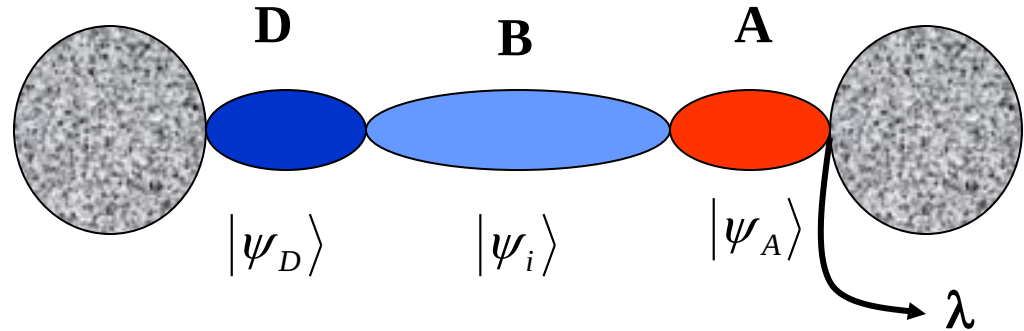
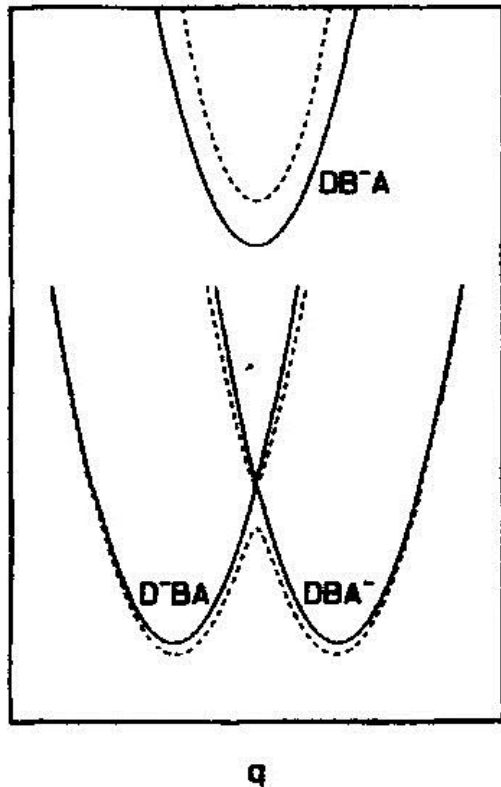


Eletrônica e Fotônica molecular

Introdução

Transferência de elétrons em dispositivos moleculares



$$H = H_S + i\lambda |\psi_A\rangle\langle\psi_A|$$

Hamiltoniano do sistema

$$|\chi_j\rangle = \sum_i C_{ji} |\psi_i\rangle$$

Autofunções de H

$$P_i(t) = \left| \langle \psi_i | \exp(-iHt/\hbar) | \psi_D \rangle \right|^2$$

Probabilidade do e⁻ no estado i

$$P(t) = \sum_i P_i(t)$$

Probabilidade do e⁻ não fugir para o contato

$$\tau = \int_0^\infty P(t) dt$$

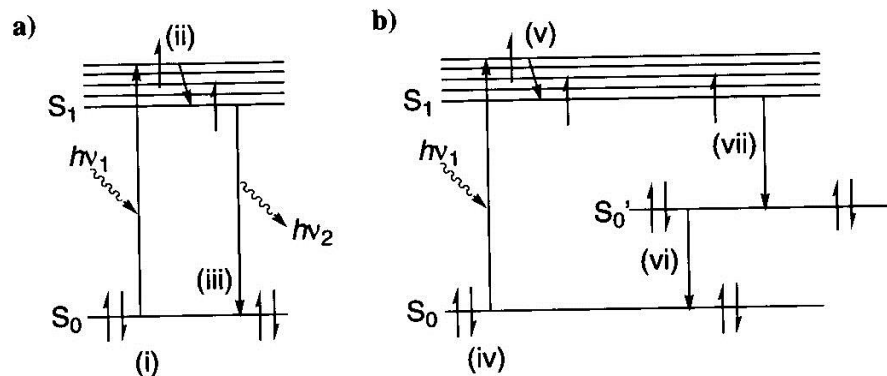
Tempo de vida do e⁻ no sistema

$$k = \tau^{-1}$$

Taxa de transferência de elétrons

Portas lógicas moleculares e sensores

1. Porta AND

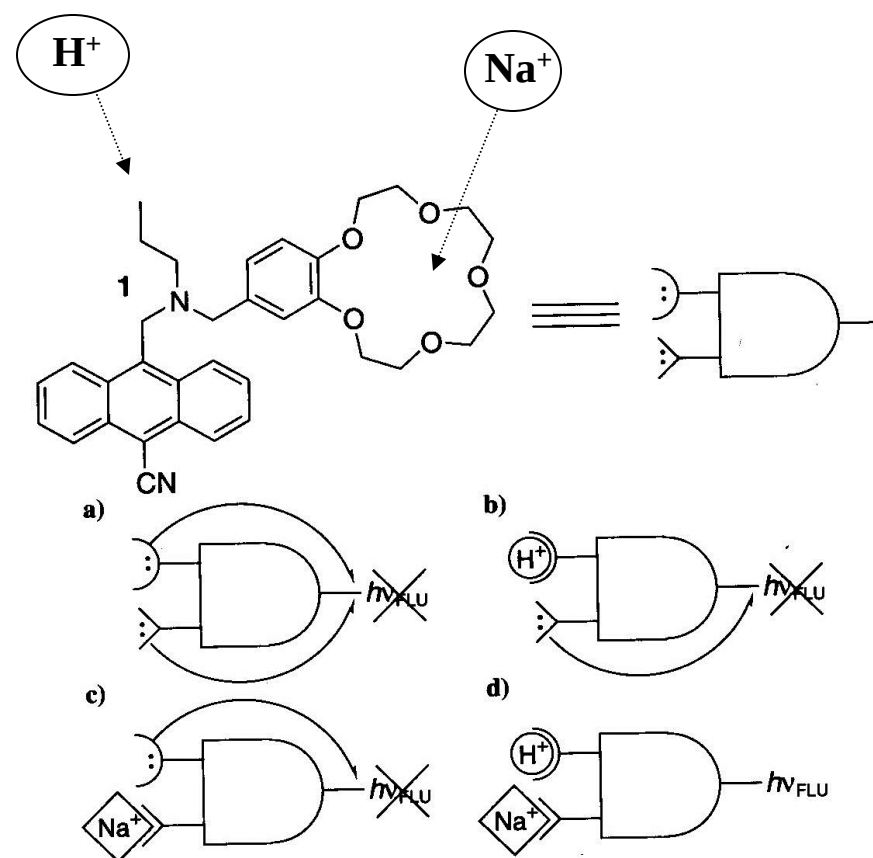


a) Transição eletrônica radiativa

b) Transição Eletrônica não radiativa

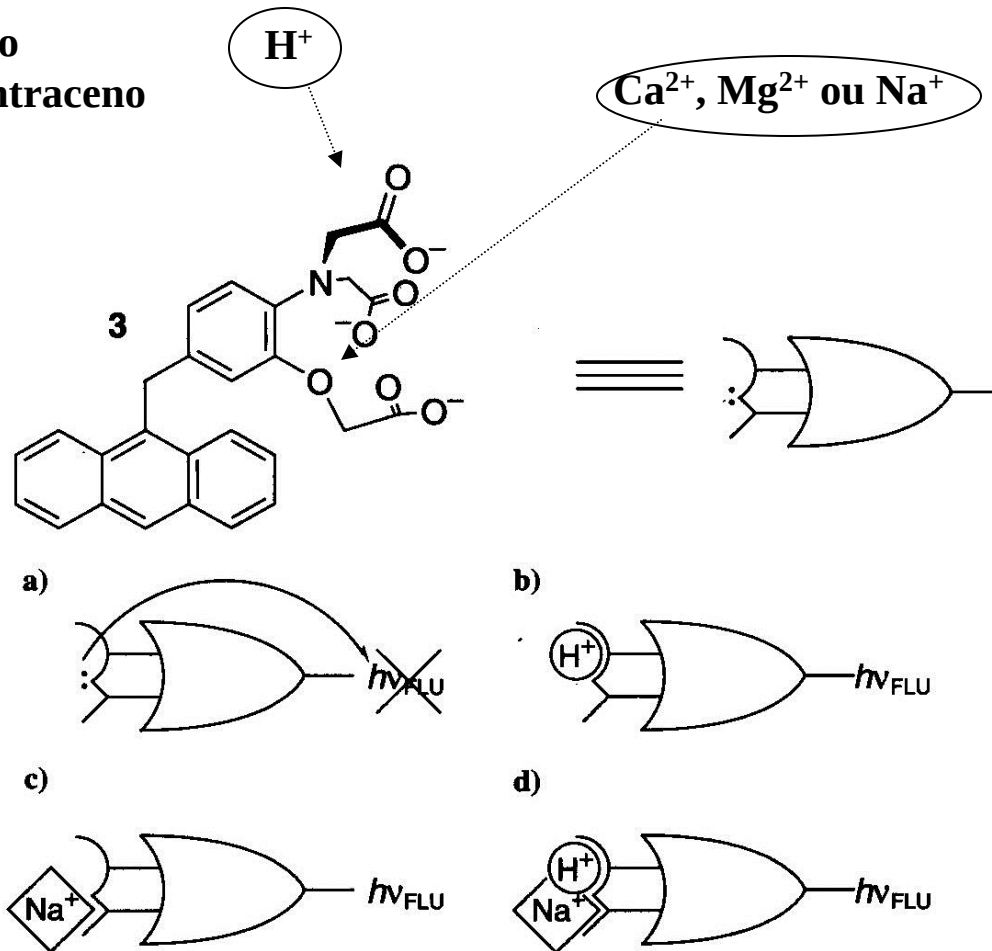
PET: “Photo induced electron transfer”

