

International Year of CHEMISTRY  
2011

100 Years of Noble Prize -  
Mme Curie - 1911

# Public Image — Media *Chemistry at a Crossroad*

*Mismatch between the rich potentialities of CHEMISTRY  
&  
The tarnished public image carried by Chemicals and Chemical  
Industries*

**“Bhopal” “Carcinogens”**

**“Toxic Brown Fumes” - fertilizer**

**Pesticides “Environmental Villain”**

**Drugs — Brown Sugars, Speed, LSD**

# *Public Image — Media*



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**New road is a rocky one cobbled with fear and Sensationalism**



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**Sponsored & Stimulated by well meaning but half informed environmentalist & single issue advocates who are well versed in exploiting media**



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**Who in turn are searching for “Newsworthy” & Sensational stories TV Viewers**

**Life saving Medicines, Polymers, Gasoline, Coal**  
**Morning to Night — CHEMISTRY**

**A message of alarm has that Quality,  
a message of reassurance does not !!!**



**Missing the Exciting Frontiers on Horizon**

# From Morning to Night, From our FIRST cup of tea

Soap  
Toothpaste  
Toothbrush  
Tea, Coffee  
Milk, Sugar  
Newspaper  
Ink, Fruit  
Juice

Office Bag  
Plastics  
Sun mica table  
Shoes – PVC  
Paints, petrol  
Gas

New  
Materials  
“Rockets”  
Nose Cap  
“POKHRAN”

All the Drugs  
Antibiotics,  
Anti HIV,  
Sleeping pills,  
Vitamin Tabs  
Battery in your  
watch

“NO”..... VIAGRA

It is CHEMISTRY &  
CHEMISTRY

# Image

**CHEMISTRY**

**Stinky Science**

**Air Pollution, Toxic Chemicals**

**Bhopal Tragedy**

**Water pollution (Dye industry in Kalyan)**

**CHEMISTRY**

**Central, Useful & Creative science**

*Central role in Human well being*

**Petroleum, Gas**

**Fertilizers, Pesticides  
Herbicides**

**Drug Design**

**Revolution in clothing**

**New Construction materials  
(plastics, polymers)**

- **“CHEMISTRY is an OLD Science”**
- “Whatever was to be discovered has already been discovered”
- **“What’s New to learn in CHEMISTRY? ”**
- “CHEMISTRY is a Dry subject requiring remembering endless names, Symbols & equations”


*But*

**CHEMISTRY is Highly Systematic  
&  
Rational Subject**

# Perceptions

 Perceptions of chemistry comprise a disparate set of images and impressions from school days – Bunsen burners, long wooden benches and tall stools, blue bottles and noxious smells.

 They remember the ‘stinks and bangs’ aspects of school chemistry and some of the interesting hand – on experiments

 They may recall having heard about the periodic table and symbols, fancy names and complicated formulae, but only a few of the more technology-oriented men could remember having learned anything meaningful from these lessons





**It was too theoretical, abstract and removed from the real world. They found it too difficult – all facts with no room for creativity - badly taught, and (as far as some women were concerned) solely “for boys”.**



**Most of these people had been lost to chemistry after the early hands – on experiments, at the stage where the fundamentals begin to be taught. At that point they had found it “too difficult”, ‘irrelevant’ and boring**



**They regarded those who went on to study chemistry at a level as studious, single-minded and, let’s face it, dull.**

# **Excitement in Chemistry**

Chemistry is Exciting  
Chemistry is Exciting

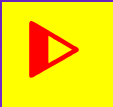
*Jai P. Mittal*

**Chemistry Group  
Bhabha atomic Research centre  
Trombay - Mumbai**

# *Excitement in Chemistry*

**Chemistry is exciting**

- 1988**      **Fusion in Test Tubes??**
- 1991**      **Fullerenes, C<sub>60</sub>, C<sub>70</sub>, C<sub>84</sub>**
- 1986**      **High Tc Superconductor**
- 1993**      **Peep at Chemical Reactions at as short time scale as 6fs (6 x 10<sup>-15</sup> Sec)**

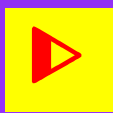


**Video of the Birth & Progress of Chemical Reactions**

⋮

**1995**      **Vision 2020**

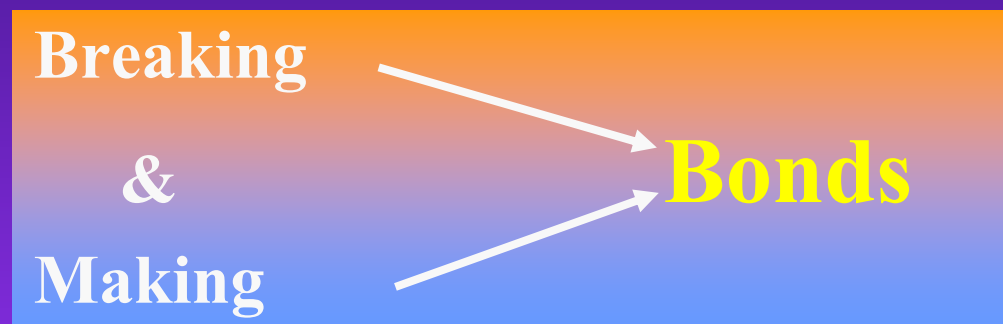
⋮  
~  
~  
⋮



**2020**      **Complete control of chemical pathways.  
Breaking Bonds to order reactions à la mode  
selective tuning the CHEMISTRY**



What the **CHEMISTRY** is all about ?



Synthesis, Structure, & Dynamics

*Question of Time? How fast bond breaks  $-\tau$  ?*  
*Which bond should break? - Equilibrium*

# *Carbon in Upper Atmosphere*

1980 – 84

Kroto (Sussex, U.K)

UV Spectra. Carbon Polymers (Telescope, observatory)

Jan 1980 – Aug 1984

Kroto writes proposal to space

Gives talk in seminars

*But*

*NO LUCK*

Sept 1984

Meets Curl & Robert Smalley at Texas

Smalley proposed the idea

Kroto again writes proposal to.....

Smalley relents for 2 weeks use of instrument

Kroto rushes to Texas

*NO*

*Money!!!*

Borrows wifes jewellery, Fly to texas

July 1985

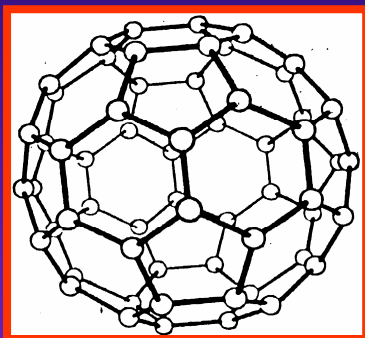
Experiment Starts,

July 15 RESULTS

July 18, 1985

*Letter to Nature*

# What kind of 60 C atom structure gives rise to Super stable species ?



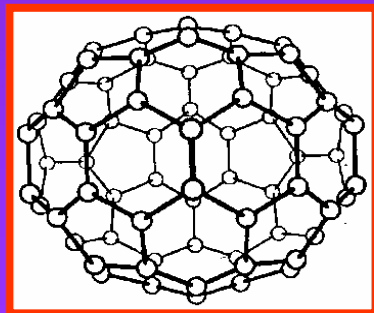
Symmetry group  $I_h$  (truncated icosahedron) a polyhedron with 60 vertices & 32 faces (12, pentagonal and 20, hexagonal)

