Molecular Recognition: Storage and Processing of Molecular Information

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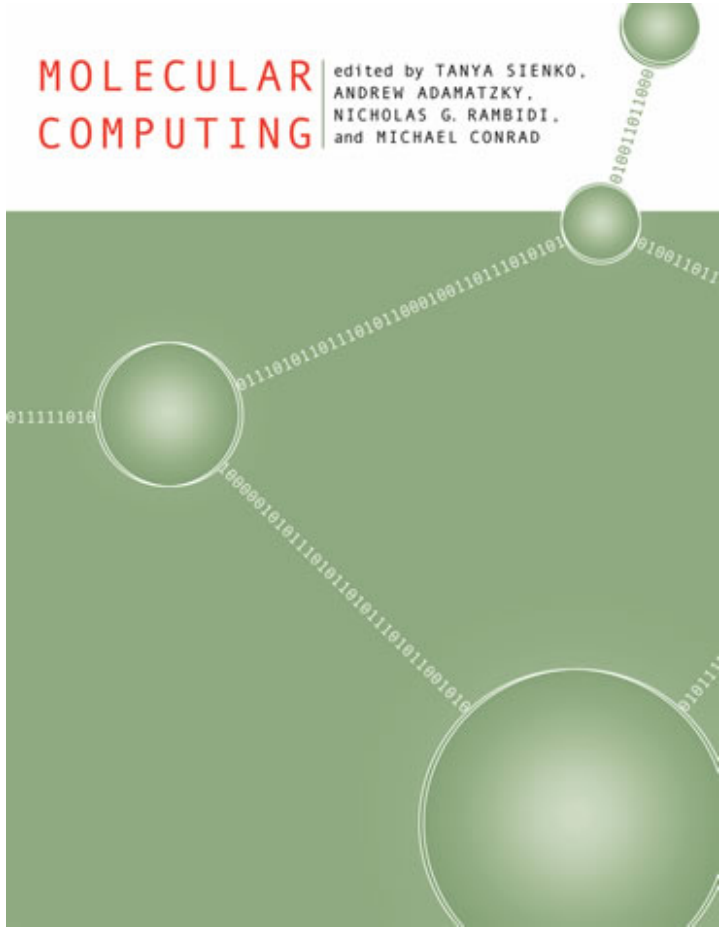
- Thermodynamics, Information, and Entropy

Authors (1)

- Jean-Marie Lehn
  - Winner of The Nobel Prize in Chemistry 1987

Authors (2)

- Tanya Sienko
  - Coauthor of “Molecular Computing”



Molecular Computing Basics (1)

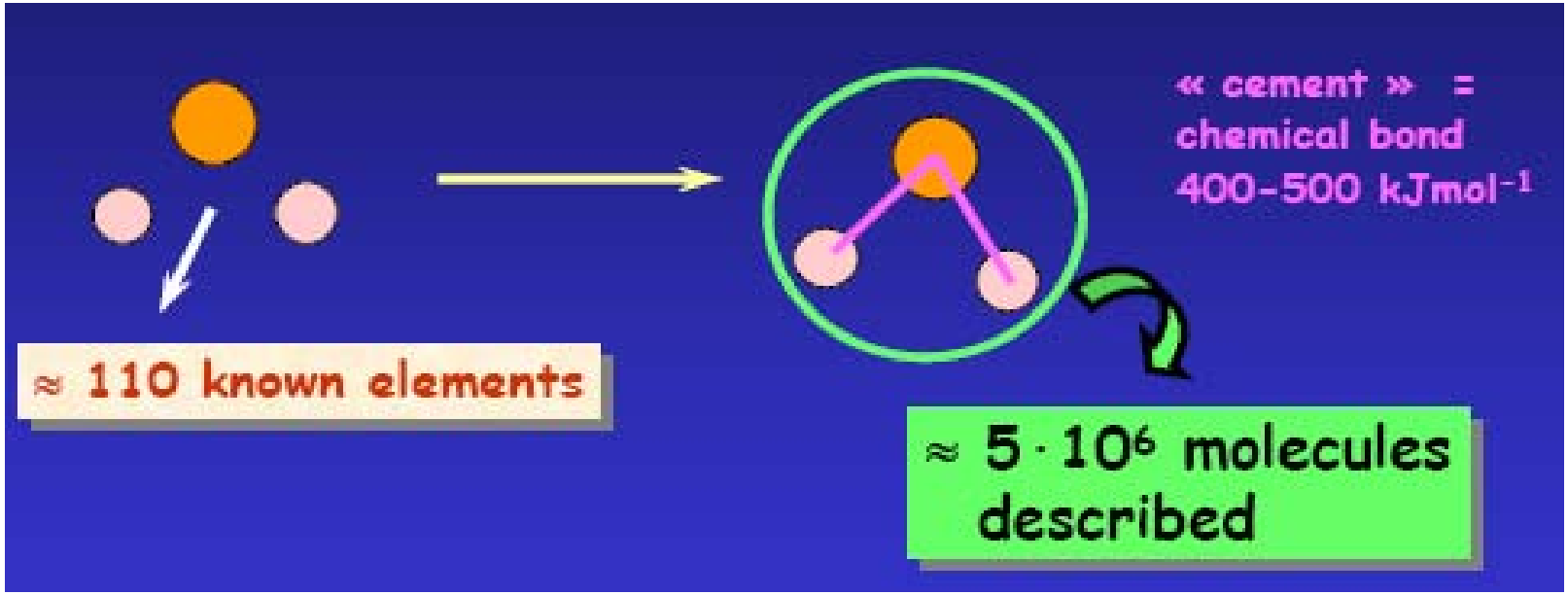
- physical base underlying every computing system
  - semi-conductor material
  - more complicated organic chemical
- Reverse the demarcation of computing into “hardware” and “software”
  - cannot make a distinction
- instead of “programmability”,
  - “evolution”,
  - “adaptability,”
  - and “informed materials”

Molecular Computing Basics (2)

- “information” lie in
  - chemical
  - supramolecular attributes and behavior
- gains ability of implementing
  - “recognition,”
  - self-organization,
  - and other “high-level” behaviors
- molecular recognition
  - supramolecular interaction algorithms

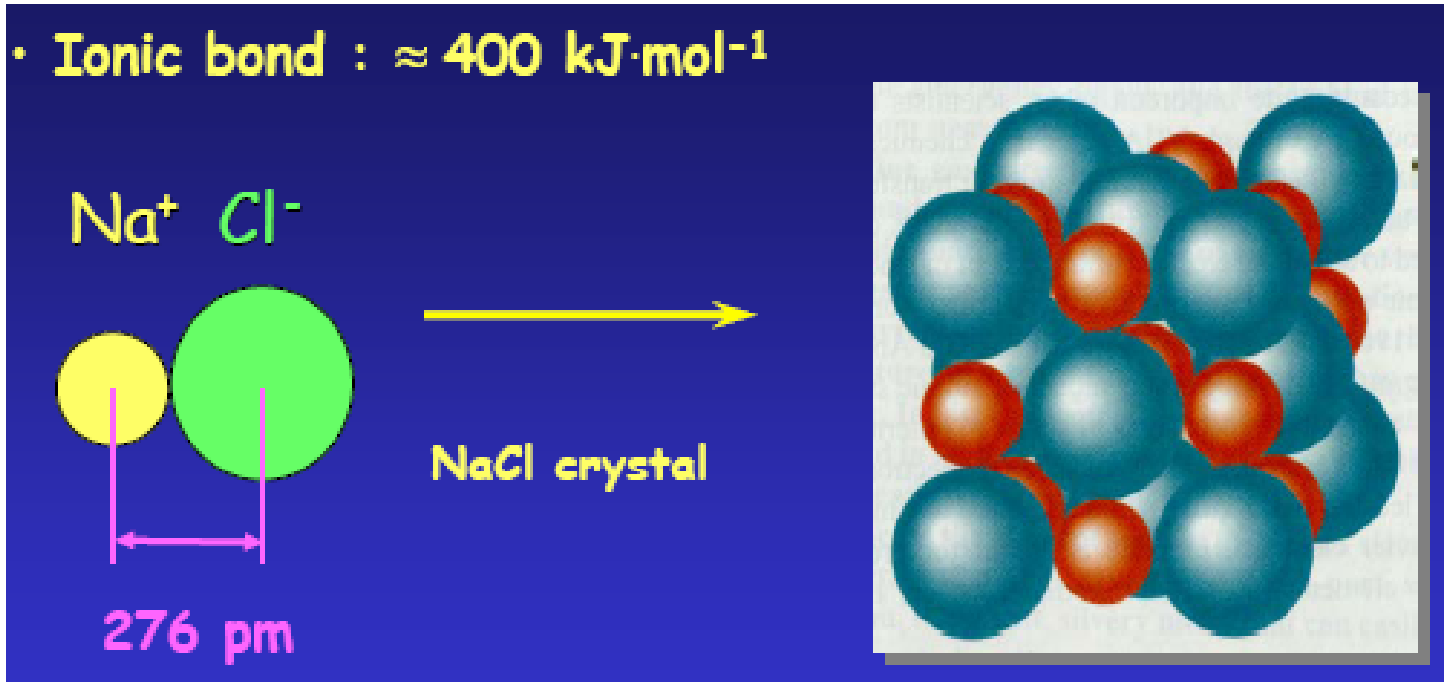
Covalent Chemistry (1)