**PET desde o amino terciário para o antraceno
ou desde o Eter Crown para o antraceno**

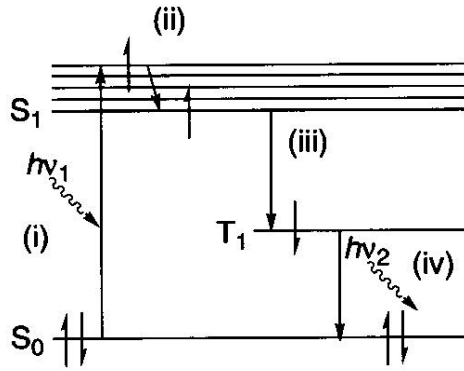


Porta Or

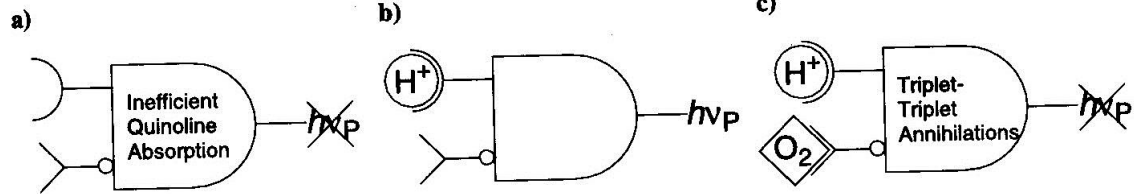
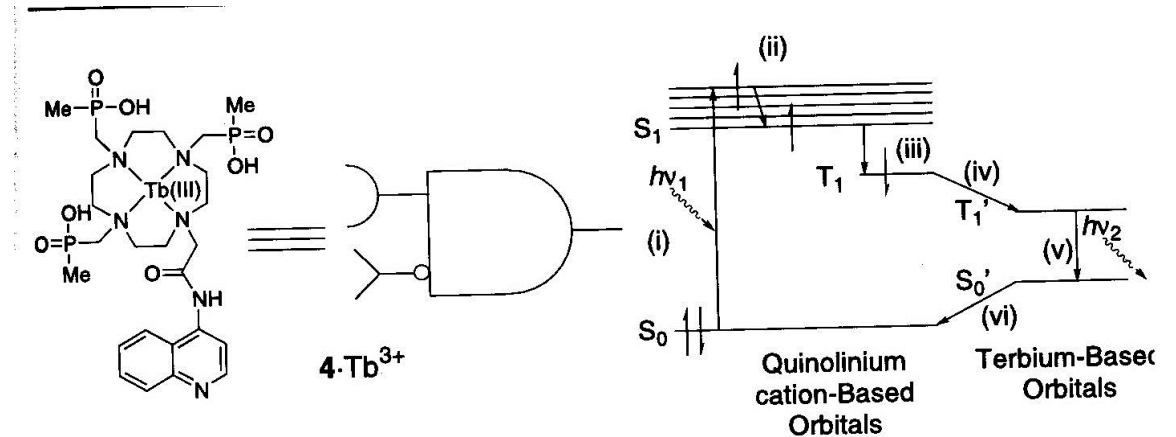
PET desde o amino
terciário para o antraceno



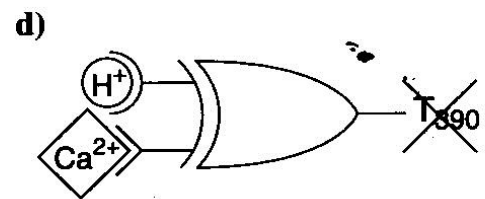
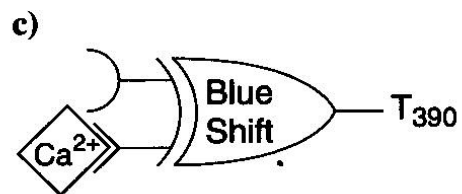
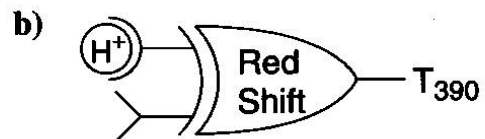
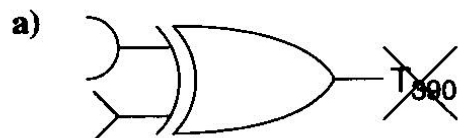
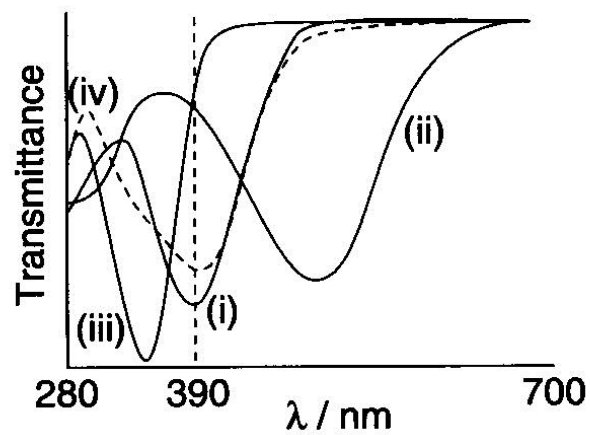
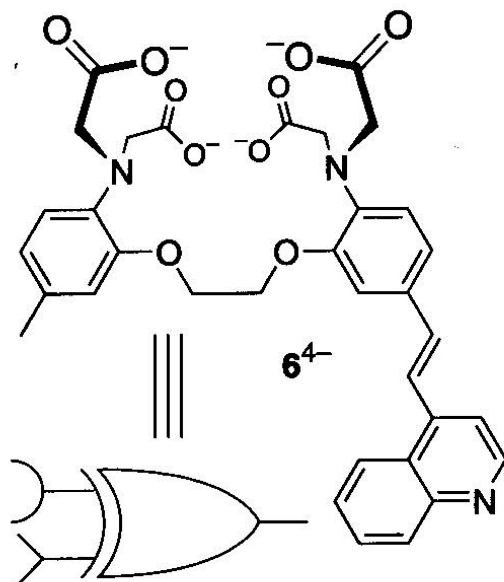
Porta inibidora



