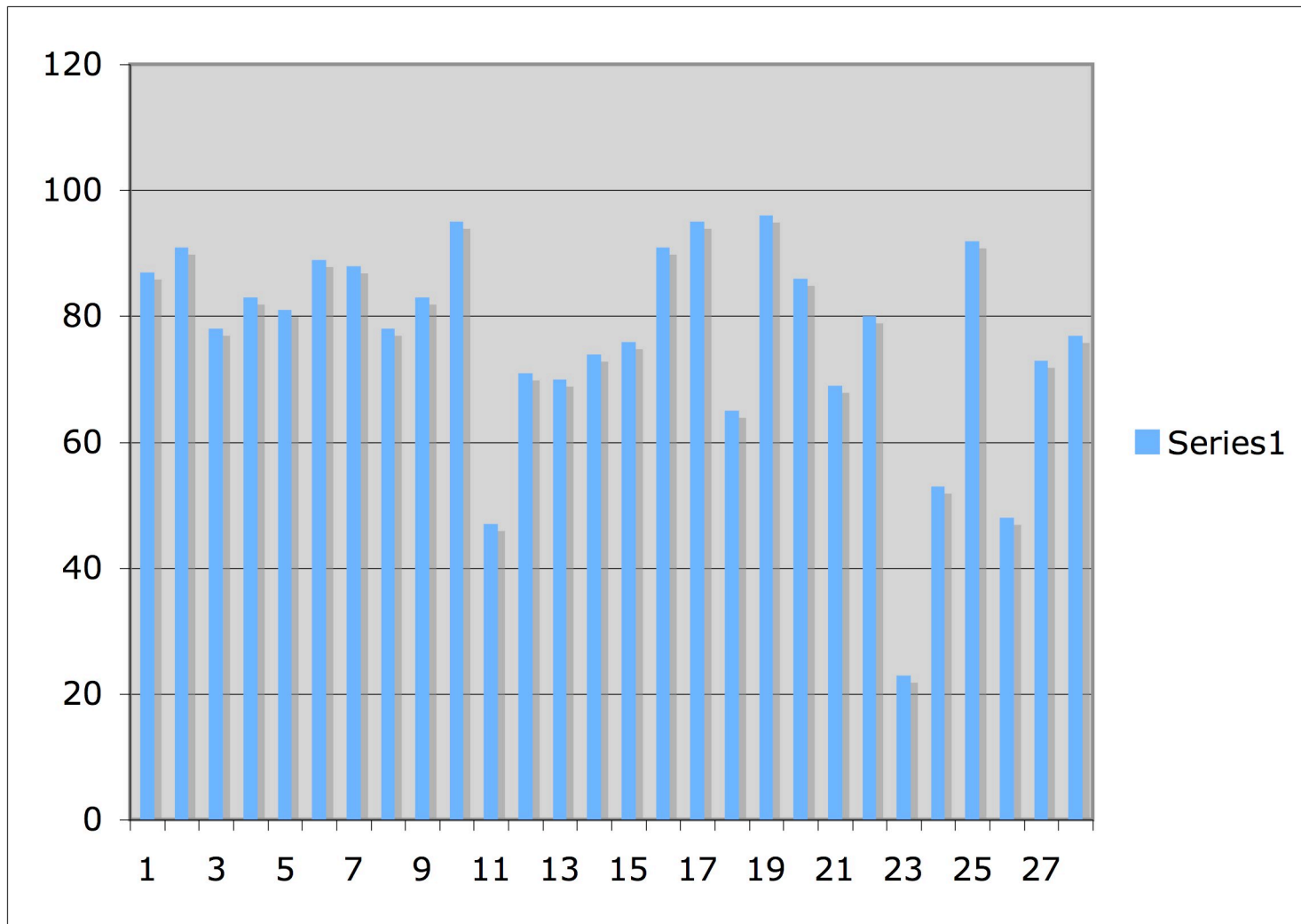


Results for Exam 2_C1403_05: Mean grade = 80, Median grade = 82
For any questions on the exam, please post on the discussion board.



Results of Course evaluation after exam 2

Test: Class Survey after Exam 2

N/A: No Answer

Helpfulness

Please rank the following in terms of their assistance to you in preparing for the exam.

Question 1: Class Lectures

a: very useful 69%

b: useful 17%

c: not useful 13%

Question 2: Homework assignments from the text

a: very useful 20%

b: useful 63%

c: not useful 17%

Question 3: Multiple choice homework assignments

a: very useful 47%

b: useful 39%

c: not useful 13%

CourseWorks

N/A

Question 1: Courseworks worked well for me to obtain information on the course syllabus and exam materials.

a: strongly agree 54%

b: agree 41%

c: disagree 5%

Question 2: The quicktime movies were useful in clarifying and reinforcing concepts related to the course content in the book and lectures.

a: Strongly agree 22%

b: agree 58%

c: disagree 18%

Question 3: The powerpoint presentations were useful in clarifying and reinforcing concepts related to the course content in the book and lectures.

a: strongly agree 30%

b: agree 61%

c: disagree 7%

Exam

N/A

Question 1: On the average, how many hours per week have you spent preparing for the course by reading, studying for quizzes or completing homework assignments?

- a: Less than 5 h 15%
- b: 5-10 h 45%
- c: 11-15 h 28%
- d: 16-20 h 7%
- e: More than 20 h 6%

Question 2: Please indicate your opinion of the exam.

The exam covered materials that were stressed in the homework.

- a: strongly agree 17%
- b: agree 65%
- c: disagree 14%
- d: strongly disagree 4%

Question 3: The exam covered materials that were stressed in the lectures.

- a: strongly agree 25%
- b: agree 63%
- c: disagree 8%
- d: strongly disagree 3%

Question 4: The exam covered materials that were stressed in the practice multiple choice questions.

- a: strongly agree 29%
- b: agree 60%
- c: disagree 8%
- d: strongly disagree 4%

Question 5: The exam covered materials that were stressed in the recitation sections.

- a: strongly agree 8%
- b: agree 49%
- c: disagree 30%
- d: strongly disagree 11%

Question 6: Based on the information presented concerning the exam, the exam was fair.

- a: strongly agree 26%
- b: agree 60%
- c: disagree 11%
- d: strongly disagree 3%

Ratings

N/A

Question 1: Instructor: Organization and Preparation

a: excellent 39%

b: very good 44%

c: satisfactory 16%

d: poor 2%

Question 2: Instructor: Approachability

a: excellent 36%

b: very good 42%

c: satisfactory 19%

d: poor 2%

Question 3: Course: Amount Learned

a: excellent 20%

b: very good 49%

c: satisfactory 25%

d: poor 4%

Question 4: Course: Appropriateness of Workload

a: excellent 19%

b: very good 49%

c: satisfactory 27%

d: poor 5%

**Question 5: N/A 0%
Course: Overall Quality**

a: excellent 18%

b: very good 52%

c: satisfactory 25%

d: poor 4%

Question 6: Quality of Textbook

a: excellent 8%

b: very good 33%

c: satisfactory 36%

d: poor 15%

Chapter 18 Molecular orbitals and spectroscopy

18.1 Diatomic molecules

18.2 Polyatomic molecules

18.3 Conjugation of bonds and resonance structures

18.4 The interaction of light and matter (spectroscopy)

18.5 Photochemistry Atmospheric photochemistry

Special Topic: Buckyballs (C_{60}) and molecules@ C_{60}

18.3 Conjugation of bonds. Resonance structures

Conjugation: delocalization from overlap of π orbitals

Connection between MO theory and Lewis resonance structures

MOs of conjugated molecules

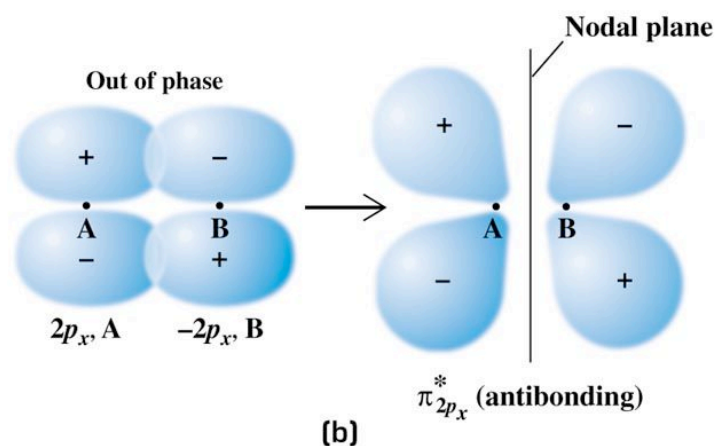
Conjugation of π orbitals and resonance

Resonance: 1,3-butadiene and benzene

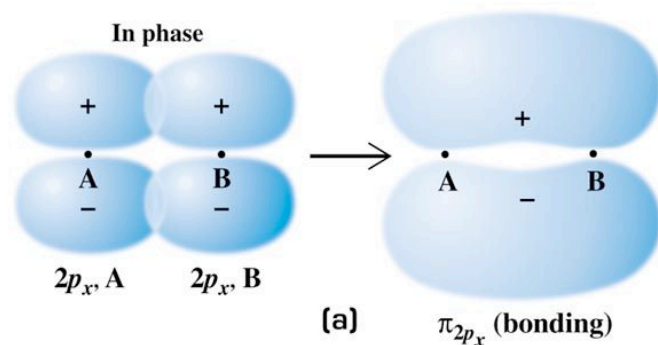
Conjugation and light absorption

Two atoms: Ethylene

(1) Lowest MO has no nodes; (2) each higher MO has one more node; (3) each MO has the symmetry of the molecule

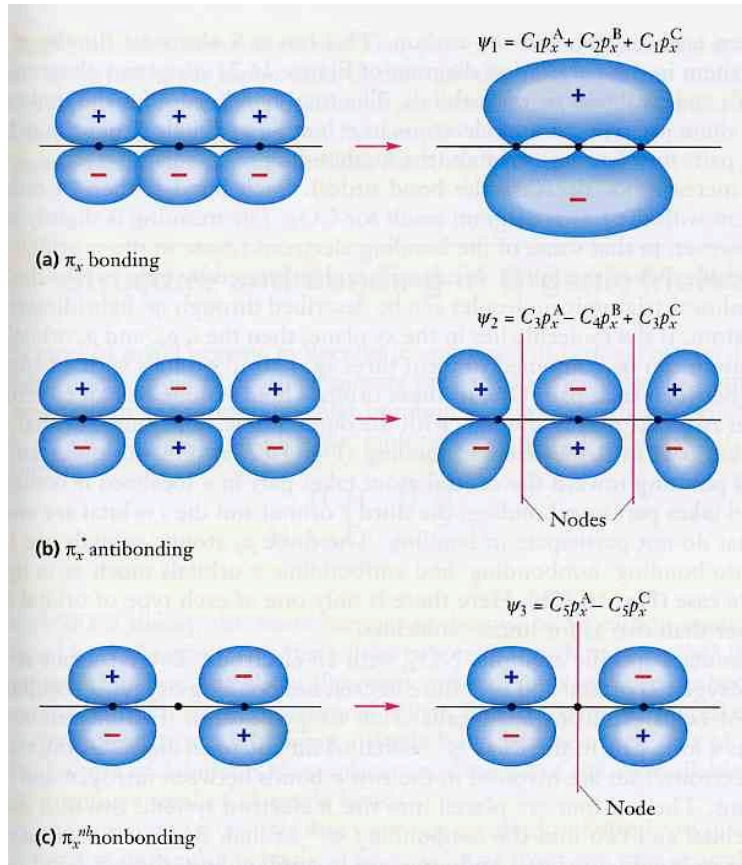


One node



No nodes

Three atoms: Molecular pi orbitals



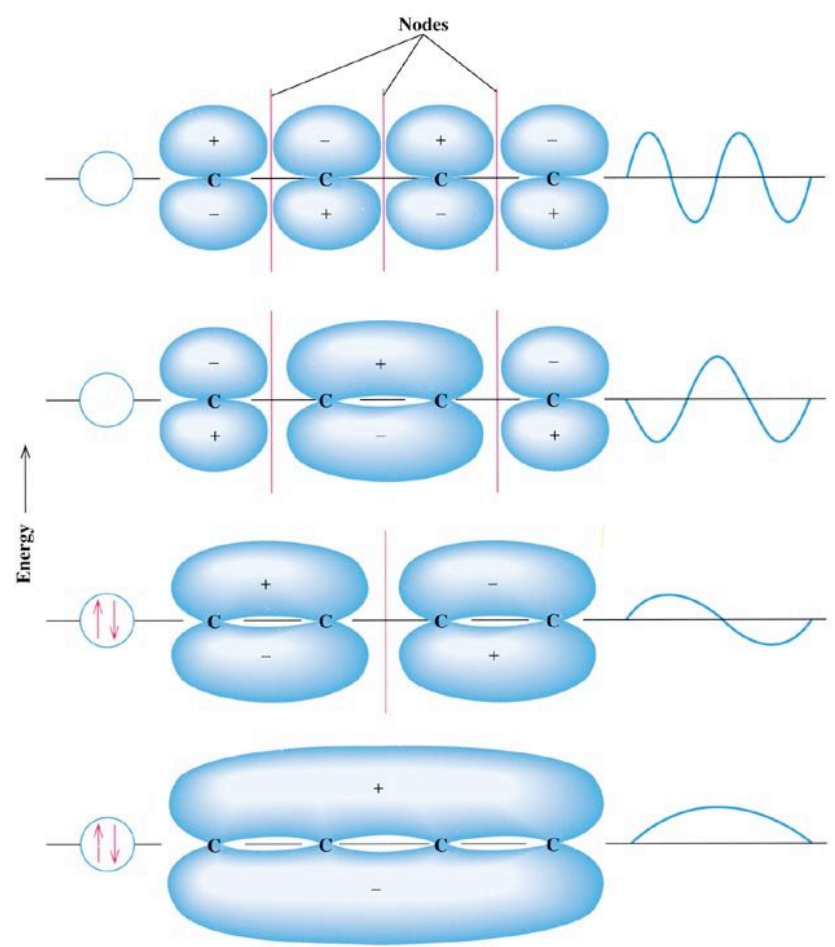
No nodes (π)

