CHEM2100J
Chemistry
Autumn 2024

Chapter 01
Atomic Theory

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Atomic Theory Overview

The goal of this chapter is to help you understand the reason why we need a theory of the "small-world" and the successes of quantum mechanics.

We will see how classical Newtonian mechanics failed, meaning we needed a new type of physics.

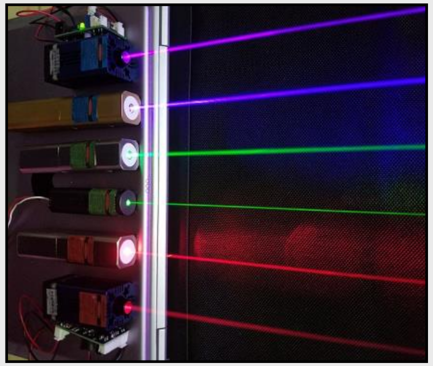
We will see experiments showing how photons and electrons can behave as both waves and particles.

The ultimate success of quantum mechanics was its explanation of the wave–particle nature of matter.

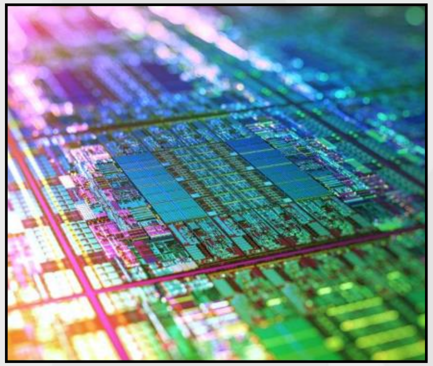
Applications of Quantum Mechanical Theory

Quantum mechanical theory helped bring about the discovery of many important technologies.

Quantum mechanics tells us how to predict or handle small objects like electrons and photons.



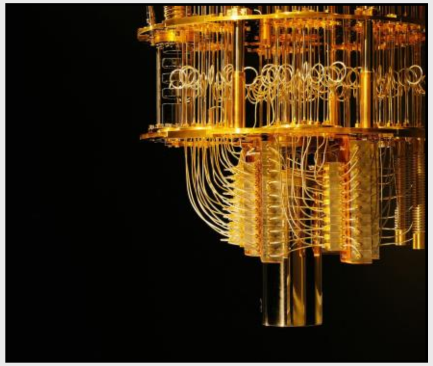
Lasers



Transistors (radios, televisions, and computers)

Solar panels

LCD, LED, OLED

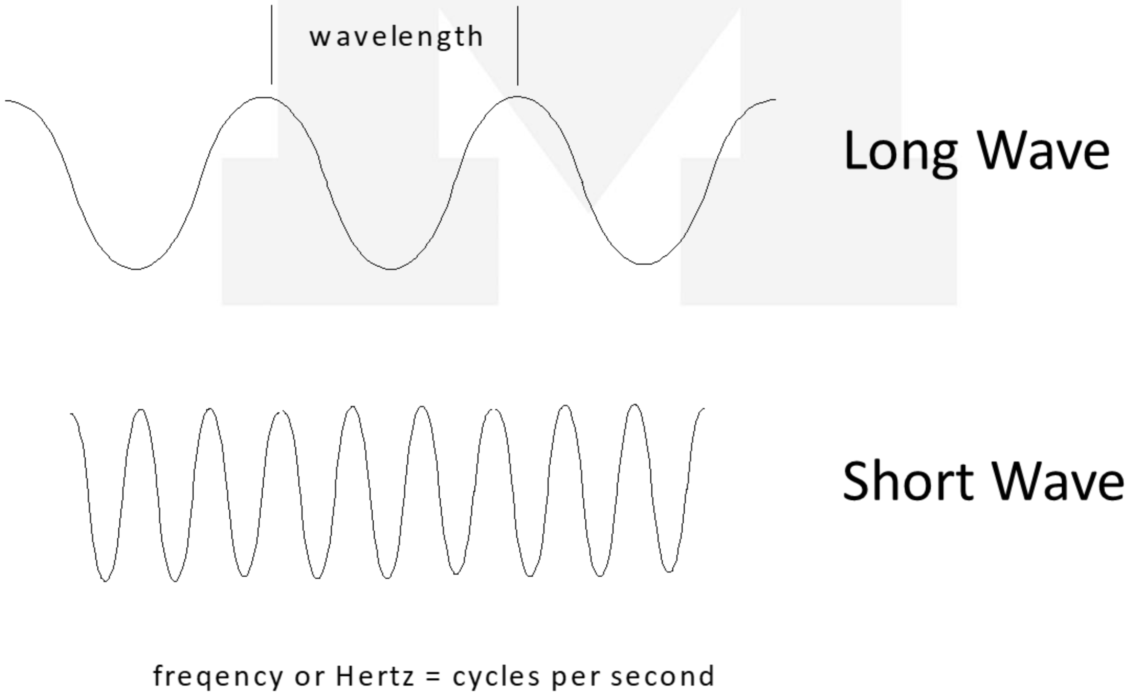


Quantum computers

https://en.wikipedia.org/wiki/Laser#/media/File:Lasers.JPG
https://www.samtec.com/industries/computer-semiconductor/
https://3dprintingindustry.com/wp-content/uploads/2020/03/IBMs-quantum-computer-one-of-the-first-quantum-computers-developed.-Photo-via-IBM.jpg
http://www.nzxsolar.com/
https://cdn.arstechnica.net/wp-content/uploads/2016/12/GettyImages-612898744.jpg