Transição eletrônica de fosforescência



Porta XOR



Nano células moleculares programáveis

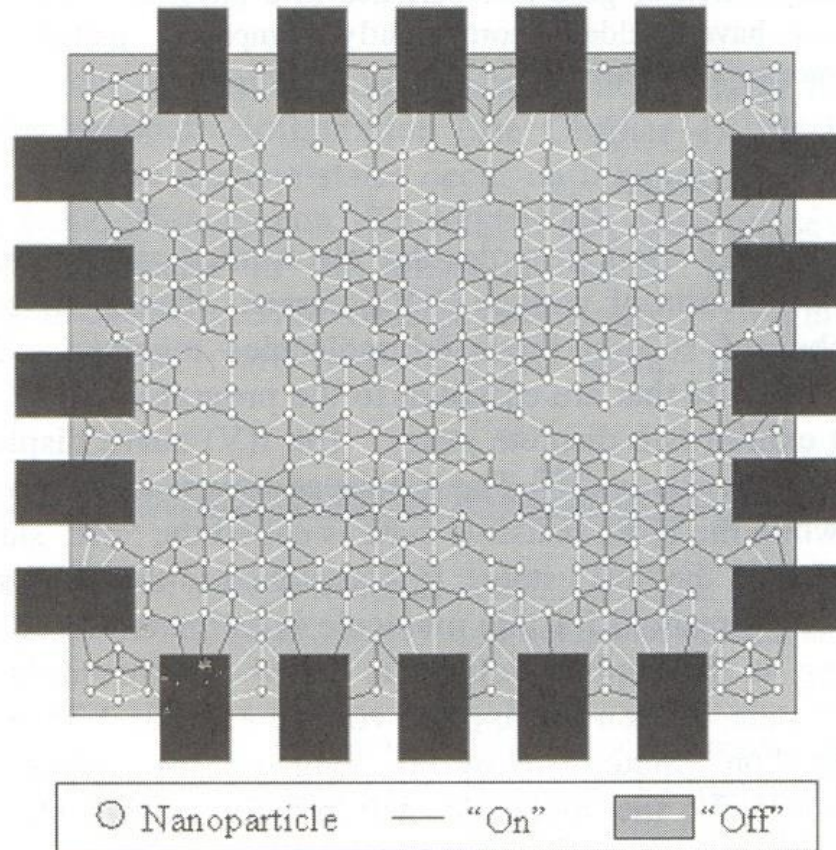
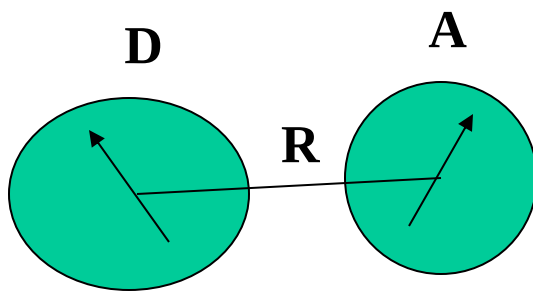


Figure 6.1 This is a simulated NanoCell with five I/O leads on each side. Within the cell is a planar array of metallic nanoparticles and molecules (dark and light lines). The molecules can be in a high conducting state (dark lines) or a low conducting state (white lines).

Transferência de Energia



$$H = H_{rad} + \sum_X H_{Mol}(X) + \sum_X H_{Int}(X)$$

$$H_{int} = -\epsilon_0^{-1} \mu(X) \cdot d^\perp(R_X)$$

$$d^\perp(R) = i \sum \left(\frac{\hbar c k \epsilon_0}{2V} \right) e^{(\lambda)}(k) \left\{ a^{(\lambda)}(k) e^{ik \cdot R} - a^{(\lambda)+} e^{-ik \cdot R} \right\}$$

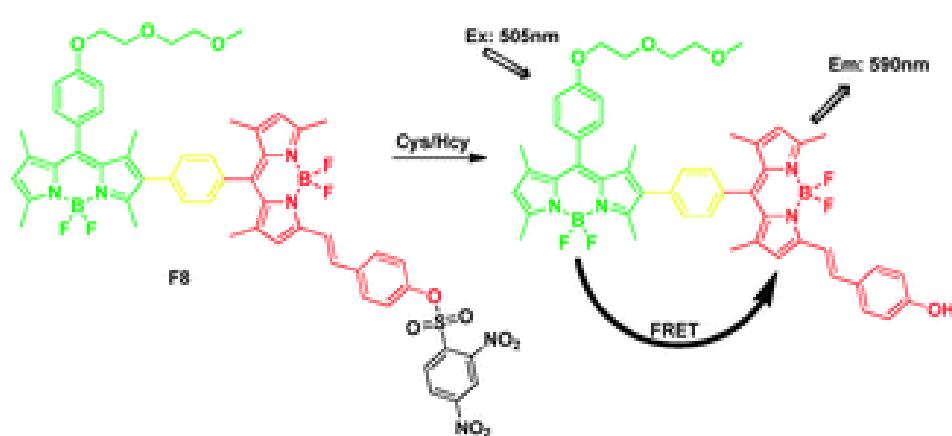
$$|I\rangle = |D^*\rangle |A\rangle |0\rangle$$

$$|F\rangle = |D\rangle |A^*\rangle |0\rangle$$

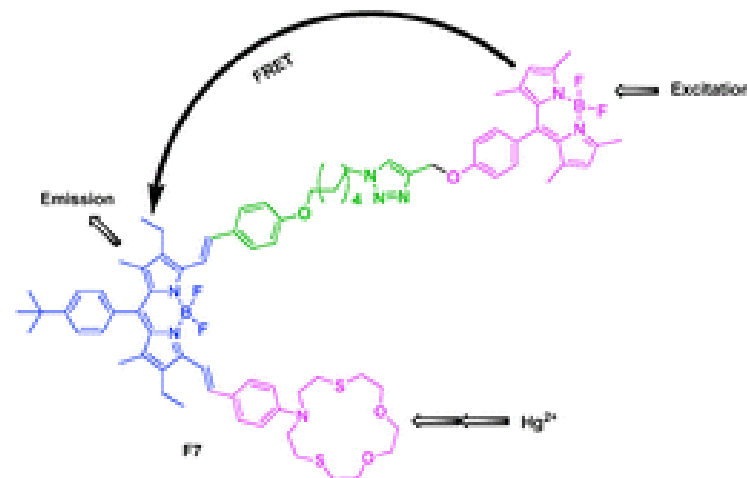
$$W_{FI} = \frac{2\pi}{\hbar} |\langle F | T | I \rangle| \delta(E_I - E_F)$$

$$W_{DA} = \frac{9}{8\pi c^2 \tau_D} \int_0^\infty F_D(\omega) \sigma_A(\omega) \omega^2 g^{vac}(\omega, R) d\omega$$

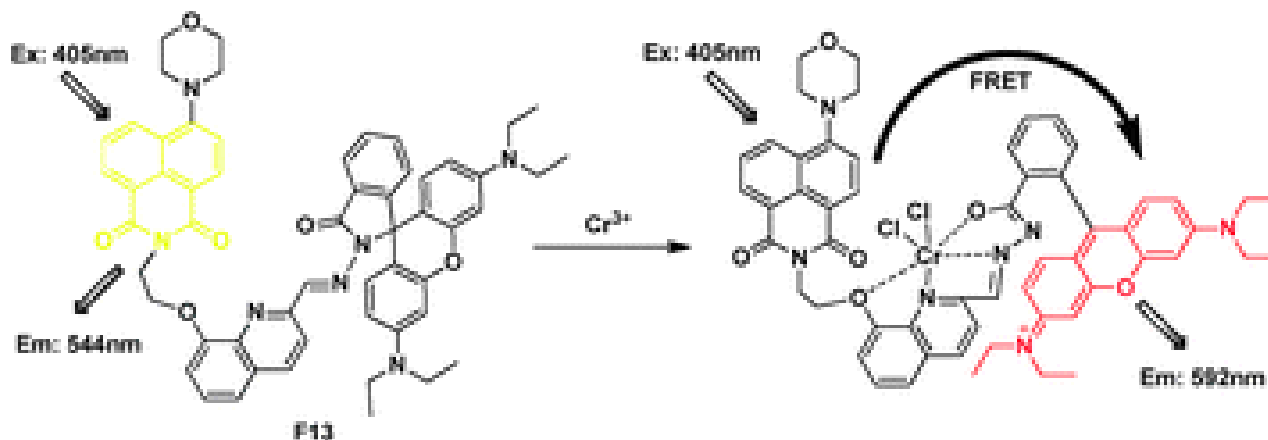
Transferência de Energia: Dispositivos



FRET chemosensor for detection of thiol



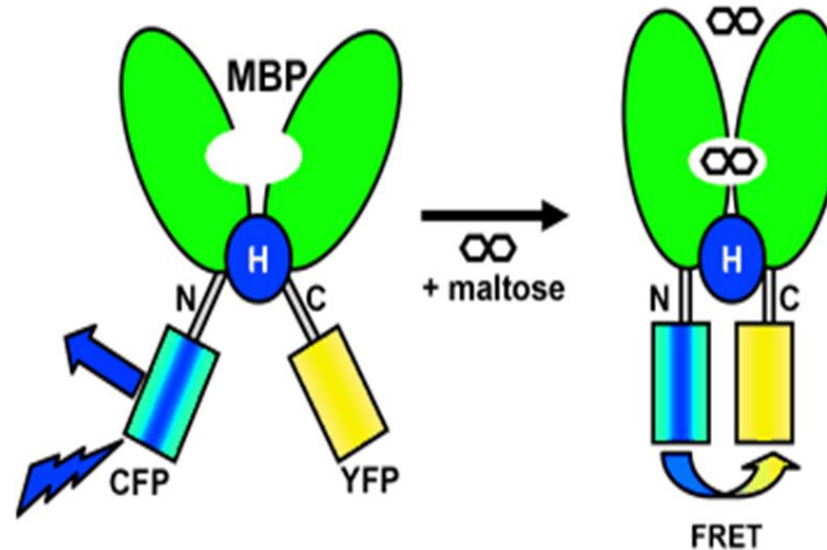
Fluorescent probe for Hg²⁺ based on FRET



