

28-11-19
Thursday

4. ADVANCED CONCEPTS / TOPICS IN CHEMISTRY

Supramolecular chemistry: The chemistry concern in chemistry systems composed of a discrete no. of molecules in which the strength of the forces responsible for special organisation of system. These forces range from weak molecular forces, electrostatic ^{charge} hydrogen bonding to strong covalent bonding provided the electronic coupling strength remains small relative to the energy parameters of the component is called supramolecular chemistry. 04-1 Wed

Supramolecular chemistry: weaker and reversible non-covalent interactions. hydrogen bonding, metal coordination, hydrophobic forces, van der Waals forces, π - π interactions, electrostatic effects.
Traditional chemistry:
Covalent - bond.

Concepts involved in supramolecular chemistry:

1. Molecular assembly.
2. Molecular folding.
3. Molecular recognition
4. Host-guest chemistry.
5. Mechanically interlocked locked molecular architectures.
6. Dynamic covalent chemistry.

* Supramolecular chemistry roots is developed by Nobel Laureate Rurmann Emil Fischer in 1894

* Host guest chemistry is developed by Donald J. Cram, Jean Marie Lehn and Charles J. Pedersen won nobel prize in 1987.

* Molecular machines and highly self assembly structures developed by James Fraser Stoddart in 1990.

* Miller develops sensors and methods of electronic and biological interfacing.

Self Assembly:

04-12-11
Neha

Orderly (or) disorder arrangement.

Inter-folding Intra-self assembly.

Applications:

1. Thin film self assembly mono layers (SAM) are expensive and widely used biology and electronics non-electromechanical^{4th} house hold goods, studying membranes properties of cells.

2. For coating moulding tools for polymer replication, self assembly mono layers are used.

Characteristics of molecular motors:

Molecular motors are biologically molecular machines that essentially agent of movement in living organisms.

A motor is a device that consumes energy in one form and converts into mechanical work.

Ex: Protein based molecular motors use of chemical free energy released by like the hydrolysis of ATP to mechanical work.

Types of Motors:

1. Cytoskeletal motors: myosins, kinesin, dyoem.

2. Polymerisation motors: actin, microtubules, dynamin.

3. Rotary motors: F_0F_1 -ATP synthase, ATP synthase.

4. Nucleic acid motors: RNA polymerase, helicases.

5. Enzymatic motors: catalase, urease, adolase, hexokinase etc.

6. Synthetic rotary molecular motors: chemically driven rotary molecular motors (reported by Kelly and co-workers in 1999).

* light driven ^{rotation} rotary molecular motors (reported by Ben in 1999).

Molecular Machines; Nanites of Nanomachines:

10-12-19
Tuesday

A molecular machine is a molecular compound that produces quasi mechanical movements, in response to specific stimulus.

Jean-Pierre Sauvage, Sir J. Fraser Stoddart and Bernard L. Feringa → were awarded Nobel Prize in 2016 (synthetic molecular machines)

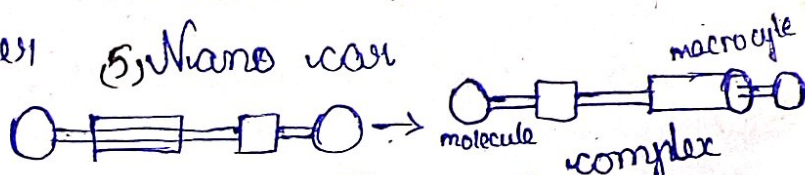
Synthetic molecular machines: (simple & small).

J. F. Stoddart

1) Molecular motors 4) Molecular shuttle

2) Molecular propeller 5) Nano car

3) Molecular switch

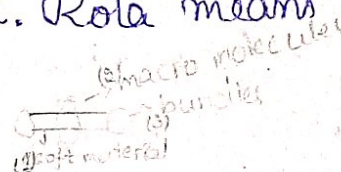


Biological molecular machines: The most

molecular machines are found with in cells, often in the form of multi protein complexes.

A rotaxane is a mechanically interlocked molecular architecture consisting of a dumbbell shaped molecule which is threaded through a macrocycle. Which is derived from Latin. Rota means wheel, axis means axle

1) Capping (soft material)



2) clipping (half part)

3) slipping (direct) (bangle)

Applications:

1) Molecular machines.

Potential use of protoxides in molecular electronic switching elements and molecules shuttle.

