

**M5052**  
**CHARACTERIZATION OF MATERIALS AND NANOMATERIALS**  
*Graduate Program in Nanotechnology*

**INTERACTIONS OF LIGHT AND MATTER AND THEIR USE IN  
MATERIALS AND NANOSTRUCTURE ANALYSES**

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The book cover features a close-up photograph of water droplets on a surface, showing a vibrant rainbow of colors through dispersion. To the right of the image, the title "THE ELECTROMAGNETIC SPECTRUM" is written in large, white, sans-serif capital letters. Below it, the subtitle "A Light Introduction to Instrumental Analysis" is written in a smaller, black, sans-serif font, enclosed within a circular gradient graphic that transitions from red at the top to green at the bottom. At the very bottom of the page, the Tec de Monterrey logo and name are repeated, along with the course code "M5052 - Characterization of Materials".

**THE**  
**ELECTROMAGNETIC**  
**SPECTRUM**

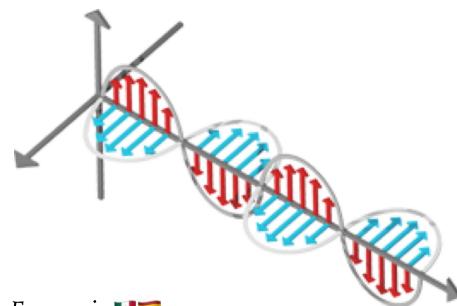
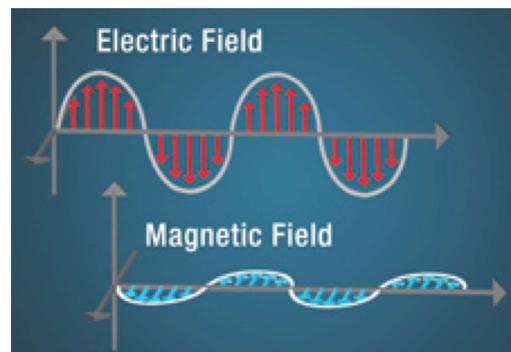
A  
Light  
Introduction  
to  
Instrumental  
Analysis

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# LIGHT IS ELECTRO-MAGNETIC RADIATION

- Light behaves as waves of **electric** and **magnetic** fields
- Both fields oscillate in unison, perpendicular to each other
- Different colors of light correspond to light of different wavelengths ( $\lambda$ , the distance between peaks)
- The speed of light is given by the frequency ( $v$ , in Hertz, 1/s) and the wavelength ( $\lambda$ , in meters)

$$c = v\lambda = 299,792,458 \text{ m/s}$$



Wavelength = Longitud de Onda

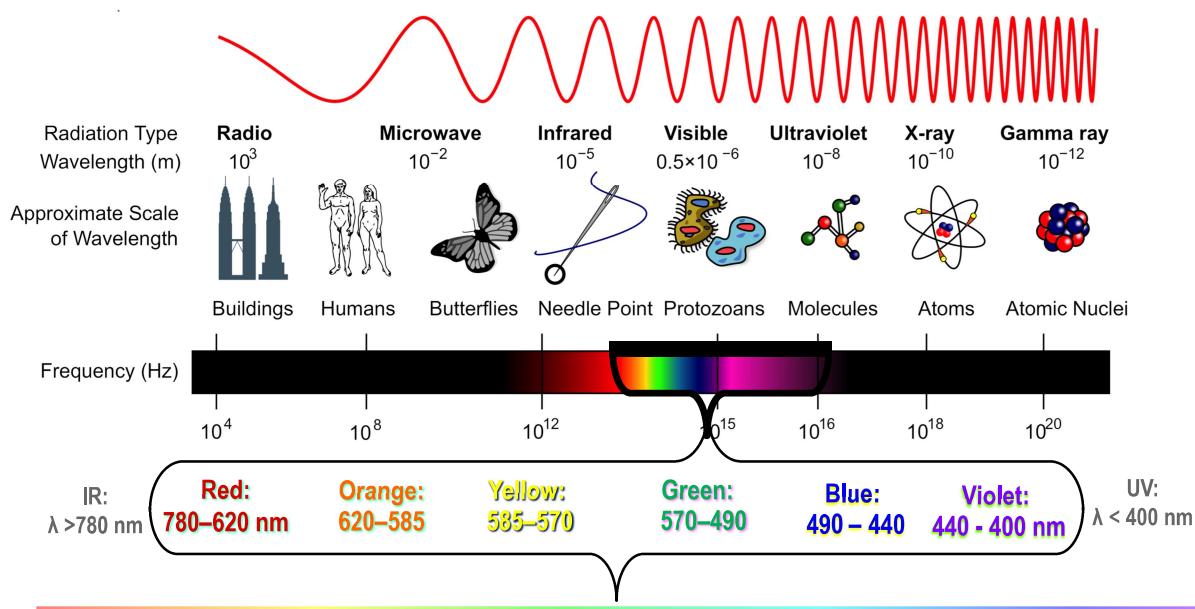
Frequency = Frecuencia



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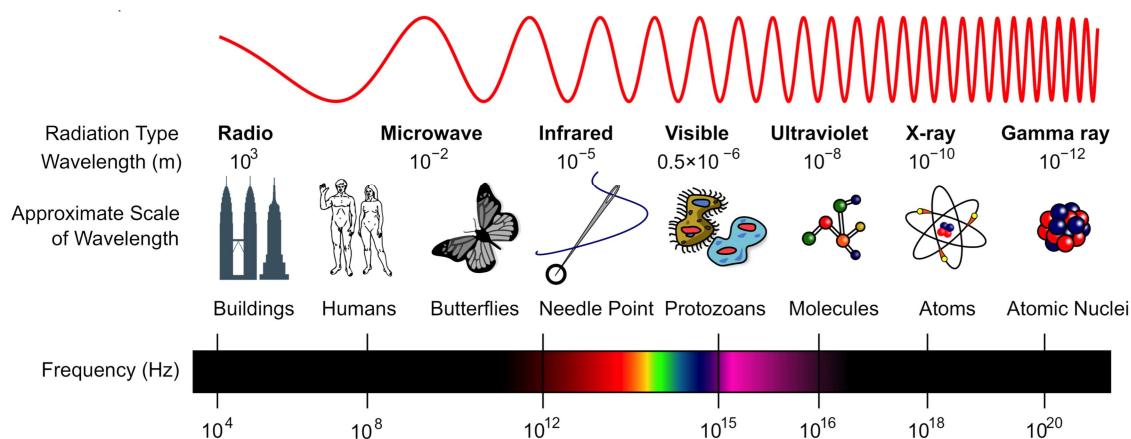
## THE ELECTROMAGNETIC SPECTRUM



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# THE ELECTROMAGNETIC SPECTRUM



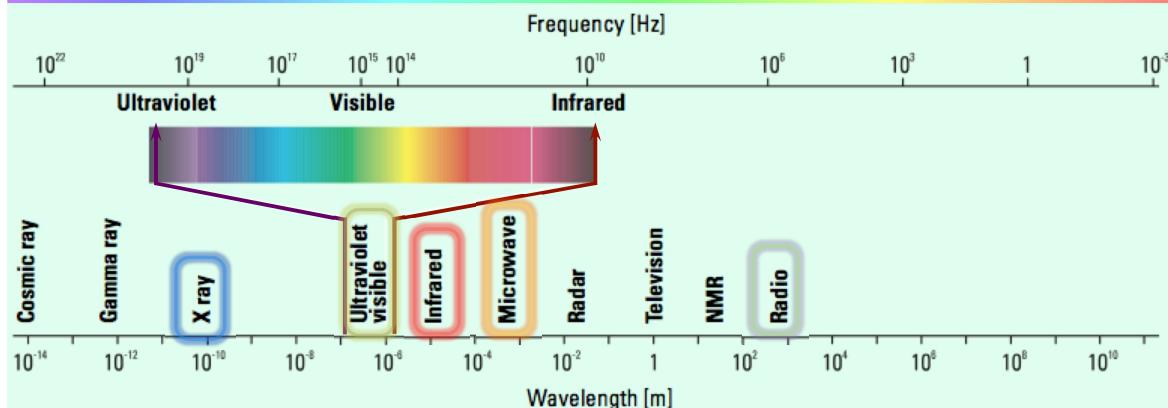
- We can use different regions of the spectrum for different uses.
- We can use instruments to generate and measure light of almost all wavelengths, even those we can not see with our own eyes