- assemble molecules from atoms or smaller molecules

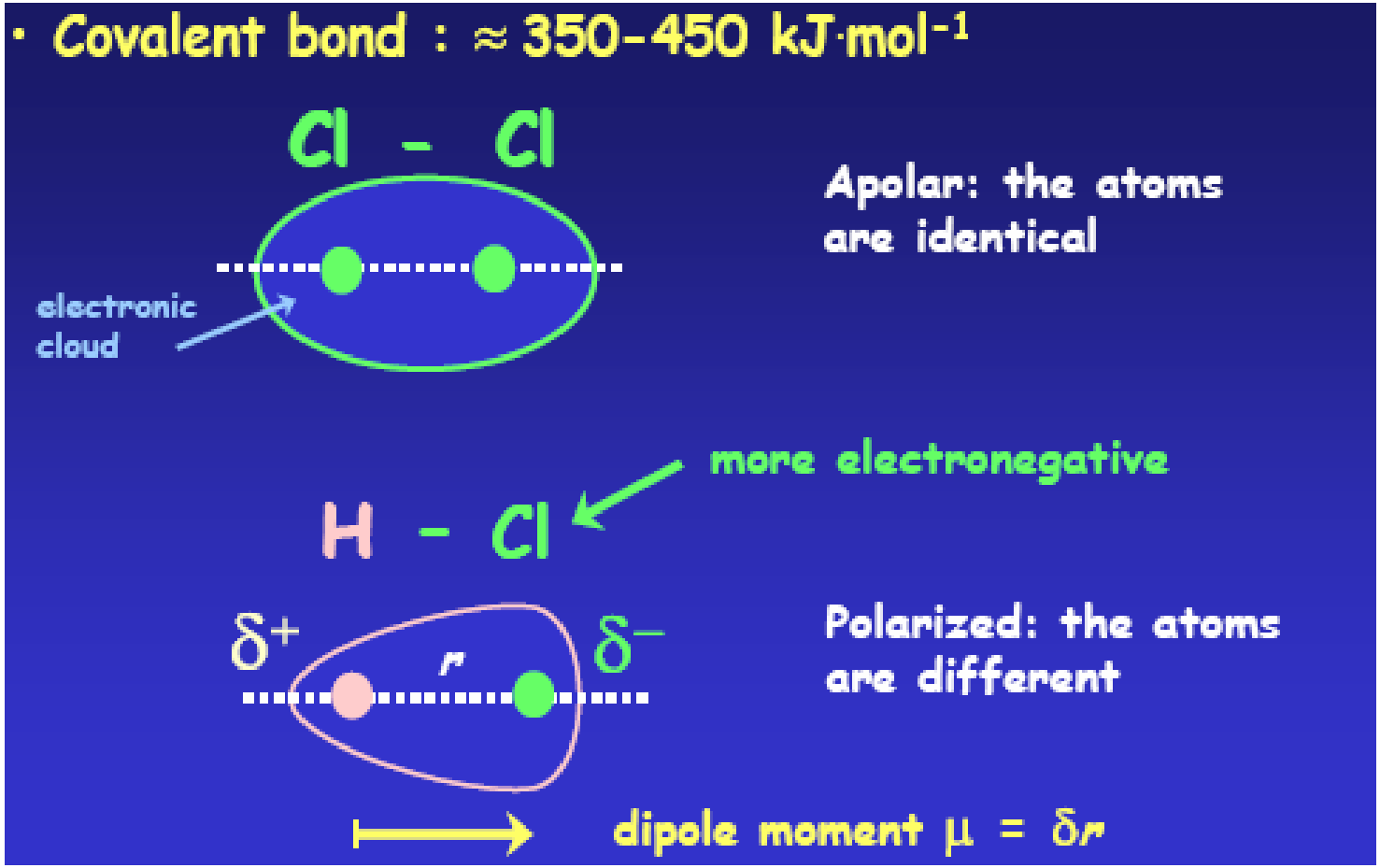


- Structure and functionality depend on the anture of the atoms and on their geometrical arrangement

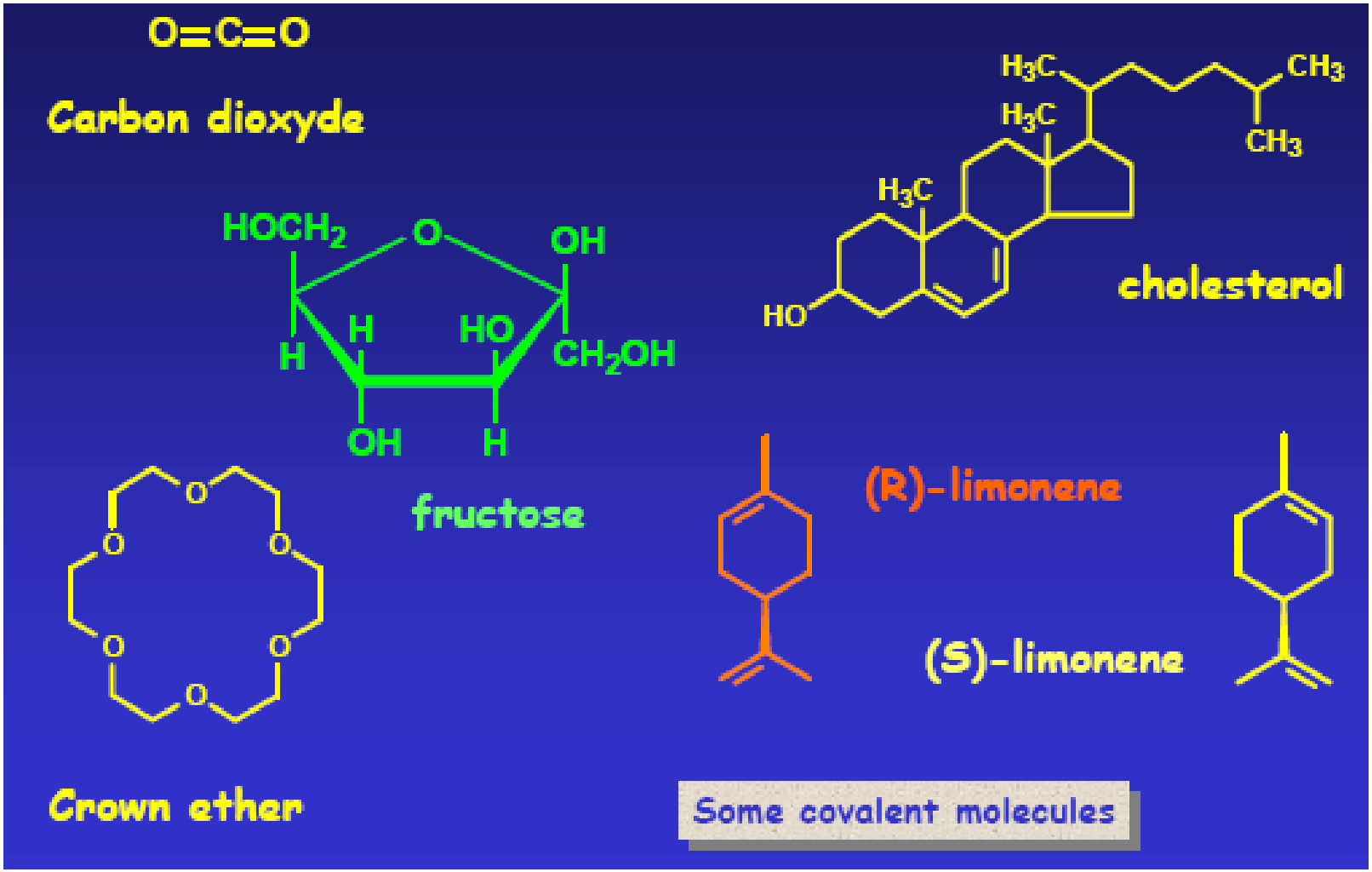
Covalent Chemistry (2)



Covalent Chemistry (3)



Covalent Chemistry (4)



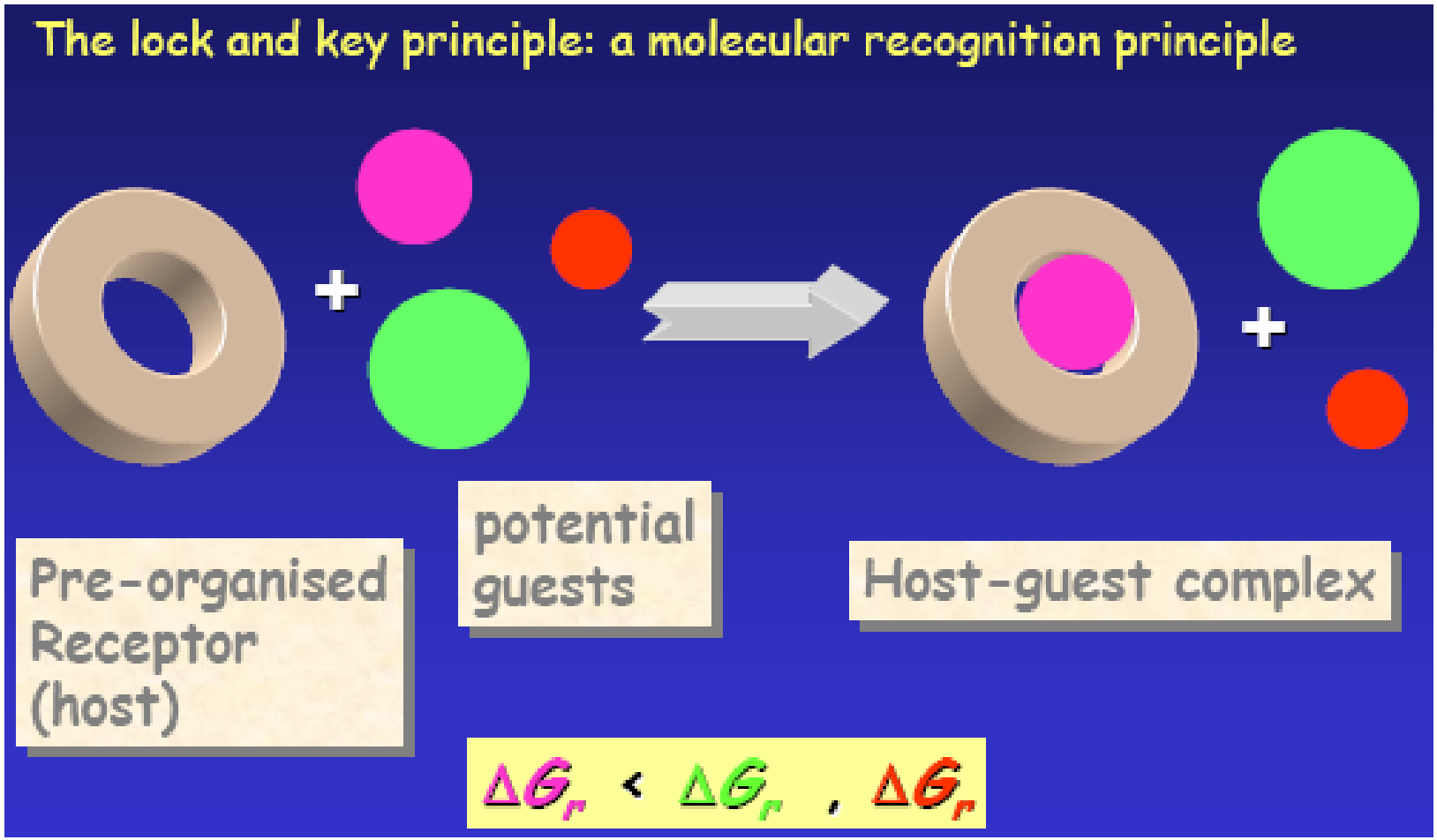
Molecular Recognition – Definition (1)