The inner and outer surfaces are covered with a sea of  $\pi$  electrons, diameter for  $C_{60} = 7.1 \text{ \AA}$

Density of  $C_{60} = 1.65 \text{ gm/cm}^3$

► Appears to be capable of holding a variety of atoms

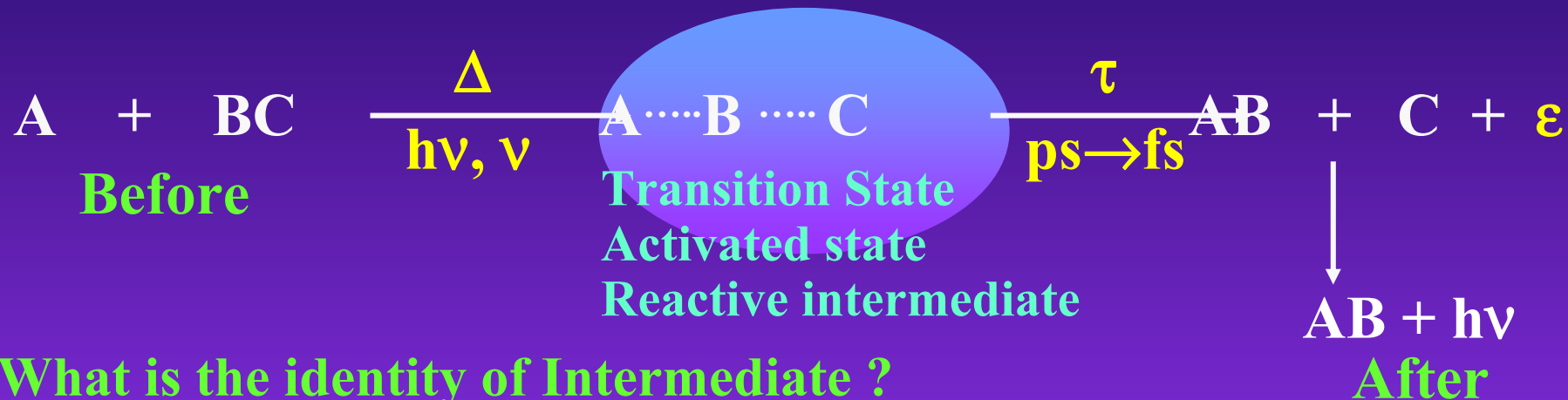
X-ray diffraction: hexagonal packing of these 7.1 Å diameter spheres with 10 Å separations between the centres.



For  $C_{70}$  symmetry group is  $D_{5h}$

# What the CHEMISTRY is all about ?

Breaking & Making  $\rightarrow$  Bonds



What is the identity of Intermediate ?  
 What is the lifetime of Intermediate ?

Temporal  
Spectral

$\mu\text{sec}, \eta\text{sec}, \text{ps}, \text{fs}$   
 structural, identity

Spectroscopy

Excited states,  $S_1, T_1$   
 Free radicals  
 radical cations, radical anions

Lasers  $\rightarrow$  Control of chemical reactions  
 Laser flash photolysis - pump & Probe

coherence  
 IR laser, MPE

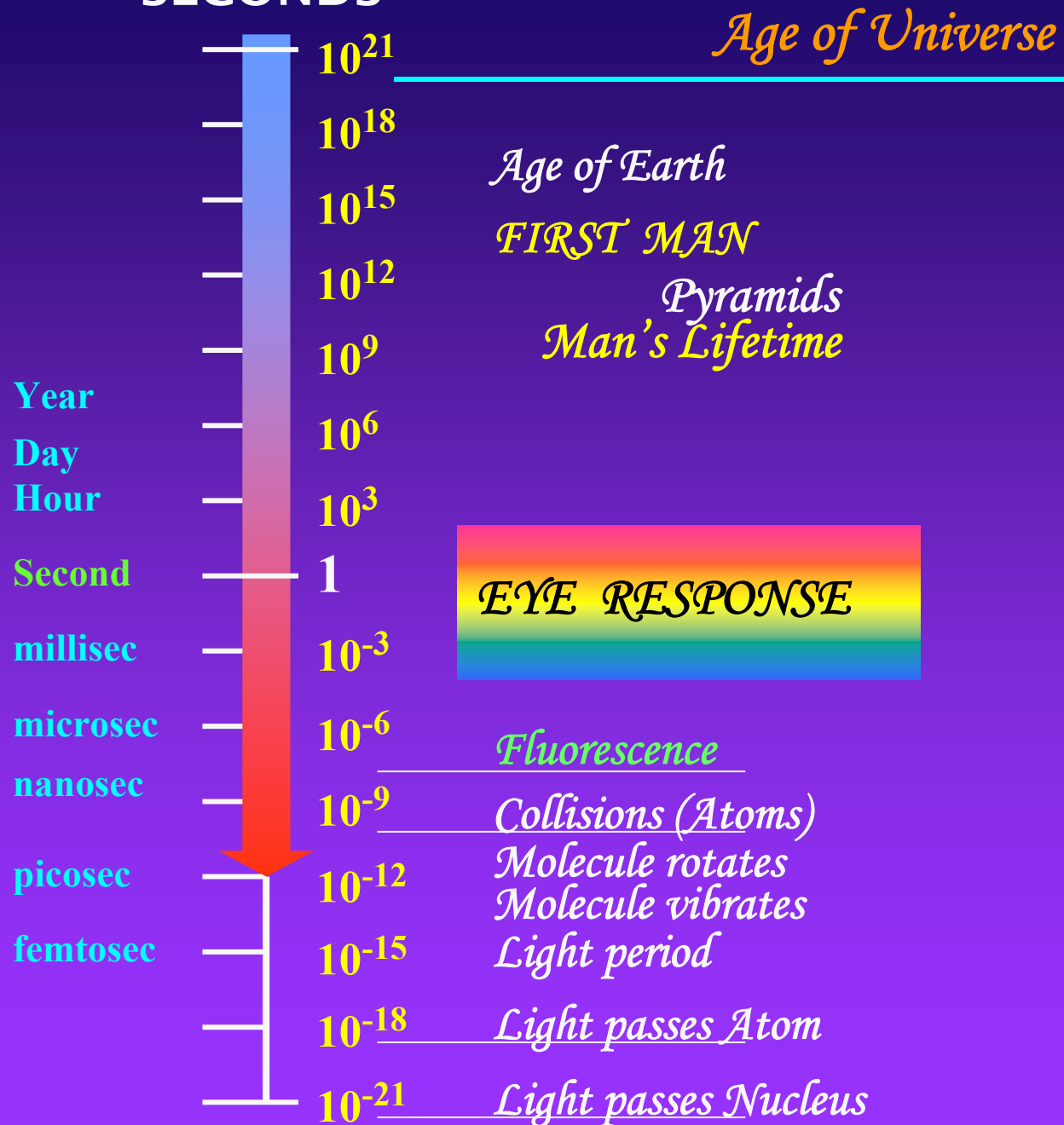
# How Fast is Fast ?