Two nodes (π^*)

One node
(Non bonding, nb)

Energy ranking: $p < nb < \pi^*$ (order of nodes)

Four atoms: The π molecular orbitals for a 1,3-diene



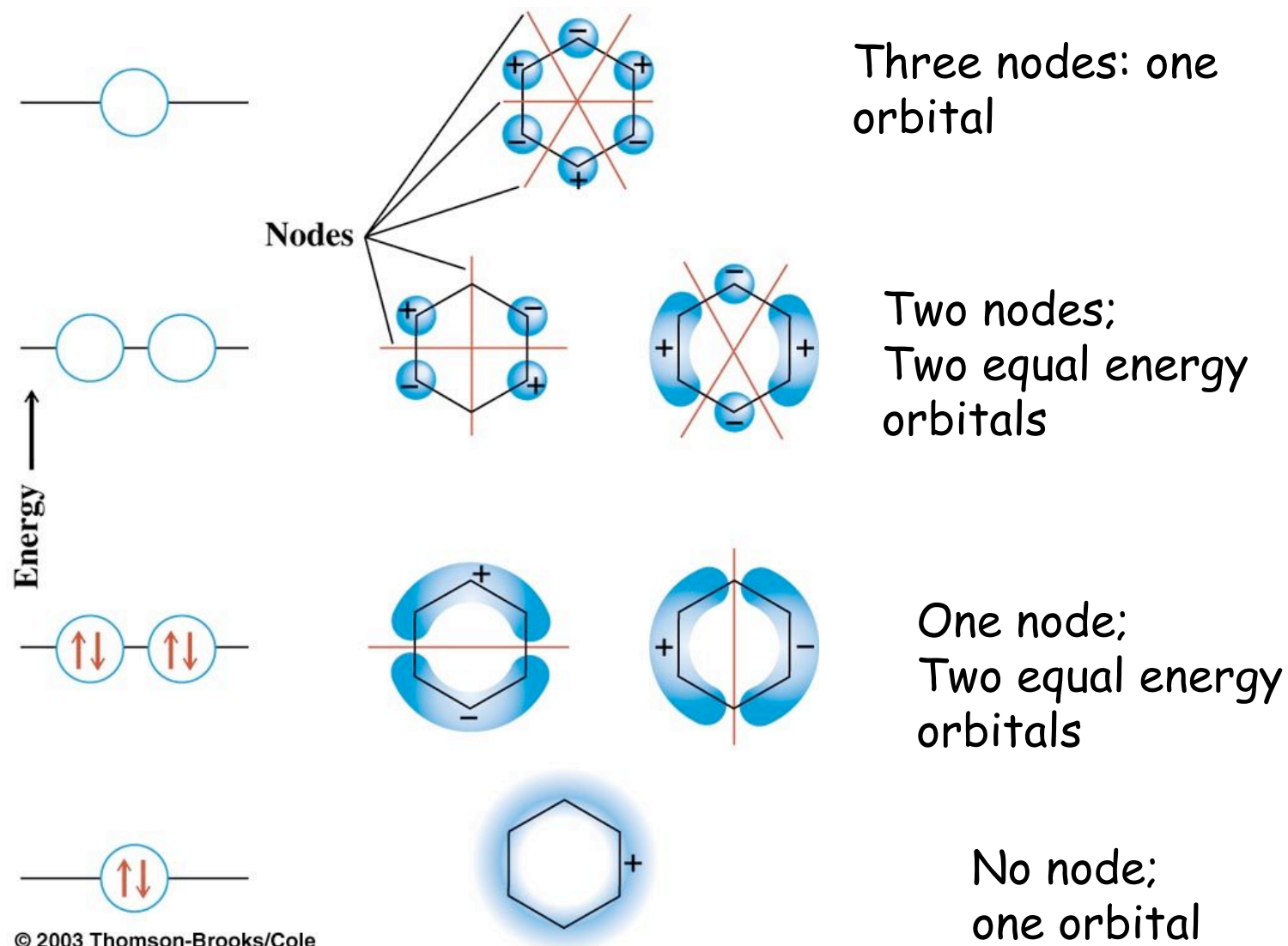
Three nodes

Two nodes

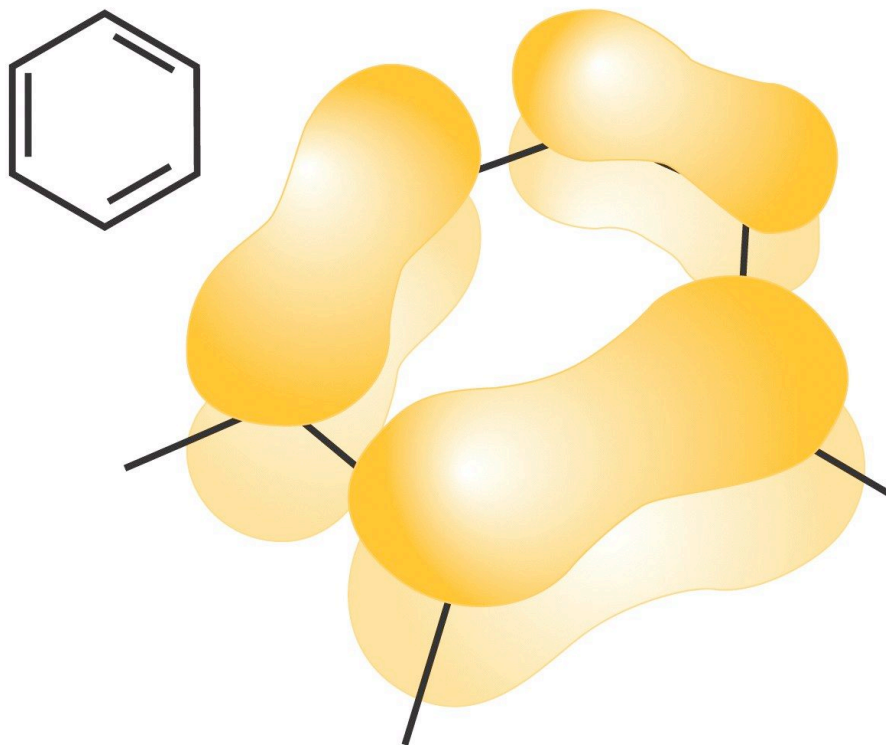
One node

No nodes

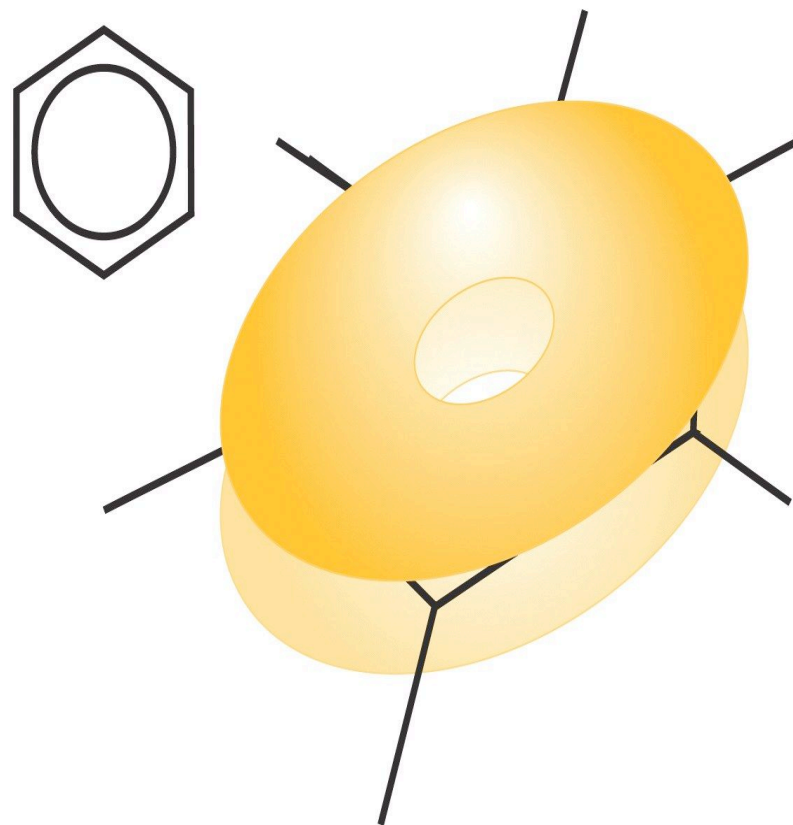
Benzene: A closed ring has some special properties



Two descriptions of benzene



Valence bond:
 π bonds localized



Molecular orbital:
 π bonds delocalized

18.4 The interaction of light and molecules. Molecular spectroscopy

Classifications of electromagnetic radiation:

Spectral classification: X-ray, Ultraviolet, Visible, Infrared, Microwave, Radio

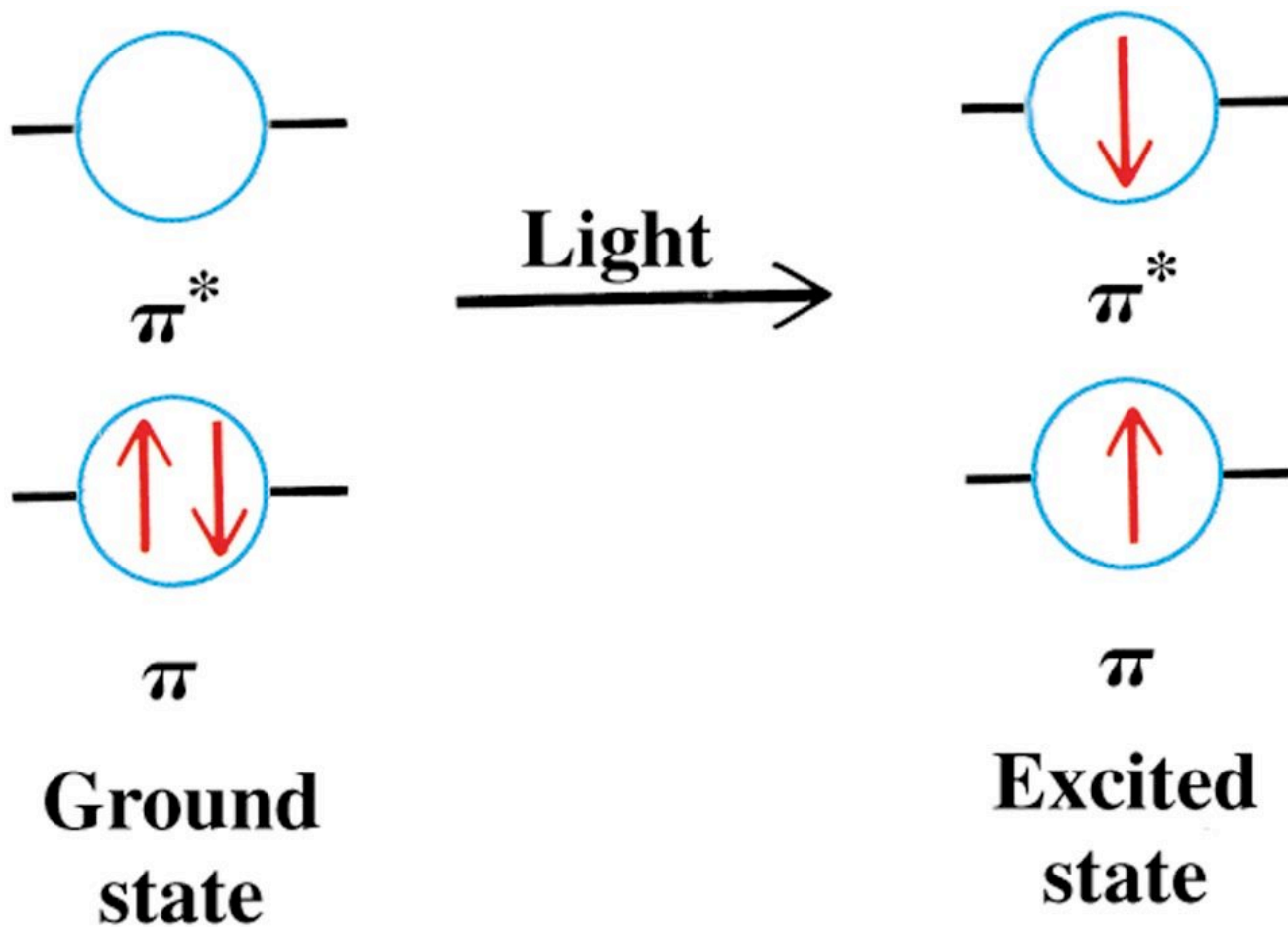
Spectroscopic classification

Electronic spectroscopy, Vibrational spectroscopy, Spin spectroscopy (Magnetic resonance)