- Is the binding and specific selection of substrates by a given receptor molecule
  - binding forms a complex, or supramolecule
- Pattern-recognition process
- Major difference – types of bond
  - molecular chemistry - covalent bond
  - supramolecular chemistry - noncovalent types of binding
    - eletrostatic interactions
    - hydrogen bonding
    - van der Waals forces
    - etc

Molecular Recognition – Definition (2)

- has a critical role to play in
  - catalytic activity
  - membrane trasport
- self-assembly and self-organization
- most, if not all, biological processes involve a molecular recognition event at some stage

Molecular Recognition Basic



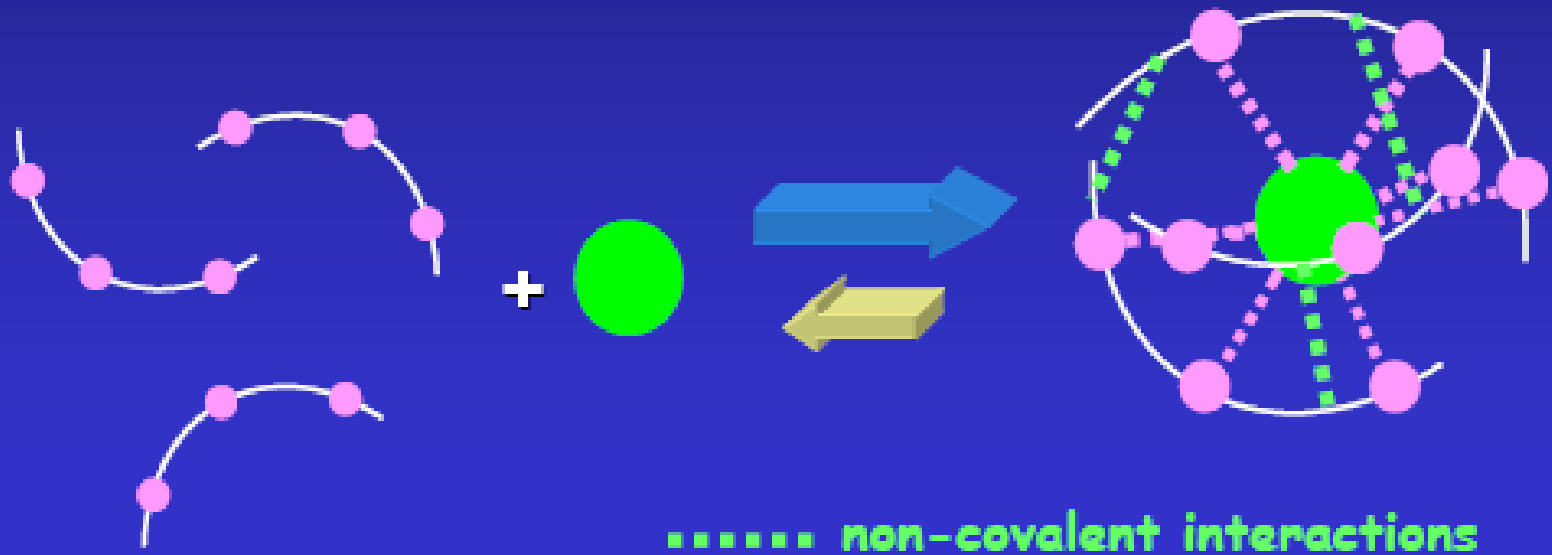
Molecular Recognition Basic

- Lock and key principle (Emil Fischer, 1894)
  (and induced fit principle)
- Non-covalent interactions: $kJ \cdot mol^{-1}$
  - Electrostatic interactions:
    - ion-ion, ion-dipole: 200-400
    - hydrogen bonds, dipole-dipole: 20-60
    - dispersion, induction forces (van der Waals interactions): 5-20

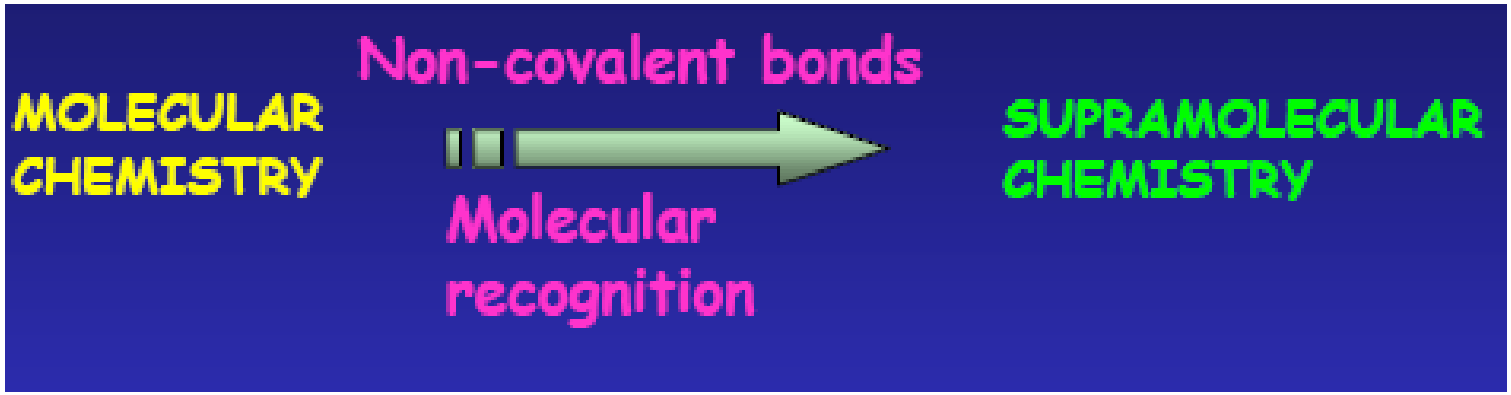
Molecular Recognition Basic

- π–π stacking interactions
- hydrophobic effects or solvent effects
- steric effects

♣ Self-assemby processes



Molecular Recognition Basic



Molecular Recognition Basic

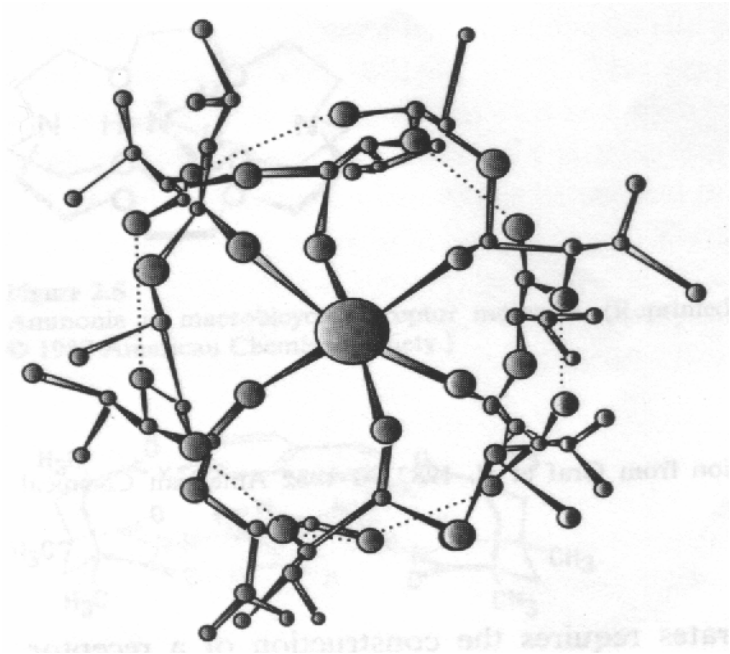
- Factors
  - Steric (shape and size) complementarity
  - Interactional complementarity
  - Large areas of contact between receptor and substrate
  - Multiple interaction sites
  - Strong overall binding
  - Inclusion and Dynamics
  - Medium effects on molecular recognition

Contents

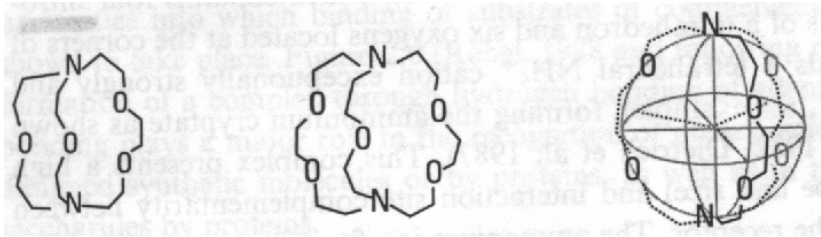
Examples (1)

- Exoreceptors
  - analogous to enzymes
- the active sites are containes inside the cavity of a large protein molecule,
- then binds a smaller substrate fitting into the cleft
- most cavities range from approximately 2 to 15 angstroms

Examples (2)