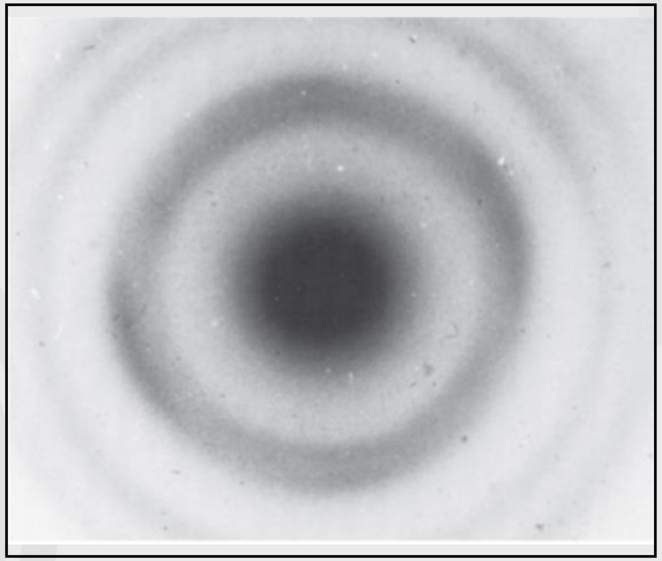
Photons as Waves

One property of a photon is that it acts like a **wave** (proven by both Faraday and Maxwell in the 1850s). Each gave us new sets of equations unrelated to Newtonian physics.



Photons as Waves

Evidence of the **wave** nature of light, diffraction patterns showing interference patterns from a **single-slit** experiment



Created by nickel atoms spaced 250 pm apart

A drop of water sends out ripples across the surface.

Blue water droplet by Adrian von der Hoh

Photons as Waves

Evidence of the **wave** nature of light, diffraction patterns showing interference patterns from a **closely spaced slits** experiment:

It shows that photons are at "certain," predictable locations.

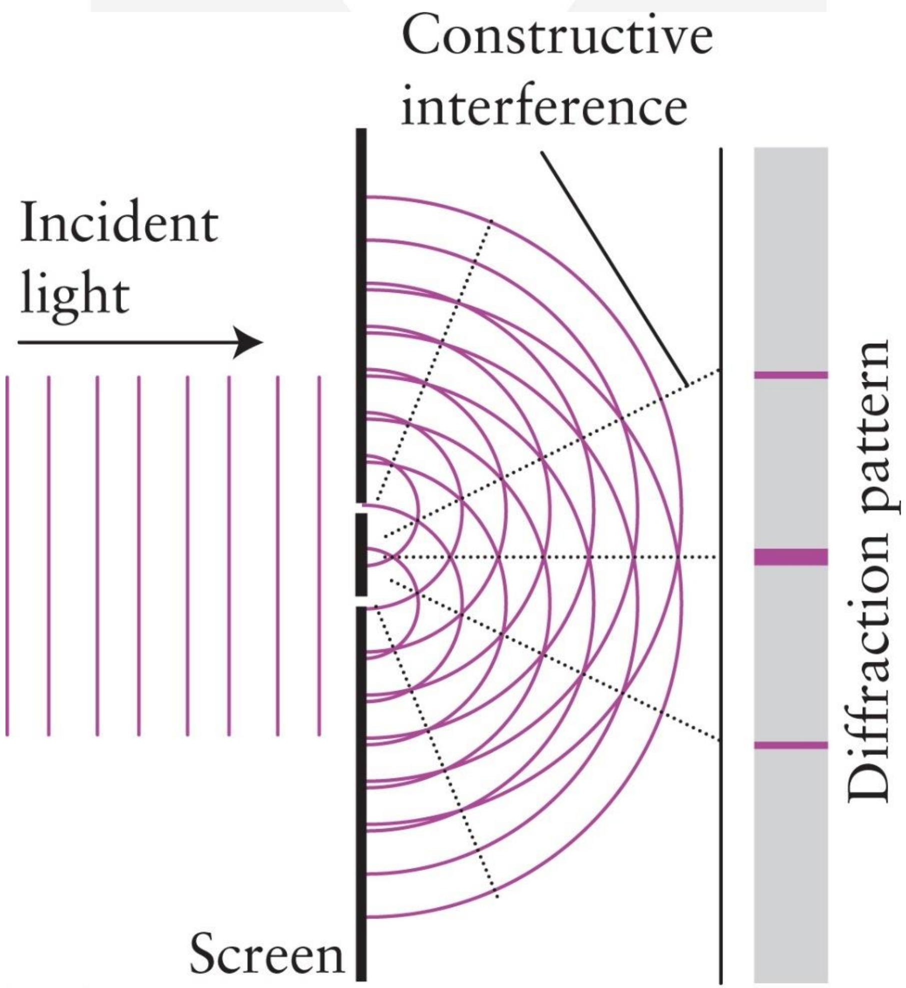


Figure 1B.8
Atkins, *Chemical Principles: The Quest for Insight*, 7e
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Electromagnetic Waves

Snapshot of an electromagnetic wave traveling at $3.00{\times}10^{8}\ \mathrm{m{\cdot}s^{-1}}$