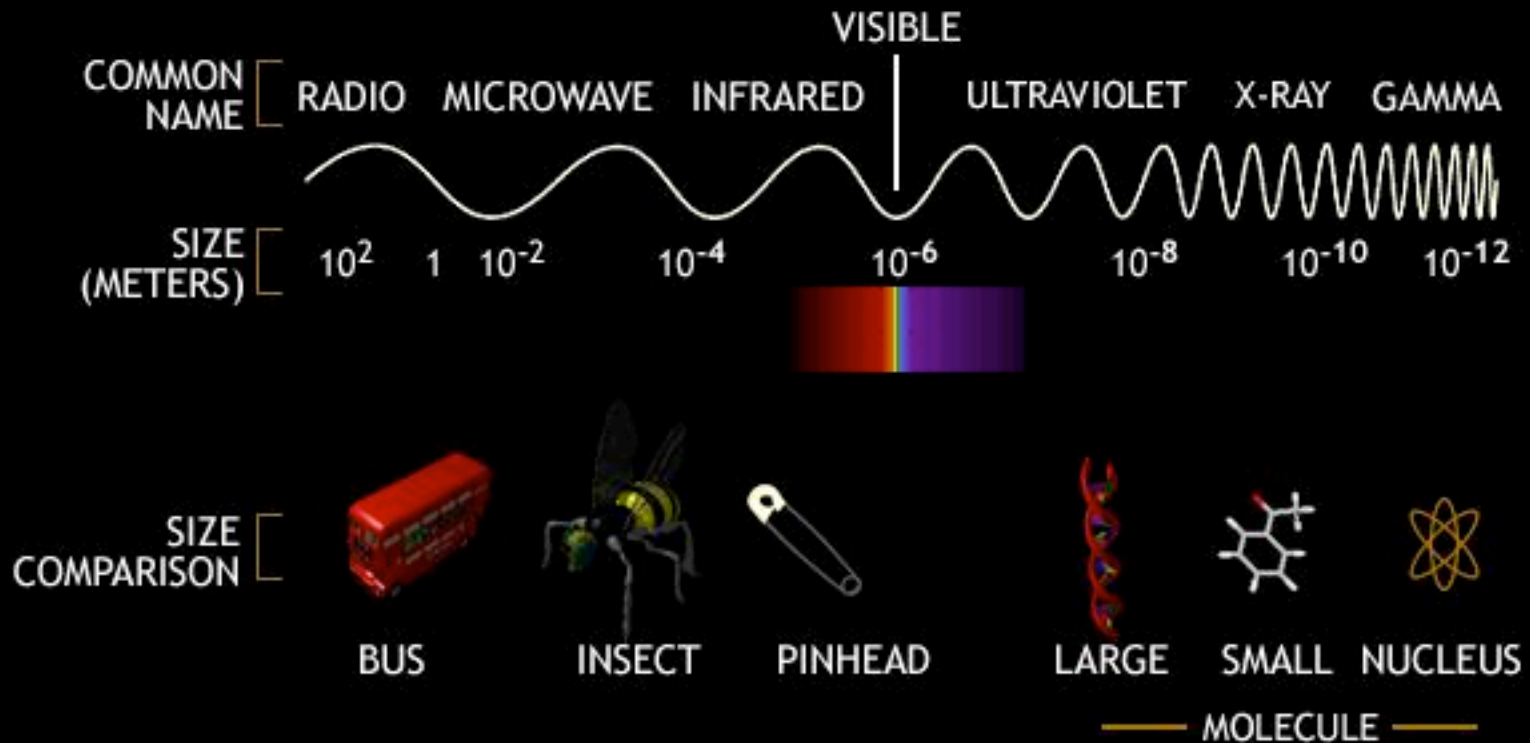
Absorption of light and color

Photochemistry: photosynthesis, vision, atmospheric, toxic, therapeutic

Photochemistry: involves electronically excited states



The distance and size scales of the electromagnetic spectrum

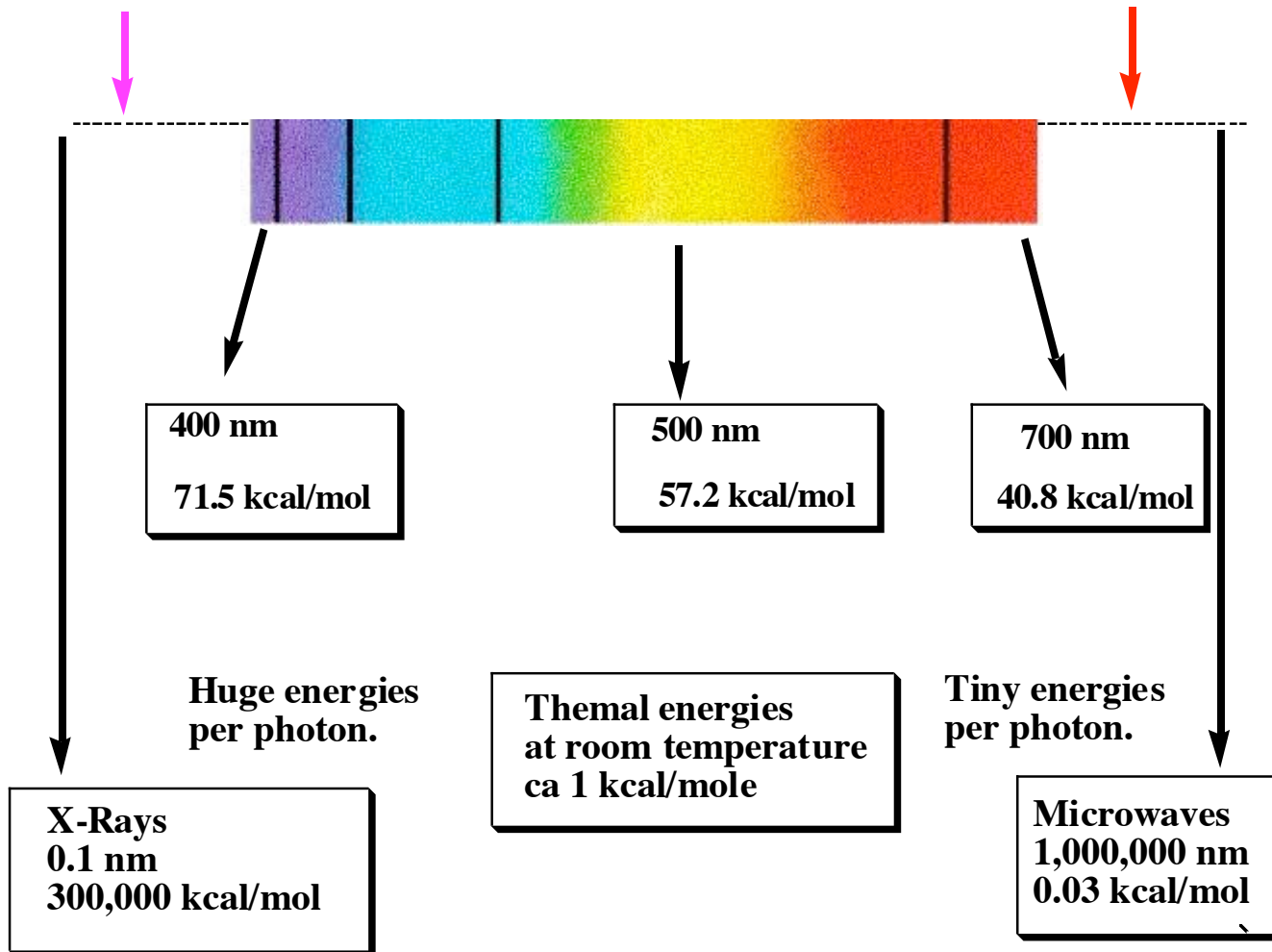


THE ELECTROMAGNETIC SPECTRUM

Energy Scales: Why the visible region works for vision

Ultraviolet Region
Chemical Bonds of
DNA and Proteins
Damaged

Infrared Region
Chemical Bonds Energy
too low to make or break
chemical bonds.

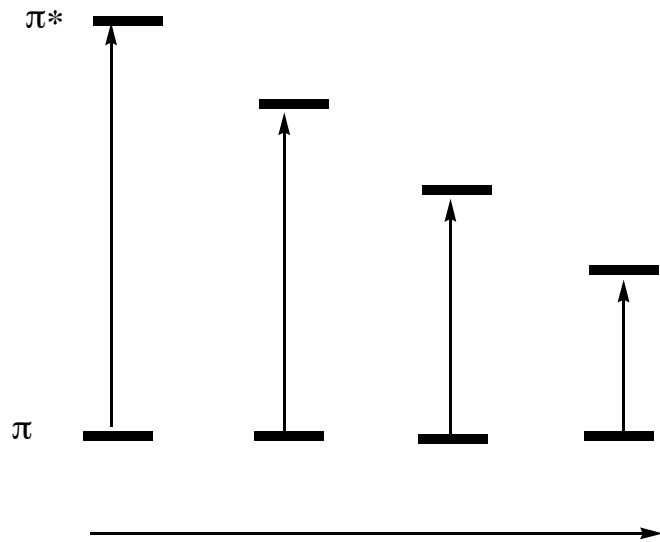


Photochemistry and spectroscopy both involve the absorption of photons to change a structure

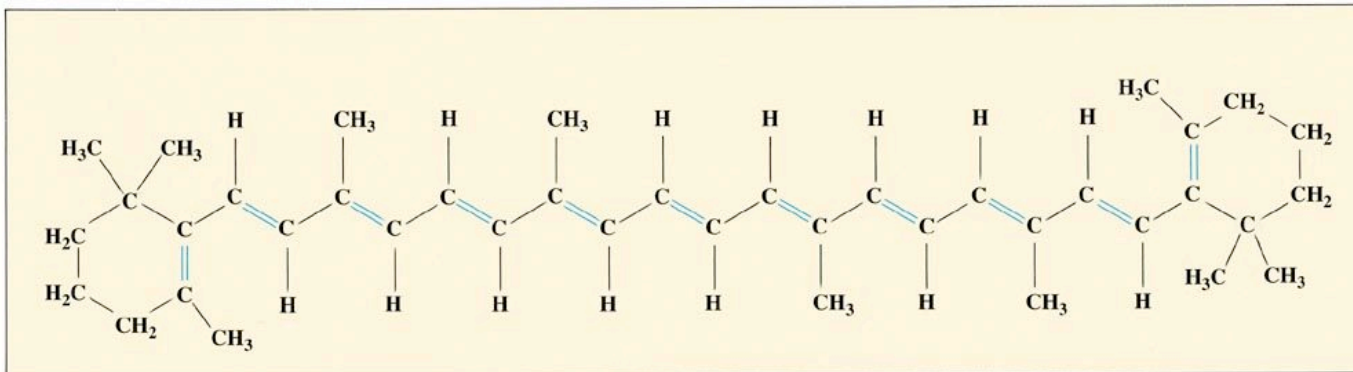
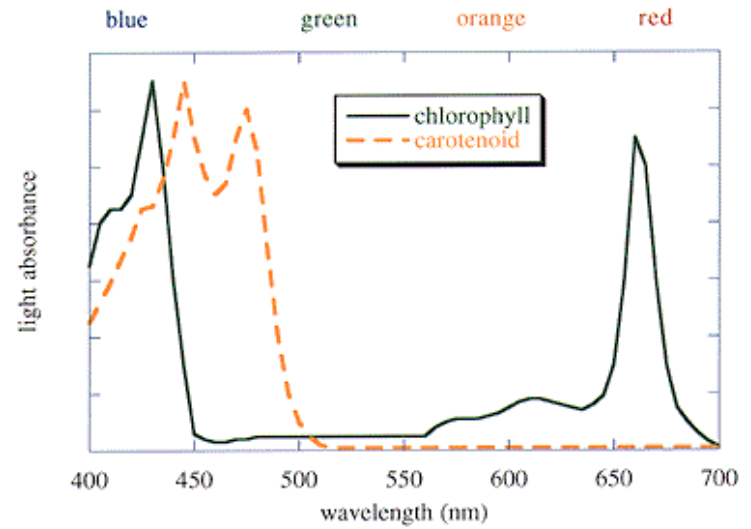
The configurations of electron, the vibrations of atoms, the orientation of spins

Name	Region of Spectrum	Approximate Frequency Range (s^{-1})	Approximate Energy ($kJ\ mol^{-1}$)	Energy Levels Involved	Information Obtained
Nuclear magnetic resonance	Radio	10^7 – 10^9	5×10^{-6} to 5×10^{-4}	Nuclear spin states	Connectivity of atoms in molecules
Microwave	Microwave	10^9 – 10^{12}	0.001 to 1	Rotational	Bond lengths and bond angles
Infrared	Infrared	10^{13} – 10^{14}	2 to 150	Vibrational	Stiffness of bonds, identification of compounds
Ultraviolet-visible	Visible, ultraviolet	10^{14} – 10^{15}	150 to 1200	Valence electron	Electron configurations
X-ray absorption spectroscopy	X-ray	10^{16} – 10^{19}	>10,000	Core electron	Core-electron energies

As conjugation is extended, the wavelength of absorption increases

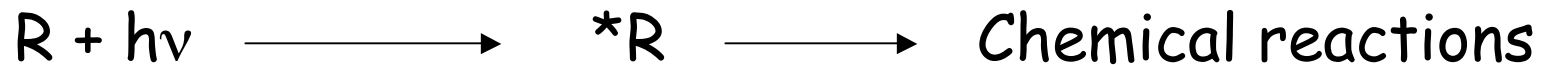


Energy gap decreases: Wavelength increases



beta Carotene

Photochemistry: the science of chemical reactions which occur from electronically excited states of molecules



*R is an electronically excited state

Some important photochemical events:

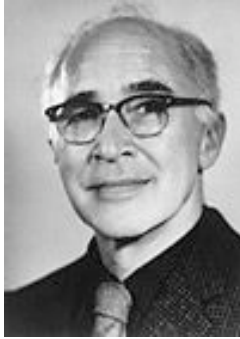
Photosynthesis (electron transfer)

Vision (cis-trans isomerization)

Atmospheric: ozone layer (dissociation)

Vision: Early theories of light were theories of vision.