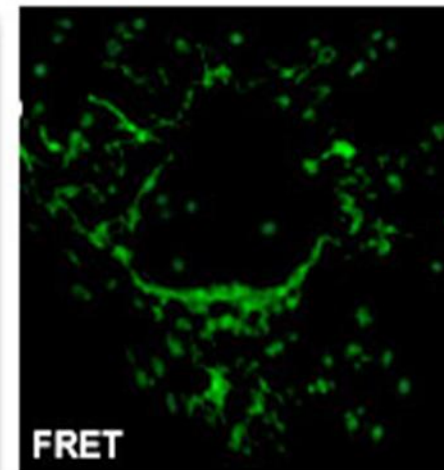
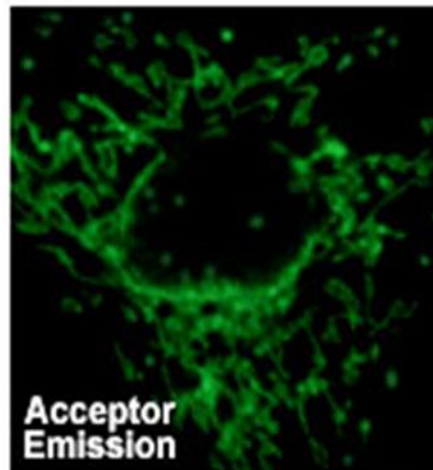
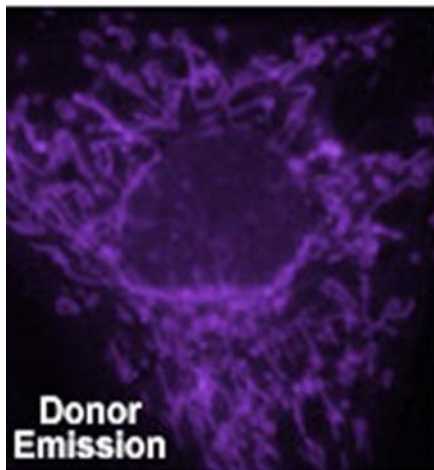
Fluorescent probe F13 for Cr³⁺ detection based on FRET

Transferência de Energia: Dispositivos

maltose-FP sensor

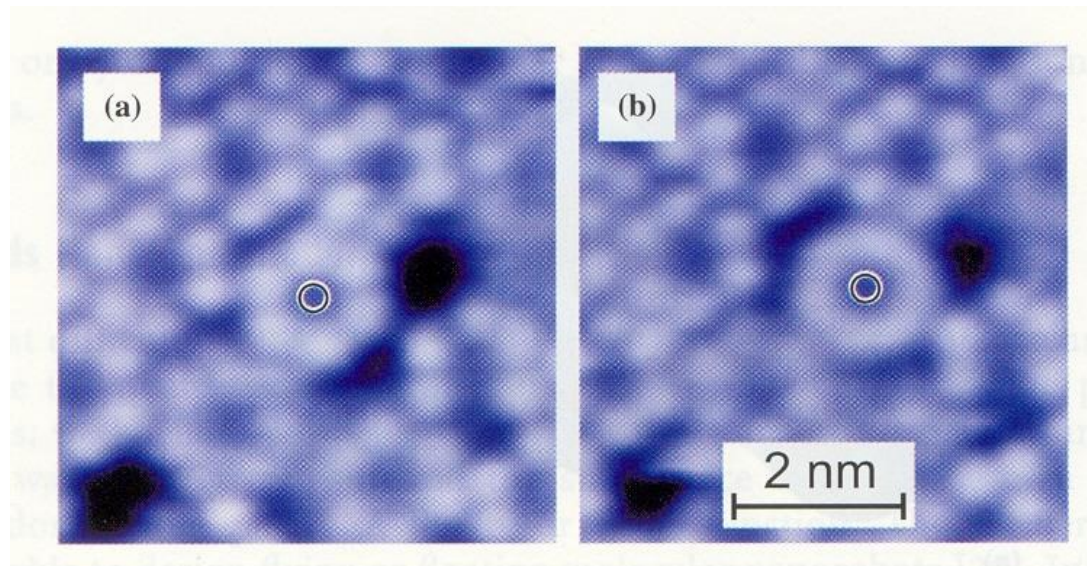


Mitochondrial Protein-Protein Association with FRET



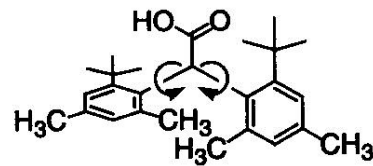
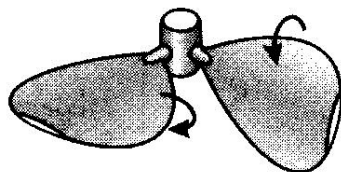
Maquinas moleculares

Maquina Browniana



Propulsor molecular

a



2

Sistema de engrenagem molecular

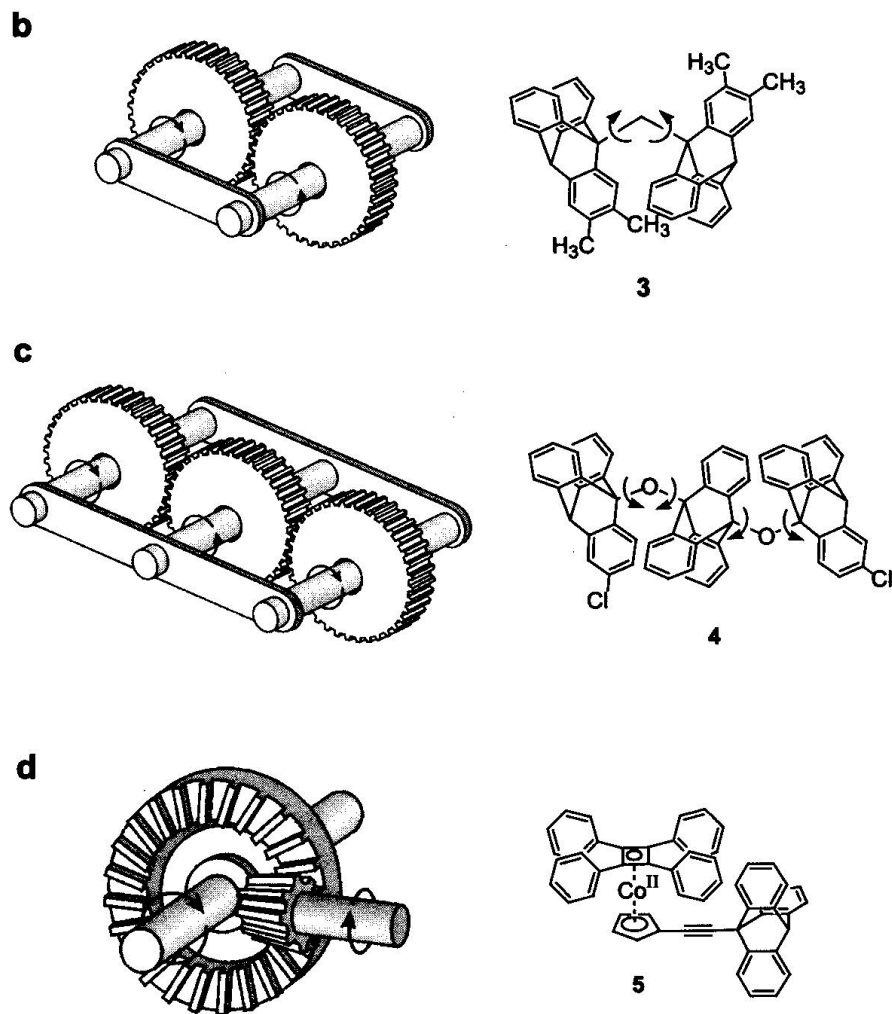
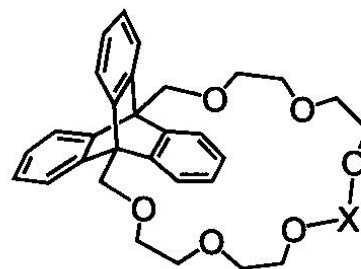
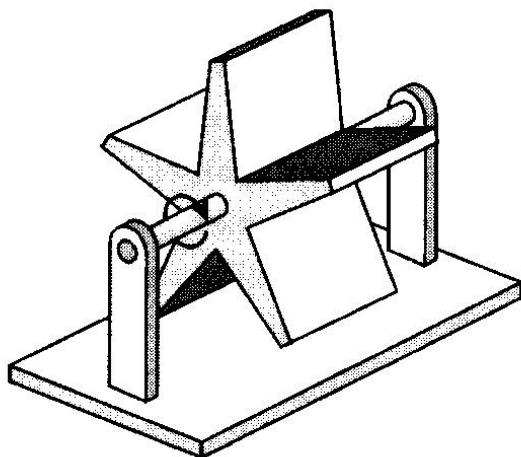
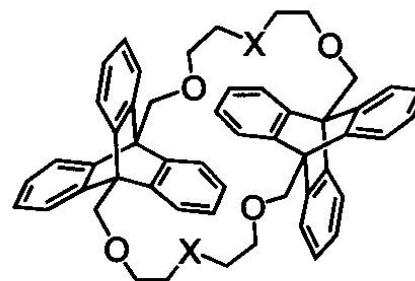
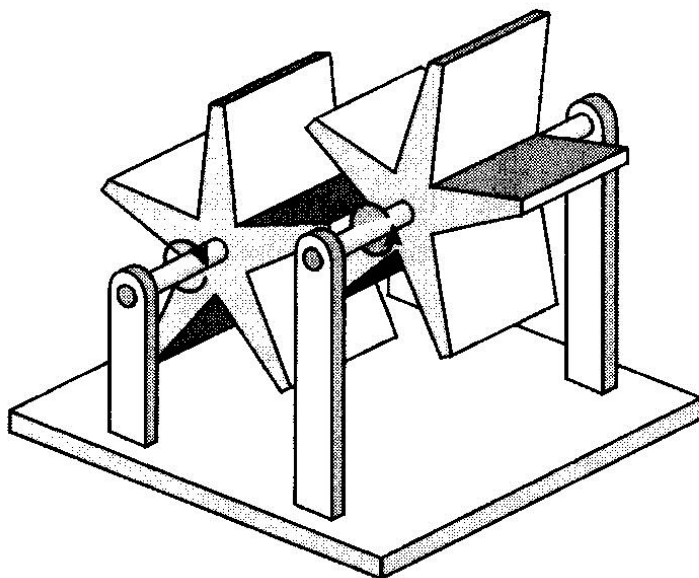