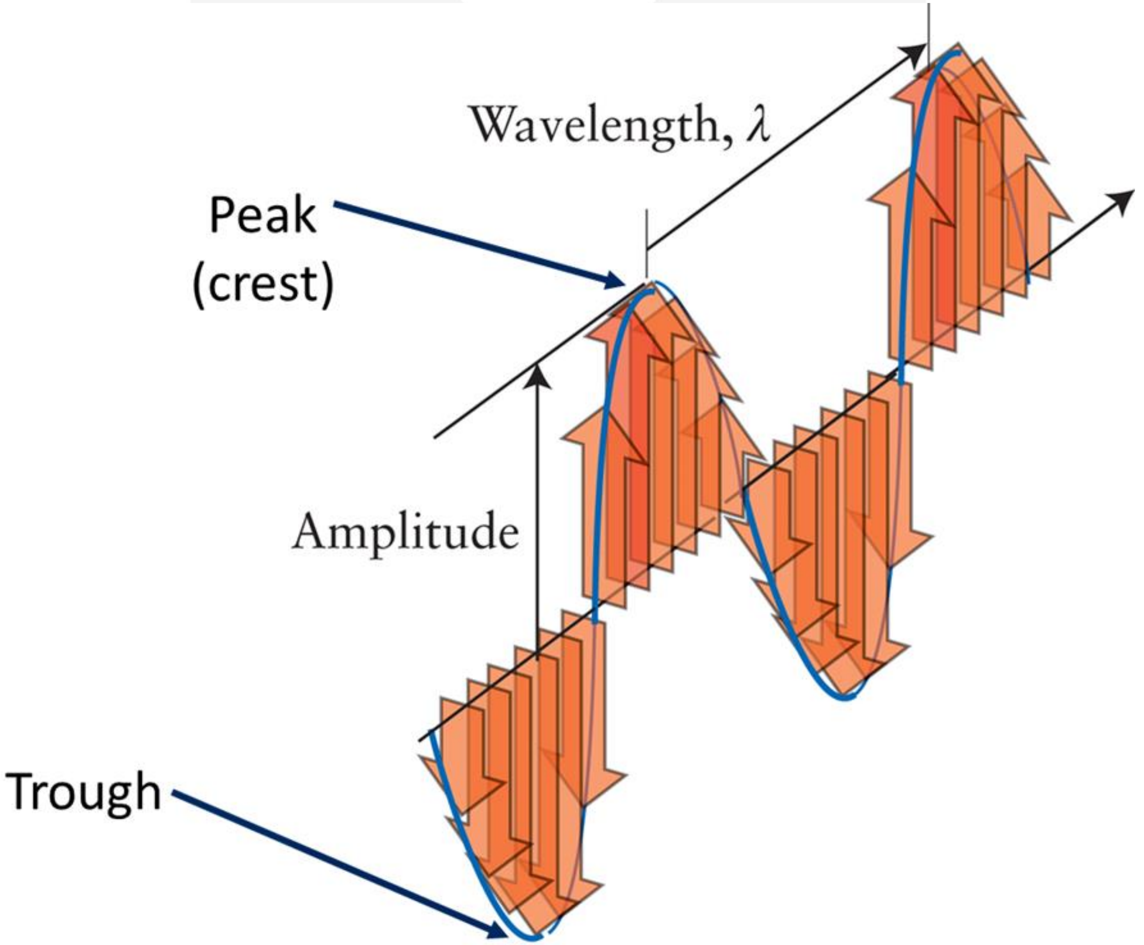

Figure 1A.7
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Wavelength and Frequency

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Radiation Type	Frequency / 10^{14} Hz (s^{-1})	Wavelength / nm	Energy per Photon / 10^{-19} J
X-rays and γ-rays	$\geq 10^3$	≤ 3	$\geq 10^3$
Ultraviolet	8.6	350	5.7
Visible light			
Violet	7.1	420	4.7
Blue	6.4	470	4.2
Green	5.7	530	3.8
Yellow	5.2	580	3.4
Orange	4.8	620	3.2
Red	4.3	700	2.8
Infrared	3.0	1000	2.0
Microwaves and radio waves	$\leq 10^{-3}$	$\geq 3\times 10^6$	$\leq 10^{-3}$