Photosynthesis: Life requires the capture, storage and release of the sun's energy.



Wald

Nobel in Medicine
Mechanism of Vision

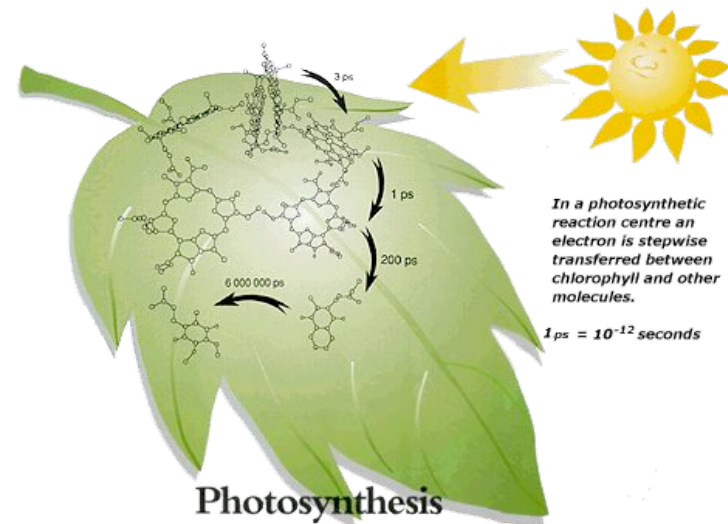
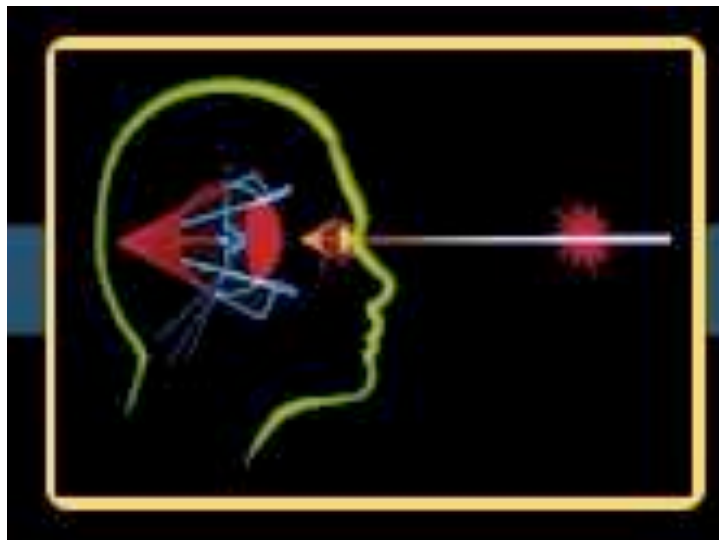


Calvin



Marcus

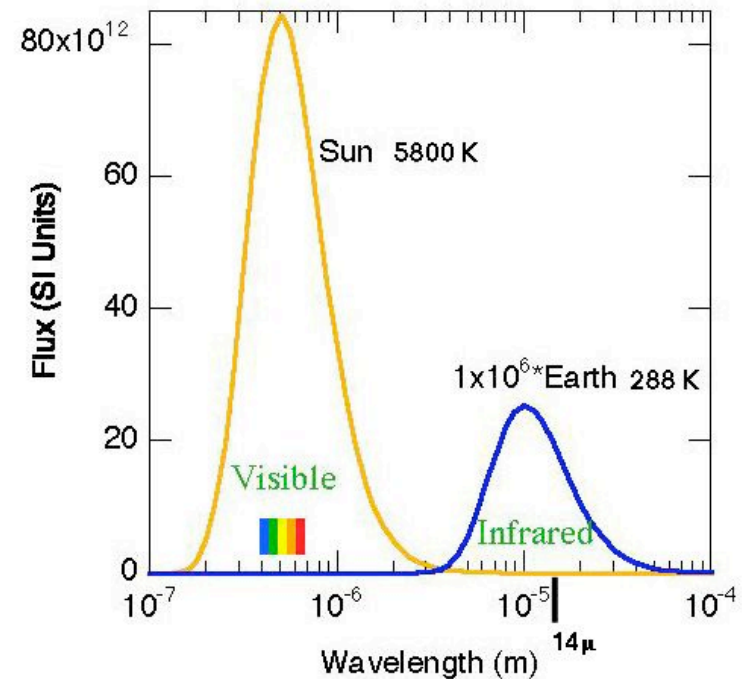
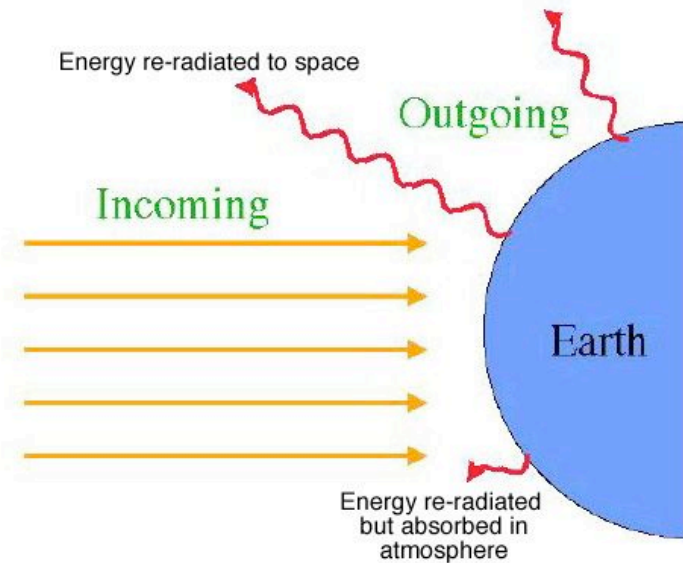
Nobels in Chemistry
Mechanism of Photosynthesis



Solar Radiation

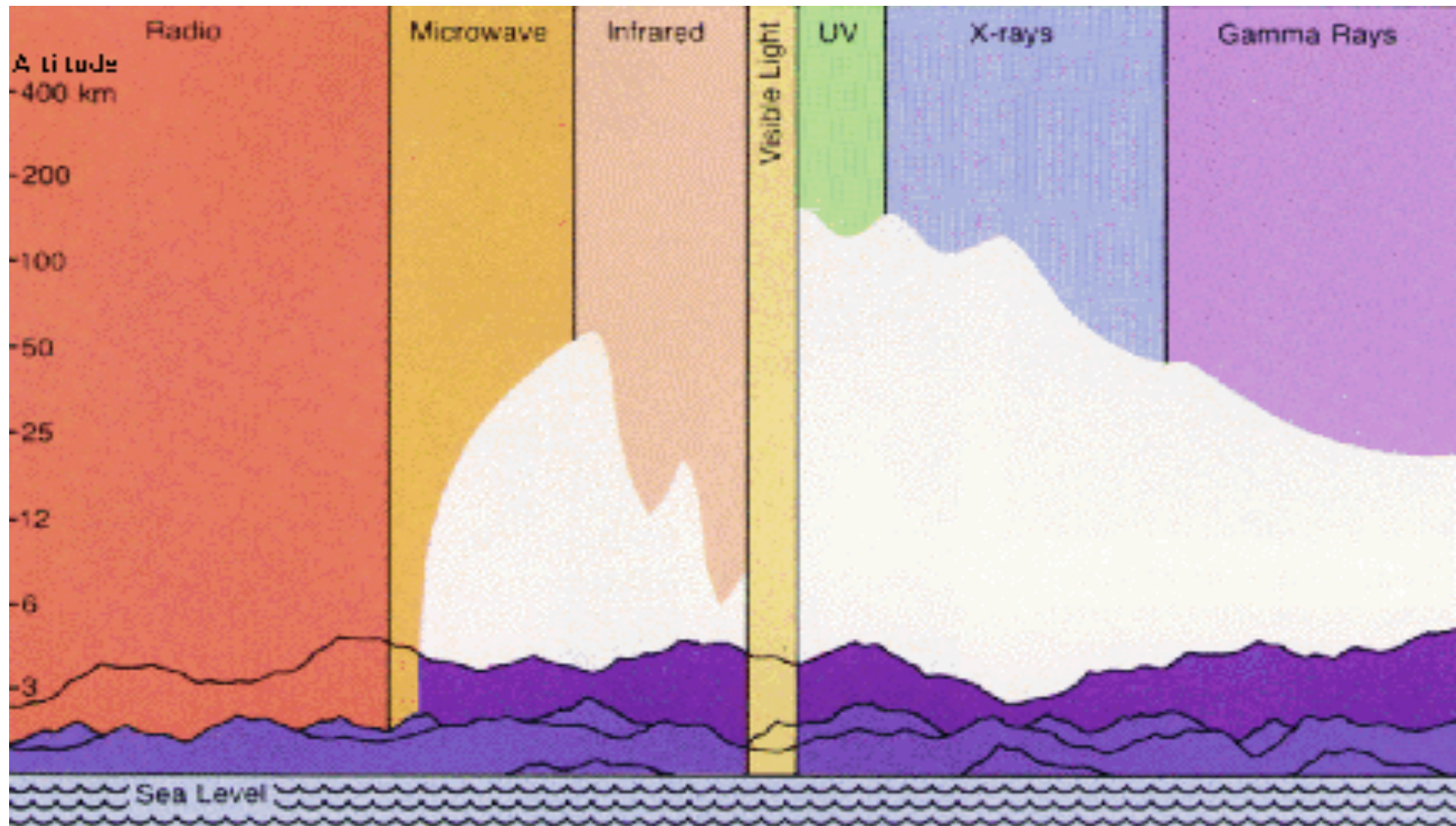
•What wavelengths are present?

This depends on the wavelengths given off by the sun AND the wavelengths absorbed by the atmosphere



Photochemistry and spectroscopy of the atmosphere

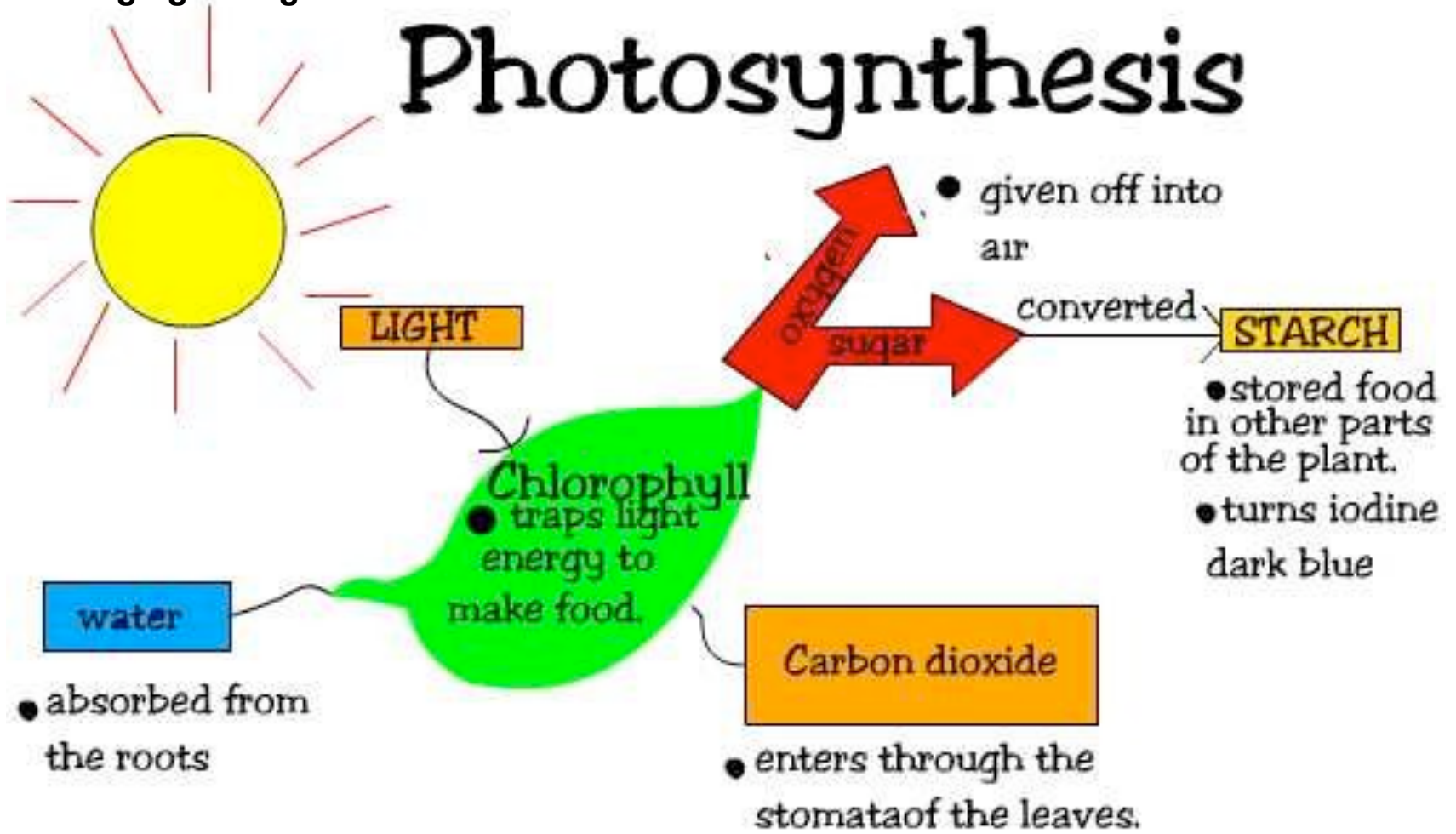
Penetration of electromagnetic radiation through the atmosphere