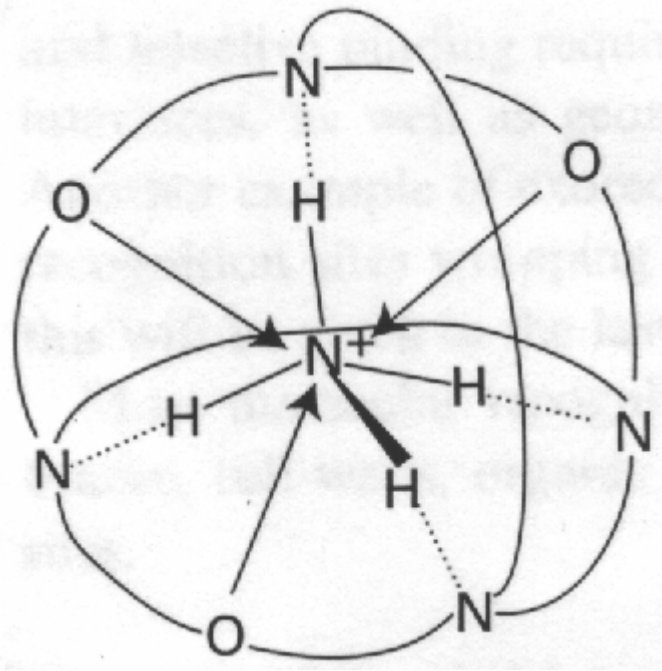


cubic binding of K^+ into valinomycin

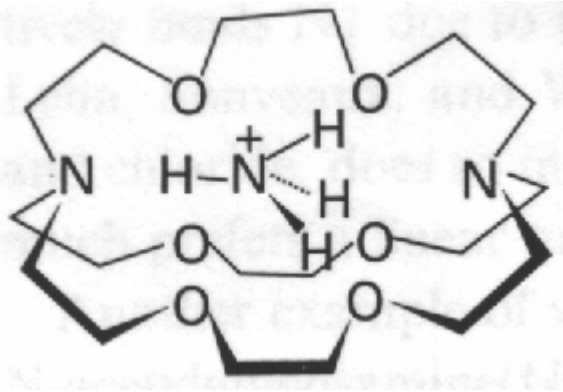


macrobicyclic ligands –
Spherical recognition

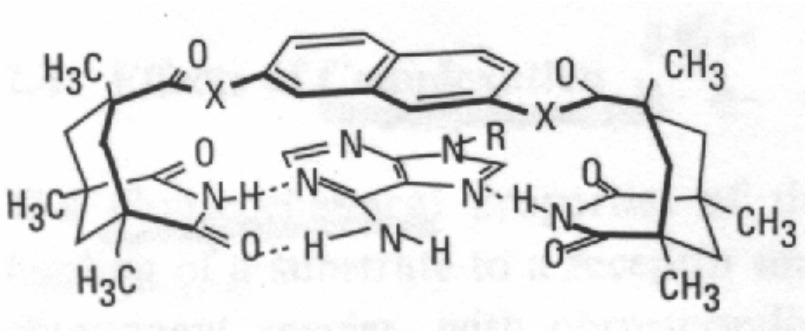
Examples (3)



ammonium cryptate - Tetrahedral Recognition



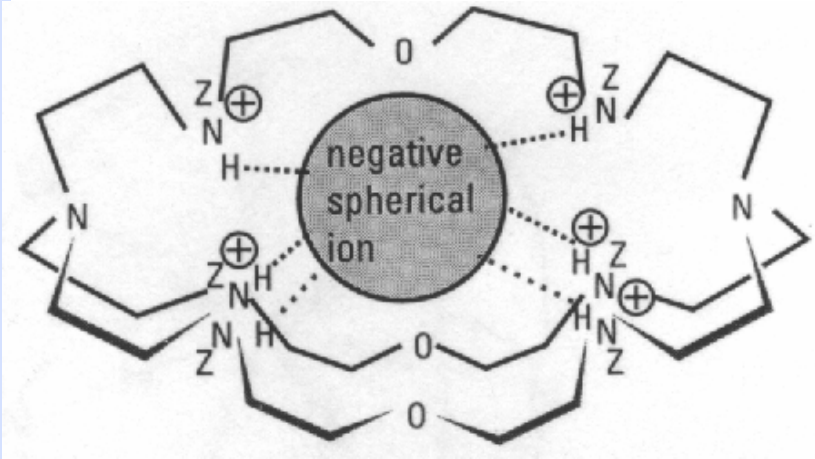
Ammonia in macrobicyclic receptor molecule

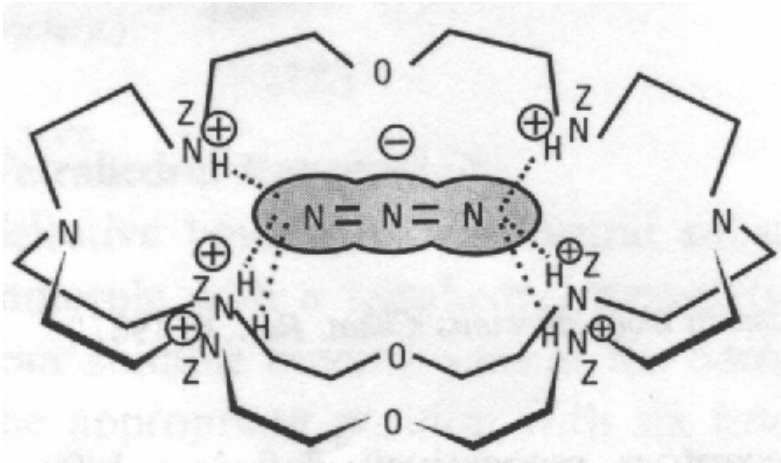


Binding of adenine in a cleft

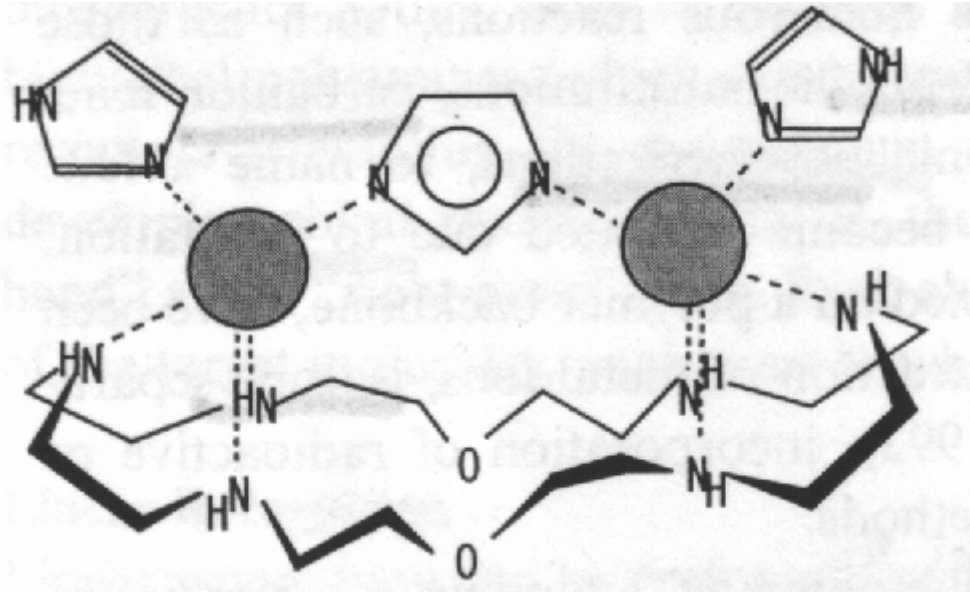
Examples (4)

- Linear Recognition





Multiple Recognition



Cascade-type dinuclear copper (II) cryptate fromed with a macrocyclic polyamine as the ligand. The copper ions bind first, followed by the imidazole groups.