$$\lambda \nu = c$$

wavelength × frequency = speed of light

Short Quiz

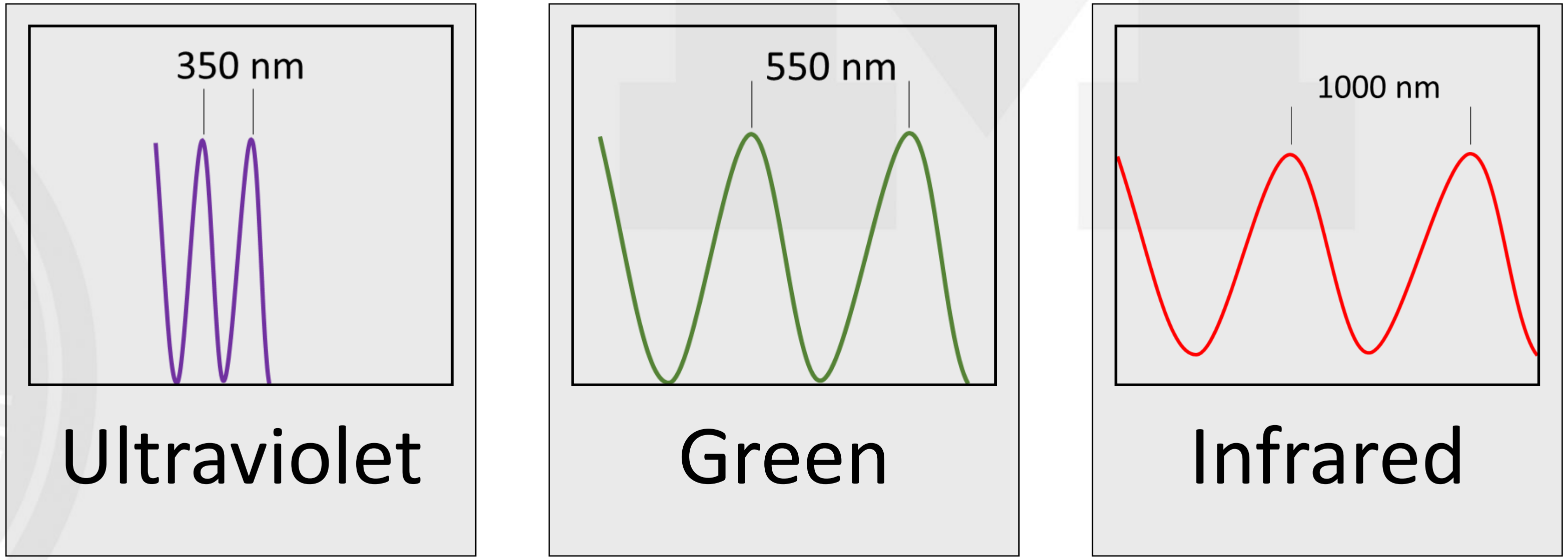
In one second, which of these photons would have the highest frequency, ν?

A. Ultraviolet (shortest wavelength)

B. Green light (medium wavelength)

C. Infrared (longest wavelength)

D. They all are all the same.



Since $\lambda\nu = c$, then $\nu = \frac{c}{\lambda}$, so for an ultraviolet photon:

$$\nu = \frac{3.00\times10^{8}\ \mathrm{m{\cdot}s^{-1}}}{3.5\times10^{-7}\ \mathrm{m}} = 8.5 \times 10^{14}\ \mathrm{s^{-1}}$$

Short Quiz

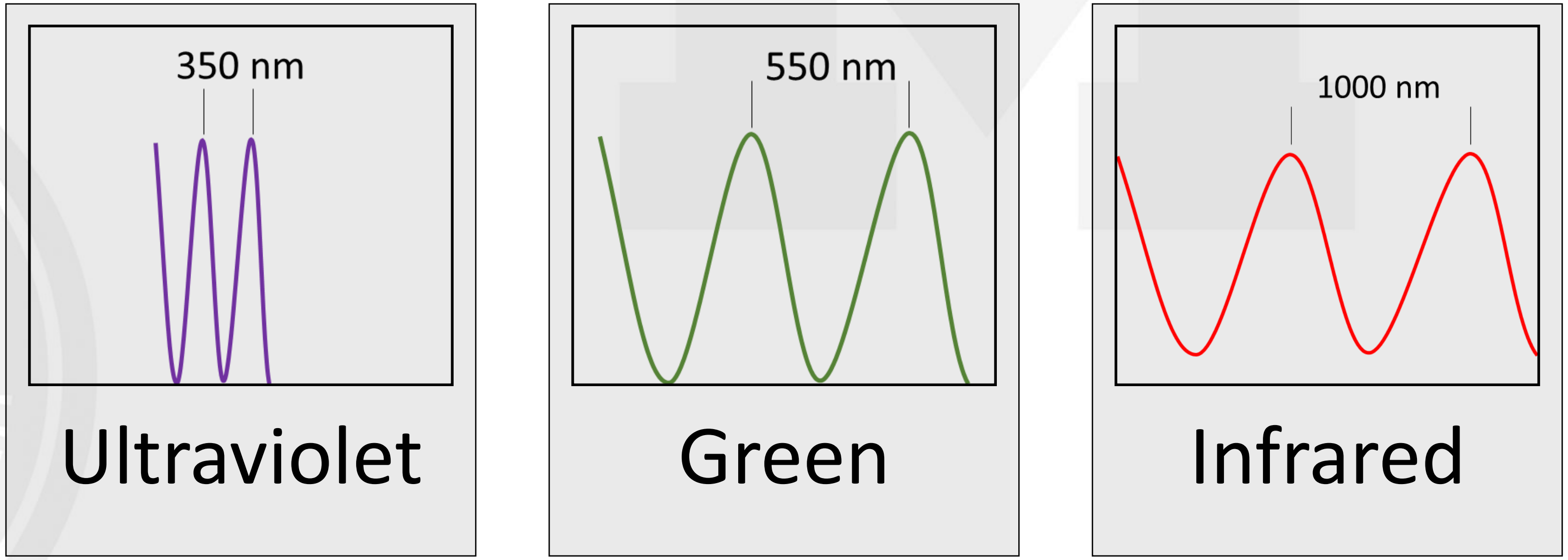
Which type of photon travels the fastest in a vacuum according to $\lambda\nu = c$?