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## SOME ANALYTICAL USES OF LIGHT



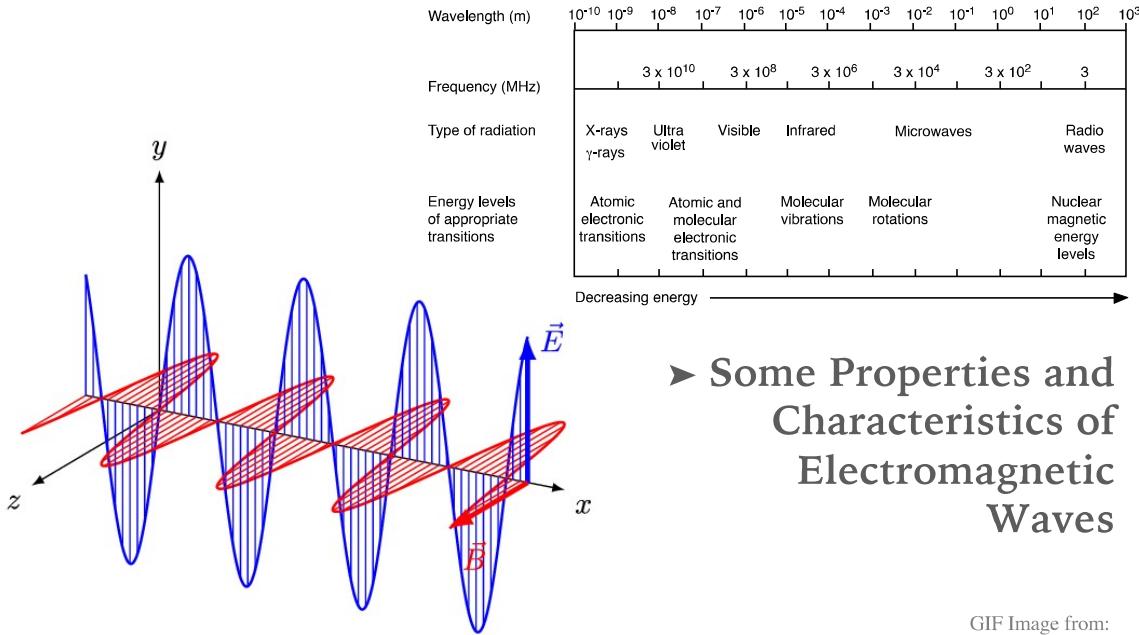
- **X-Rays:** medical imaging, crystal structure of materials by diffraction. Elemental analyses by X-ray Fluorescence (XRF), X-ray Photoelectron Spectroscopy (XPS), Energy/Wavelength Dispersive X-Ray Spectroscopy (EDS/WDS)
- **Ultraviolet-Visible:** spectroscopy for chemical analysis, including clinical analyses, and analysis of nanomaterials
- **Infrared:** Chemical analysis (FTIR)
- Terahertz Spectroscopy: photon frequencies in the region between IR and microwaves have analytical uses that are an active area of development
- **Microwaves:** preparing samples by microwave digestion (also to heat food)
- **Radiofrequency:** Magnetic Resonance Imaging (MRI) and chemical analysis by NMR (Nuclear Magnetic Resonance)



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# THE FACTS OF LIGHT



## ► Some Properties and Characteristics of Electromagnetic Waves

GIF Image from:  
<https://commons.wikimedia.org/wiki/File:EM-Wave.gif>



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## SPEED OF LIGHT IN DIFFERENT MEDIA

- The speed of light is  $299,792,458 \text{ m/s}$  only in vacuum
  - Interaction of the electromagnetic field of radiation with electrons in matter slows light down
  - *This change in speed is responsible for refraction*
  - Wavelength decreases when light enters a medium different than vacuum
  - Frequency is correlated to photon energy and does not change
  - Index of refraction ( $n$ ) is the ratio of the velocity of light in vacuum ( $c$ ) and the velocity of light in the medium ( $v$ )
  - Note: here  $v$  is the latin vee, for velocity, not the greek nu, ( $\nu$ ) used to represent frequency
  - $$n = \frac{c}{v}$$
  - Index of refraction of air is  $n = 1.00027$
- 
- Figure 6-2 Change in wavelength as radiation passes from air into a dense glass and back to air. Note that the wavelength shortens by nearly 200 nm, or more than 30%, as it passes into glass; a reverse change occurs as the radiation again enters air.

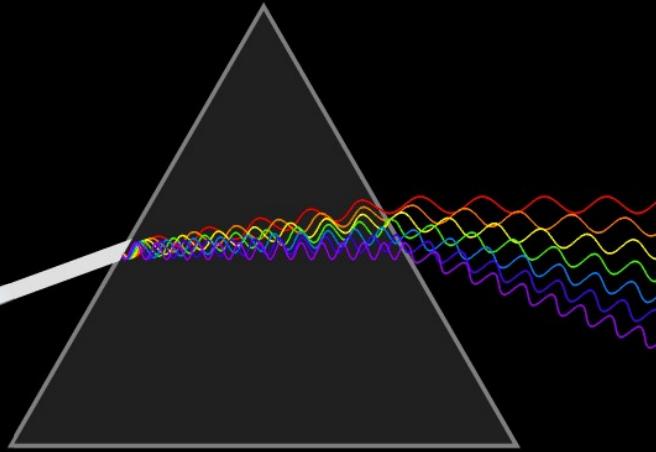


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# REFRACTION DISPERSES LIGHT BY WAVELENGTH

- Shorter wavelengths are slowed down more and are refracted (“bent”) more
- Longer wavelengths are deviated by a smaller angle

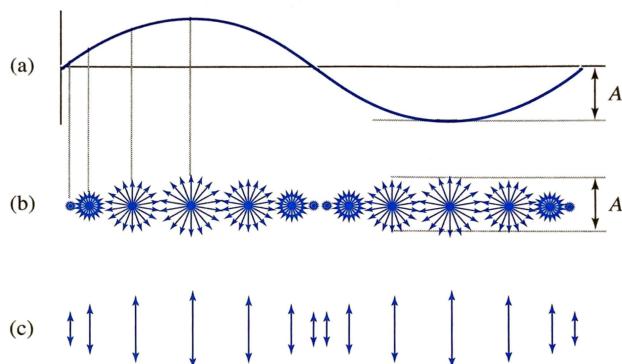


Tecnológico de Monterrey<sup>GIF</sup> Image from: [https://commons.wikimedia.org/wiki/File:Light\\_dispersion\\_conceptual\\_waves.gif](https://commons.wikimedia.org/wiki/File:Light_dispersion_conceptual_waves.gif)

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## POLARIZATION

- Polarized Light
  - The electric field vectors of all photons are aligned in the same direction when light is polarized
  - Most light is unpolarized (direction of the electric vectors of different photons is random)
- Filters can be used to select light polarized in a specific direction or plane
- Some materials can act as intrinsic polarization filters
  - *Dichroic* materials absorb preferentially light polarized in certain directions
- They transmit light of a certain polarization



**FIGURE 6-11** Unpolarized and plane-polarized radiation:  
(a) cross-sectional view of a beam of monochromatic radiation,  
(b) successive end-on view of the radiation in (a) if it is unpolarized,  
(c) successive end-on views of the radiation of (a) if it is plane polarized on the vertical axis.