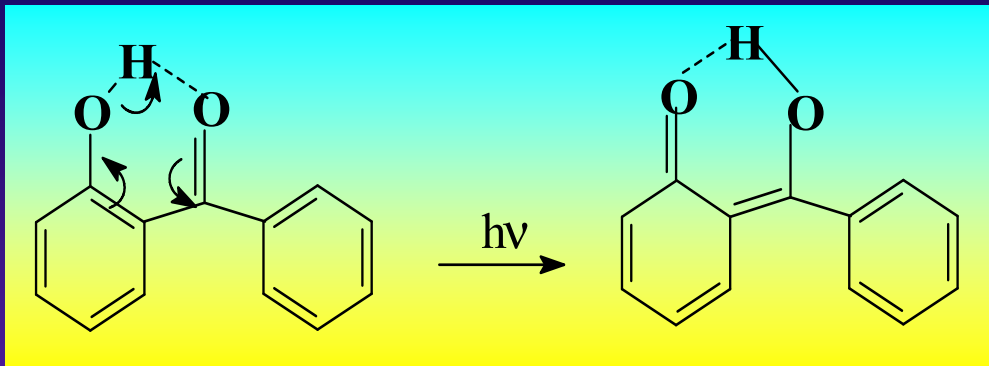
<b>1 Second</b>	<b>1 Sec</b>	<b>Fast</b>
<b>Millisecond</b> (Fast flow, 1941)	<b><math>10^{-3}</math> Sec</b>	<b>Very Fast</b>
<b>Microsecond</b> (Norish & Porter, 1960) Flash photolysis	<b><math>10^{-6}</math> Sec</b>	<b>UltraFast</b>
<b>Nanosecond</b> (Q-switched laser)	<b><math>10^{-9}</math> Sec</b>	<b>“SuperFast”</b>
<b>Picosecond</b> (mode locked laser)	<b><math>10^{-12}</math> Sec</b>	<b>“Damn Fast”</b>
<b>Femtosecond</b> (Ippen & Shank, 1993, 6fs)	<b><math>10^{-15}</math> Sec</b>	<b>“Damn Fast Indeed”</b>
<b>Attosecond</b>	<b><math>10^{-18}</math> Sec</b>	<b>Who Cares ?!!</b>

**In last 5 year ability to time resolve molecular events has improved by roughly  $10^{-6}$  times as in last preceding 50 years.**

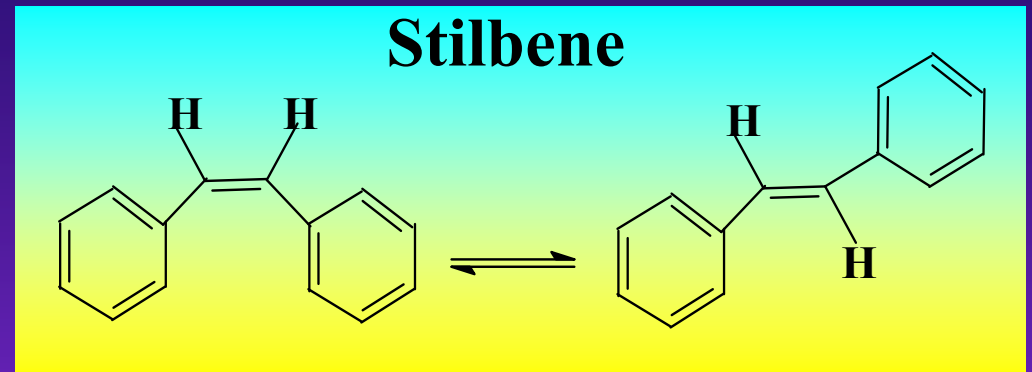


# SECONDS

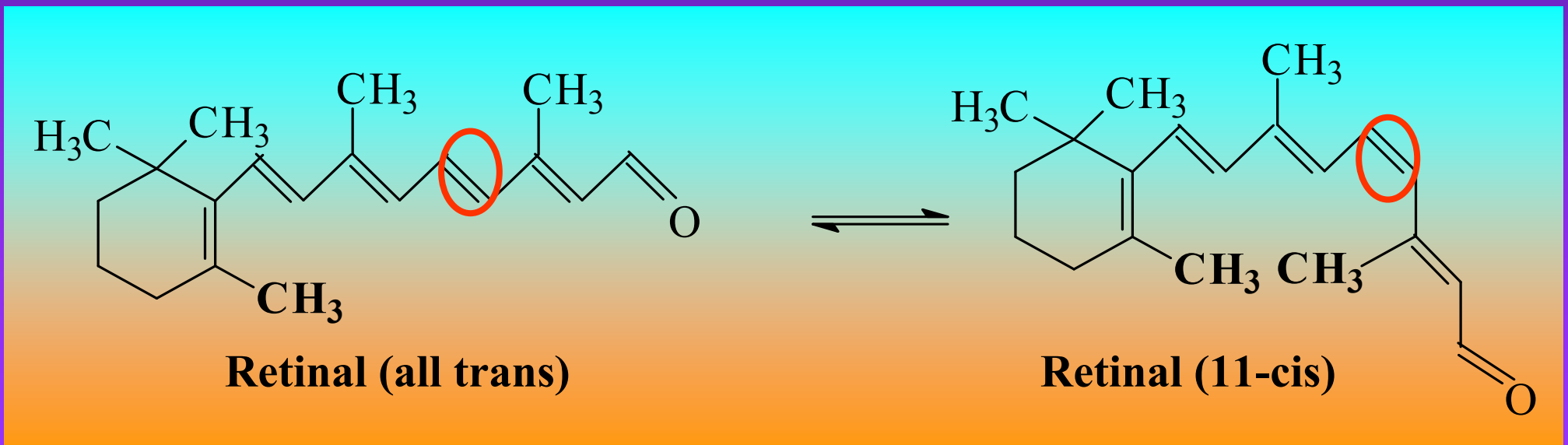




This swap round  $\approx 0.1$  Pico sec



cis      100p sec      trans



Retinal (all trans)

Retinal (11-cis)

## *CHEMISTRY in a "Jiffy"*

**G.N. Lewis:** He was also a great wit who often coined delightful phrases, such as the "Jiffy"

🕒 The time taken by a photon to travel 1cm, or 33 pico seconds.

*But*

🕒 When the phrase was coined in 1920's, Chemistry was done on a time scale some hundred million times slower than a "Jiffy".

🕒 In 1941 the fastest process studied in the laboratory was on a milli second scale, gas kinetics in flow systems.


🕒 In last five years ability to time resolve molecular events has improved by roughly the same factor ( $10^6$ ) as in last 50 years

★ Latest is 0.06 pico second or 6 femto second.

# *Transition States in chemistry*

## *Its where the action is*

 The ability to observe them has added immeasurable power to the chemist's arsenal

 Time zero for chemistry. The clock starts, & in an unimaginably short period of time – on the order of a millionth of a millionth of a second — atoms change partners, chemical reactions take place and new molecules are born.

Before & After pictures were easy to get but there were no Eye witness account.

 Sort of freeze frame pictures or even better.

Just a peep at the “ Activated Complex”.