A. Ultraviolet

B. Green light

C. Infrared

D. They all travel at the same speed.



They all travel at the same speed in a vacuum, 3.00×10^{8} m·s^{-1}.

Electromagnetic Spectrum

What is the wavelength of the signal from a radio station transmitting at 98.4 MHz?

$$\lambda = \frac{c}{\nu} = \frac{3.00 \times 10^{8}\ \mathrm{m \cdot s^{-1}}}{9.84 \times 10^{7}\ \mathrm{s^{-1}}} = 3.05\ \mathrm{m}$$

Calculate the wavelength of 5.75×10^{14} Hz.

$$\lambda = \frac{3.00 \times 10^{8}\ \mathrm{m \cdot s^{-1}}}{5.75 \times 10^{14}\ \mathrm{s^{-1}}} = 522\ \mathrm{nm}$$

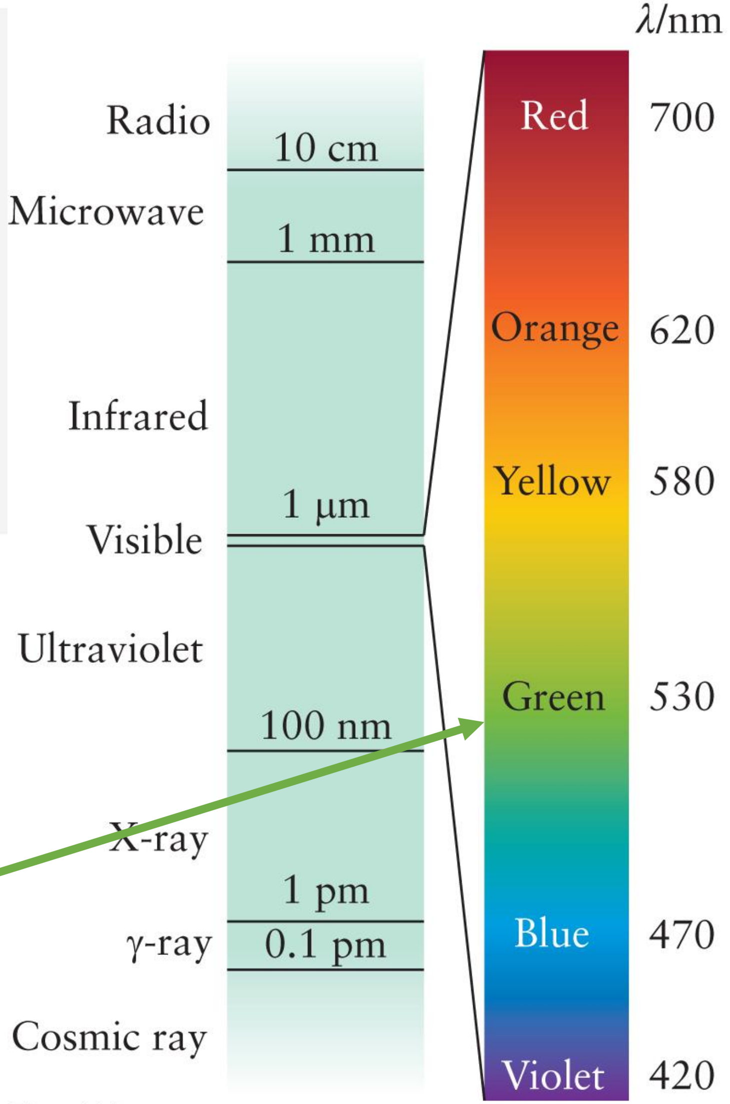


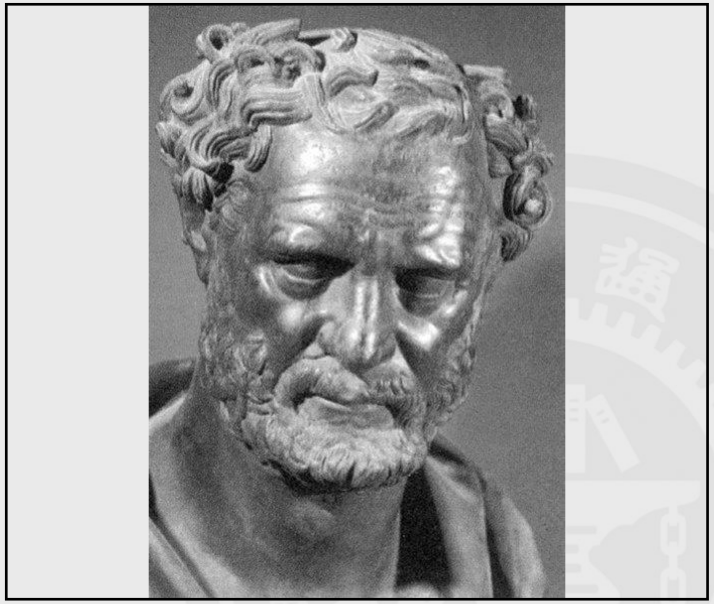
Figure 1A.9
Atkins, *Chemical Principles: The Quest for Insight*, 7e

The Atomic Nucleus

Once electromagnetic wave mechanics was mastered, scientists turned their attention to studying radioactive decay.