Figure from Skoog, Holler, Crouch,  
*Principles of Instrumental Analysis*, 7th ed.  
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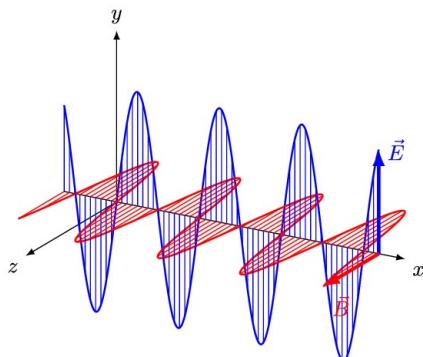
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# LINEAR POLARIZATION

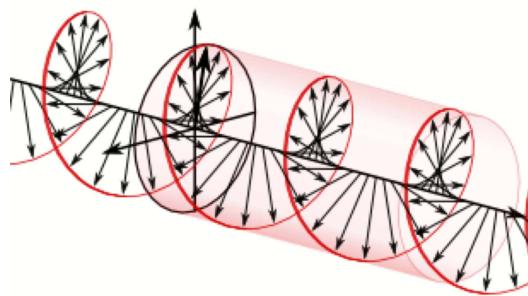
VS.

# CIRCULAR POLARIZATION

- In linear polarization the electric vector of the electromagnetic wave is aligned to a plane



- In circular polarization the electric vector of the electromagnetic wave rotates

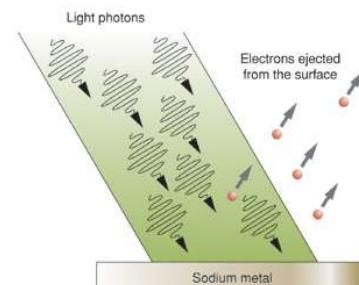


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## WAVE-PARTICLE DUALITY

- Light behaves as a wave, but is composed of individual particles called Photons
- Diffraction is a wave-related phenomenon, but can also be observed for single-photon experiments
- The energy of photons is quantized, all photons of a same frequency have the same energy
- The energy of each photon is given by the frequency ( $\nu$ ) and Planck's constant ( $h$ )
- $E = h\nu = h\frac{c}{\lambda}$
- Photons are particles with spin of 1
- Particles with integer spin (bosons) are not affected by Pauli's exclusion principle
- Quantization of light explains the photoelectric effect
- Einstein won the Nobel Prize in Physics for his work on the photoelectric effect



Photoelectric effect, for each photon (with a minimum energy) one electron is ejected

Image from: [http://www.daviddarling.info/encyclopedia/E/Einstein\\_and\\_photoelectric\\_effect.html](http://www.daviddarling.info/encyclopedia/E/Einstein_and_photoelectric_effect.html)

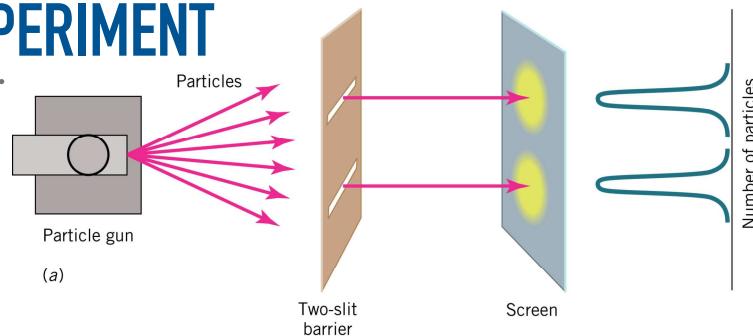


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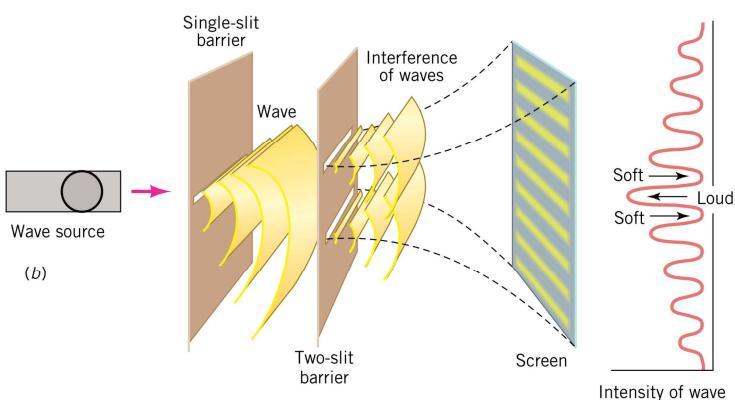
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# DOUBLE SLIT EXPERIMENT

- Classical particles and classical waves behave differently



- Particles go only through one of the two slits
- Waves diffract and show an interference pattern



Images from: <http://www.cas.miamioh.edu/~yarrisjm/S05101incl.html>

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## WAVE-PARTICLE DUALITY: DOUBLE SLIT EXPERIMENT

- Quantum particles can always show wave behavior
- Sending individual photons, one by one, through a double slit results in an interference pattern
- Sending particles with mass (electrons, protons, full atoms, etc.) through a double slit or diffraction grating also produces an interference pattern
- Oscillations at the quantum level can correspond to a “virtual” particle

- NOTE: even large molecules (particles) can behave as waves in certain conditions

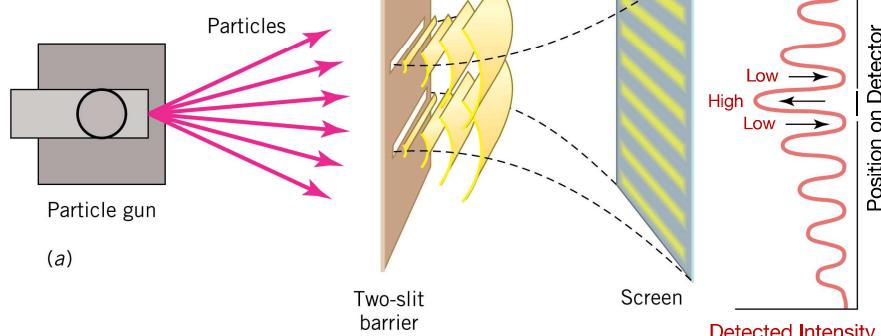


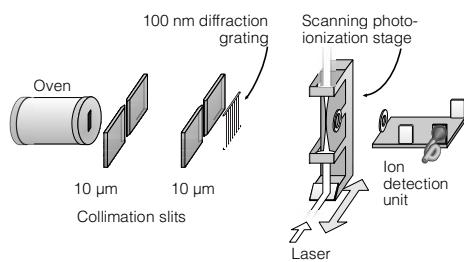
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## Parenthesis:



- Wave-particle duality was shown with a molecular beam of C<sub>60</sub> vapor
- About 1.3x10<sup>6</sup> times heavier than an electron
- Nature 401 (1999) 680-681

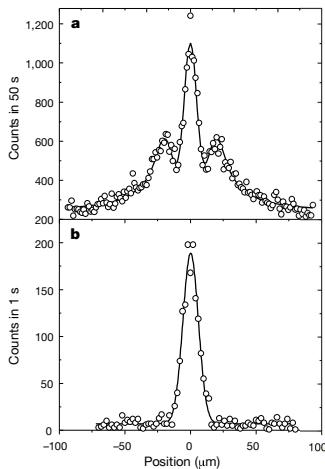
## WAVE-PARTICLE DUALITY WITH A 0.5 NM WIDE MOLECULE

**Figure 1** Diagram of the experimental set-up (not to scale). Hot, neutral C<sub>60</sub> molecules leave the oven through a nozzle of 0.33 mm × 1.3 mm × 0.25 mm (width × height × depth), pass through two collimating slits of 0.01 mm × 5 mm (width × height) separated by 1.04 m, traverse a SiN<sub>x</sub> grating (period 100 nm) 0.1 m after the second slit, and are detected via thermal ionization by a laser 1.25 m behind the grating. The ions are then accelerated and directed towards a conversion electrode. The ejected electrons are subsequently counted by a Channeltron electron multiplier. The laser focus can be reproducibly scanned transversely to the beam with 1-μm resolution.