Fig. 11.2. (a) A macroscopic and a molecular [8] propeller-shaped entity; (b) a macroscopic and a molecular [15c] gear; (c) a macroscopic and a molecular [18] gear train; (d) a macroscopic and a molecular [19] bevel gear.

Sistema de paletas moleculares



- | | |
|---|--|
| 6 | $X = (\text{CH}_2\text{CH}_2)_2\text{O}$ |
| 7 | $X = \text{CH}_2\text{CH}_2$ |



- | | |
|---|---------------------------------------|
| 8 | $X = \text{O}$ |
| 9 | $X = \text{OCH}_2\text{CH}_2\text{O}$ |

Fig. 11.3. Macroscopic and molecular [17] paddle wheels.

Porta giratória molecular

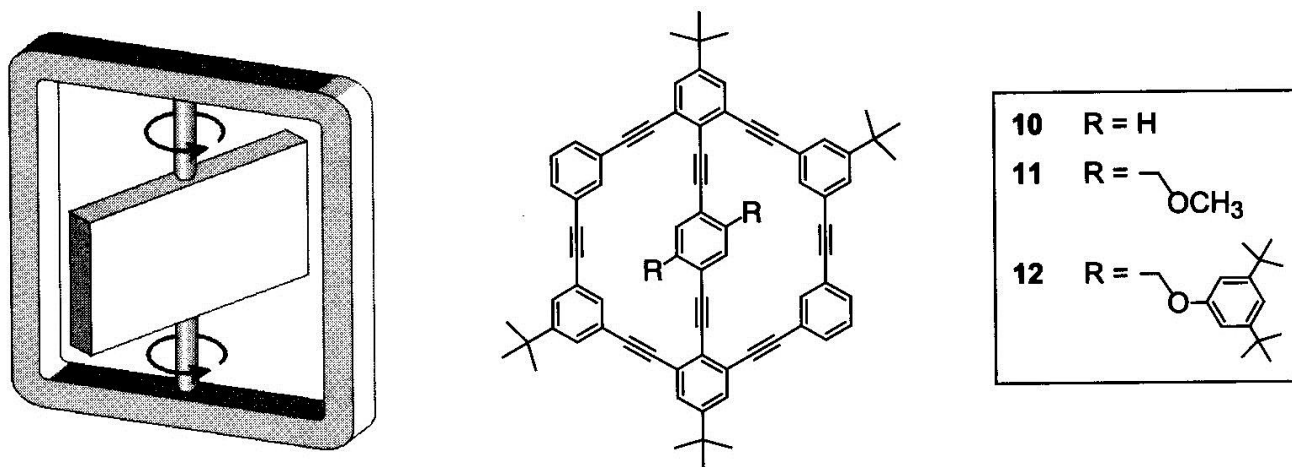
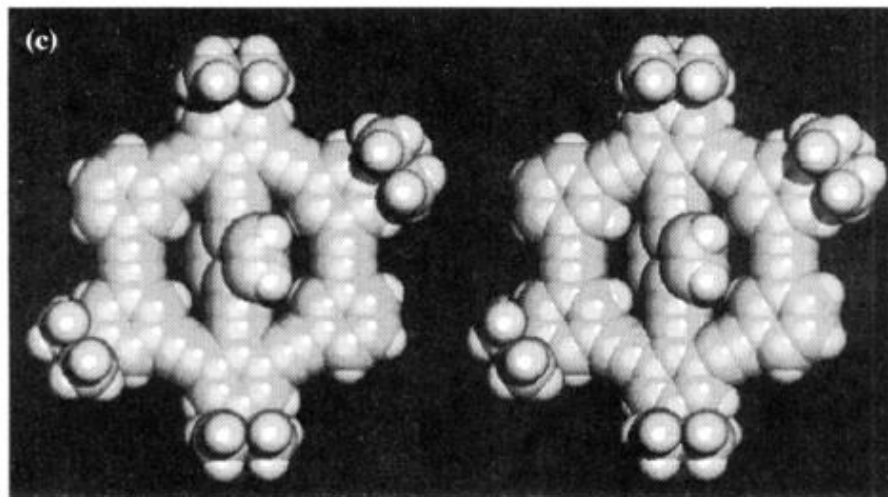


Fig. 11.4. Macroscopic and molecular [24] turnstiles.