Water + Carbon dioxide = Food (carbohydrates) + Oxygen

Sun: like a bell ringing out light

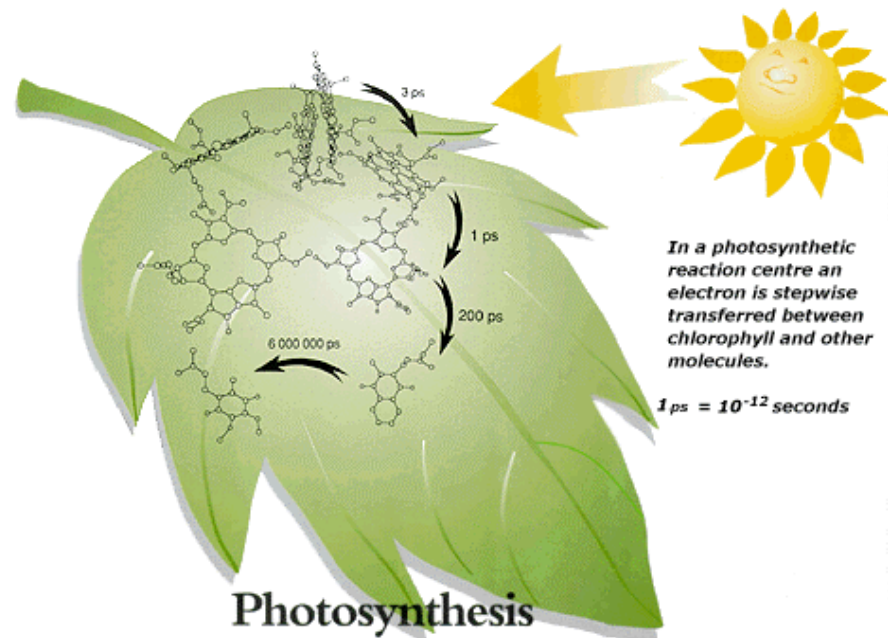
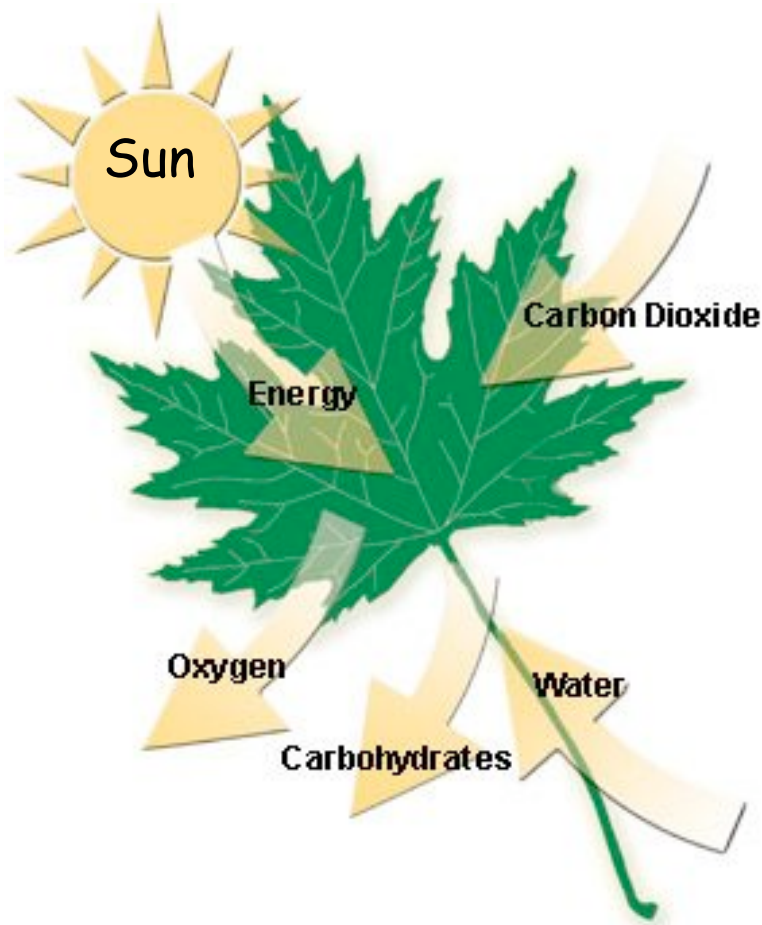
Photosynthesis



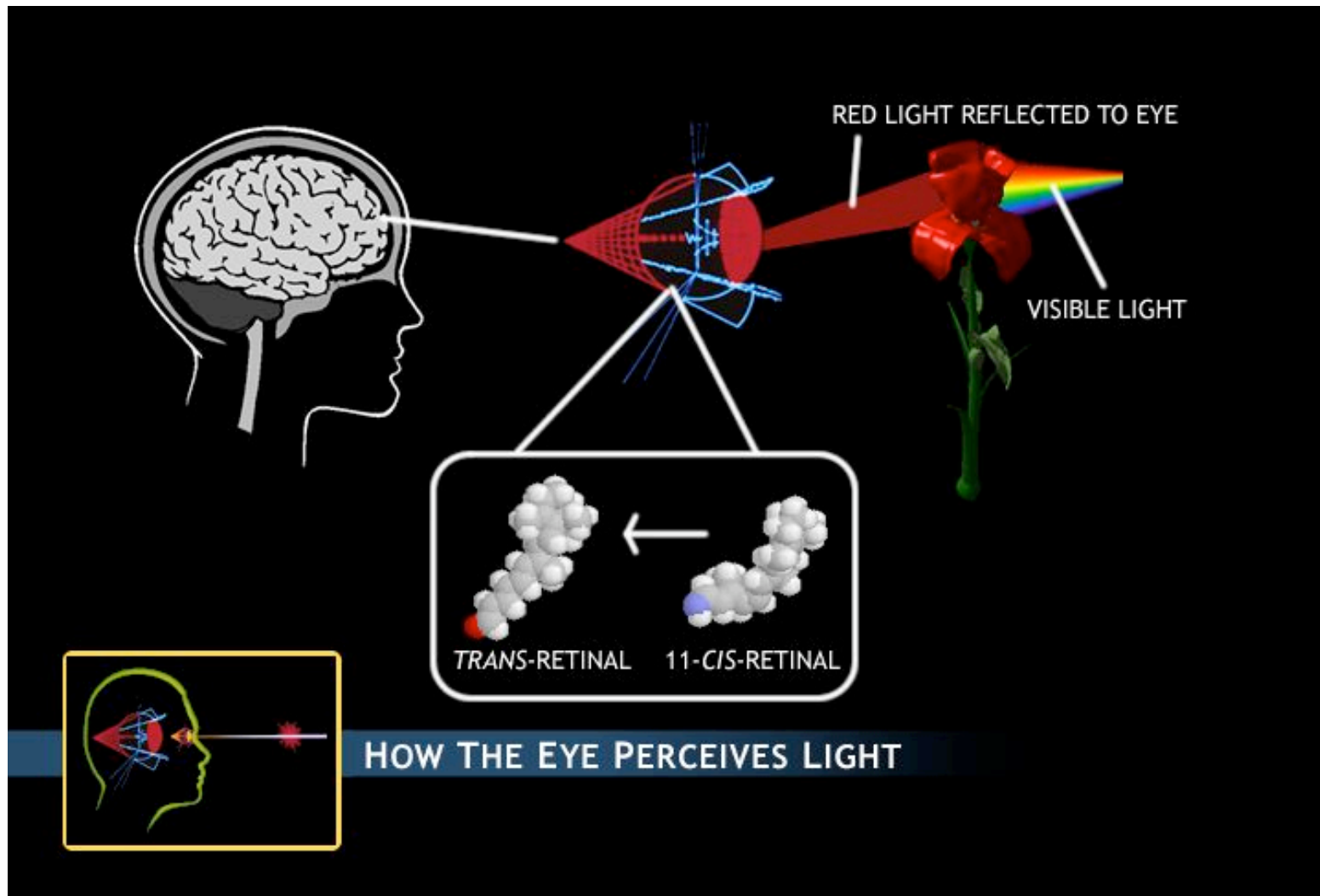
Photosynthesis: $Ch + h\nu \longrightarrow *Ch$ (electrically excited)

$*Ch + Q \longrightarrow Ch^+ + Q^-$ (electron transfer)

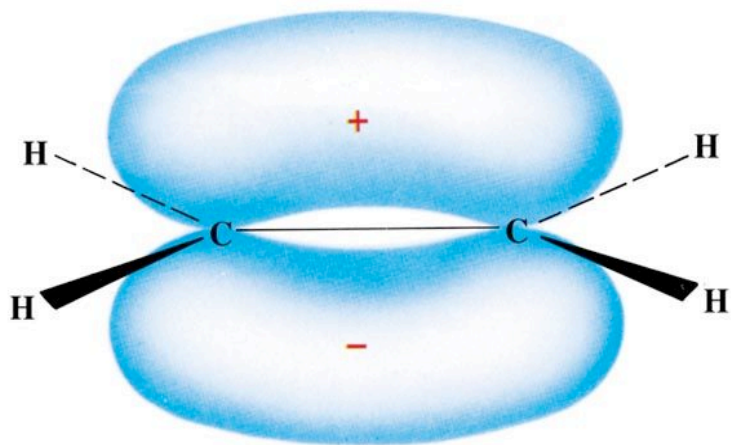
Photosynthesis: $6 H_2O + 6 CO_2 = C_6H_{12}O_6 + 6 O_2$



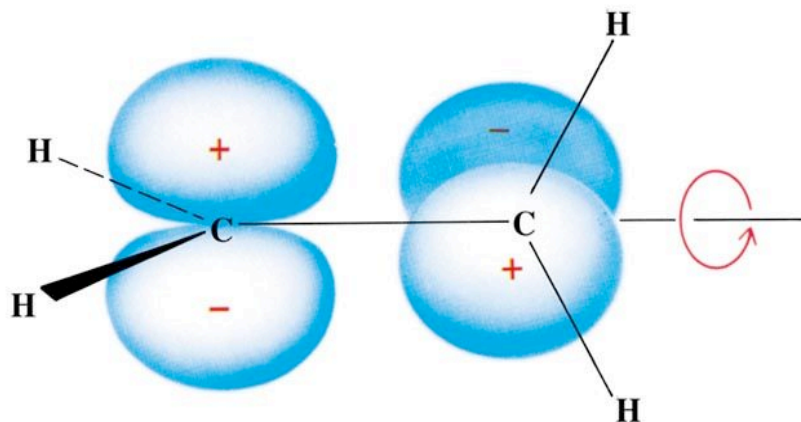
Vision: triggered by a photochemical reaction



The effect of photoexcitation of a π electron to a π^* orbital: the double bond is broken



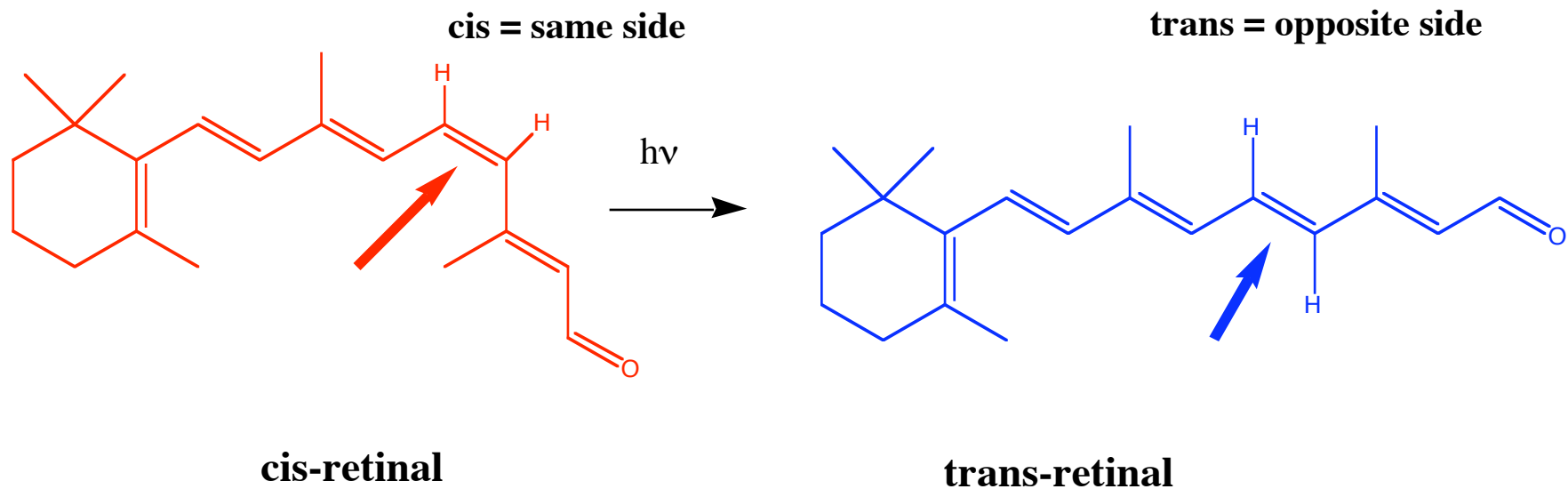
π^2 electronic configuration:
double bond keeps the
molecule planar and
prevents twisting about the
C=C bond