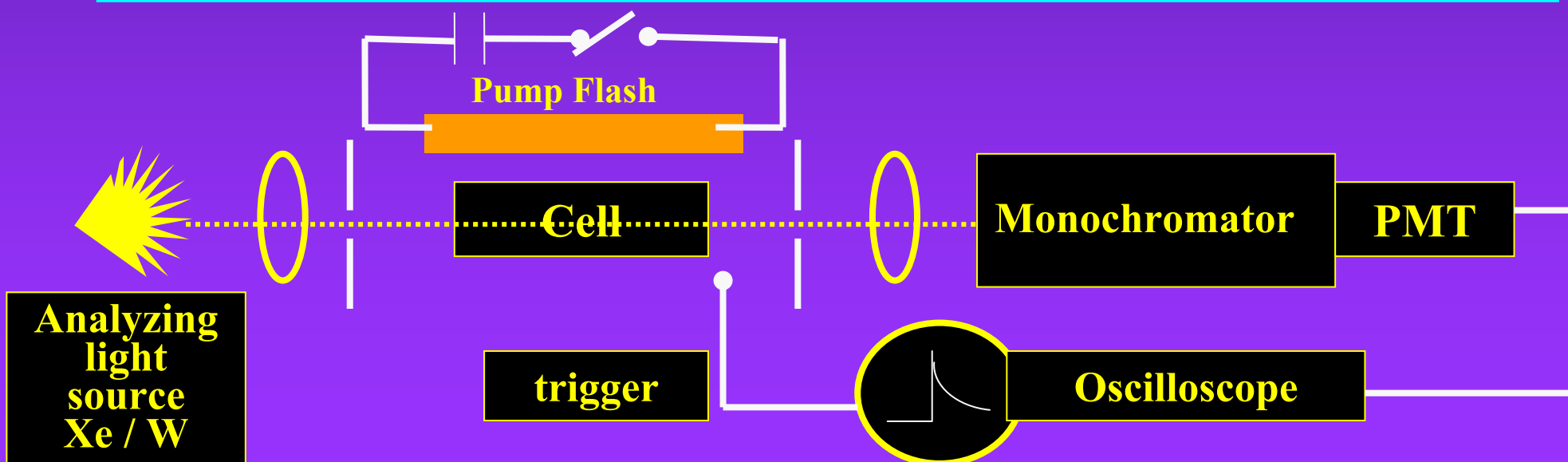
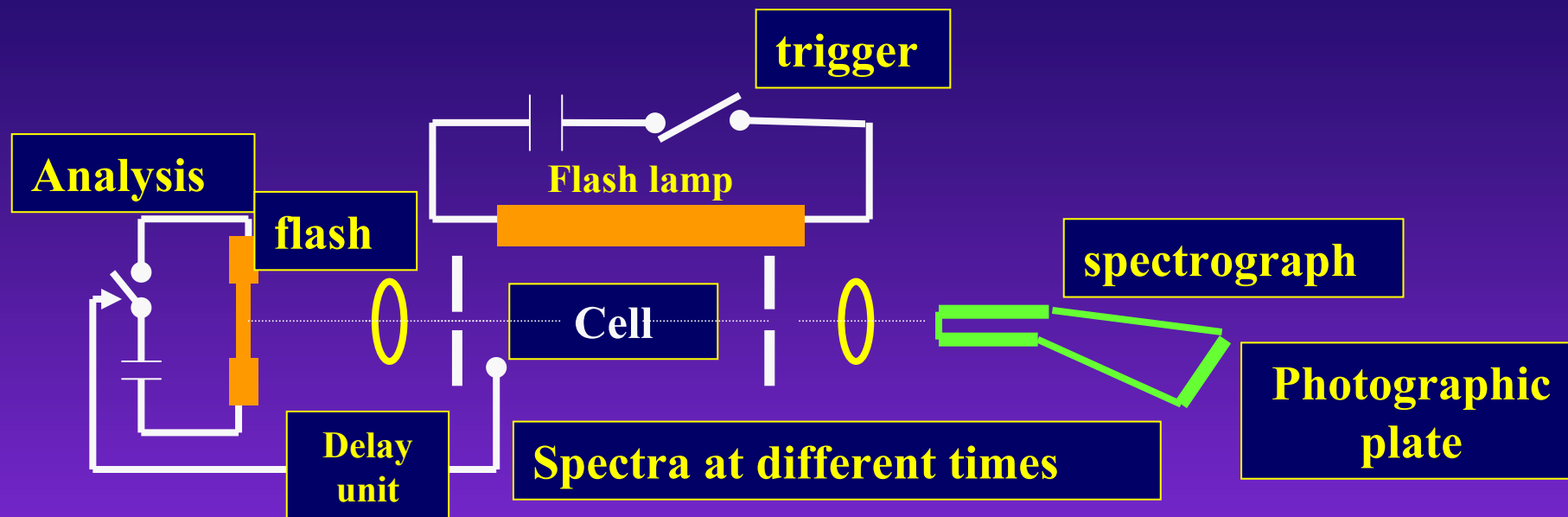
Penetrating the black box — “Transition State”

 “ Lasers, Beams & Molecular dreams”

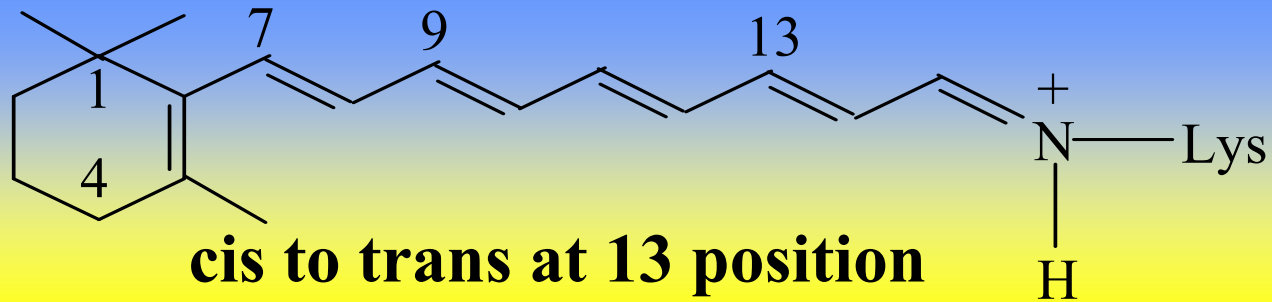
George Porter (1962)

to

Ahmed Zewail (1999)