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  - **Chemical Systems**
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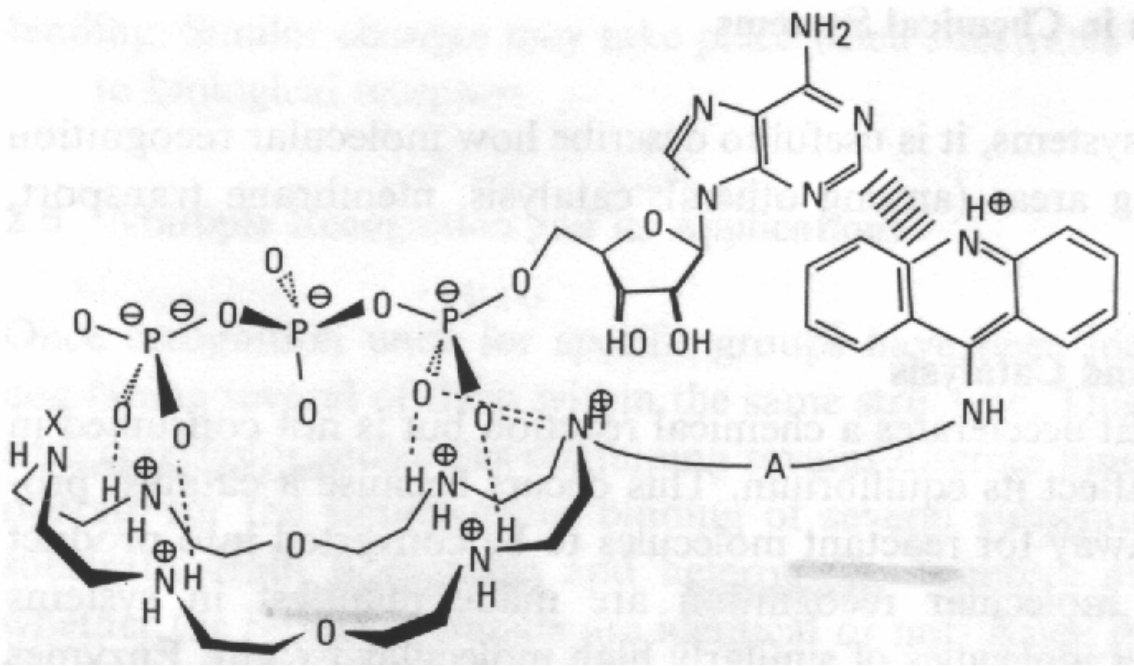
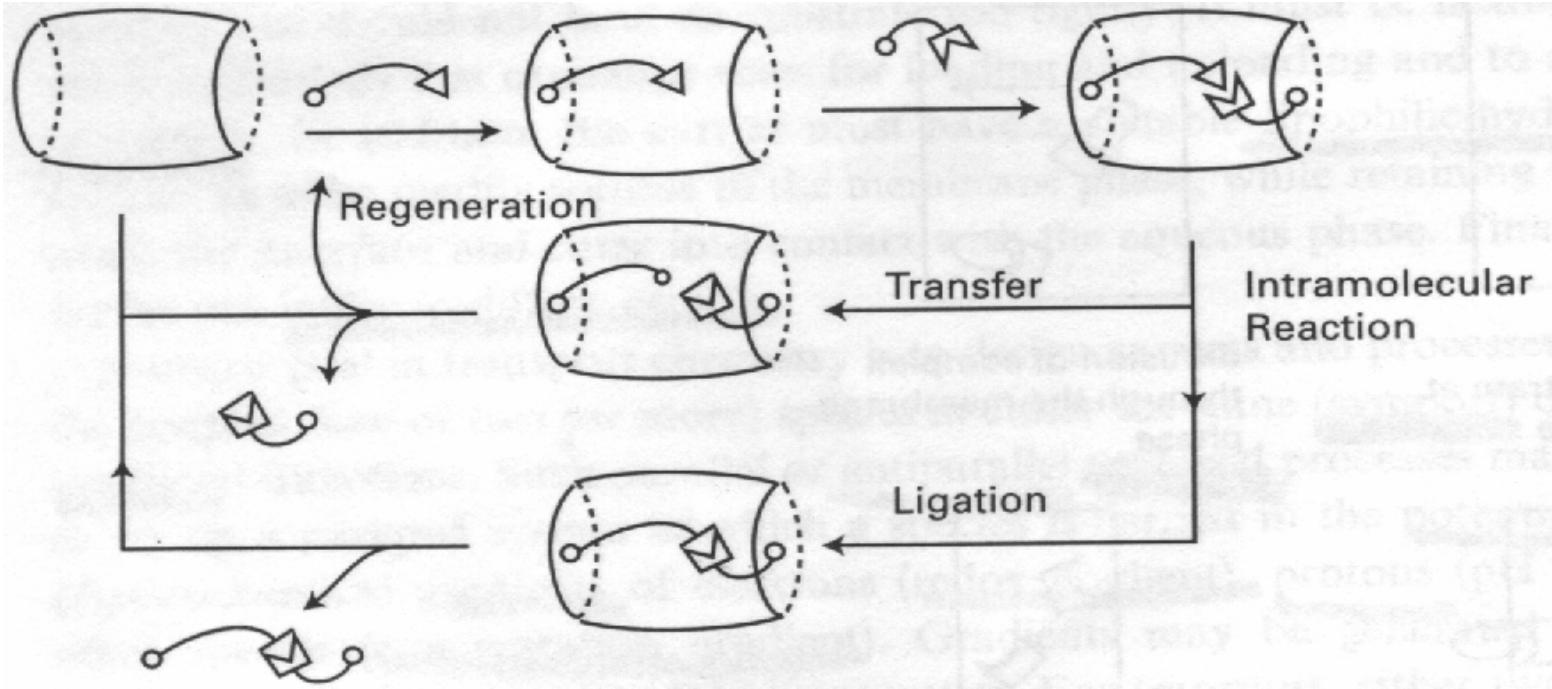
    - Carrier-Mediated Transport
    - Photonic Molecular Devices
  - Self-Assembly, Self-Recognition, and Self-Organization
    - Micelles and LB Films
- Thermodynamics, Information, and Entropy

Supramolecular Reactivity and Catalysis (1)



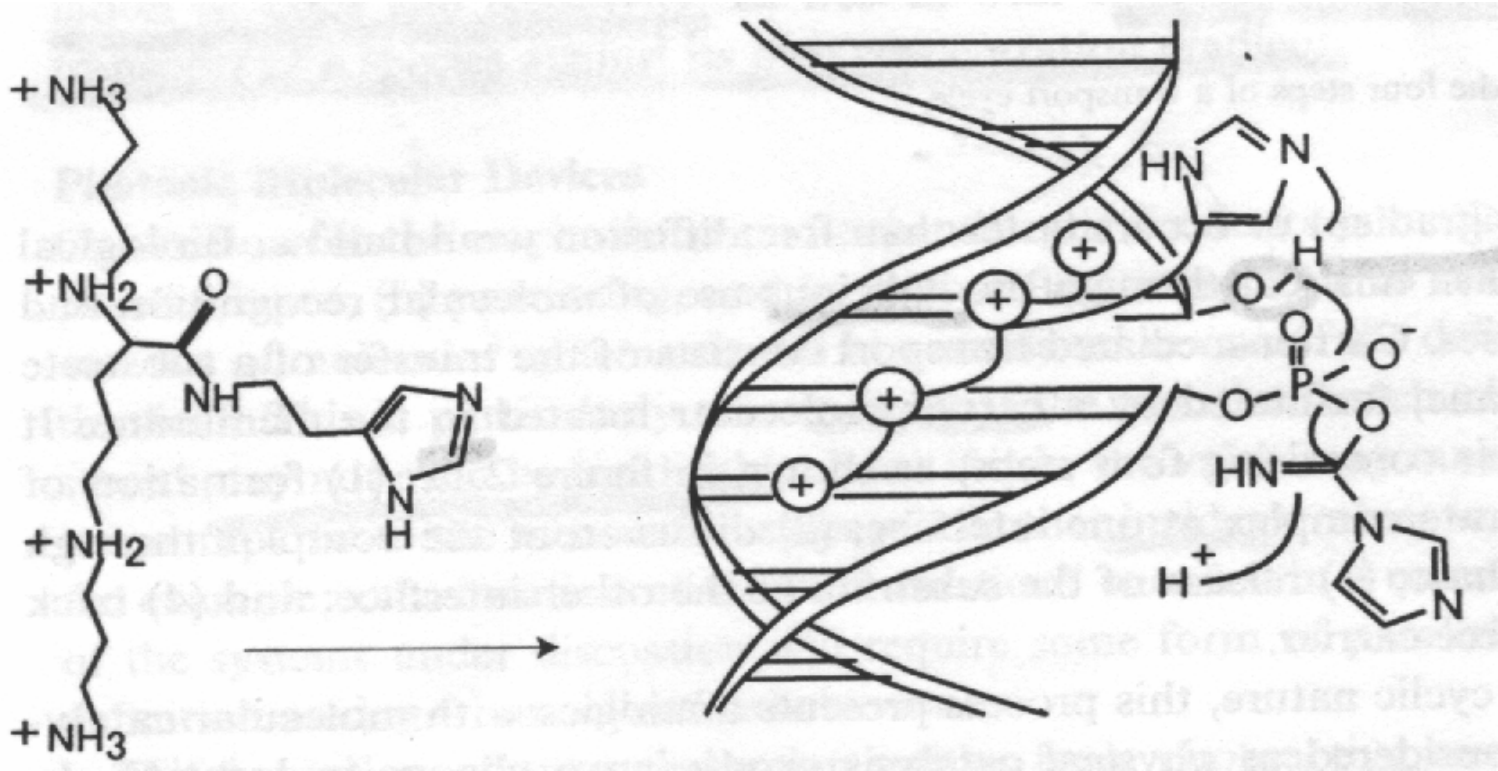
Hypothetical structure of the ATP complex in the catalysis of ATP hydrolysis

Supramolecular Reactivity and Catalysis (2)



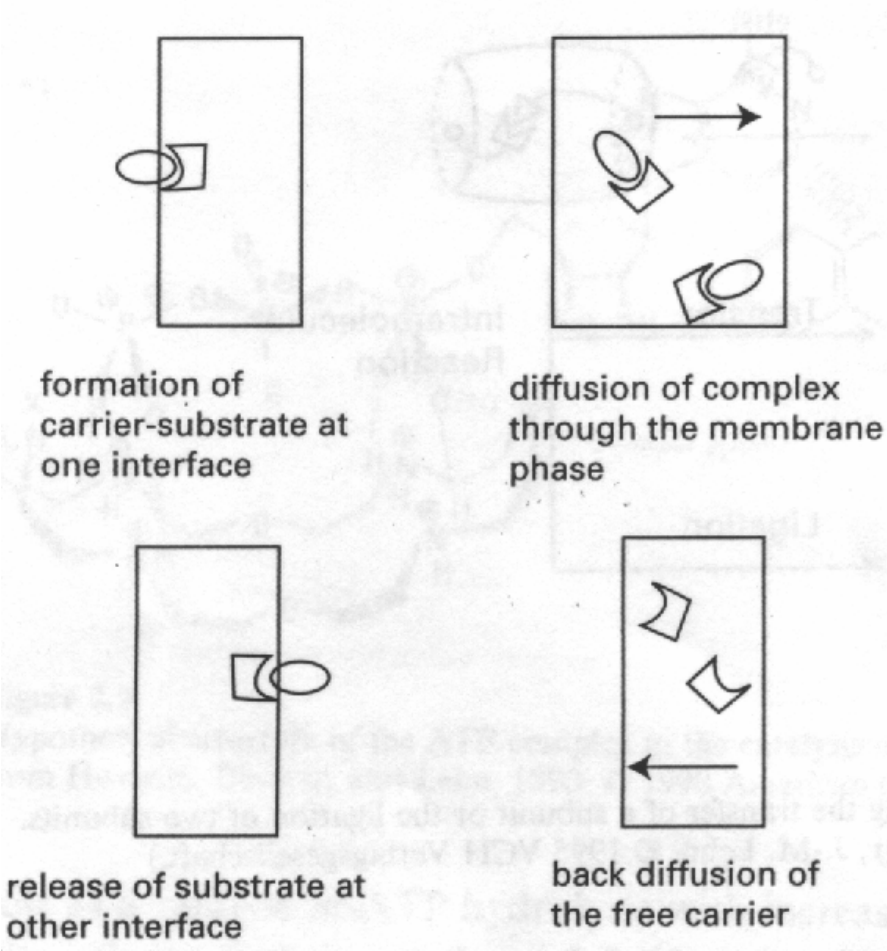
Cocatalysis cycle, with final products either being the transfer of a subunit or the ligation of two subunits.