$(\pi)^1(\pi^*)^1$ electronic
configuration:
double bond broken and
twisting occurs about
the C-C bond

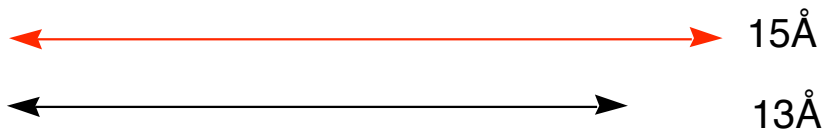
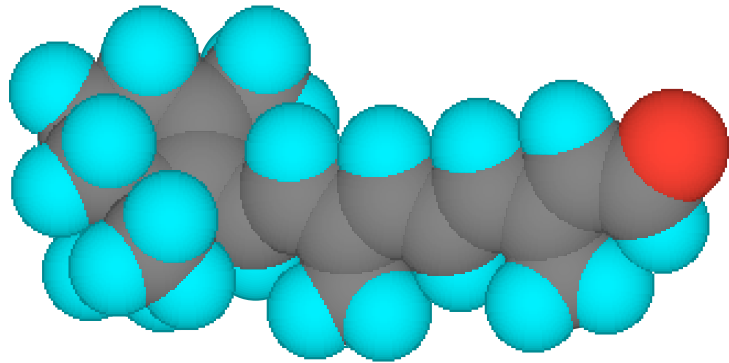
Rotation about a $C=C^*$ bond causes cis-trans isomerization

**The photochemical change which triggers vision.
A simple cis-trans isomerization: rotation about a double bond.**

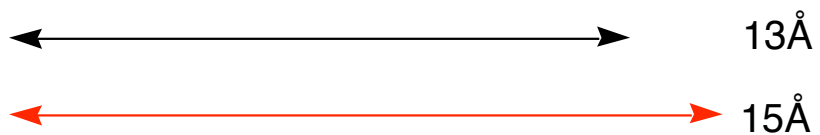
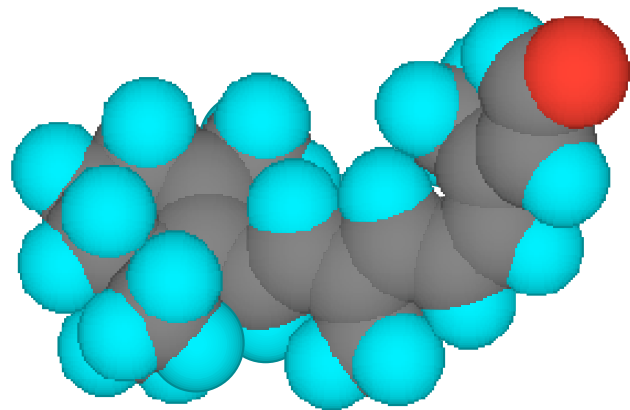


The cis to trans isomerization triggers vision

Vision results from the change of a shape of ca
.2 nm = 0.2×10^{-9} m

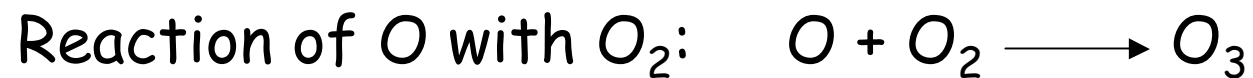
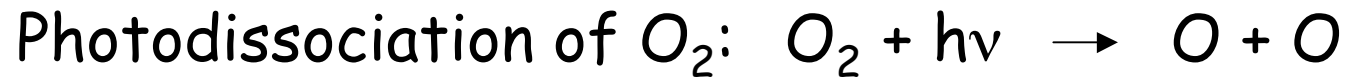


trans-retinal



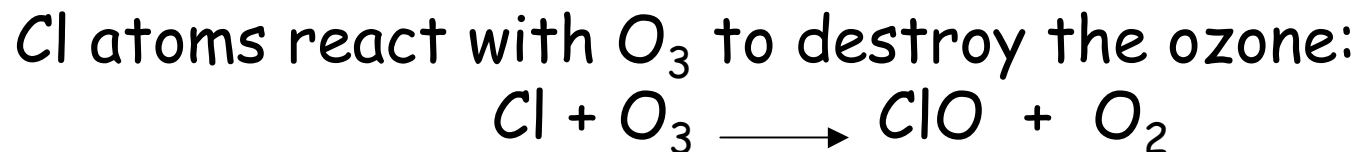
cis-retinal

Atmospheric photochemistry: production and destruction of ozone



Ozone protection: O_3 absorbs light whose wavelength is in the 200-350 nm region of the spectrum

Fluorocarbons absorb light and produce Cl atoms



Photochemistry and biology

Photons can be toxic (cause DNA bases to dimerize)

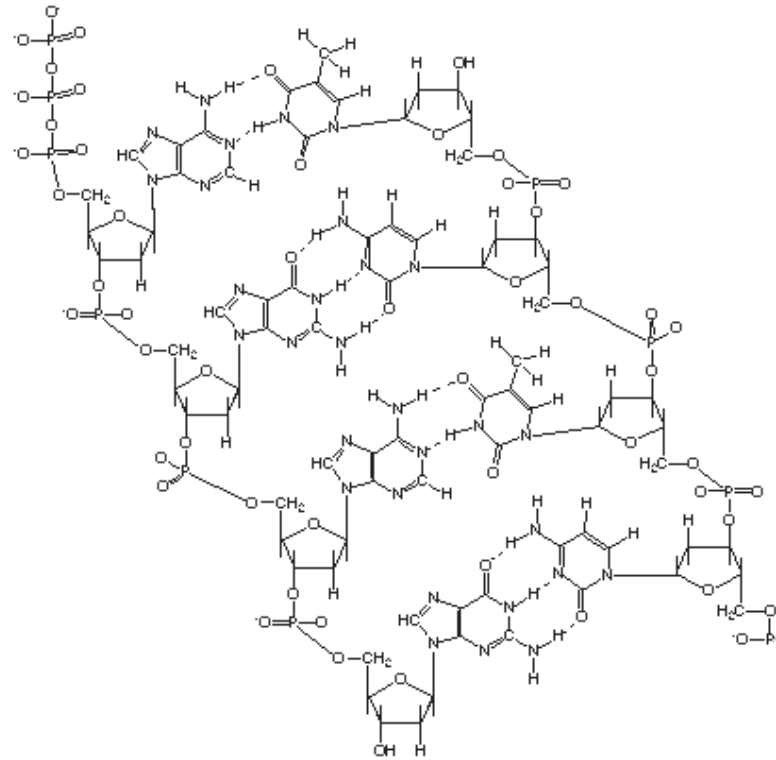
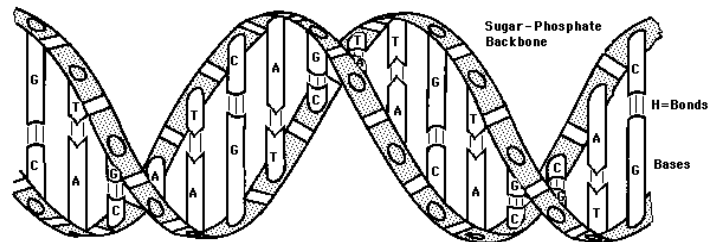
Photons can be therapeutic: phototherapy

Photons can track thoughts, one molecule at a time

Photons can image whole bodies and search for disease

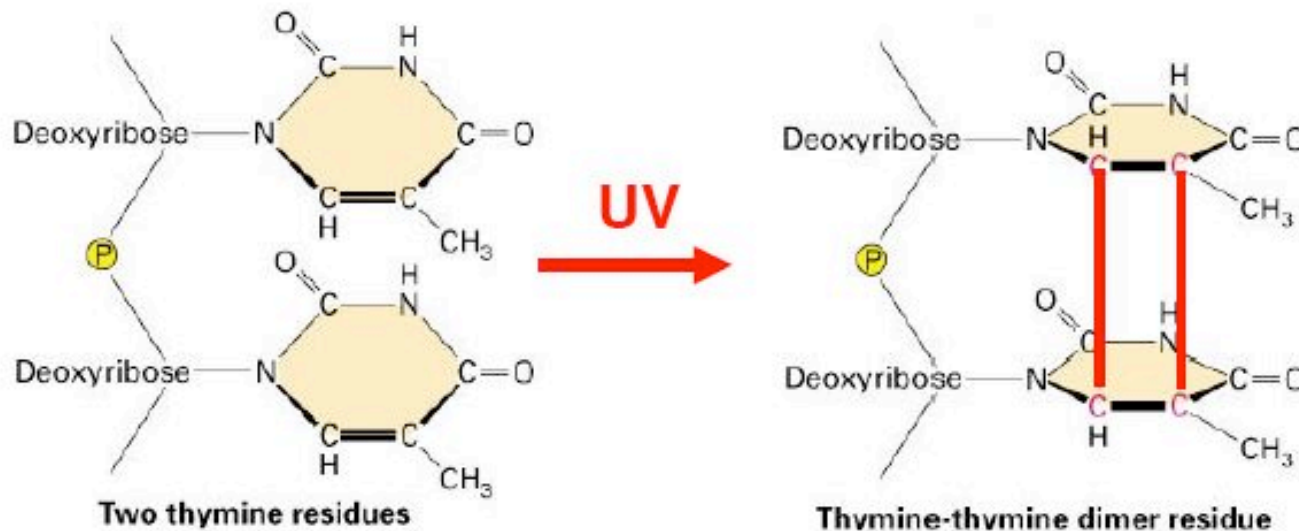
Phototoxicity: Damage to DNA

- DNA
- 2' Deoxyribo Nucleic Acid



DNA: UV photochemistry

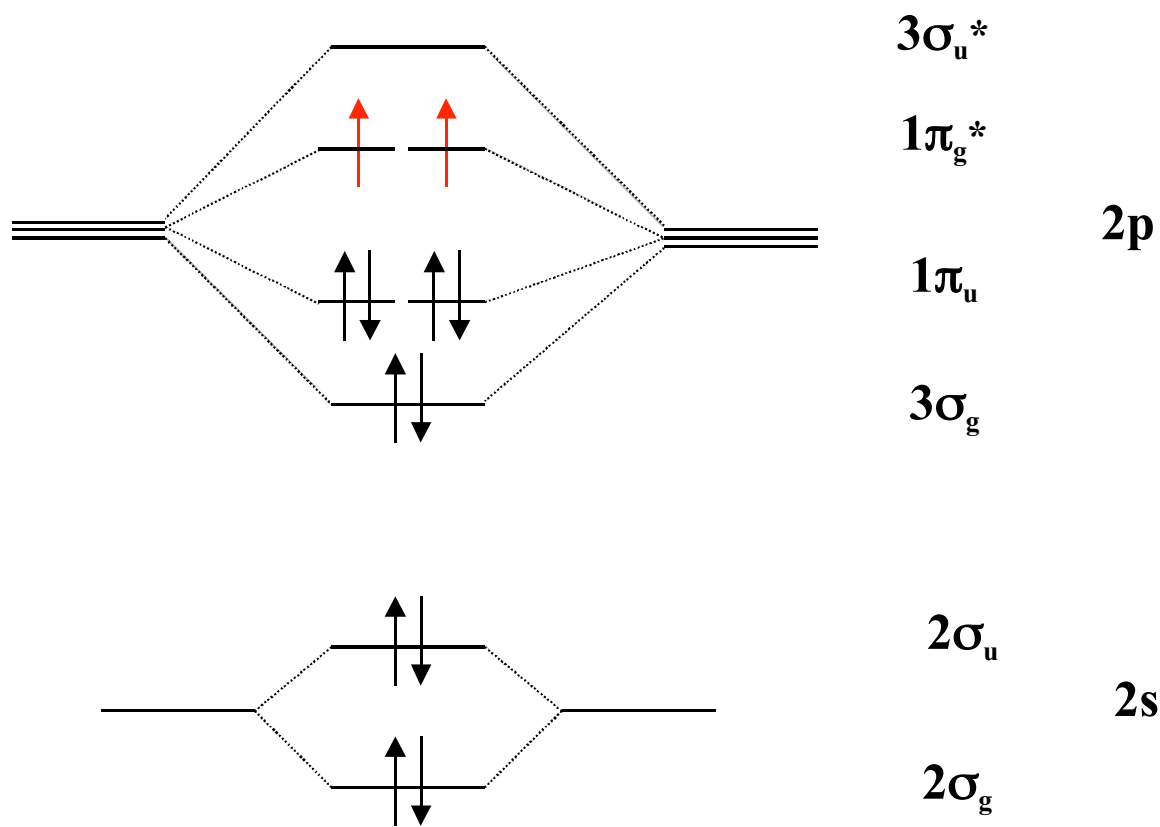
Thymidine dimers are generated by exposure to UV light