## letters to nature

### Wave-particle duality of C<sub>60</sub> molecules

Markus Arndt, Olafair Nairz, Julian Vos-Andreae, Claudia Keller, Gerbrand van der Zouw & Anton Zeilinger



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## FREQUENCY AND ENERGY OF PHOTONS

- Speed of light relates frequency and wavelength

$$c = \nu\lambda$$

- Energy of a photon is directly proportional to the frequency

$$E = h\nu$$

- Energy of a mole of photons:

$$E = h\nu N_A$$

- Energy of a photon is inversely proportional to its wavelength

### ► Wavenumber:

$$\bar{\nu} = \nu/c = 1/\lambda$$

- Reciprocal of wavelength in centimeters, units: cm<sup>-1</sup>
- Number of waves in 1 cm
- Directly proportional to energy

Frequency ( $\nu$ ) (Hz)	Wavelength ( $\lambda$ ) (m)	Energy (kJ mol <sup>-1</sup> )
$3.33 \times 10^{14}$	$9.0 \times 10^{-7}$	137.5 (infrared)
$4.29 \times 10^{14}$	$7.0 \times 10^{-7}$	171.2 (red light)
$7.50 \times 10^{14}$	$4.0 \times 10^{-7}$	299.3 (blue light)
$1.58 \times 10^{15}$	$1.9 \times 10^{-7}$	630.5 (ultraviolet)

$c$  = speed of light in vacuum       $h$  = Planck constant

$\nu$  = frequency in Hz (s<sup>-1</sup>)      ( $h = 6.63 \times 10^{-34} \text{ J}\cdot\text{s}$ )

$\lambda$  = wavelength (m)       $N_A$  = Avogadro constant  
( $N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$ )



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# HOW DOES LIGHT INTERACT WITH MATTER?



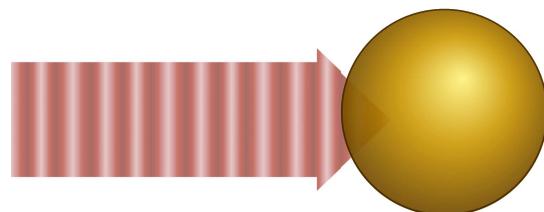
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## INTERACTIONS OF LIGHT WITH MATTER

### ► Absorption

- Absorción  
- Absorbed Light can be re-emitted
- Photoluminescence (light emission after exposure to light)



### ► Fluorescence

- Fast re-emission of absorbed light
- Almost immediate, fluorescence ceases when exciting light is interrupted
- Emitted photons have lower energy
- Lower frequency / Longer wavelength

### ► Phosphorescence

- Slow re-emission of the absorbed light
- Similar to fluorescence but with longer timescales
- Phosphorescence can continue for hours after excitation light is interrupted
- The absorbed light is stored in long-lived excited states of the molecules or atoms



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# INTERACTIONS OF LIGHT WITH MATTER: FLUORESCENCE

- Example: Quantum Dots in Colloidal suspension

- Illuminated with visible light, they absorb different colors



- Illuminated with UV light, Quantum Dots glow in the dark



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## CREATIVE INTERACTIONS OF LIGHT WITH MATTER: FLUORESCENCE

- Example: Decorative vases, in exhibition at the Montreal Museum of Fine Arts

Illumination with white light excites molecules that glow pink or yellow



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## INTERACTIONS OF LIGHT WITH MATTER: PHOSPHORESCENCE

- Examples: Glow in the dark safety signs

- Phosphorescent materials absorb UV and blue light (300-450 nm) and at night, or in a blackout, emit yellow or green light (500-600 nm)

- Emission of phosphorescence can last for more than one hour



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Video taken from <http://uk.everlux.eu/en/videos/detalhes.php?id=49>



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## CREATIVE INTERACTIONS OF LIGHT WITH MATTER:

### PHOSPHORESCENCE

- Example:
- 2017 Canadian silver coin



Image source

[http://www.mint.ca/store/dyn/html/proudlycanadian/  
img/product/160837\\_glow-1198.jpg](http://www.mint.ca/store/dyn/html/proudlycanadian/img/product/160837_glow-1198.jpg)

- “Fireworks” and Canadian flag glow in the dark



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# INTERACTIONS OF LIGHT WITH MATTER

► Absorption

► Reflection

►  Reflexión

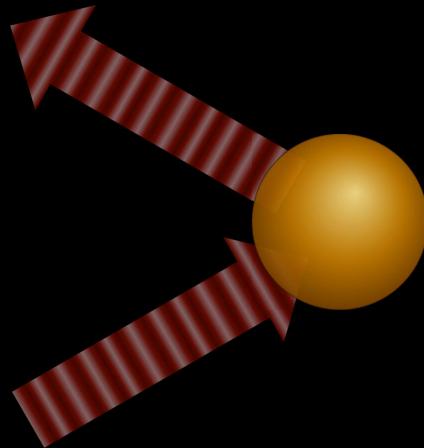


Photo of mirror taken at the Montreal Museum of Fine Arts  
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## WHY DOES LIGHT SEPARATE INTO DIFFERENT COLORS WHEN IT GOES THROUGH WATER DROPLETS?



Niagara Falls Photo © Fernando JRM, usage granted under a CC-BY-NC-SA license



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# INTERACTIONS OF LIGHT WITH MATTER

► Absorption

► Reflection

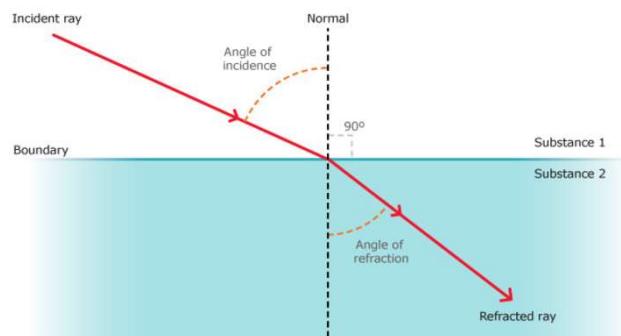
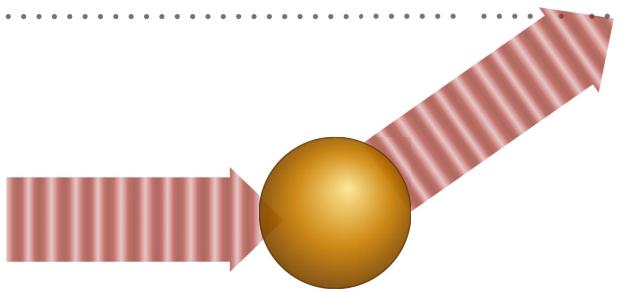
► Refraction

►  *Refracción*

► Change in direction of a beam of light

► Angle of deviation depends on a parameter called *index of refraction*

► Refraction is used to focus light with lenses in microscopes (and cameras)



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Figure taken from  
<https://www.sciencelearn.org.nz/images/49-refraction-of-light-in-water>  
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## INTERACTIONS OF LIGHT WITH MATTER:

### REFRACTION

► Refraction by a prism can separate the colors of white light if the index of refraction is different for different wavelengths