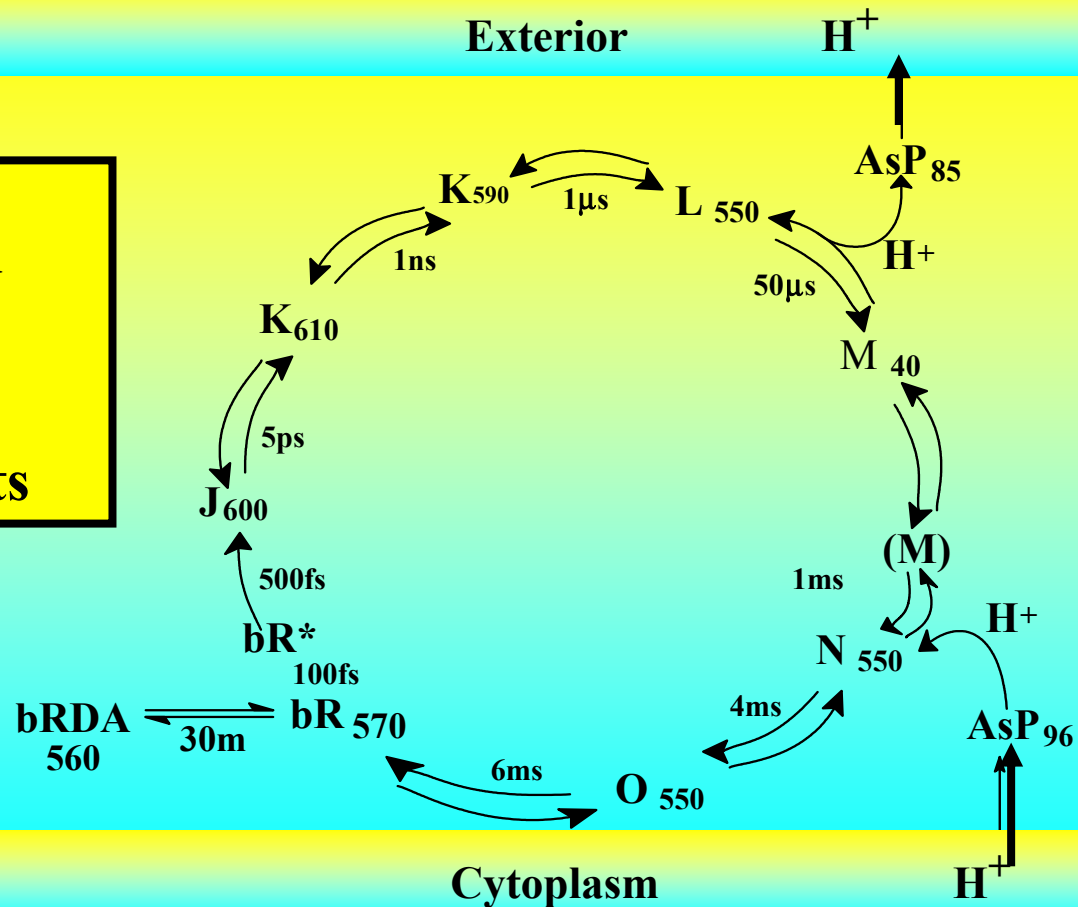


# Vision CHEMISTRY



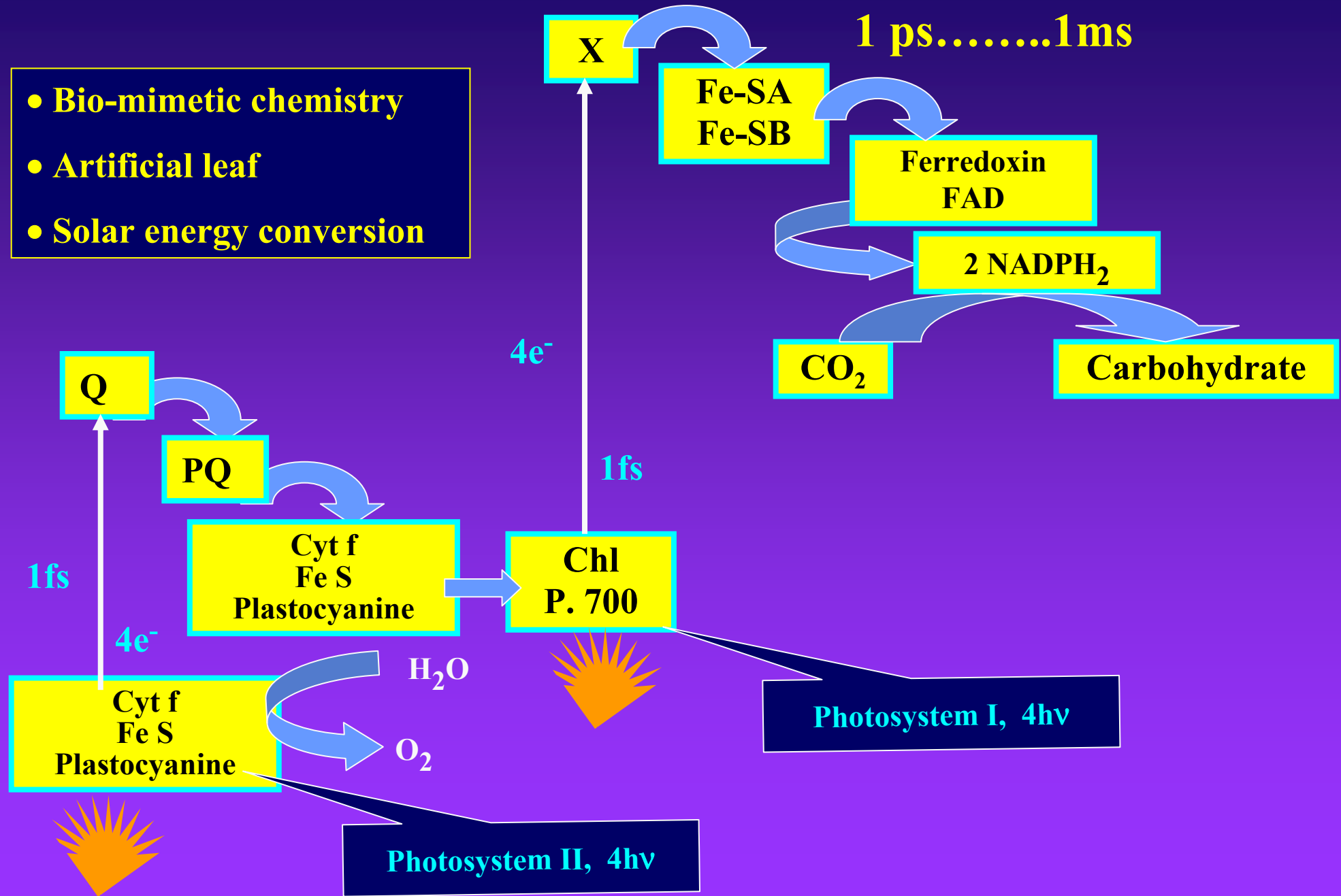
Bacteriorhodopsin, Purple membrane bacteria

- ◆ Ultra fast processes in vision not fully understood
- ◆ Role of  $H^+$  transfer
- ◆ Correcting vision defects



# Photosynthesis *Z - Scheme*

- Bio-mimetic chemistry
- Artificial leaf
- Solar energy conversion



# *Excitement in chemistry*

**Chemists have long been tantalized by the dream of altering the probabilities, or choosing themselves the bonds within a molecule to vibrate and break to order**