Supramolecular Reactivity and Catalysis (3)

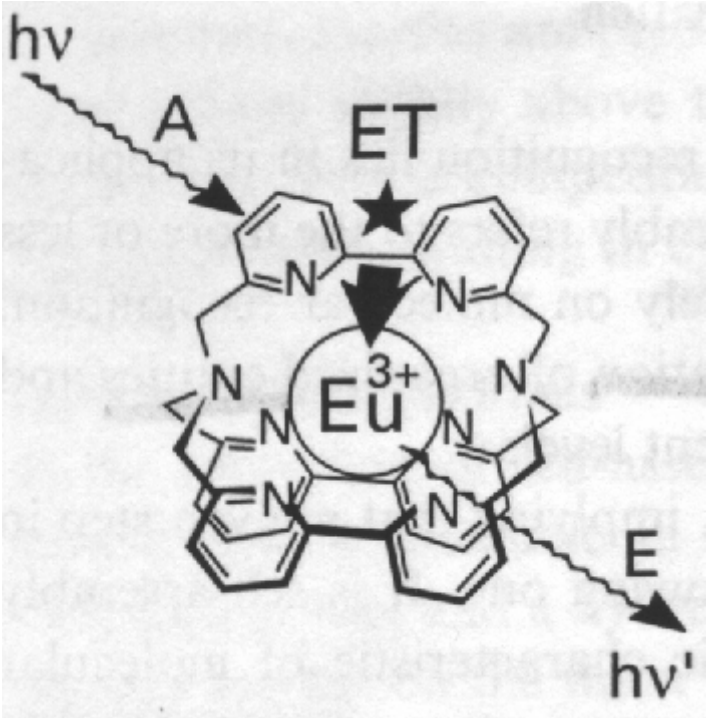


Enhancement of ligation of DNA as effected by an imidazole-functionalized spermine binding in the minor groove of the double helix

Carrier-Mediated Transport

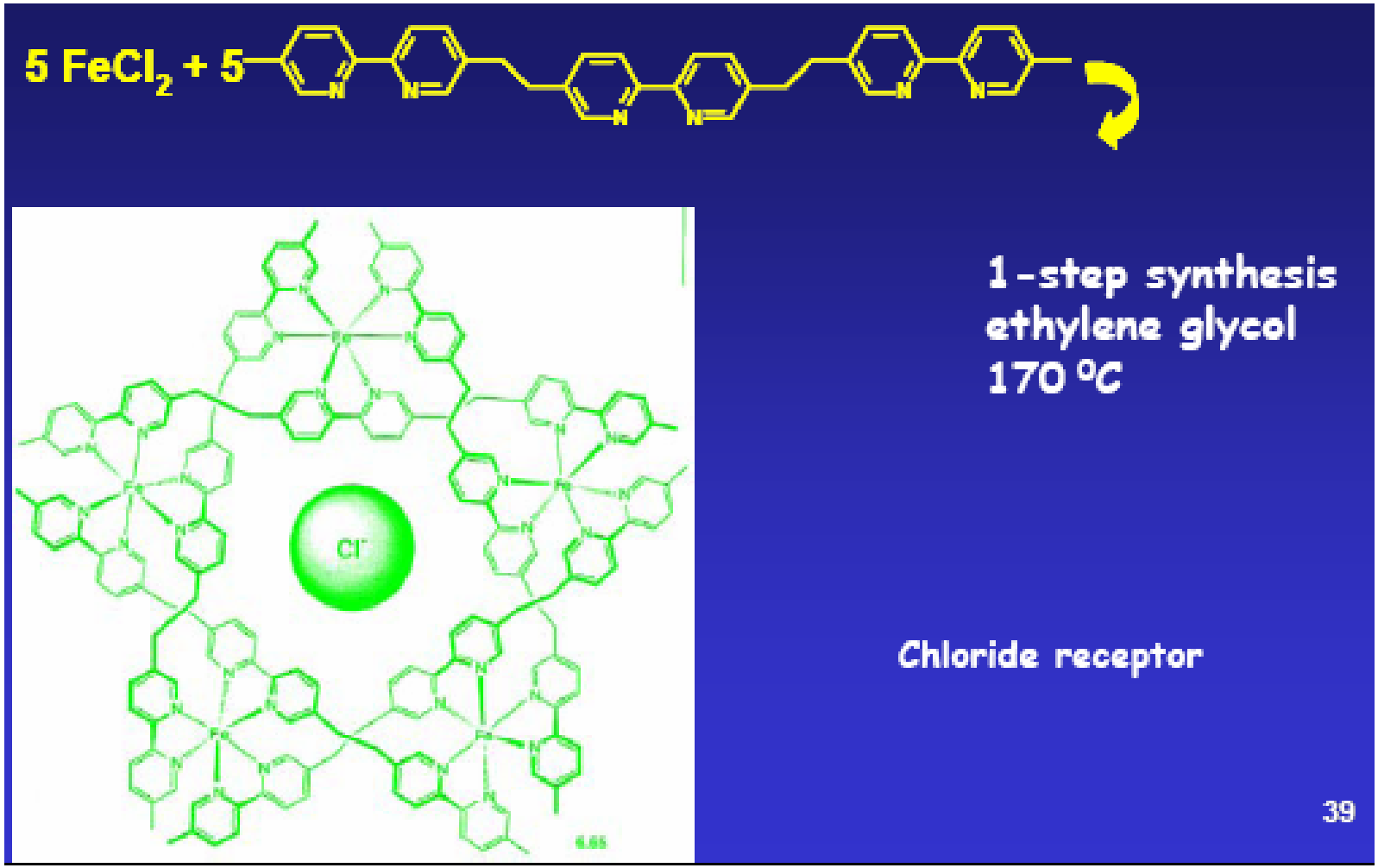


Photonic Molecular Devices

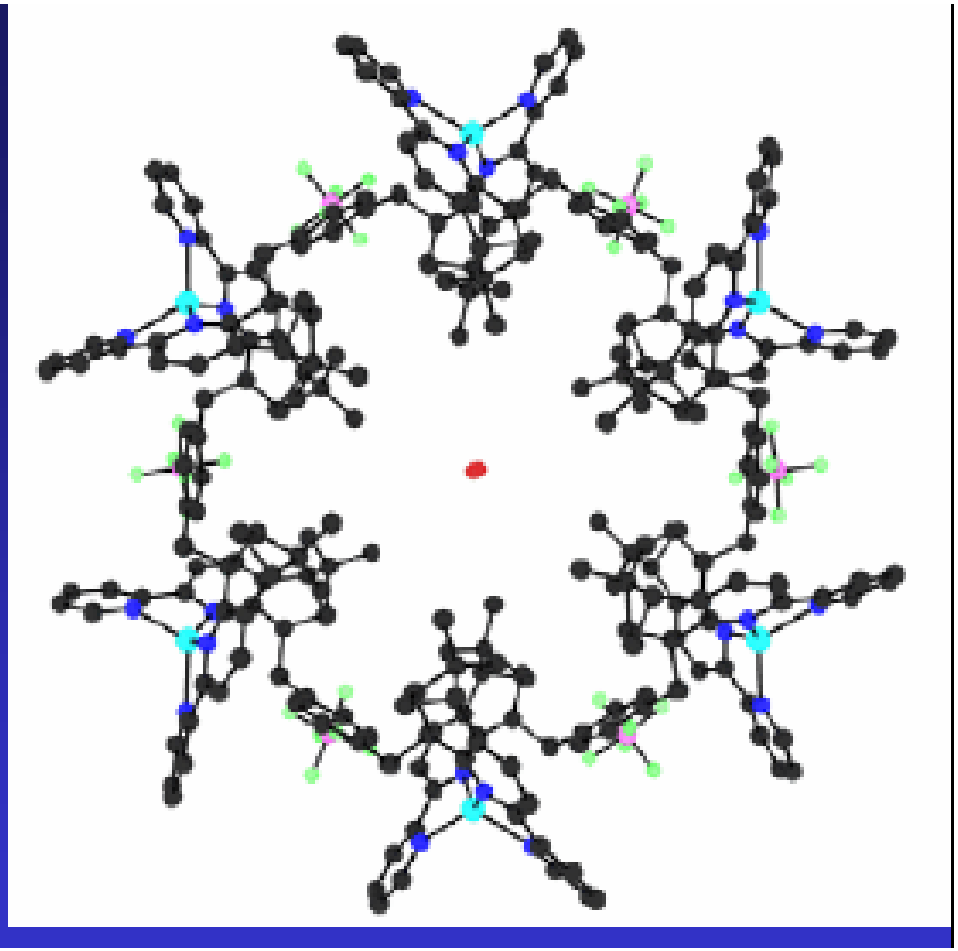


Eu(III) cryptate showing the three steps (absorption, energy taransfer, and emission) in light conversion