Sistema Moleculares de Frenagem

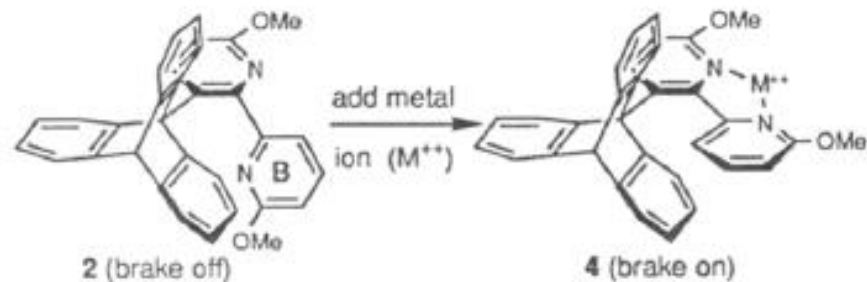
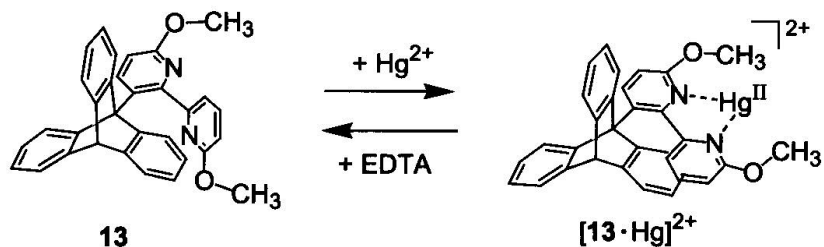
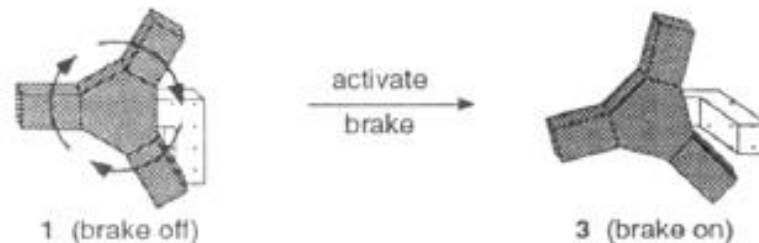
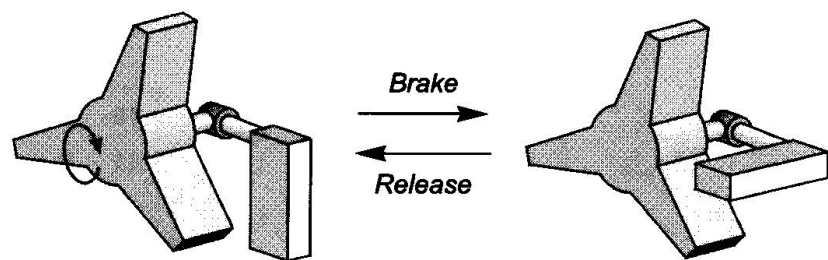
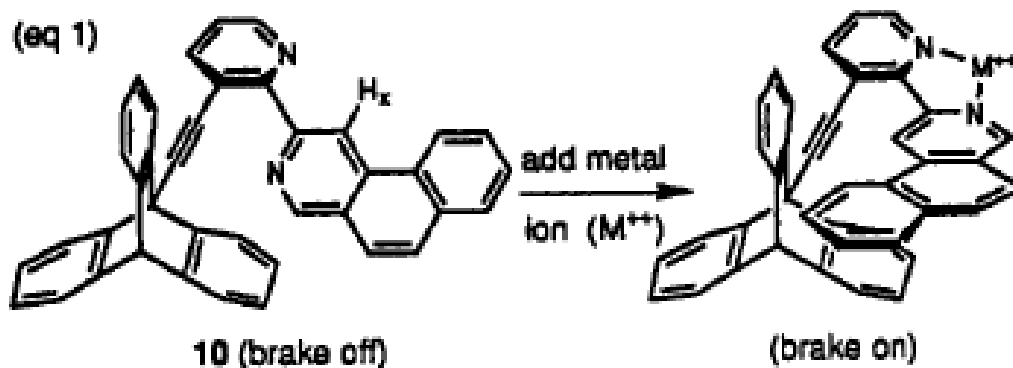
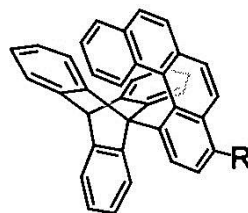
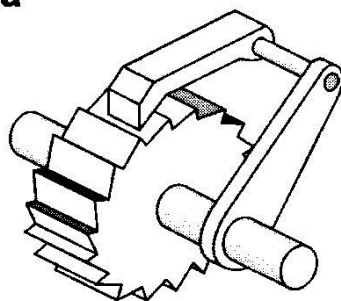


Fig. 11.5. Macroscopic and molecular [26] brakes.



Maquina molecular com giro unidirecional

a



14	R = H
15	R = CH ₃

b

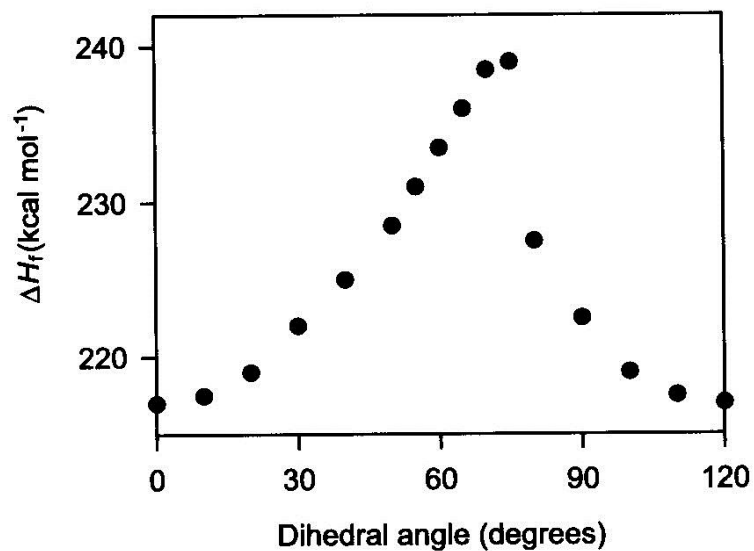


Fig. 13.6 (a) Mechanism and molecular [27] rotaxane; (b)

Giroscópio molecular

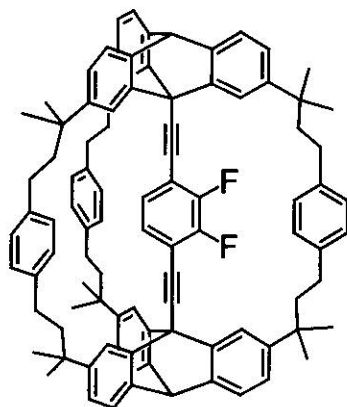
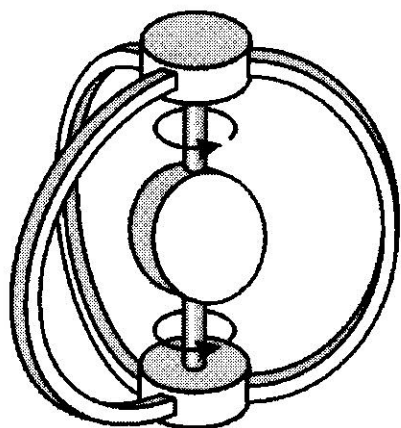
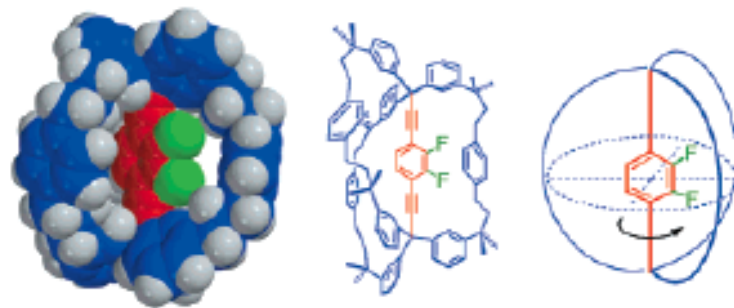
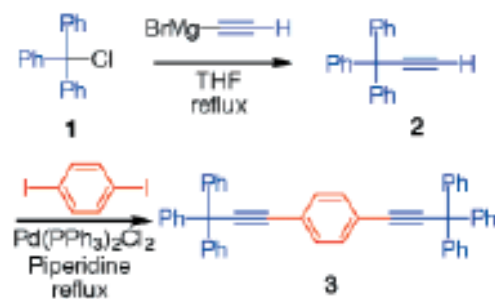


Fig. 11.7. Formula of a 1,4-bis[(9-triptycyl)ethynyl]-2,3-difluorobenzene and schematic illustration of its shape and functional similarity with a macroscopic gyroscope [34].