**Chemists are trying to realize this, knowing all the while, that it may be like Don Quixote's, be an impossible One.**

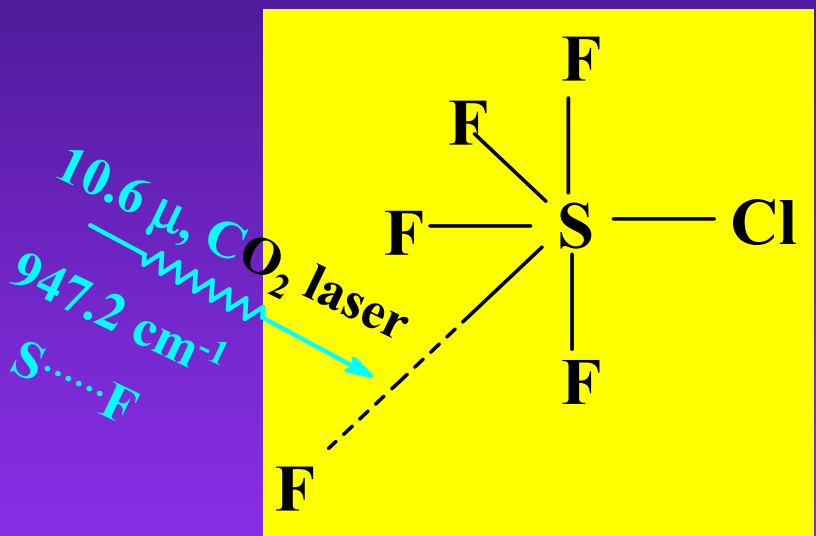
*But*

**Now they have a new mighty Sword to use in their quest, One that was not available very recently**

**The FAST EXCITATION by INFRA RED LASERS  
INFRA RED PHOTOCHEMISTRY  
(PHOTOCHEMISTRY in ELECTRONIC GROUND STATE**



# New Chemistry



||  
?

“Bond Selective”

CHEMISTRY ?!

“Mode Selective”

CHEMISTRY ?!

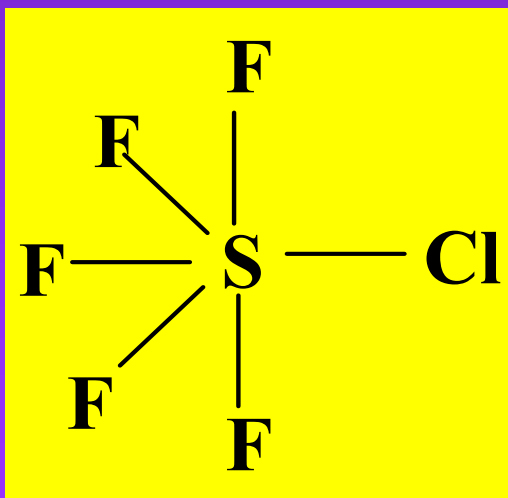
Since the days of **ALCHEMY**, sluggish reactions have been prodded to occur more readily by the application of **HEAT**

————— **THERMAL CHEMISTRY**

Then came irradiation with visible or UV light to generate electronically excited states which frequently undergo unique transformations

————— **PHOTO CHEMISTRY**

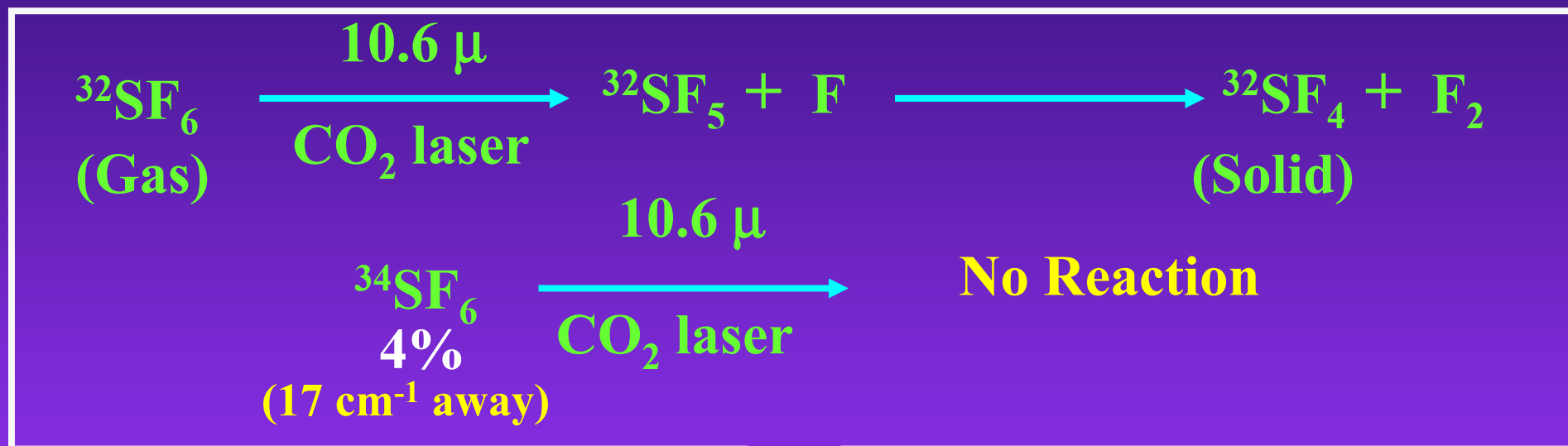
But Synthetic Chemists still had to live with the idea of  
—————→ Reaction occurring predominantly via  
**LOWEST ENERGY REACTION CHANNEL**



# ISOTOPE SPECIFIC

## INFRA RED LASER CHEMISTRY (PHOTOCHEMISTRY IN ELECTRONIC GROUND STATE)

### Accidental Discovery



34S isotope  $\approx$   
\$ 1000/gm

By laser method  $\approx$   
\$ 0.30/gm

**NEW METHOD FOR ISOTOPE SEPARATION**

# How? What is the CHEMISTRY

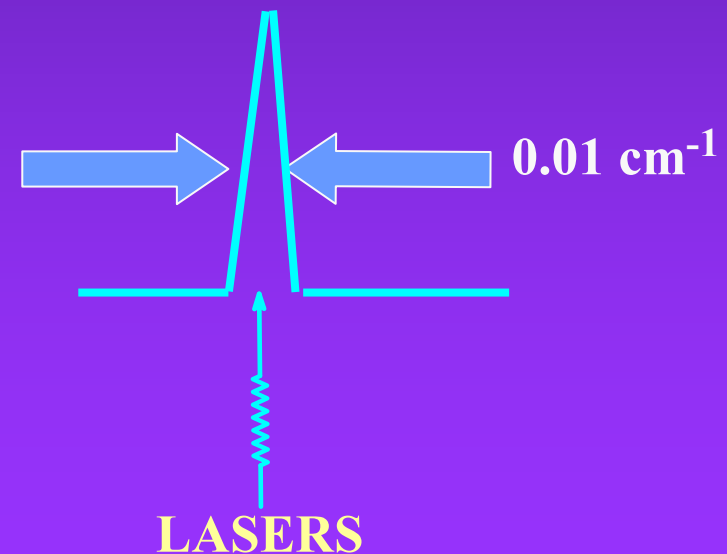
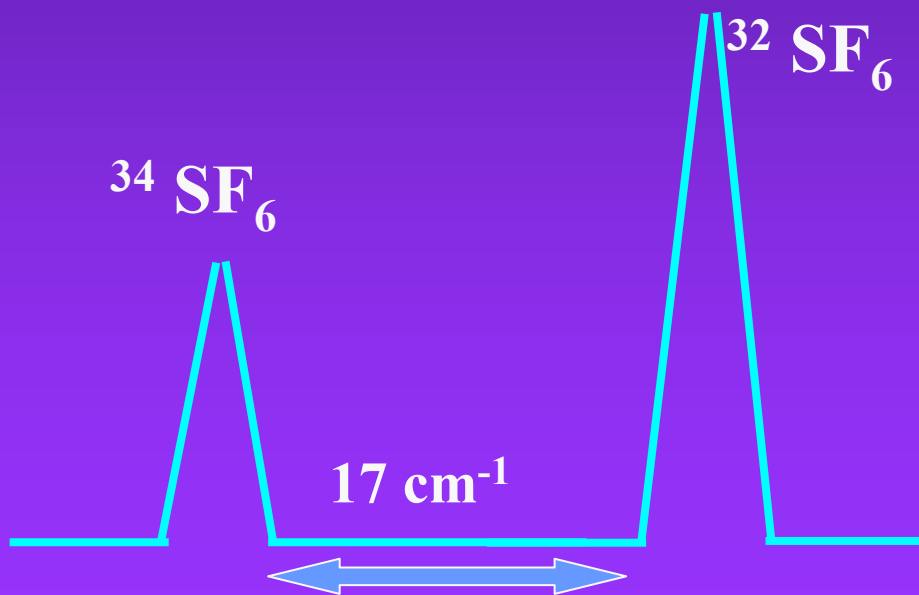
S-F,  $\approx 90$  Kcal/mole  
& Energy of a 10.6 m  $h\nu \approx 2.86$  Kcal/mole  
 $\approx 30$  IR photons required to break the bond