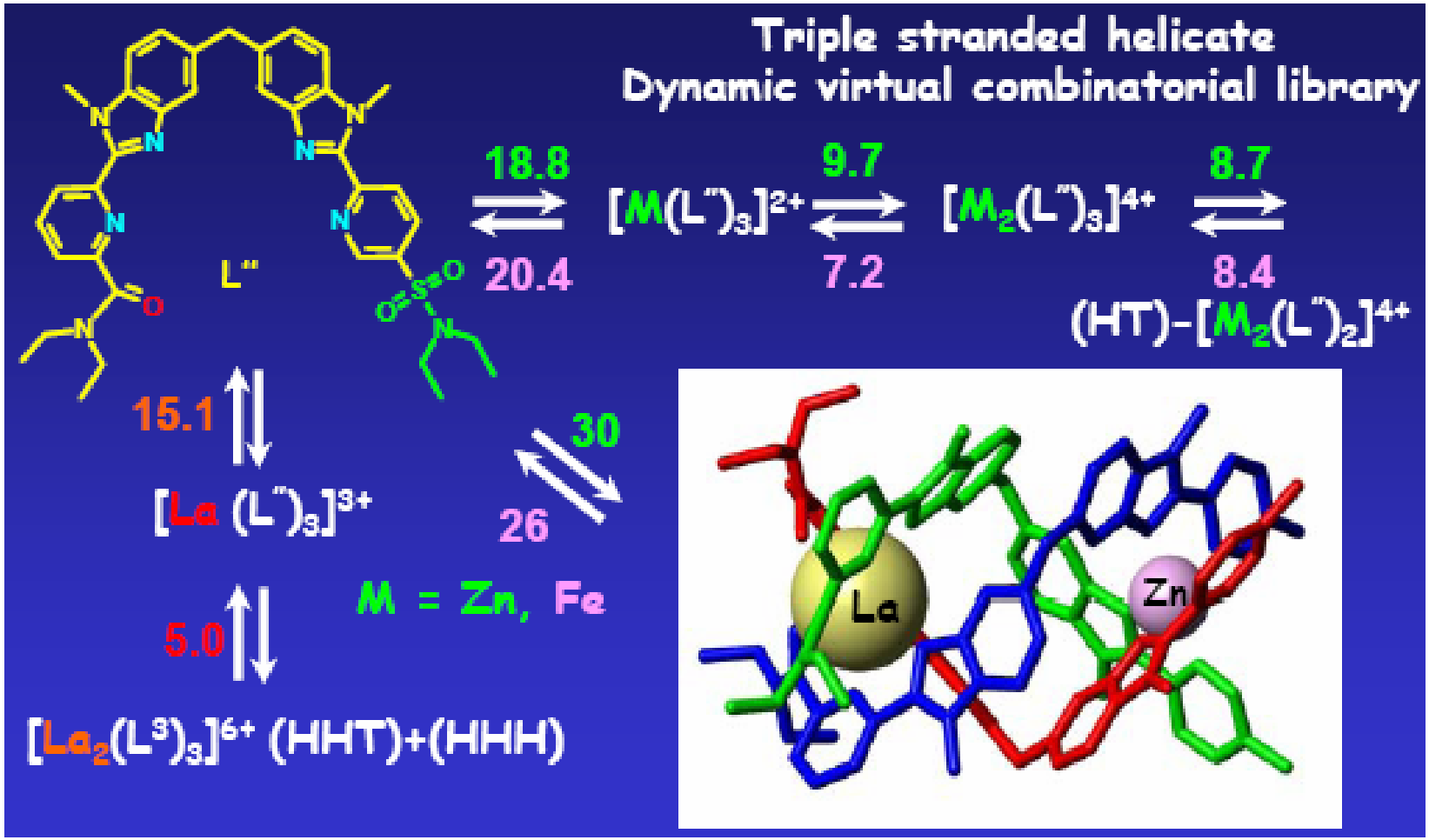
Self-Assembly, Self-Recognition, and Self-Organization (1)



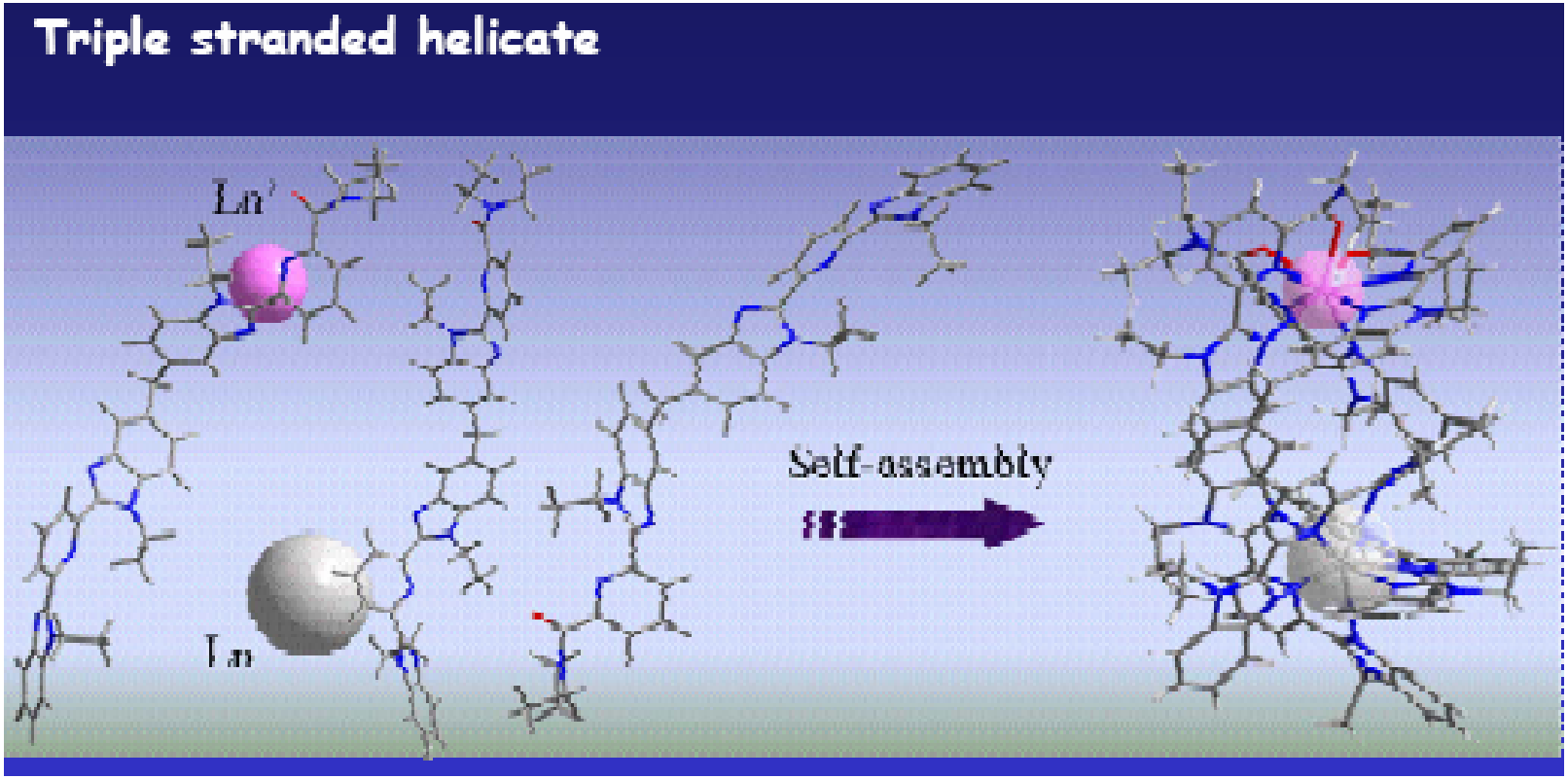
Self-Assembly, Self-Recognition, and Self-Organization (2)



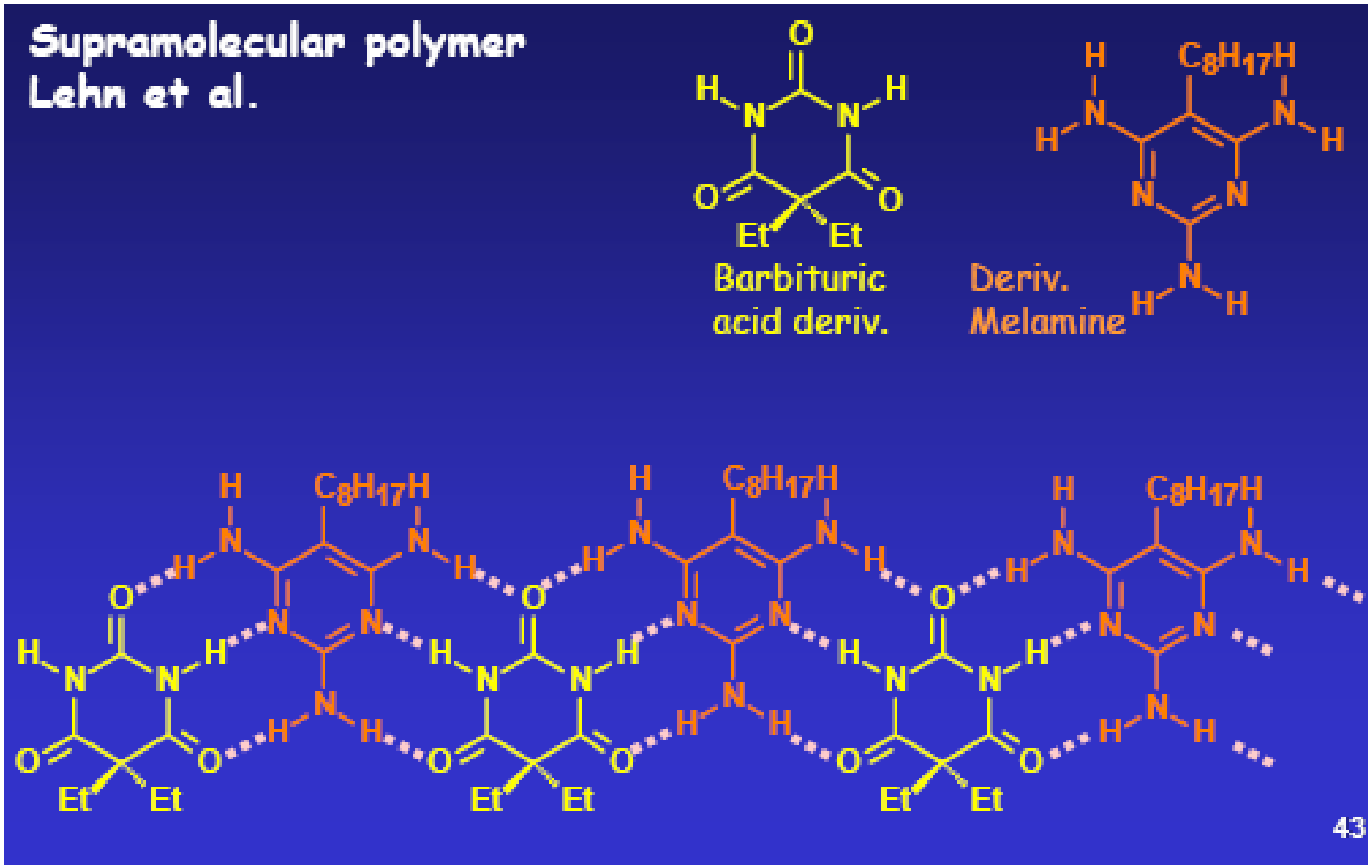
Self-Assembly, Self-Recognition, and Self-Organization (3)