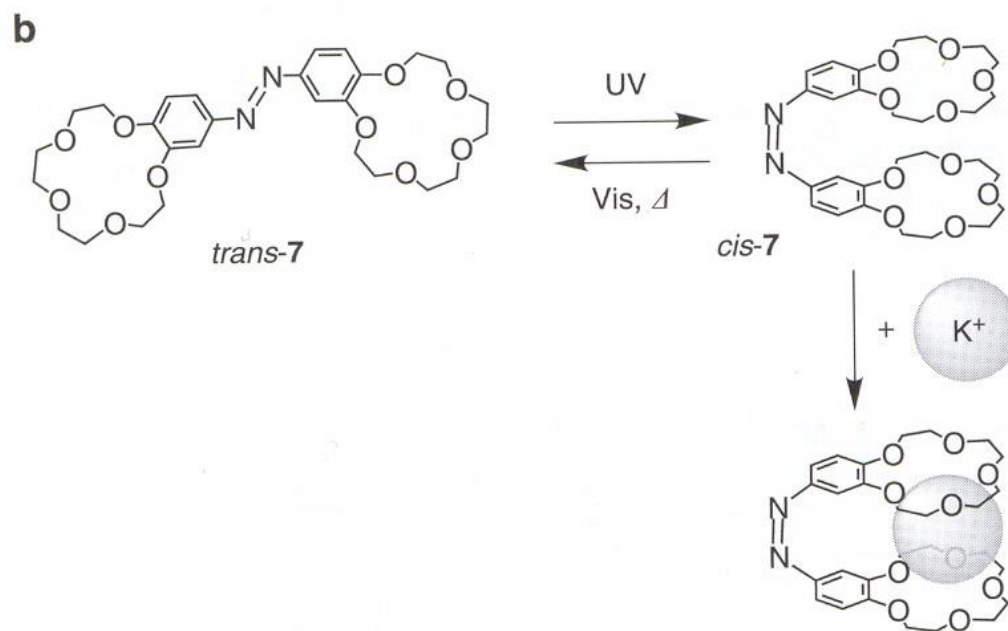
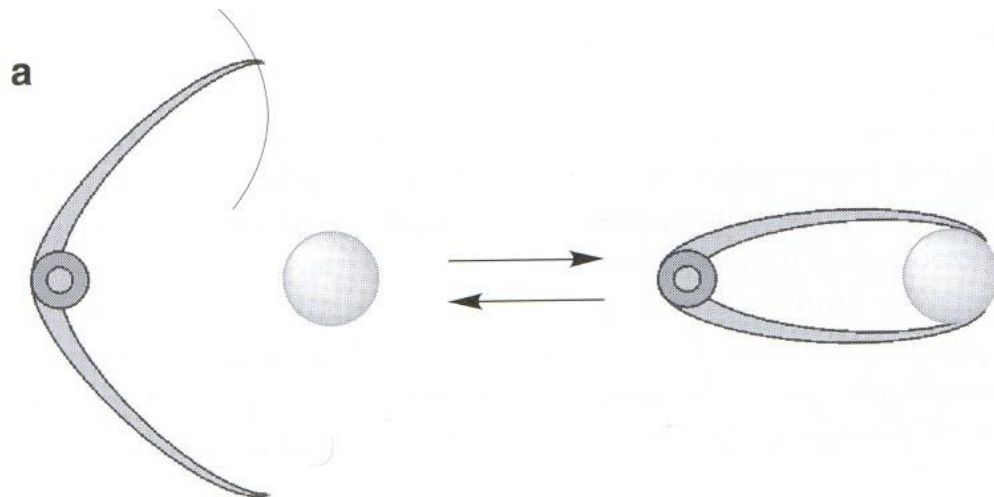
Scheme 1