► We can use this phenomenon in spectroscopy

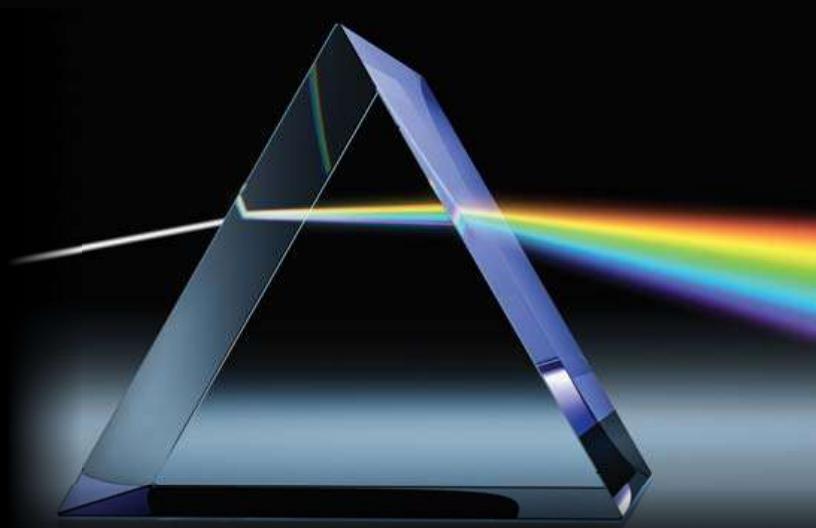


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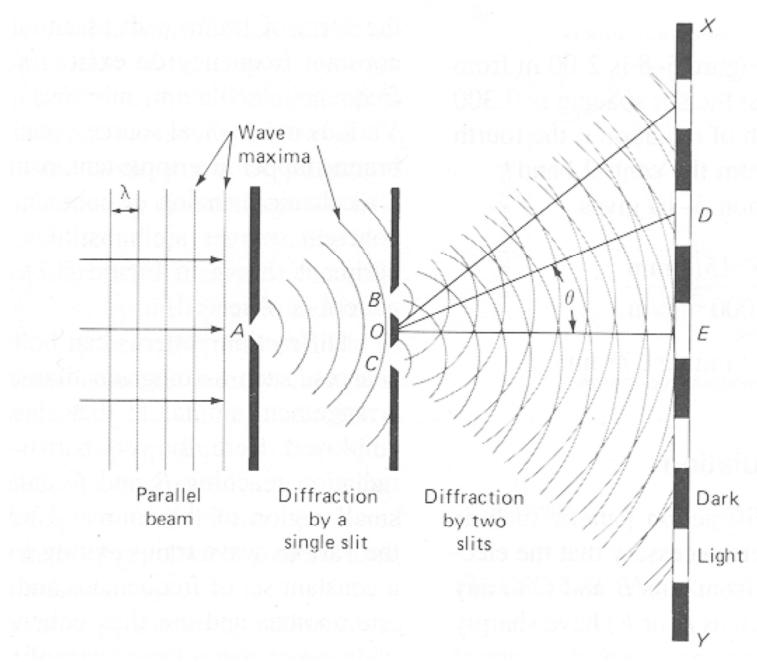


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# INTERACTIONS OF LIGHT WITH MATTER

- Absorption
- Reflection
- Refraction
- **Diffraction**
-  *Difracción*



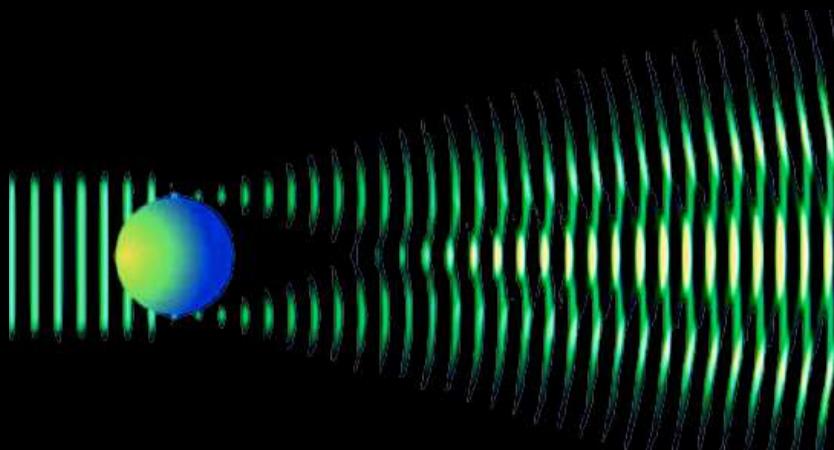
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## INTERACTIONS OF LIGHT WITH MATTER:

### DIFFRACTION

- Constructive and Destructive interference of light results in a pattern of light and dark regions
- Diffraction gratings are used to separate light by wavelength in spectroscopy



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# INTERACTIONS OF LIGHT WITH MATTER: DIFFRACTION

- Examples:
- Compact Disc acts as diffraction grating
- The reflection of a halogen light bulb over the screen of a tablet shows diffraction due to the square grid of pixels on the screen
- Reflection of a laser pointer from the screen of a smartphone or tablet can also show a square diffraction pattern
- The proper angle for diffraction has to be used



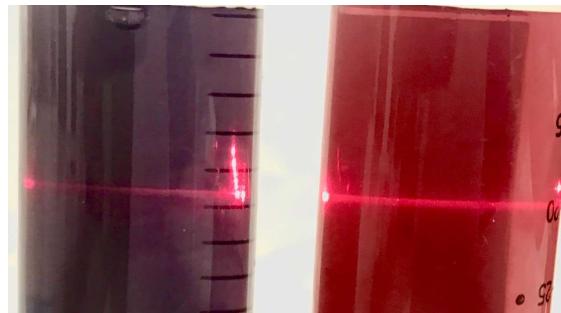
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## WHY IS THE LASER BEAM VISIBLE AS IT GOES THROUGH THE SOLUTIONS IN THESE TUBES?

- A. These are not actually solutions, they are colloidal suspensions of gold nanoparticles dispersed in water

(The difference in color is due only to differences in nanoparticle size changing how they absorb and scatter light)



- Q. Why can you even see the green beam of the “lighthouse of commerce” (*Faro del Comercio*) when it goes through the air in Monterrey?

- A. Because of suspended particles in the air scattering the beam,  
(this photo was taken in a foggy and rainy night, making it even more visible)

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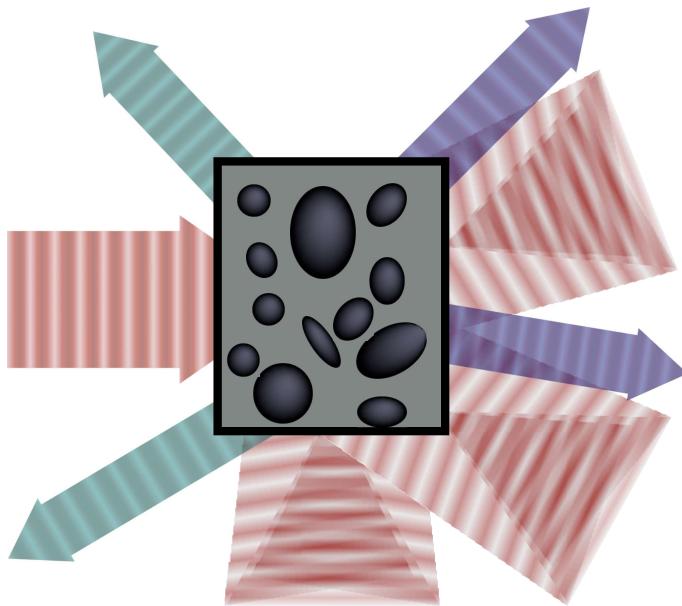


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# LIGHT IS SCATTERED BY INTERACTIONS WITH PARTICLES IN SUSPENSION

- ▶ Scattering has contributions from Absorption, Refraction, Reflection and Diffraction in addition to pure scattering
- ▶ Colloids (e.g. suspended particles in a fluid) are very effective at scattering light
- ▶ Dynamic Light Scattering (DLS) is used to measure nanoparticle sizes

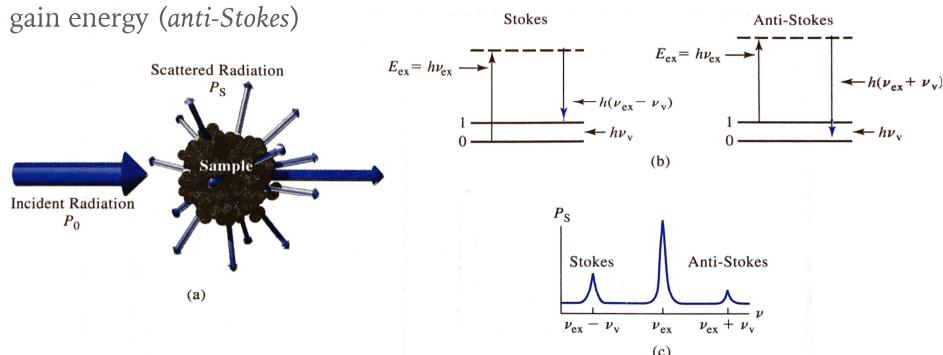


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## INTERACTIONS OF LIGHT WITH MATTER: SCATTERING

- ▶ Photons can keep the same energy when scattered (Rayleigh or Elastic Scattering)
- ▶ Some photons loose energy when being scattered by matter (*Stokes* scattering)
  - ▶ The energy difference is called *shift*
  - ▶ There is a *shift* in the peak position [ES: : desplazamiento en la posición del pico]
- ▶ Other photons gain energy (*anti-Stokes*)



**FIGURE 6-18** Inelastic scattering in Raman spectroscopy. (a) As incident radiation of frequency  $\nu_{ex}$  impinges on the sample, molecules of the sample are excited from one of their ground vibrational states to a higher so-called *virtual state*, indicated by the dashed level in (b). When the molecule relaxes, it may return to the first vibrational state as indicated and emit a photon of energy  $E = h(\nu_{ex} - \nu_v)$  where  $\nu_v$  is the frequency of the vibrational transition. Alternatively, if the molecule is in the first excited vibrational state, it may absorb a quantum of the incident radiation, be excited to the virtual state, and relax back to the ground vibrational state. This process produces an emitted photon of energy  $E = h(\nu_{ex} + \nu_v)$ . In both cases, the emitted radiation differs in frequency from the incident radiation by the vibrational frequency of the molecule  $\nu_v$ . (c) The spectrum resulting from the inelastically scattered radiation shows three peaks: one at  $\nu_{ex} - \nu_v$  (Stokes), a second intense peak at  $\nu_{ex}$  for radiation that is scattered without a frequency change, and a third (anti-Stokes) at  $\nu_{ex} + \nu_v$ . The intensities of the Stokes and anti-Stokes peaks give quantitative information, and the positions of the peaks give qualitative information about the sample molecule.