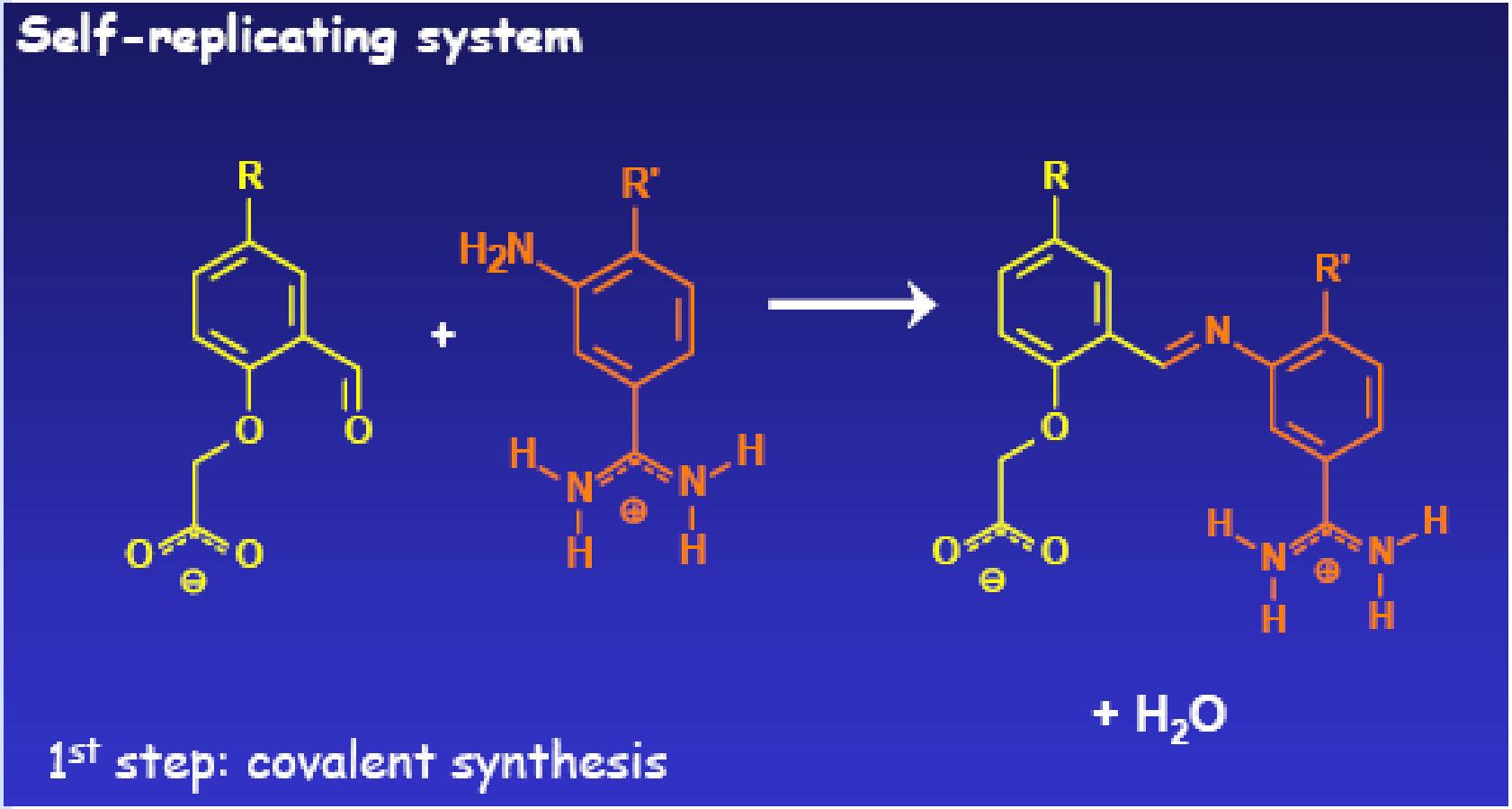
Self-Assembly, Self-Recognition, and Self-Organization (4)



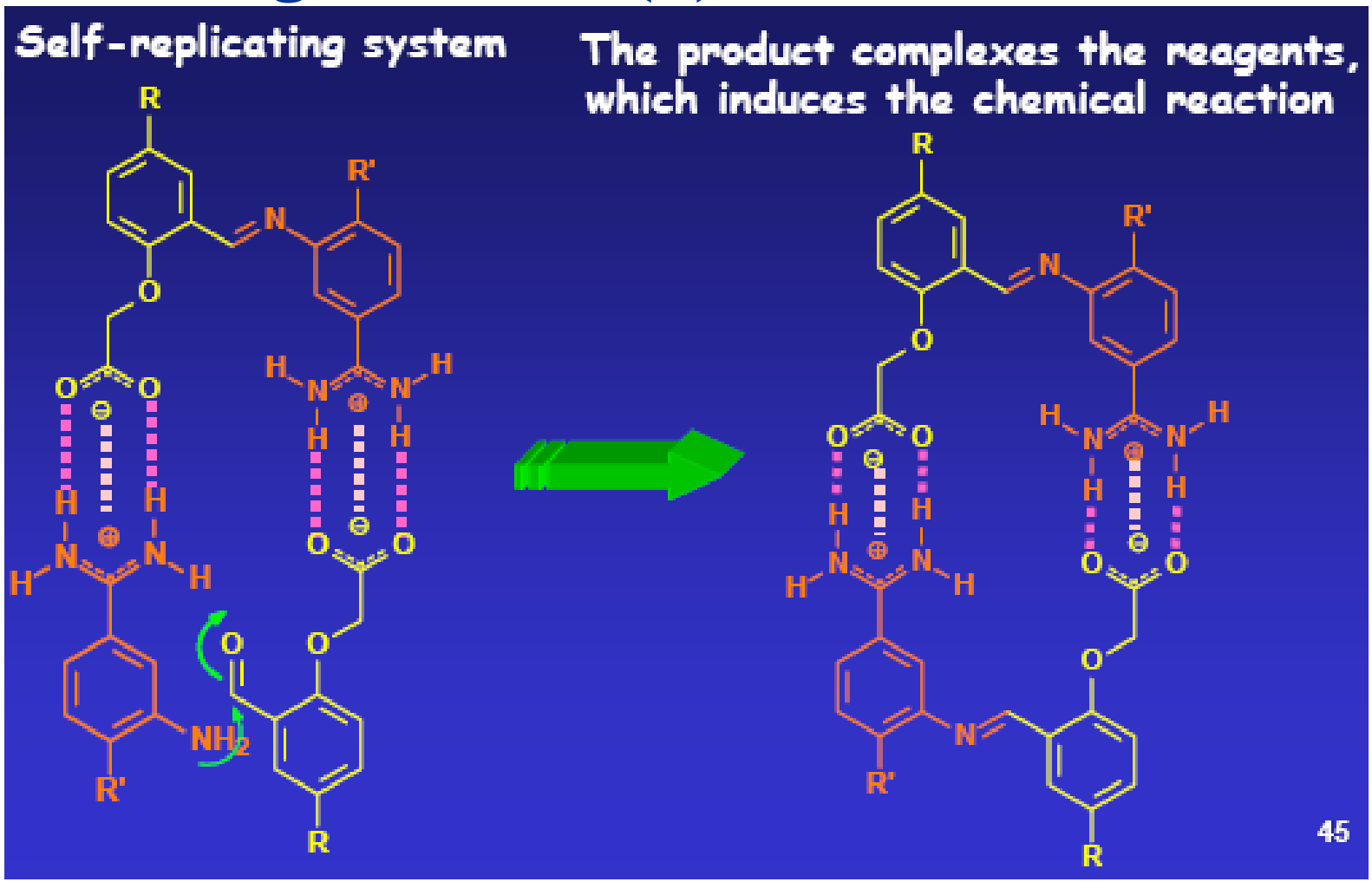
Self-Assembly, Self-Recognition, and Self-Organization (5)



Self-Assembly, Self-Recognition, and Self-Organization (6)



Self-Assembly, Self-Recognition, and Self-Organization (7)



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  - Chemical Systems
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- **Thermodynamics, Information, and Entropy**

Thermodynamics, Information, and Entropy (1)

- Factor must be considered
  - the interplay of limitations on information
  - entropy
  - whereas not about most present computer systems
- How to read information in and out
  - self-organizing behavior may work
  - it may be impossible to easily access the information without
    - erasing it
    - perturbing it
  - regeneration of the data
    - may negate putative advantages

Thermodynamics, Information, and Entropy (2)

- Chemical systems may store information either
  - in an anlog fashion; size, shape, nature, and disposition
  - or in a digital fashion; states, connections
- Recognition is a relative notion
  - results from the structural information stored in the parners
  - which rests on the difference in free energy of interaction between states
  - depends on, consequently, temperature

Thermodynamics, Information, and Entropy (3)

- these are all natural process
  - entropy always increases
- information transfer and self-replication
  - a molecule catalyzes its own formation by acting as template
  - contituents react to generate a copy of it
  - may be termed informational

Thermodynamics, Information, and Entropy (4)

- Another good features
  - self-correction
  - adaptation
- pure compounds → instructed mixtures
- unicity → multiplicity + information
- Next step! “learning” systems
  - not only instructed but can be trained
- Third basic feature of chemical systems: information
  - in addition to matter and energy