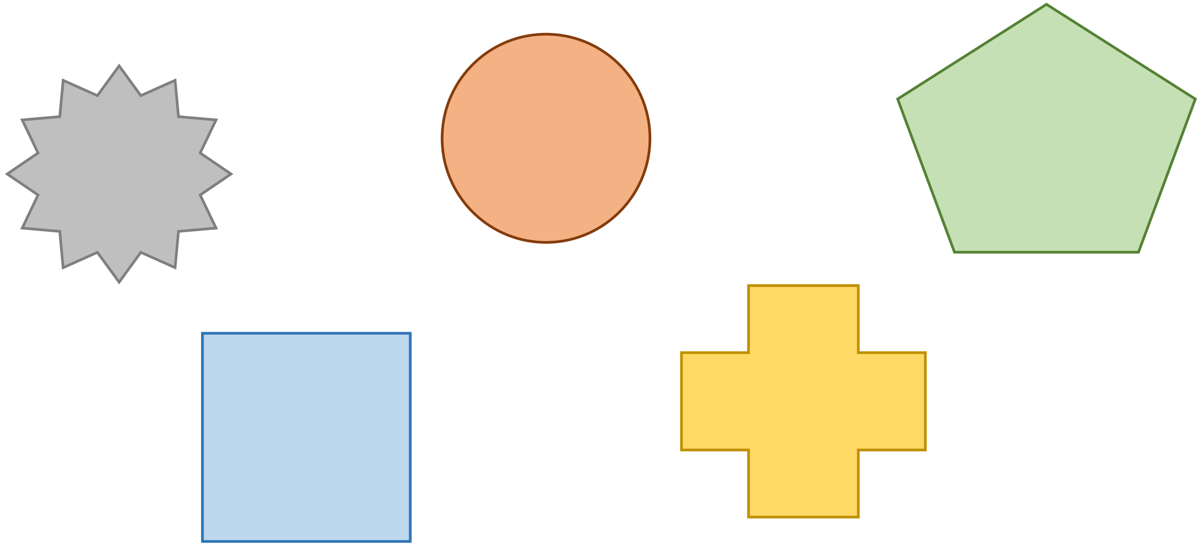
Next, we see how the nucleus of the atom was found.

The Atomic Model



Democritus
~400 BCE

Matter consists of indivisible building blocks, the "atomos". Each matter is built from different atomos with different shapes. The shapes influence the properties, e.g., sharp atomos make things sour, round atomos sweet, and metals are made from hard atomos.