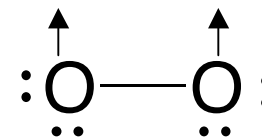
Photons cause two DNA bases to link: this kills the cells containing the irradiated DNA

Singlet molecular oxygen: and excited state of ordinary oxygen

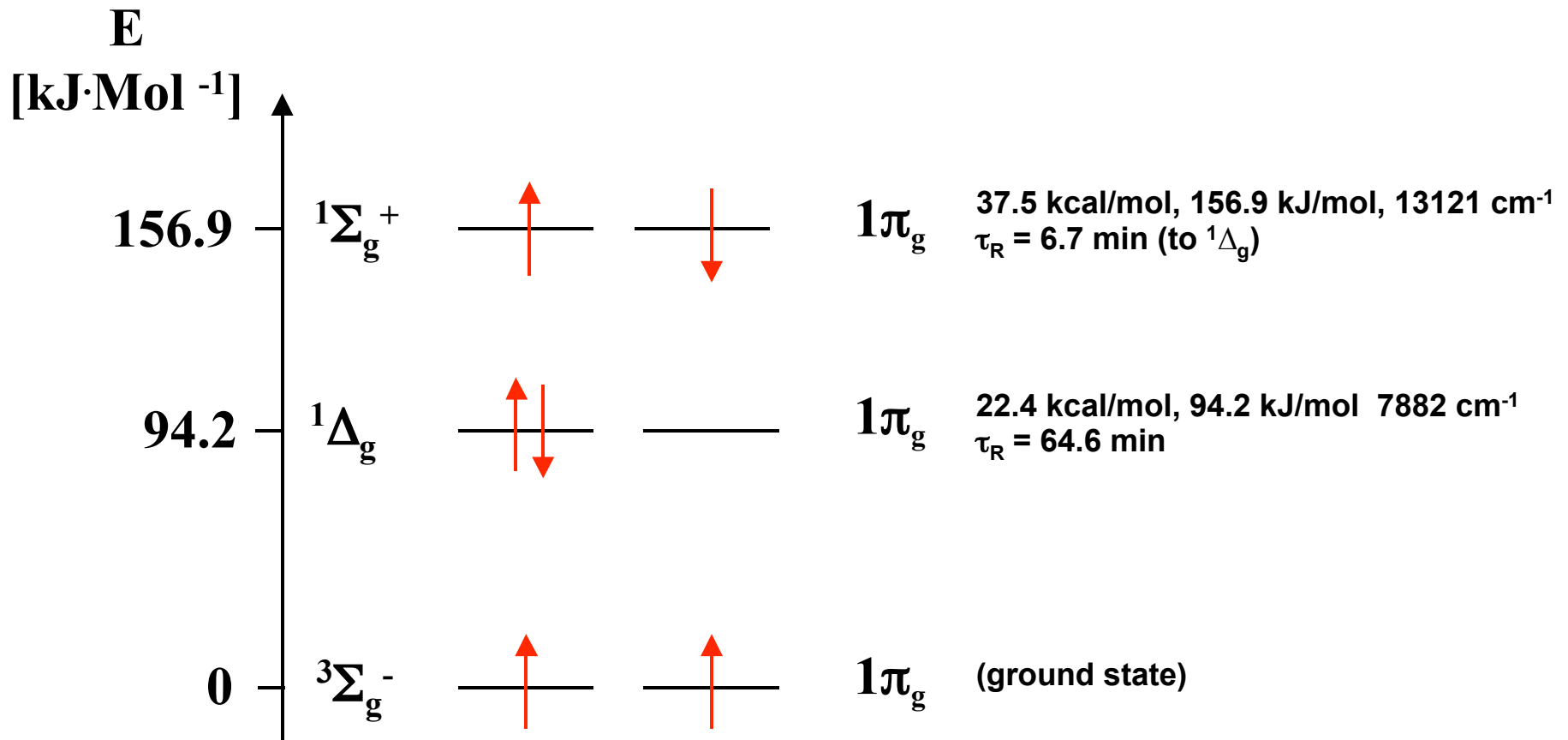
The Aufbau of the MOs of O₂



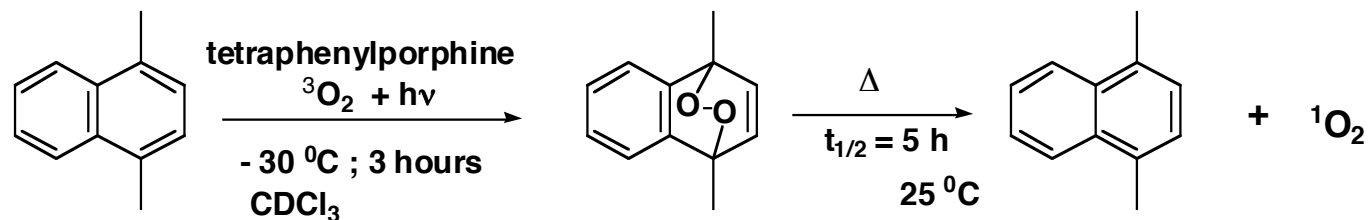
Hund's rule states: When there are two electrons to be placed in two orbitals of equal energy, the lowest energy configuration places one electron in each orbital with parallel spins, a triplet state



Electronic states of molecular oxygen: two low lying **singlet** states

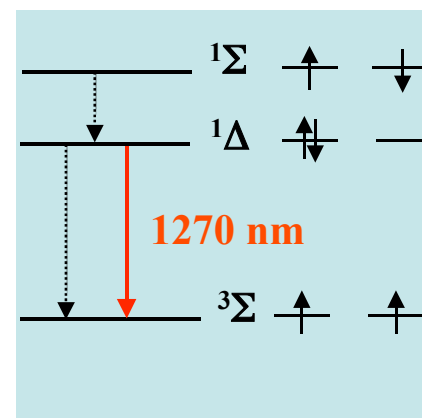
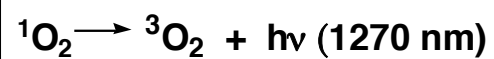
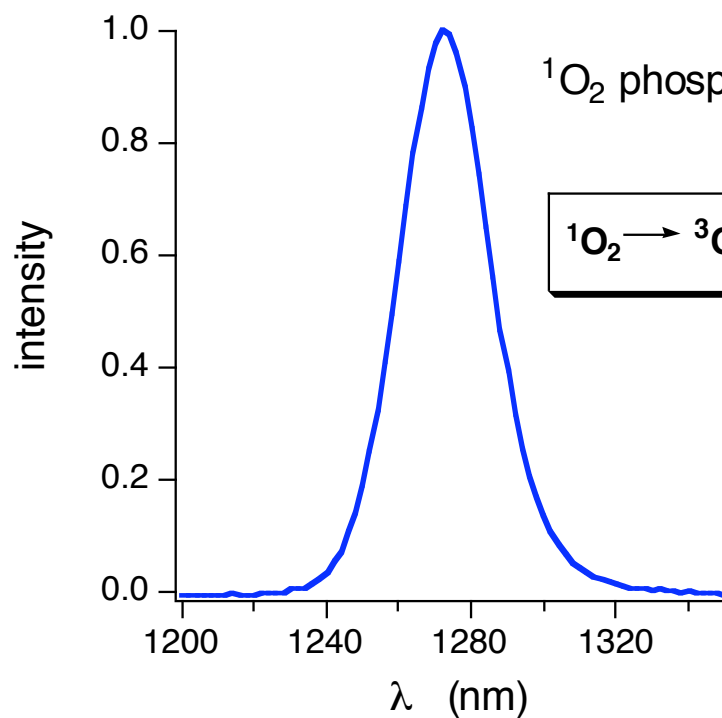


Direct spectroscopic detection of ${}^1\text{O}_2 \rightarrow {}^3\text{O}_2 + h\nu$: *phosphorescence at 1270 nm*

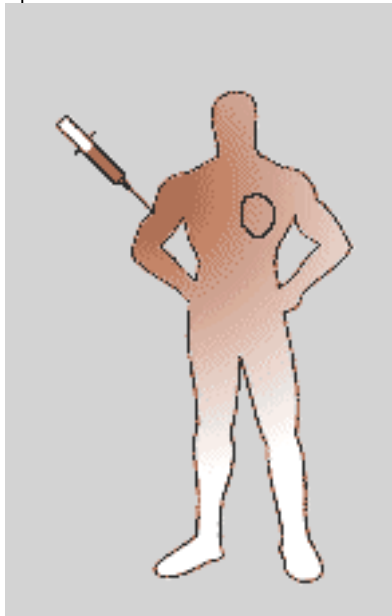


Photochemical generation
of endoperoxide

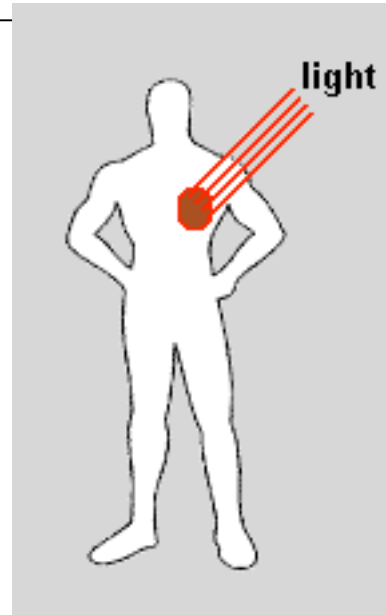
Thermal decomposition
of endoperoxide



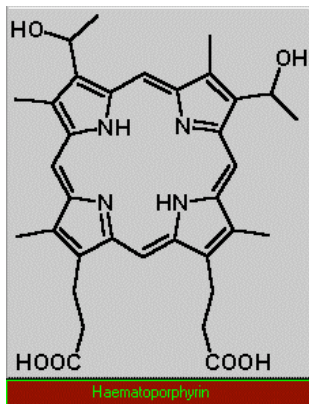
Photodynamic Therapy using singlet oxygen



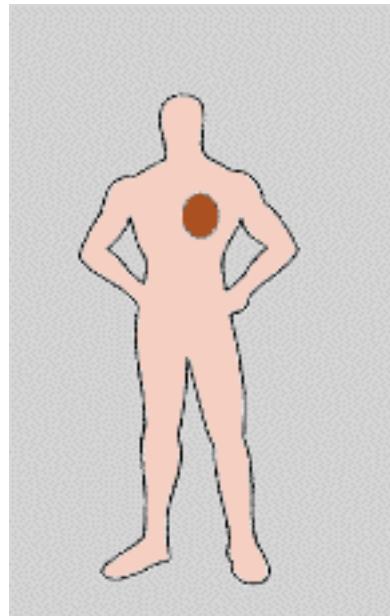
Porphyrin injected into patient



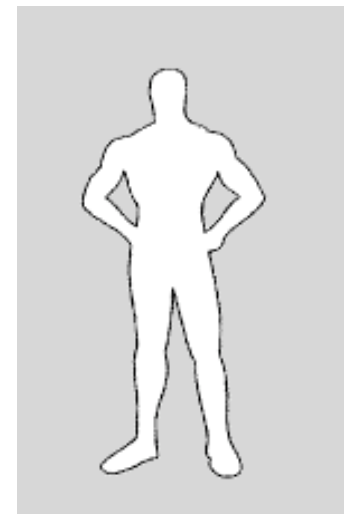
Only the affected organ irradiated with light



(Abs 390 - 450 nm)