## Birth of New Chemistry

New concepts of multi photon  
Dissociation Dynamics

Application to many isotopes?! But  
Isotope Specific

Thermal ??? Strong Bunsen Burner



As **Edward Teller** puts it Laser Chemistry can be linked to a Chemist *“Reaching into Molecular Structure with his own hands and rearranging the Structures at will”*

Chemistry is undergoing a Laser revolution

Time of intellectual ferment in chemistry

Pimental report (1986)

Pico second Femto second Chemical Kinetics  
State to State Chemistry

Implications are Staggering

Newer compounds, Rate enhancement, Exotic materials with unusual properties

Future is Theirs

We may now dream of Orchestrated trains of **ACCELERATOR, SYNCHROTRON and LASER PULSES** which prepare reactants to our highly selective specifications, monitor all intermediates in direct time domain and probe all nascent products & their final conditions with complete specificity.

It is perhaps too early to speculate, but it seems that for the first time we are on the threshold of being able to probe specific steps on the potential energy surface

**Truly a DREAM come true for a CHEMIST !!!**

Most of these discoveries needed a complete  
**PARADIGM SHIFT**

**and not just extension of Existing info .....**

**(1) Needs – Element of Creativity  
Plus little beat of Serendipity**

**Looking for a needle in Haystack  
And  
Finding the beautiful daughter of farmer**

**(2) Or systematic Questioning about Reaction  
Mechanism both temporal & structural details.**

**None of these discoveries came via any  
Planned & structural projects**

**No project was submitted or approved.**

**No proposal, No paper work & NO FUNDING**

*Except*

**Generous Dose of Curiosity**

*Science on sly*

*Bootleg Science*

**But not the band wagon Science**

**No milestones were projected, No Schedules,**

**No bar charts**

**&**

**No promises were made**



If God was to submit a new research

proposal today to the  
funding agencies

regarding creation of  
world

It would certainly be rejected  
on all the 3 criteria most often applied

1. Past Track Record : Not published in journals

2. God has not been active for millions of years

**NO**

3. We don't fund old research

# CHEMISTRY in 21<sup>st</sup>. Century

*Chemistry at a Crossroad*

## Challenges for Chemists

Chemistry pollutes!! But Chemistry only will fight pollution



Environmentally benign Chemistry

**GREEN CHEMISTRY**

Low temperature reactions- Room temp. Chemistry  
What happens to Activation Energy? How to Overcome?

- Unraveling Nature
- Learning from nature
- Enzymes role
- No more organic Toxic Solvents
- Aqueous chemistry
- Use hv s as Chemical reagents
- Use membranes
- Understand Interfacial Chemistry
- Photosynthesis mystery
- Alter the route

Eco-friendly, Less energy, intensive

Learn Biology → Instead of FOOD make FUEL

# NEW MATERIALS

- ▶ Molecular Recognition
- ▶ Non Covalent Bond Chemistry
- ▶ Supra molecular Chemistry
- ▶ Molecular Electronics
- ▶ nano particles Chemistry
- ▶ Clusters
- ▶ Organic Super Conductors
- ▶ Organic Ferro magnets
- ▶ Chemionics
- ▶ Conducting Polymers
- ▶ Smart Materials

**LEARN MATERIAL SCIENCE**

Not metallurgy

- ▶ Control of CHEMICAL Equilibria
- ▶ Breaking and Forming Bonds to Order
- ▶ Tuning the CHEMISTRY
- ▶ No Unwanted Bonds
- ▶ No waste Disposal Problem
- ▶  $R_0$  - Vibrational Excitation
- ▶ Lowest Energy Channel need not guide us
- ▶ Understanding of Transition states

**LEARN SPECTROSCOPY**

**LEARN PHYSICS**

**COMPUTERS**

**Not just an analytical tool  
but as Energetics, dynamics and  
Excited States**

# Dream of Chemists

Mystery of photosynthesis

Why Max efficiency ~ 1%?

Can we increase it ?

Can we ask plants to produce

Energy rather than Food :  $H_2$  versus Carbohydrates

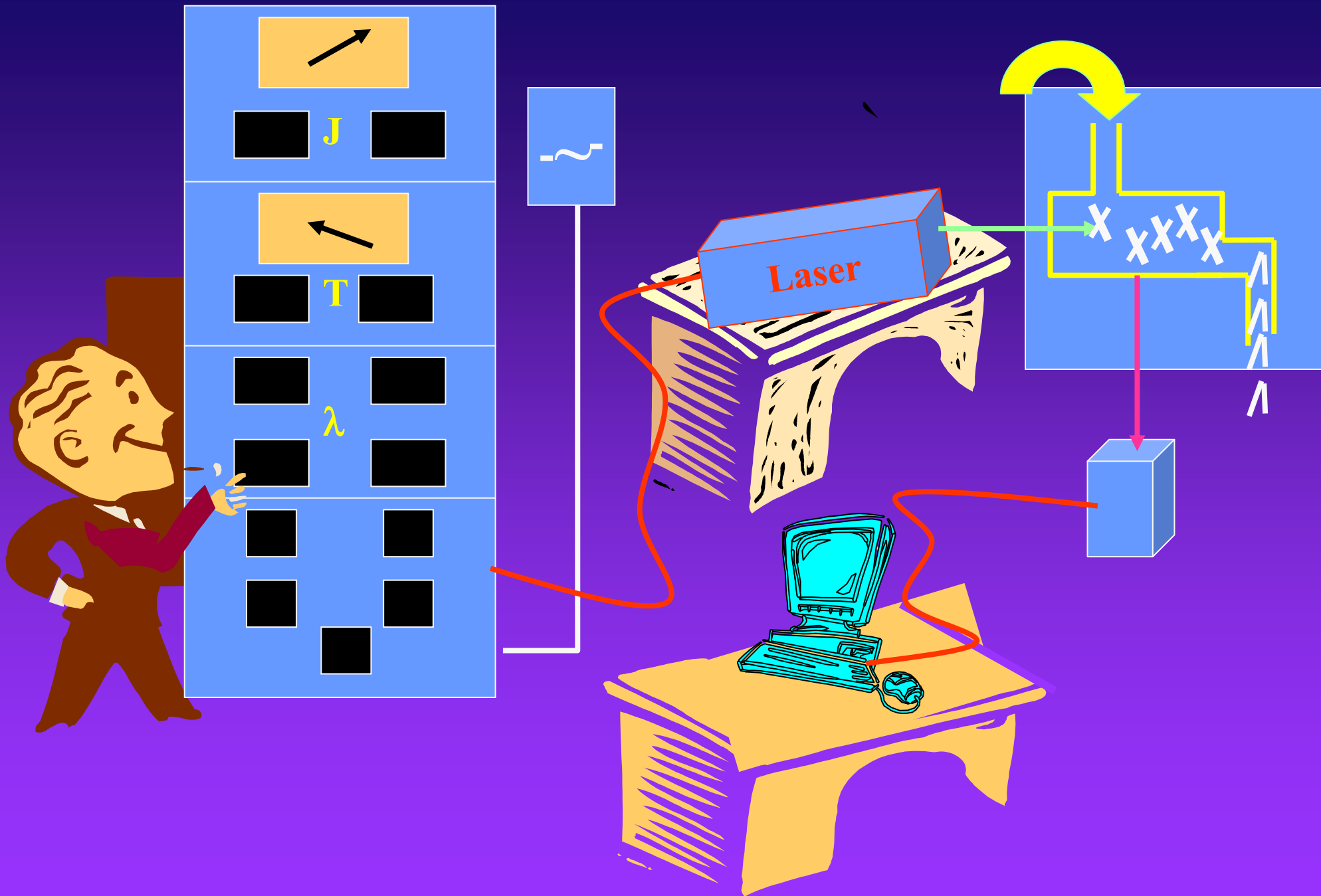
**Pesticides, herbicides, Fungicides (biodegradable) New  
Fertilizers**