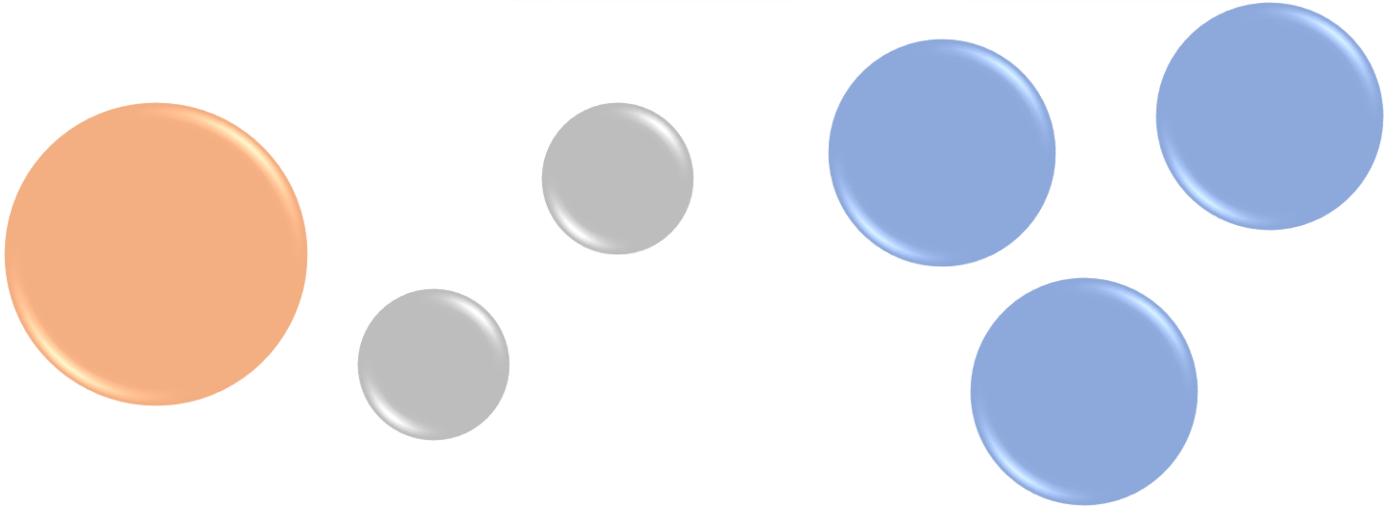


https://www.enciklopedija.hr/natuknica.aspx?id=14519

The Atomic Model

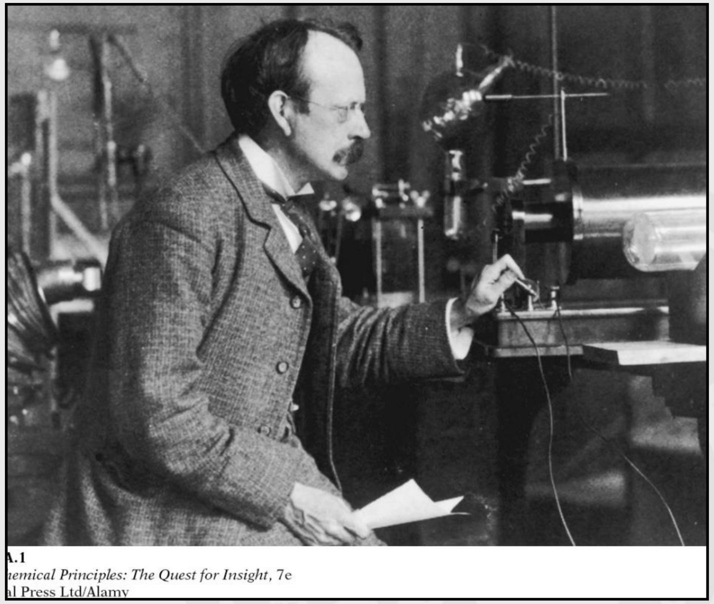
John Dalton
~1800

Each chemical element consists of a specific type of atom. These are hard spheres and cannot be altered or destroyed by chemical means. They can form compounds and react with each other in set proportions.



https://www.universetoday.com/38169/john-daltons-atomic-model/

The Atomic Model



J. J. Thomson
1897

In 1897, British physicist **J. J. Thomson** provided the earliest evidence that atoms had **internal structure**.

Thomson was able to measure the value of $\frac{-e}{m_e}$, the ratio of an electron's charge $-e$ to its mass m_e.

cathode rays

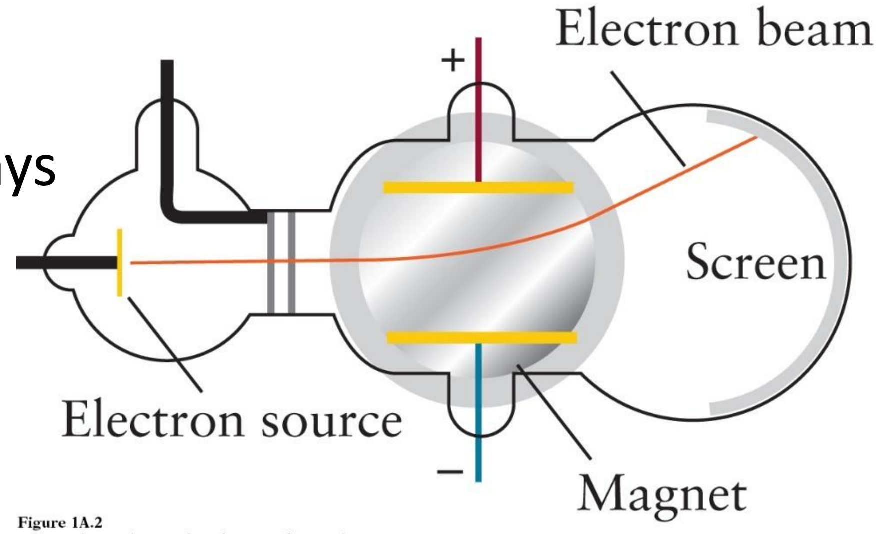


Figure 1A.2
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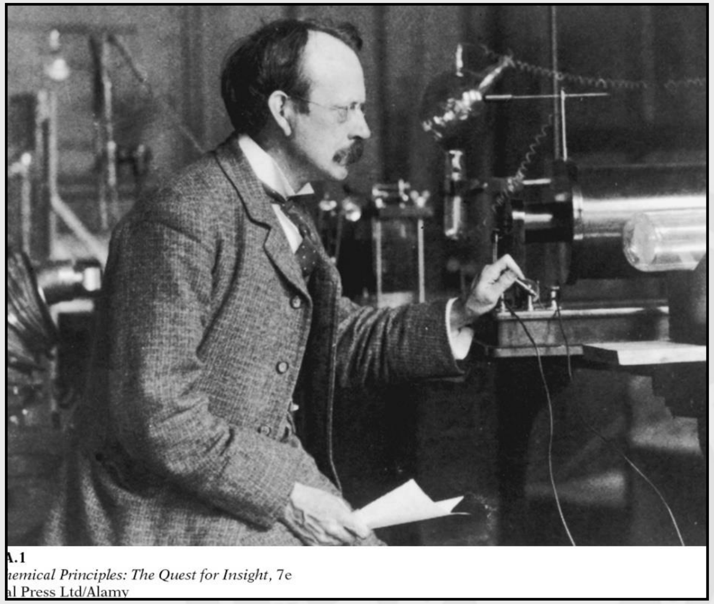
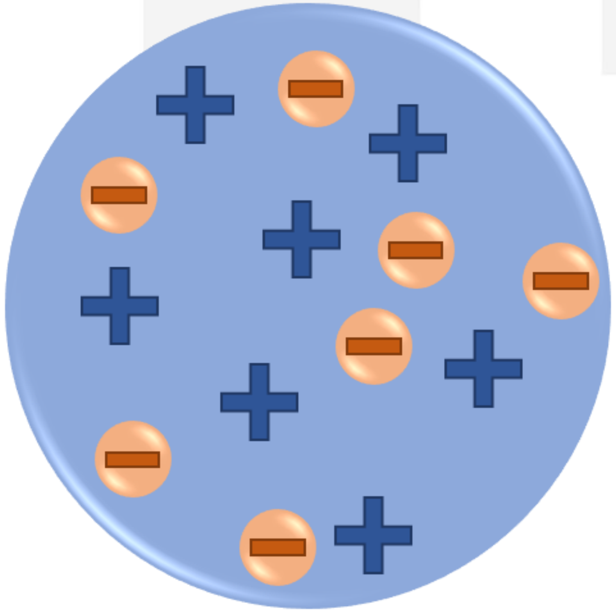
The Atomic Model