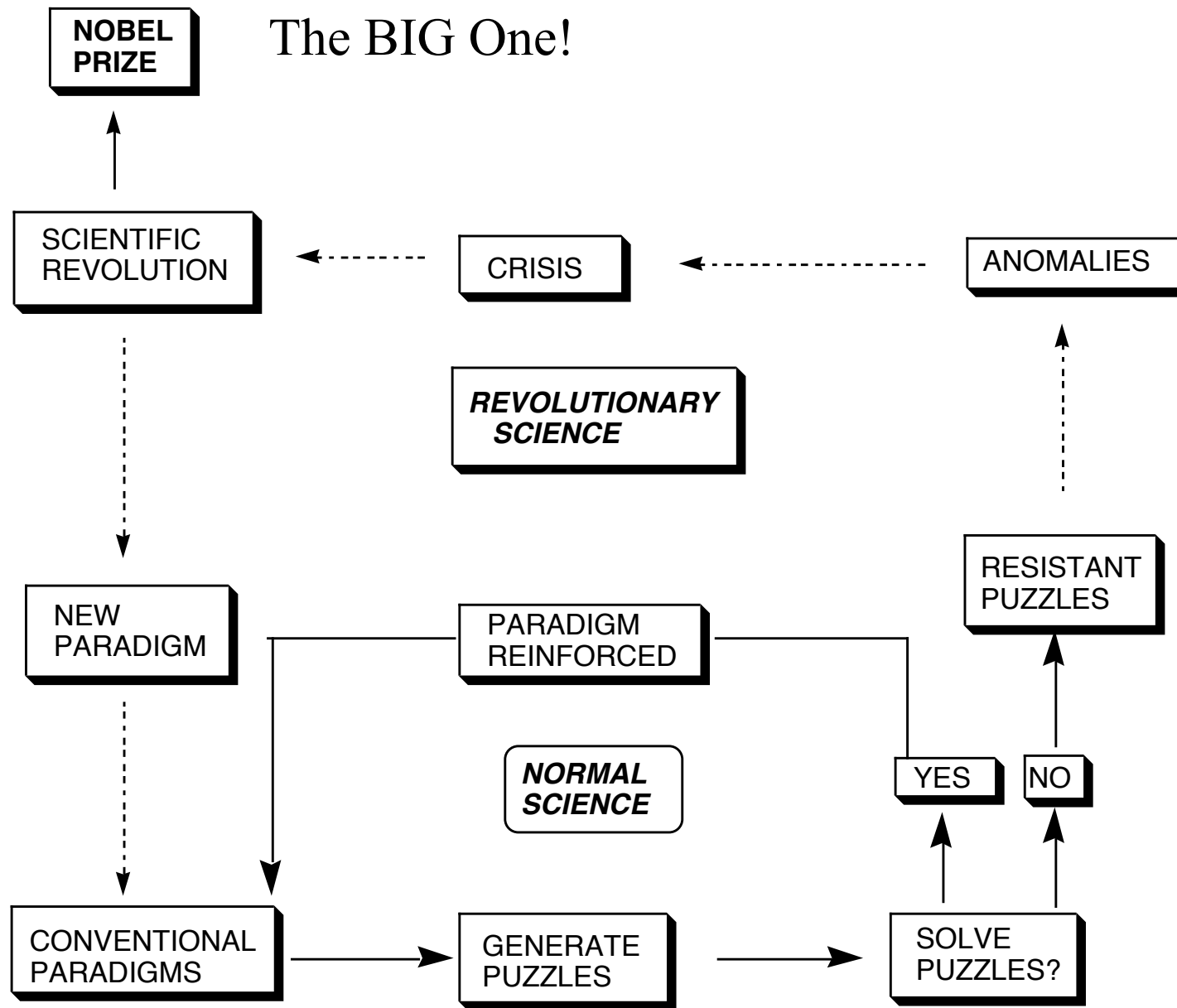
$^1\text{O}_2$ kills cancer cells in irradiated area



Patient cured!

Irradiating babies with jaundice causes a photochemical change that causes the jaundice pigment to become water soluble and to be excreted



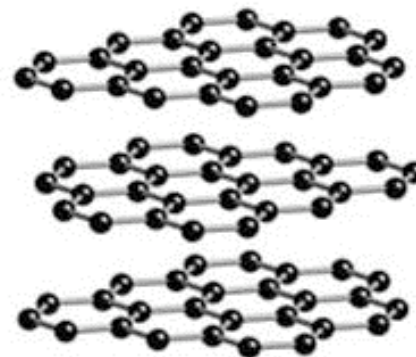


Flow diagram for revolutionary science: Extraordinary claims that become accepted and are integrated into “normal science.”

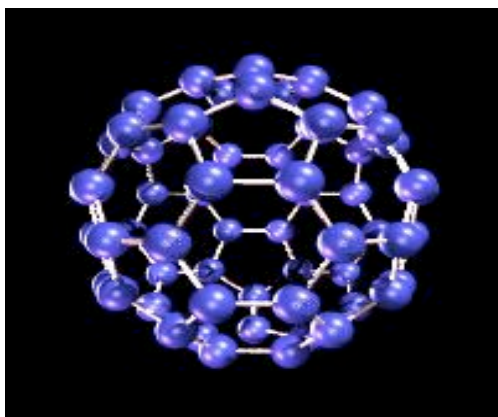
Different forms of elemental carbon: from diamond to graphite to buckyballs!



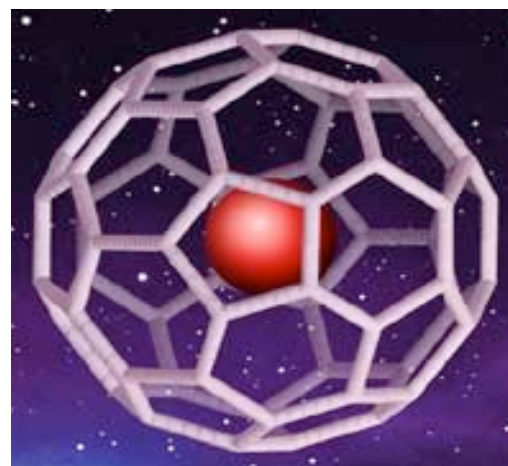
Diamond



Graphite



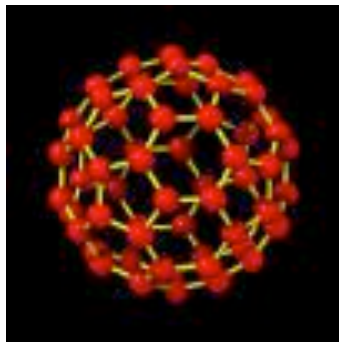
C₆₀



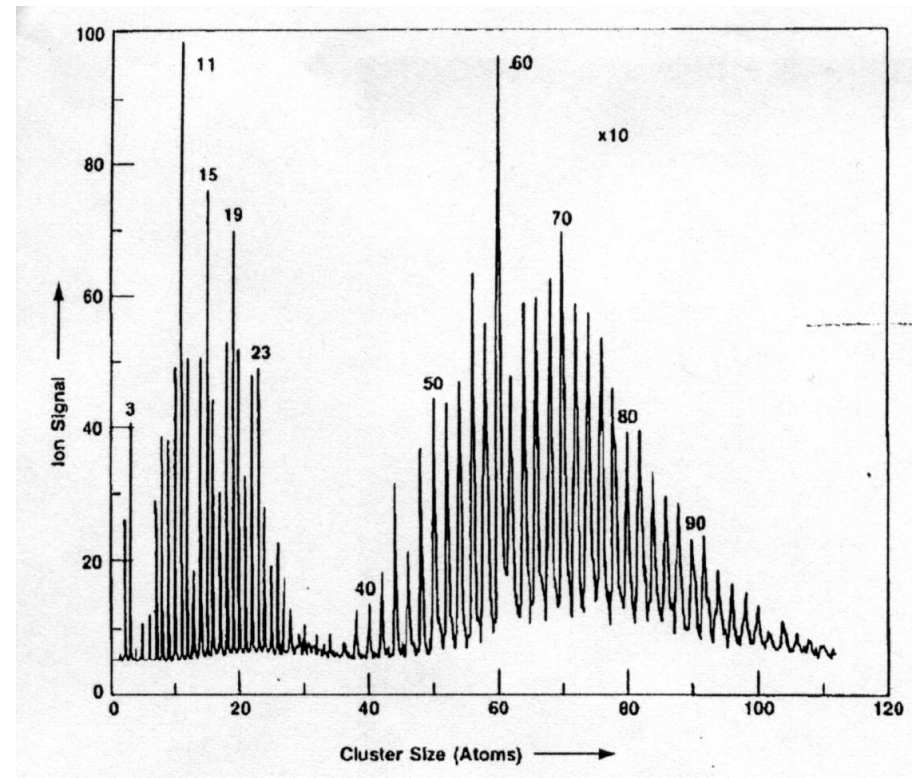
He@C₆₀

An Extraordinary Claim:
Carbon can exist in an
elemental form that has a
structure reminiscent to a
soccer ball.

Discovery of C_{60}
"Buckyballs"
Pathological Science or
Revolutionary Science?



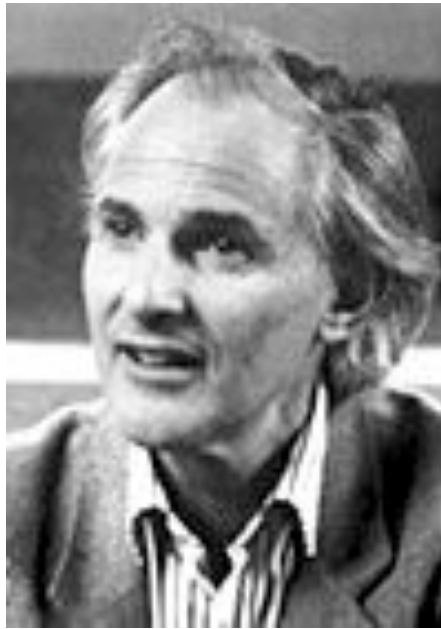
The first "evidence" for
the special stability of
 C_{60}



Would you have predicted a Nobel Prize?



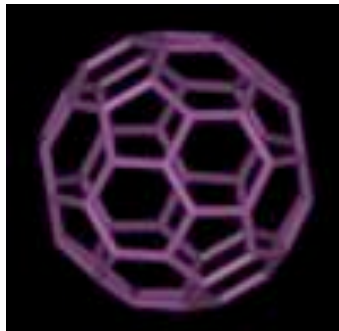
Robert Curl



Harold Kroto



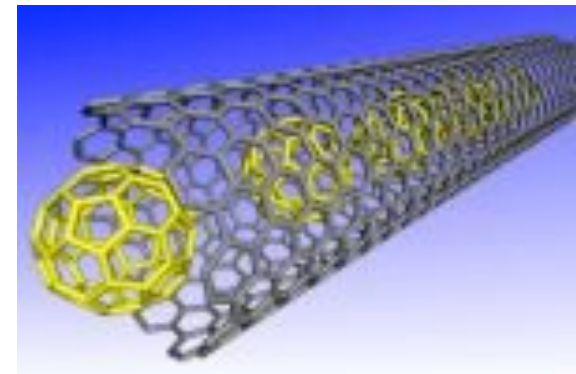
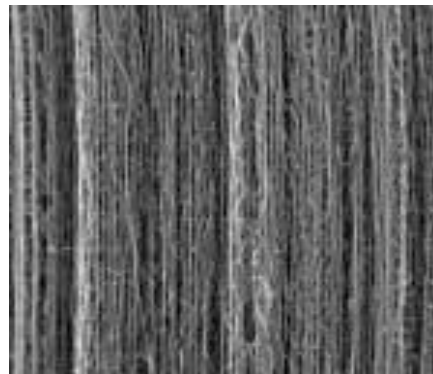
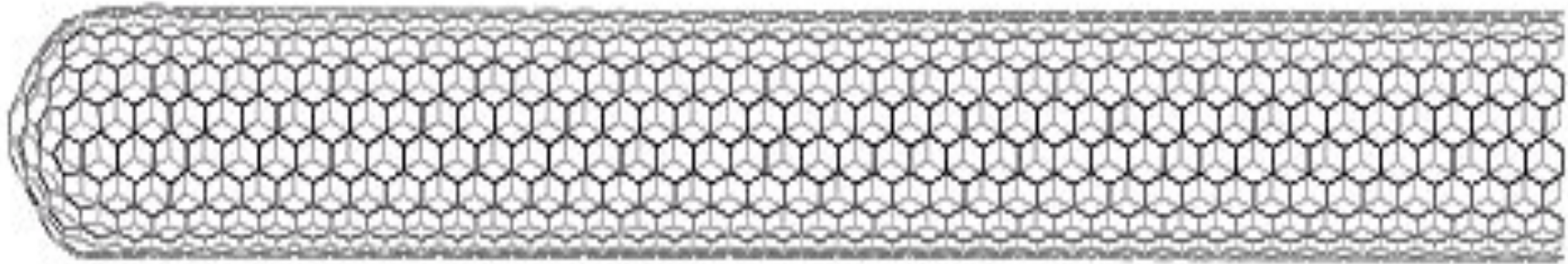
Richard Smalley



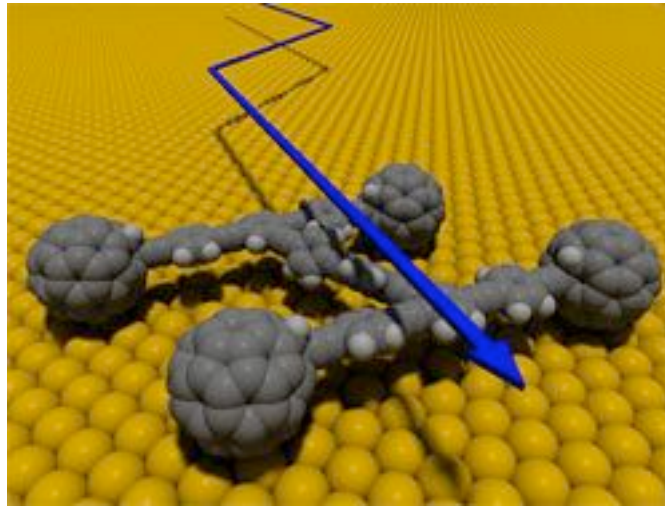
The Nobel Prize in Chemistry 1996
“for the discovery of fullerene”

The proposal of Buckeyballs turned out
to be *revolutionary* science

Buckyballs pulled into nanowires: Carbon nanotubes!



Nanodevices: A carbon nanocar rolling on a gold surface



Thanks to Whitney Zoller

Putting H₂ inside a buckyball!

Open the buckyball, pressure in gaseous H₂, close buckyball!
Professor Koichi Komatsu (Kyoto University)