2) Ultra stable

3) Nano recording.

Catenanes: It is a mechanically ^{inter}locked molecular architecture consisting of two or more interlocked macrocycles.

Synthesis: (i) Threading followed by clipping.

(ii) Double clipping.

Properties:

- 1) Many catenane is the ability ^{of the ring to rotate} with respect to one another.
- 2) Catenanes change the colour by changing the recognition sites.

Applications:

- 1) Used in molecular ^{switches} structures, motors, fabrication of molecules, molecular electronic devices, molecular sensors and chemical sensors.

Prototype (materialisation): Prototype derived from greek meaning "first impression".

A prototype is an early sample or model release built ^{of a product} to test it concept or process or to act as a thing to be replicated or ^{learned} from. It is a term ^{used in} a variety of contexts including design, electronic or software programming.

Types of prototypes:

- 1) Proof-of-principle prototype.
- 2) A working prototypes.
- 3) A visual prototype.
- 4) A user experience prototypes.
- 5) Functional prototypes.
- 6) A paper prototypes.

Applications:

- 1) Technology demonstrators in mechanical and electrical engineering.
- 2) Electronic prototypes.
- 3) Computer programming (JAVA string prototype).
- 4) Data prototyping
- 5) Scale modelling (military)
- 6) Metrology
- 7) Natural sciences

Linear motion in Rotacane:

Linear motion are also called rectilinear motion, which is one dimensional motion along a straight line describe math^{-matically} using 1-1 spatial dimension

* Uniform linear motion with constant velocity (or) zero acceleration.

* Non-uniform linear motion with variable velocity (or) non-zero acceleration.

Mathematical relation b/w position 'x' and time 't'.

The motion in which all the particles of the body move through the same distance in the same time is called

i) Rectilinear motion.

ii) Curvilinear motion.

Displacement: $\Delta x = x_2 - x_1$, Time: $\Delta t = t_2 - t_1$.

Velocity: $V_{avg} = \frac{\Delta x}{\Delta t} = \frac{x_2 - x_1}{t_2 - t_1}$

Instantaneous velocity: $V = \lim_{\Delta t \rightarrow 0} \frac{\Delta x}{\Delta t} = \frac{dx}{dt}$

Acceleration: $a_{avg} = \frac{\Delta V}{\Delta t} = \frac{V_2 - V_1}{t_2 - t_1}$

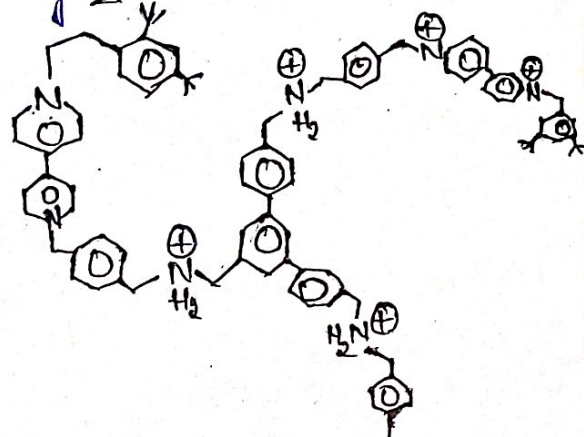
Jerk: $d = \frac{1}{2} (V_f + V_i) t$

Acid-Base Controlled molecular shuttle:

The deprotonation of ^{on} ^{nitroarene} moves the macrocycle away from this side to the other and reprotonation moves back the macrocycle ^{back}. Such molecular shuttles are called acid-base controlled molecules shuttle.

Molecular Elevator: It is a ^{molecular} machines that behaves like a nano scale elevator which is made ^{up} of a platform like component interlocked with a trifurcate sig like components which is moulding 3.5 nanometers in size.

Super bundle
+ 3,5-di-^{di}-^{di}-butyl benzoyl $\xrightarrow{+H_2O}$
+ NH_4PF_6
ammonium phosphorus
hexa fluoride



Molecular Switches:

A molecular switch is a molecule that can be reversible shifted b/w 2 or more stable states in response to environmental stimuli, changed as pH , light, temp, an micro environment in the presence of

- 1, Acetochromic molecular switches (pH)
- 2, Photochromic "
- 3, Coordination switching
- 4, Displacement "
- 5, On and off "
- 6, Rearrangement switching