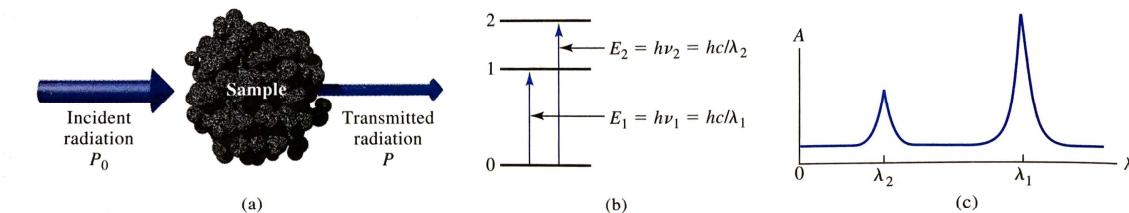


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# INTERACTIONS OF LIGHT WITH MATTER: ABSORPTION

- ▶ Only photons with energy equal to the energy difference between two energy levels of the molecule or atom get absorbed
- ▶ Absorption spectrum is obtained by measuring the power of the transmitted beam relative to the incident beam



**FIGURE 6-16** Absorption methods. Radiation of incident radiant power  $P_0$  can be absorbed by the analyte, resulting in a transmitted beam of lower radiant power  $P$ . For absorption to occur, the energy of the incident beam must correspond to one of the energy differences shown in (b). The resulting absorption spectrum is shown in (c).

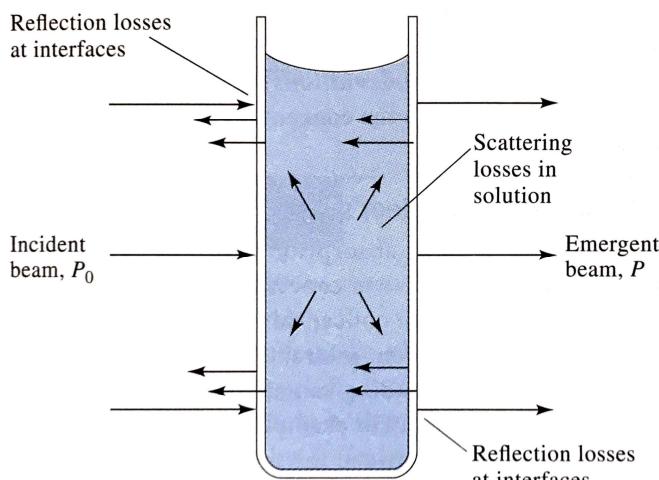
Figure from Skoog, Holler, Crouch, *Principles of Instrumental Analysis*, 7th ed. © Cengage Learning



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# TRANSMISSION



**FIGURE 13-1** Reflection and scattering losses with a solution contained in a typical glass cell. Losses by reflection can occur at all the boundaries that separate the different materials. In this example, the light passes through the air-glass, glass-solution, solution-glass, and glass-air interfaces.

- ▶ Part of the incident light beam passes through without any changes
- ▶ Light that does not get absorbed, reflected or scattered is transmitted
- ▶ **Transmittance:** ratio between the power of the incident beam and the emergent beam
  - ▶  $T = P/P_0$
- ▶ Even in the absence of an analyte, intensity will be lower due to losses by reflection at interfaces and scattering from the container
- ▶ **Important to calibrate with a blank**

Figure from Skoog, Holler, Crouch, *Principles of Instrumental Analysis*, 7th ed. © Cengage Learning

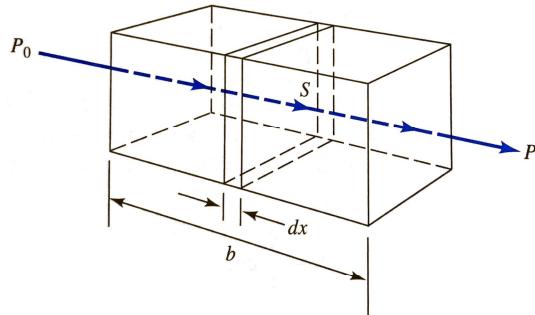


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# BEER-LAMBERT LAW: $A = \epsilon bc$

- Absorbance ( $A$ ) is proportional to concentration and path length
- The proportionality constant ( $\epsilon$  or  $a$ ) is called the absorptivity
- When concentration is expressed in units of mol/L  $\epsilon$  is called the molar absorptivity
- Molar Attenuation Coefficient is the IUPAC recommended term for molar absorptivity
  - *It has also been called "molar extinction coefficient"*
  - *"Extinction" refers to proportion of incident photons that do not reach the detector*
    - Other interactions of light and matter beyond absorption contribute to "extinction"



**FIGURE 13-2** Radiation of initial radiant power  $P_0$  is attenuated to transmitted power  $P$  by a solution containing  $c$  moles per liter of absorbing solution with a path length of  $b$  centimeters.

- For many spectroscopic measurements a sample cell with a standard path length of 1 cm is used

*Other standardized path lengths are available*



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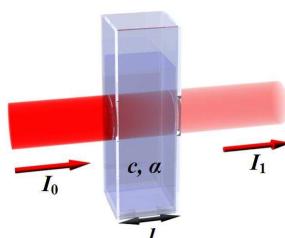
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## QUANTIFICATION IN SPECTROPHOTOMETRY

## BEER LAW

- Absorbance is proportional to concentration and path length
  - $\epsilon$  : molar absorptivity (molar attenuation coefficient)  
Units:  $L/mol \cdot cm [=] mol^{-1} \cdot dm^{-3} \cdot cm^{-1}$
  - $c$  : concentration of the absorbing chemical species ( $M$ ,  $mol/L [=] mol \cdot dm^{-3}$ )
  - $b$  : path length, distance the light travels through the sample ( $l, cm$ )
  - $\lambda_{max}$  : wavelength of maximum absorption, the one used to measure absorbance
    - Linear relation of absorbance to  $\epsilon$  means that peak of maximum absorption gives better sensitivity for quantification
  - Due to exponential relation of absorbance to transmittance: maximum absorbance in instruments is usually 4
    - This corresponds to 0.0001 transmittance
    - Dilution to absorbance below 3 is common for quantification

$$A = \epsilon bc$$



$$A = -\log_{10} T$$

$$A = \log_{10} \frac{P_0}{P}$$

Image taken from: [https://sk.wikipedia.org/wiki/S%C5%BDbor:Lambert-Beerov\\_z%C3%A1kon.png](https://sk.wikipedia.org/wiki/S%C5%BDbor:Lambert-Beerov_z%C3%A1kon.png)

