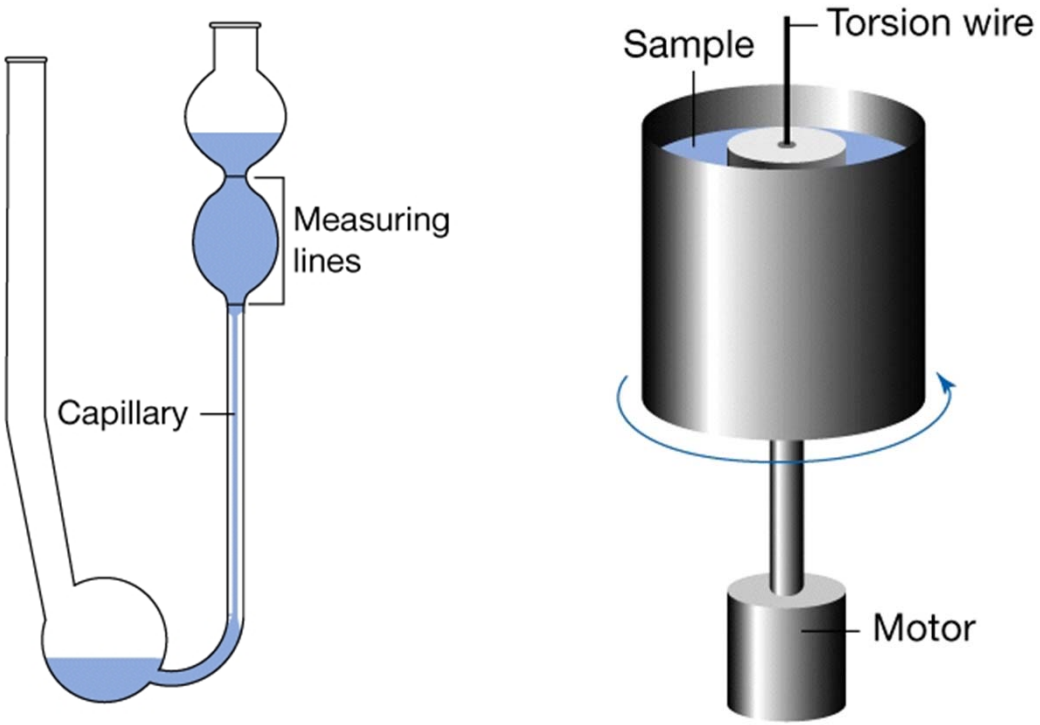


Osmometry



* number-average molar mass

Viscosity



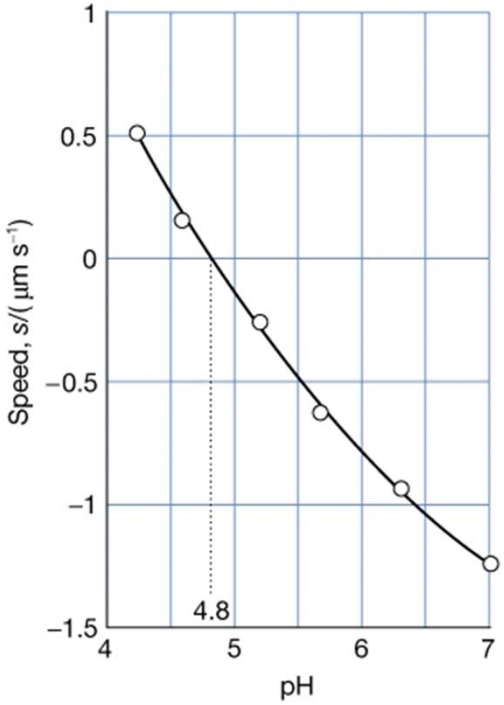
* viscosity-average molar mass

* Electrophoresis

gel electrophoresis

isoelectric focusing

capillary electrophoresis



* Size-Exclusion Chromatography (SEC)
or Gel Permeation Chromatography (GPC)