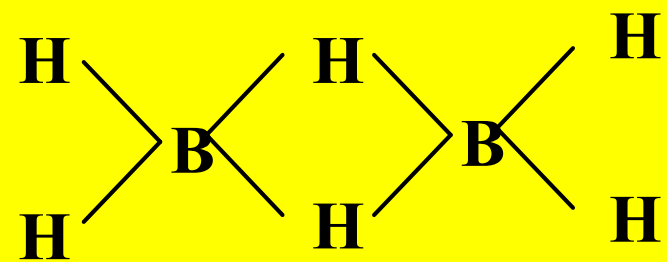
**New Materials: light in wt but strong as Steel**

**Non combustible plastics**

**Fire retardant polymers (Saris)!!**

**Can we run Car on water**





**We have done a rotten job of teaching scientists – we're quite good at that – but to equally important job of teaching science to all others, to the overwhelming 80% or more of the student population who will not enter science or engineering as a profession.  
There we have failed miserably.**

**Ray and Guzzo (1990)**  
*Trashing the planet*



## Gaseous Diffusion Separation of U isotope

**“Most inefficient activity ever devised by man”**

**3 MeV/ U atom**

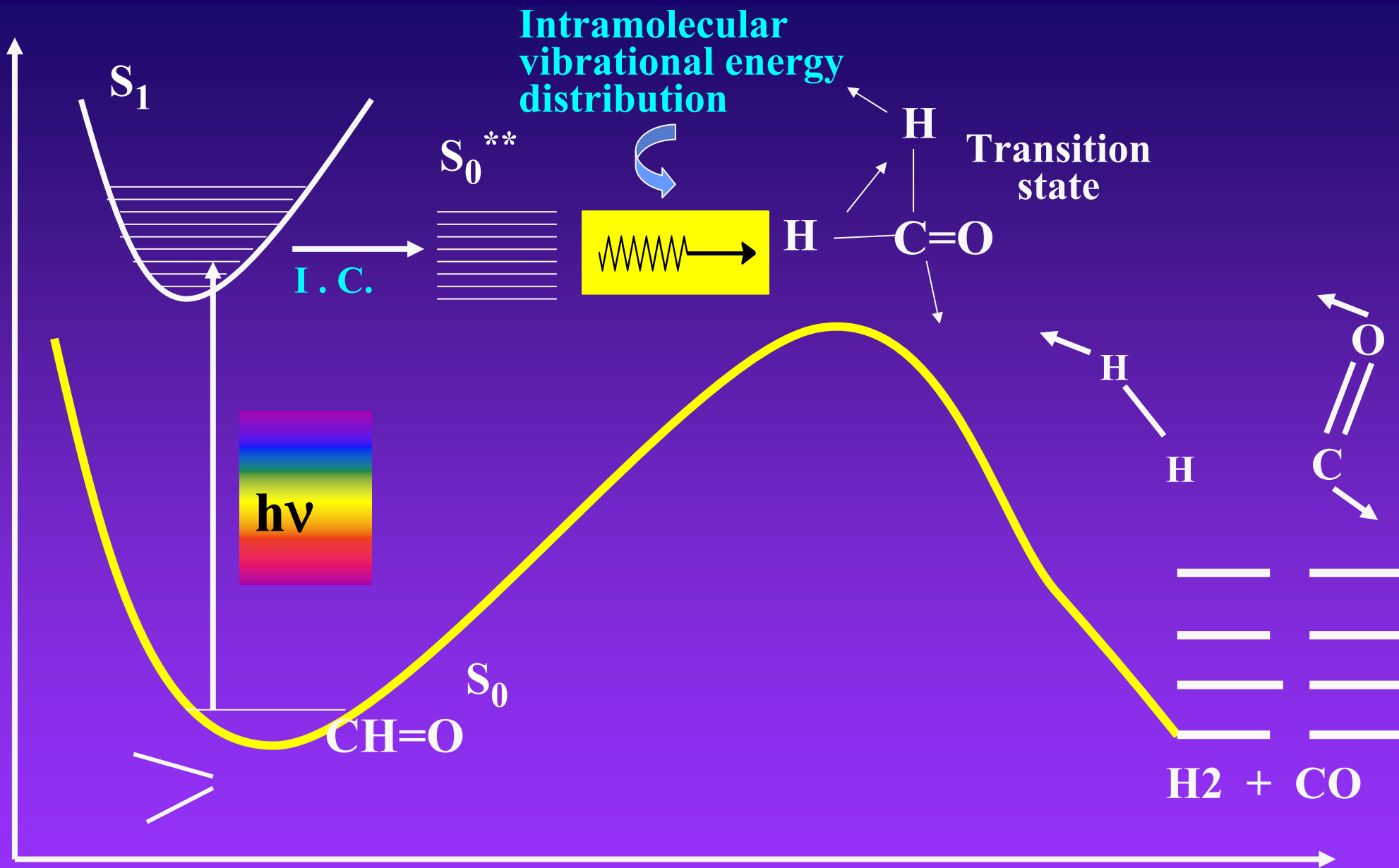
**Presently 3 diffusion plants for separation of U isotopes in  
USA cost 300 billion \$ to build and maintain**

**U<sup>235</sup> separation is  $5 \times 10^9$  \$ / yr industry**

**In a single year it consumes as much electricity as whole  
state of Minnesota**

**Or, 6 of Kalpakam plant for one year**

**WHY NOT LASERS**



*Photofragmentation of a tri-atomic molecule occurs in femtoseconds*