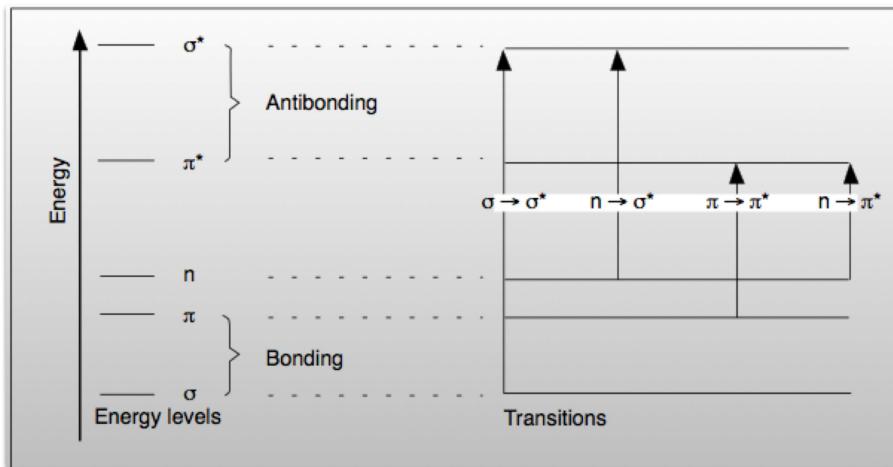


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# ABSORPTION OF PHOTONS WITH ATOMS AND MOLECULES

- Many phenomena used in analysis depend on the quantization of light
  - Wave-Particle Duality
- Energy of a beam of light is quantized (photons)
- Each photon has a specific energy dependent on the wavelength of its corresponding wave
- Absorption of light/photon with specific energy lead to electron transitions between quantized energy levels of atoms/molecules
  - Electron absorbs a photon and “jumps” to a higher energy level
  - Electron emits a photon when it jumps back to a lower level

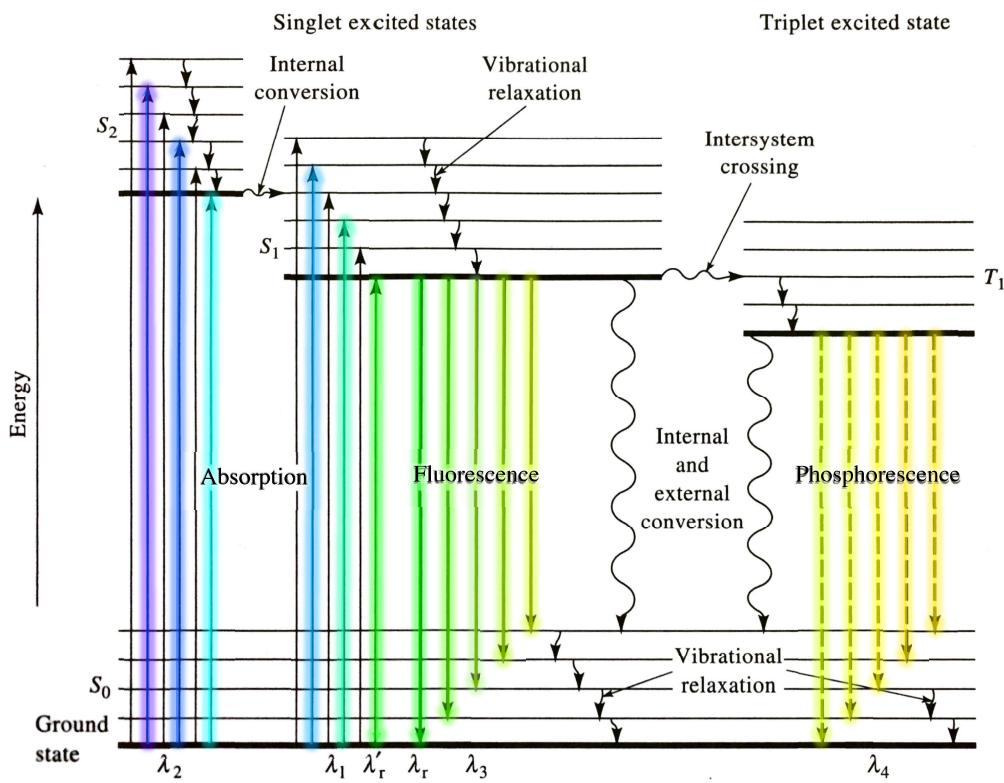


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## PARTIAL ENERGY DIAGRAM FOR A PHOTOLUMINESCENT SYSTEM

Modified from: D.A. Skoog, F.J. Holler, T.A. Nieman  
“Principles of Instrumental Analysis”, 5th Edition,  
Orlando, Florida : Harcourt Brace College Publishers, 1998.



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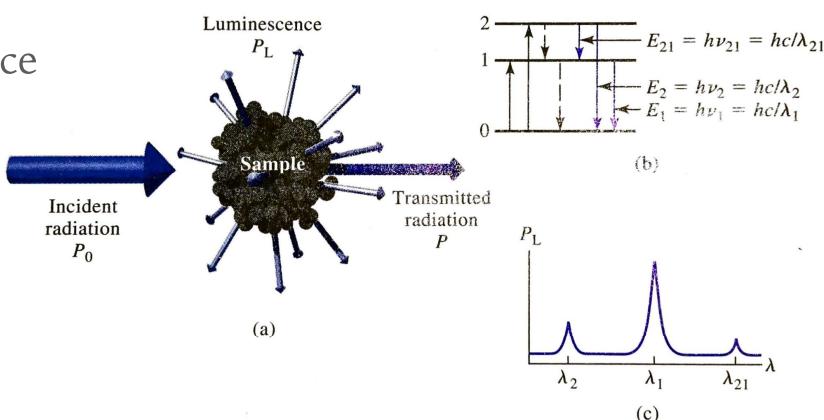
# INTERACTIONS OF LIGHT WITH MATTER: PHOTOLUMINESCENCE

►ES: :

*Fotoluminiscencia*

► Excitation source is light

- Photo-luminescence signal is usually collected at 90° from the incident beam



**FIGURE 6-17** Photoluminescence methods (fluorescence and phosphorescence). Fluorescence and phosphorescence result from absorption of electromagnetic radiation and then dissipation of the energy emission of radiation (a). In (b), the absorption can cause excitation of the analyte to state 1 or state 2. Once excited, the excess energy can be lost by emission of a photon (luminescence, shown as solid line) or by nonradiative processes (dashed lines). The emission occurs over all angles, and the wavelengths emitted (c) correspond to energy differences between levels. The major distinction between fluorescence and phosphorescence is the time scale of emission, with fluorescence being prompt and phosphorescence being delayed.

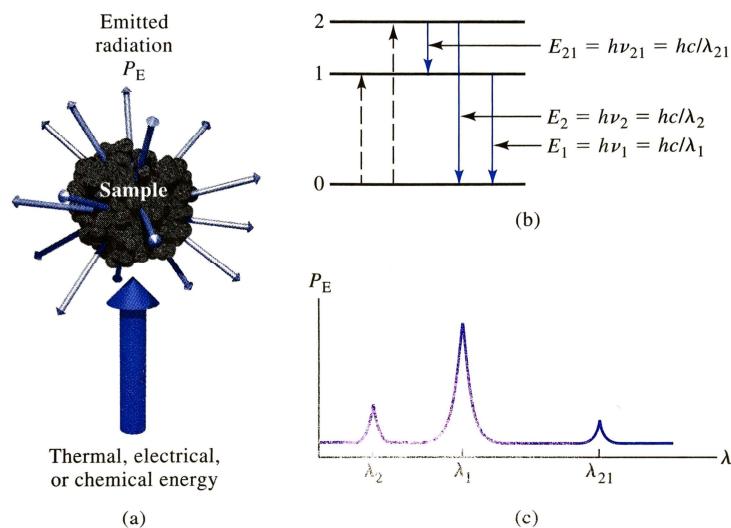
Figure from Skoog, Holler, Crouch, *Principles of Instrumental Analysis*, 7th ed. © Cengage Learning

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# INTERACTIONS OF LIGHT WITH MATTER: EMISSION

- Atoms, molecules, or nanoparticles, can emit light if their electrons are excited to a higher energy level
- Light is emitted as electrons "jump" from the excited states to the ground level
- Ground state: the lowest energy state of a quantum mechanical system
- ES: : *Estado Fundamental, Estado Basal*



**FIGURE 6-15** Emission or chemiluminescence processes. In (a), the sample is excited by the application of thermal, electrical, or chemical energy. These processes do not involve radiant energy and are hence called nonradiative processes. In the energy level diagram (b), the dashed black lines with upward-pointing arrows symbolize these nonradiative excitation processes, while the solid colored lines with downward-pointing arrows indicate that the analyte loses its energy by emission of a photon. In (c), the resulting spectrum is shown as a measurement of the radiant power emitted  $P_E$  as a function of wavelength,  $\lambda$ .