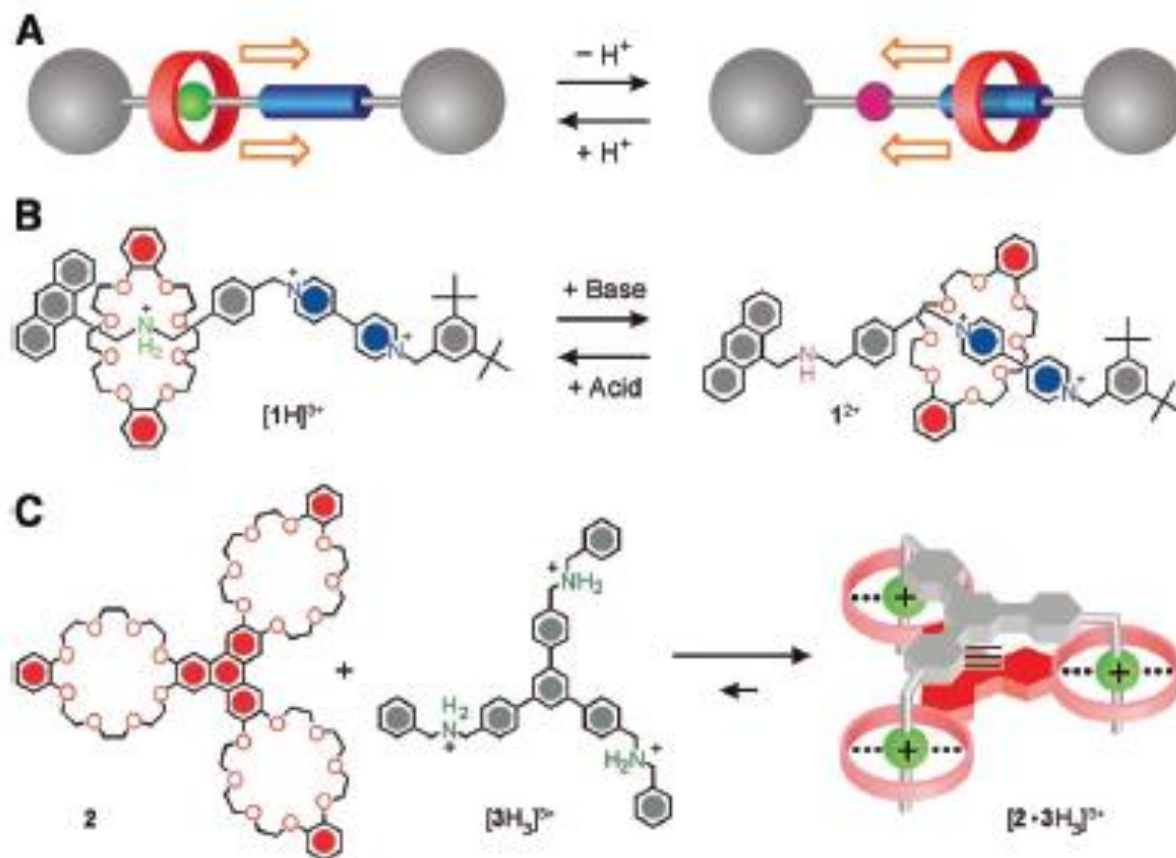
Scheme 2



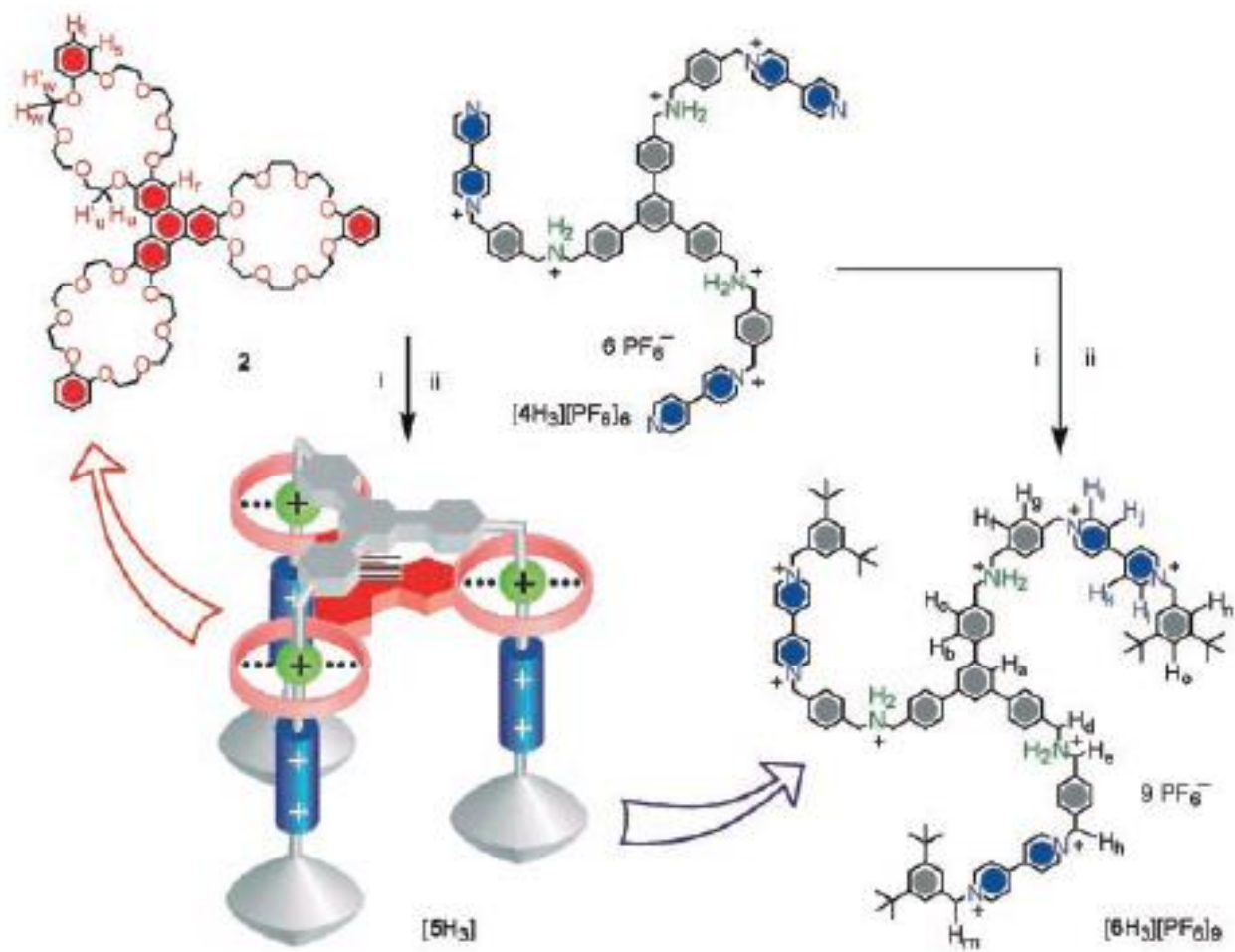
Pinça molecular



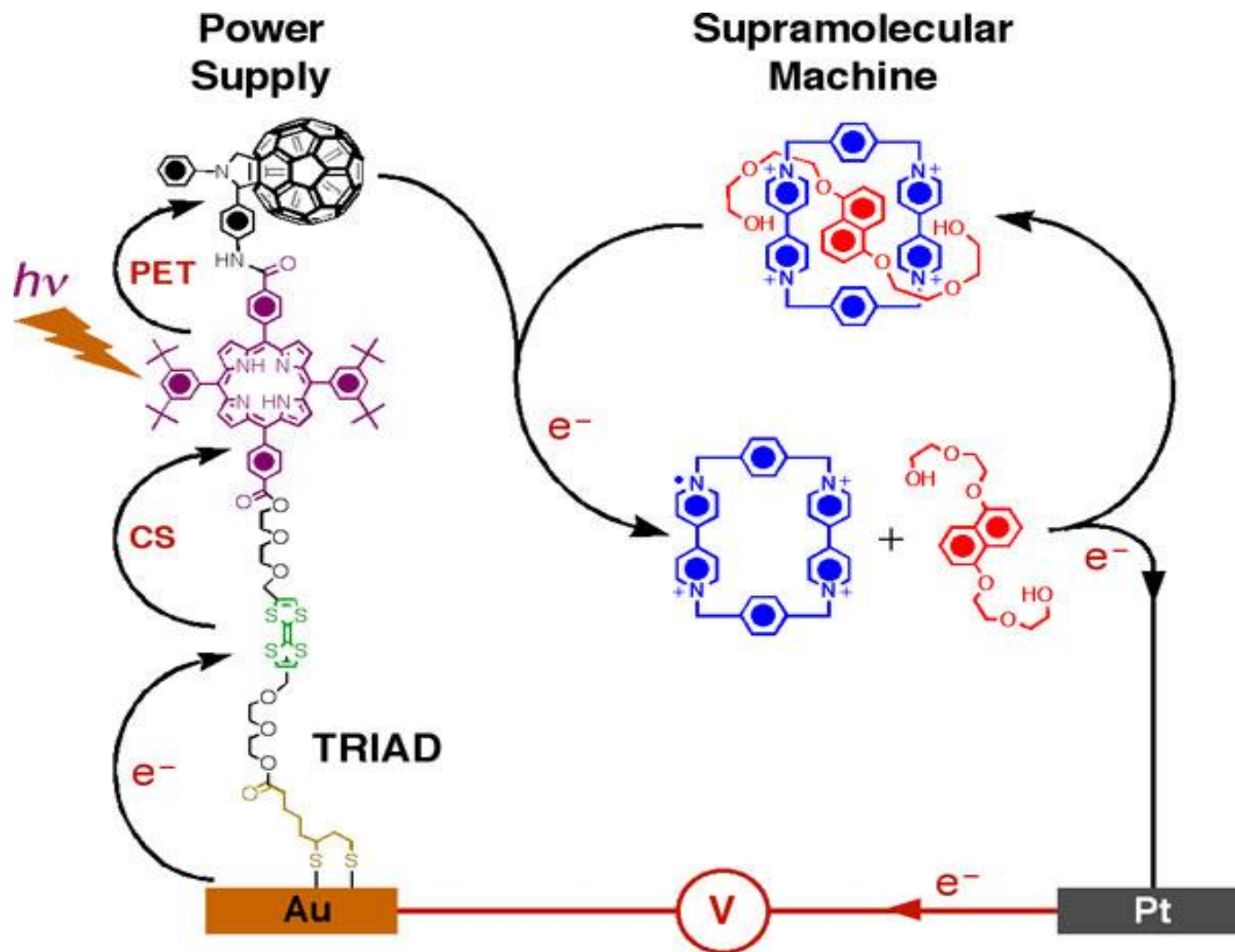
Elevador molecular

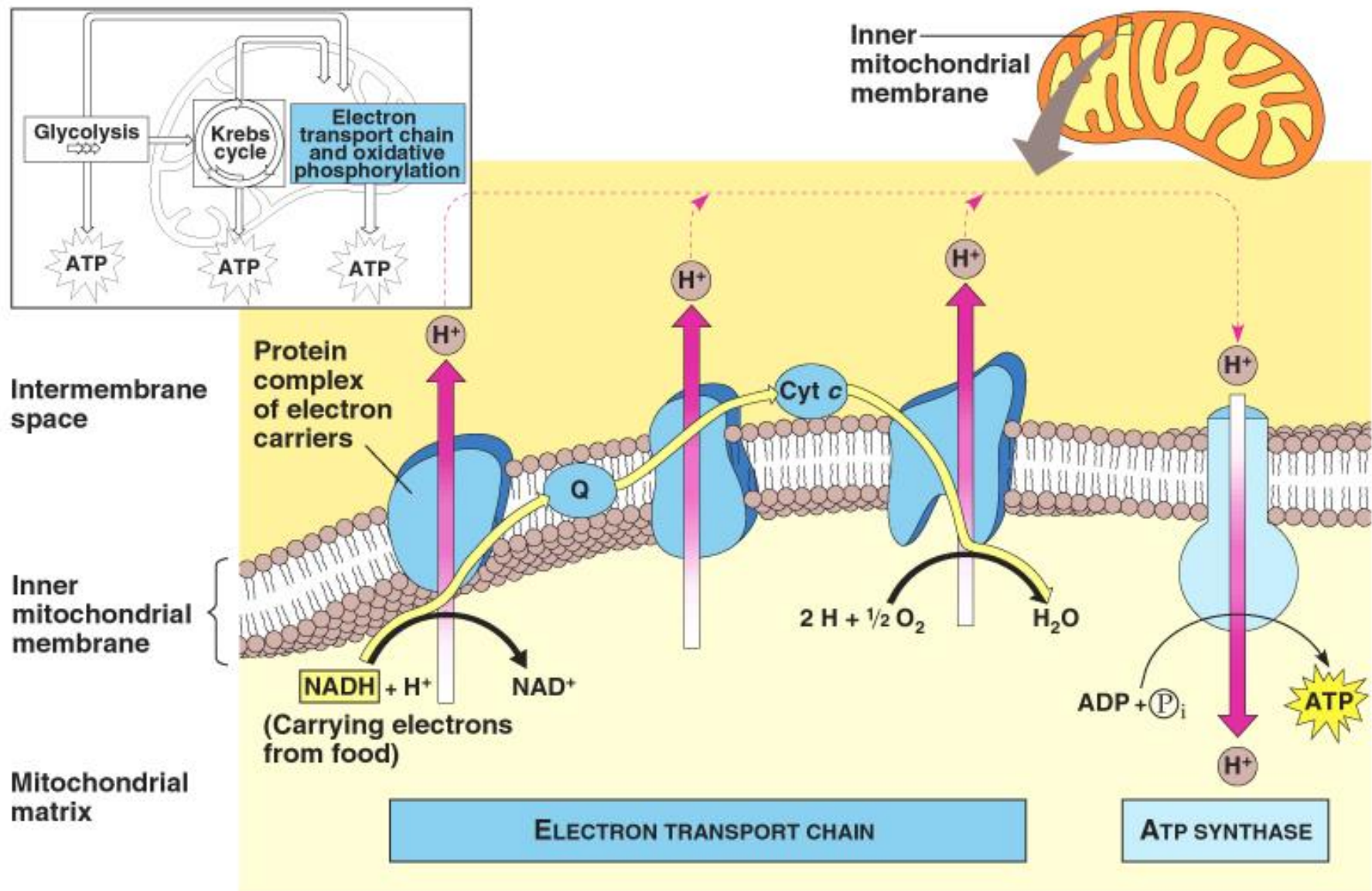


Elevador Molecular



Supramolecular Machines Powered by a Photoactive Molecular Triad





©1999 Addison Wesley Longman, Inc.

The figure is found at <http://plaza.ufl.edu/tmullins/BCH3023/cell%20respiration.html> (December 2006)