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# THERMAL EMISSION OF LIGHT

- Quartz tube in a tube furnace (at 800 °C in the photo shown) glows red hot
- Incandescent light bulbs emit light due to electric heating of a resistance

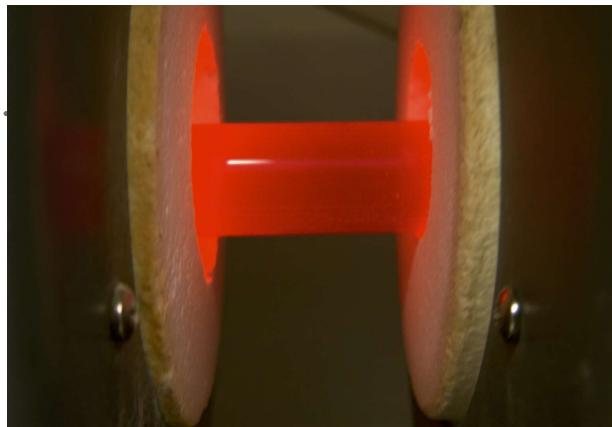


Photo of red hot quartz tube © Fernando JRM,  
usage granted under a CC-BY-NC-SA license



Photo of incandescent lamp taken from:  
<https://www.amazon.de/Globe-125-Edison-Vintage-Lampe/dp/B00SLR9780>



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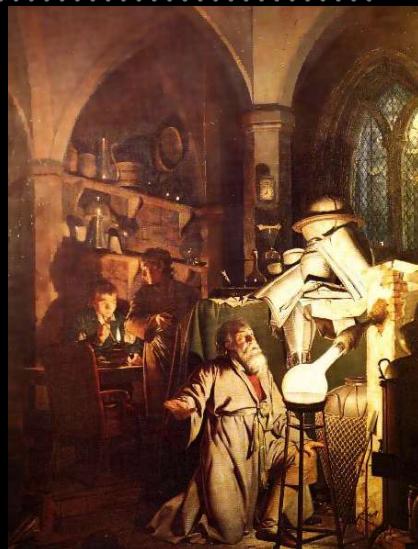
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## INTERACTIONS OF LIGHT WITH MATTER: EMISSION

- Chemiluminescence
  - When a reaction produces a molecule in an excited state the molecule releases the excess energy as light
- Bioluminescence:
  - When the reaction is made by a living being



Firefly photo from  
[http://www.alexanderwild.com/  
Insects/Stories/Fireflies/](http://www.alexanderwild.com/Insects/Stories/Fireflies/)



*Painting representing the Discovery of Phosphorus: elemental phosphorus undergoes a chemiluminescent reaction (oxidation forms transient species HPO and P<sub>2</sub>O<sub>2</sub>)*

Image taken from:  
<https://en.wikipedia.org/wiki/File:JosephWright-Alchemist.jpg>



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© Alex Wild  
[alexanderwild.com](http://alexanderwild.com)

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# USING THE INTERACTIONS OF LIGHT AND MATTER FOR INSTRUMENTAL ANALYSIS

- If a substance/material absorbs, diffracts, refracts, scatters, or emits light we can use that for analysis
- Absorption:
  - e.g. Atomic Absorption, UV-vis, Infrared
- Diffraction:
  - X-Ray Diffraction
  - Diffraction gratings for wavelength selection
- Scattering:
  - Raman spectroscopy, Dynamic Light Scattering
- Emission:
  - e.g. Atomic Emission, Fluorescence, Phosphorescence, X-Ray Spectroscopy (EDS, WDS)
- Refraction
  - Index of refraction can help identify substances, or measure concentration (e.g. of sugars)
  - Differences in index of refraction can be used to enhance contrast in microscopy
  - Lenses focus light due to refraction



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.. THE METHODS AND TECHNIQUES OF INSTRUMENTAL ANALYSIS ARE AN ESSENTIAL PART OF  
THE CHARACTERIZATION “TOOL BOX” OF MATERIALS SCIENCE AND NANOSCIENCE



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# DIFFERENT ANALYTICAL TOOLS SERVE DIFFERENT PURPOSES



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## MICROSCOPY TECHNIQUES

- Microscopy: Observation at the microscale, below the resolving power of human eyes
- Complement and extend composition analyses
  - Micro-Raman, micro-FTIR, use spectrometers in combination with an optical microscope
    - Can be used to map compositions
  - Optical Microscopy
    - Use of visible light for imaging
    - “Advanced” Optical Microscopy
      - Variations based on fluorescence or other physical phenomena to go below the diffraction limit and increase resolution
      - Advanced optical microscopy methods are called “Nanoscopy”
- Electron Microscopy (TEM/SEM)
  - Scanning Electron Microscopy SEM allows imaging surfaces with nanometer resolution
  - High Resolution Transmission Electron Microscopy (HRTEM) can provide atomic resolution
- Scanning Probe Microscopies:
  - AFM, STM, etc.
  - Both can reach atomic resolution
- Electron and probe microscopies together with advanced optical microscopies are essential for nanostructure characterization



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# SELECTING AN ANALYTICAL METHOD

- Define the problem
  - Which Type of Sample?
  - How Much sample is available?
  - How Many samples have to be analyzed?
  - What is the concentration range of the analyte?
  - Which sample components can interfere?
  - What are the physical and chemical properties of the sample matrix?
  - What methods are available?
  - What types of data need to be acquired?
  - What information can be gained by each of the available methods?
  - What are the detection limits?
- What is the desired accuracy?
- What are the achievable accuracy and precision?
- How can (or should) the sample be processed/handled before the analysis?
- Who can do the analysis?
- Is there a person qualified to use the equipment and/or with knowledge of the technique?
- And who can analyze the data?
- What is the cost?
- And how much can you pay?
- What are the consequences of a mistake?
- Both false positives and false negatives can have serious consequences

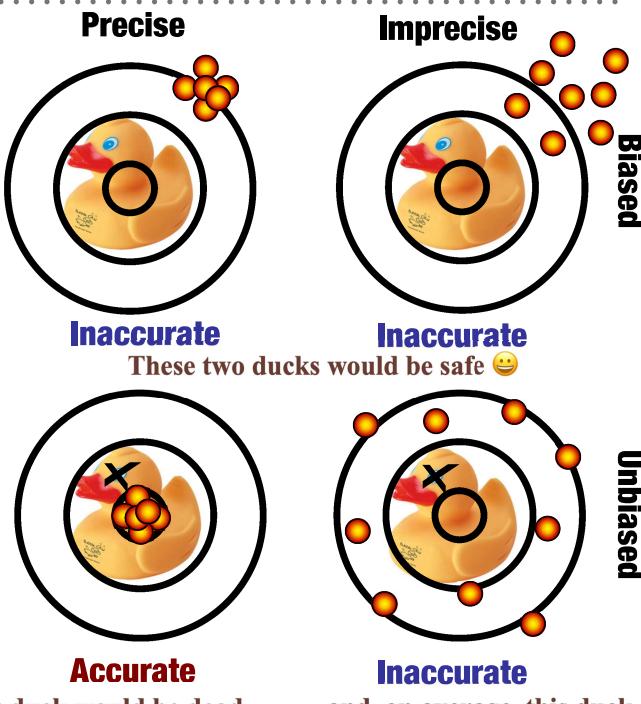


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## ACCURACY VS. PRECISION

- “Precision”
  - ( Precisión)
  - Reproducibility
- “Accuracy”
  - ( Exactitud)
  - Agreement with real value
- “Bias”
  - ( Sesgo)
  - Systematic error
  - All measurements are skewed, averaging will not remove bias
    - Calibration is necessary
- Random Error
  - Aleatory, not biased
  - With random error average of measurements can be close to the actual value
  - Repeated measurements are unavoidable



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