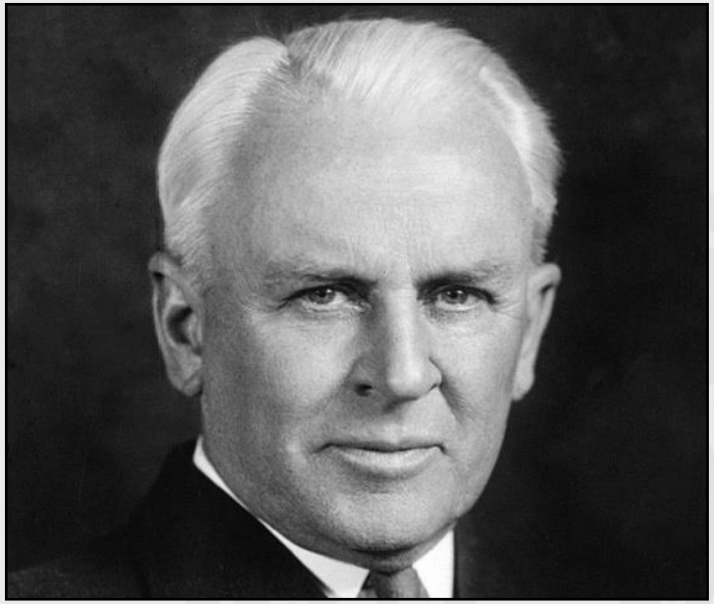


J. J. Thomson
1897

Atoms have a “jelly-like” positive part and the negative parts are scattered like plums in pudding in the positive part.



The Mass of an Electron



Robert Millikan
1909

American physicist **Robert Millikan** determines the **electrical charge** of the particles.

Electrically charged oil droplets in an electric field opposing the gravitational field.

He found the charge on one electron to be $-e$, where $e = 1.602 \times 10^{-19}$ C and is considered to be **"one unit"** of negative charge.

The combined work of J.J. Thomson and Robert Millikan:

$$\frac{m_e}{-e} \cdot -e = 9.109 \times 10^{-31}\text{kg}$$

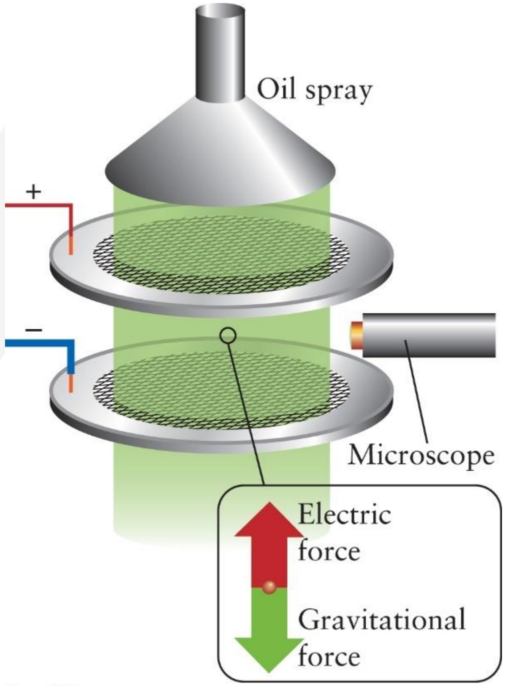


Figure 1A.3
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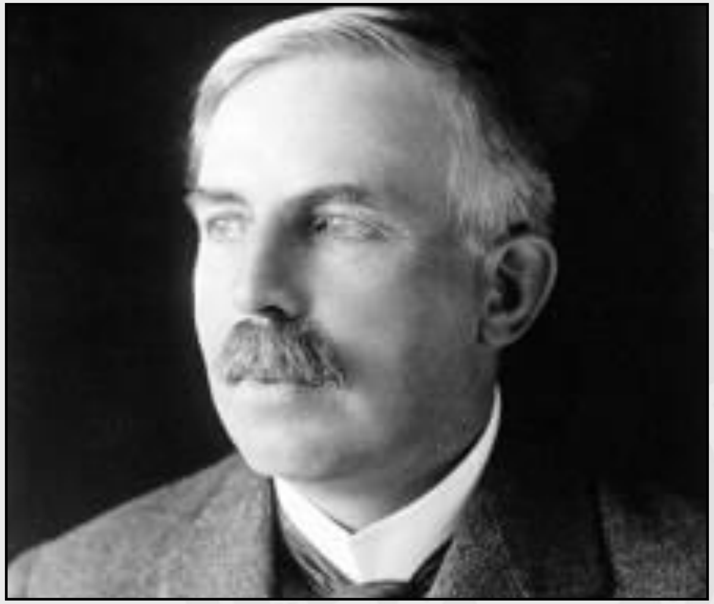
$$m_{drop} \cdot g = e \cdot E$$

m_{drop}:	Mass of selected drop
g:	Gravitational constant
e:	Charge of one electron
E:	Electric force

The Atomic Model

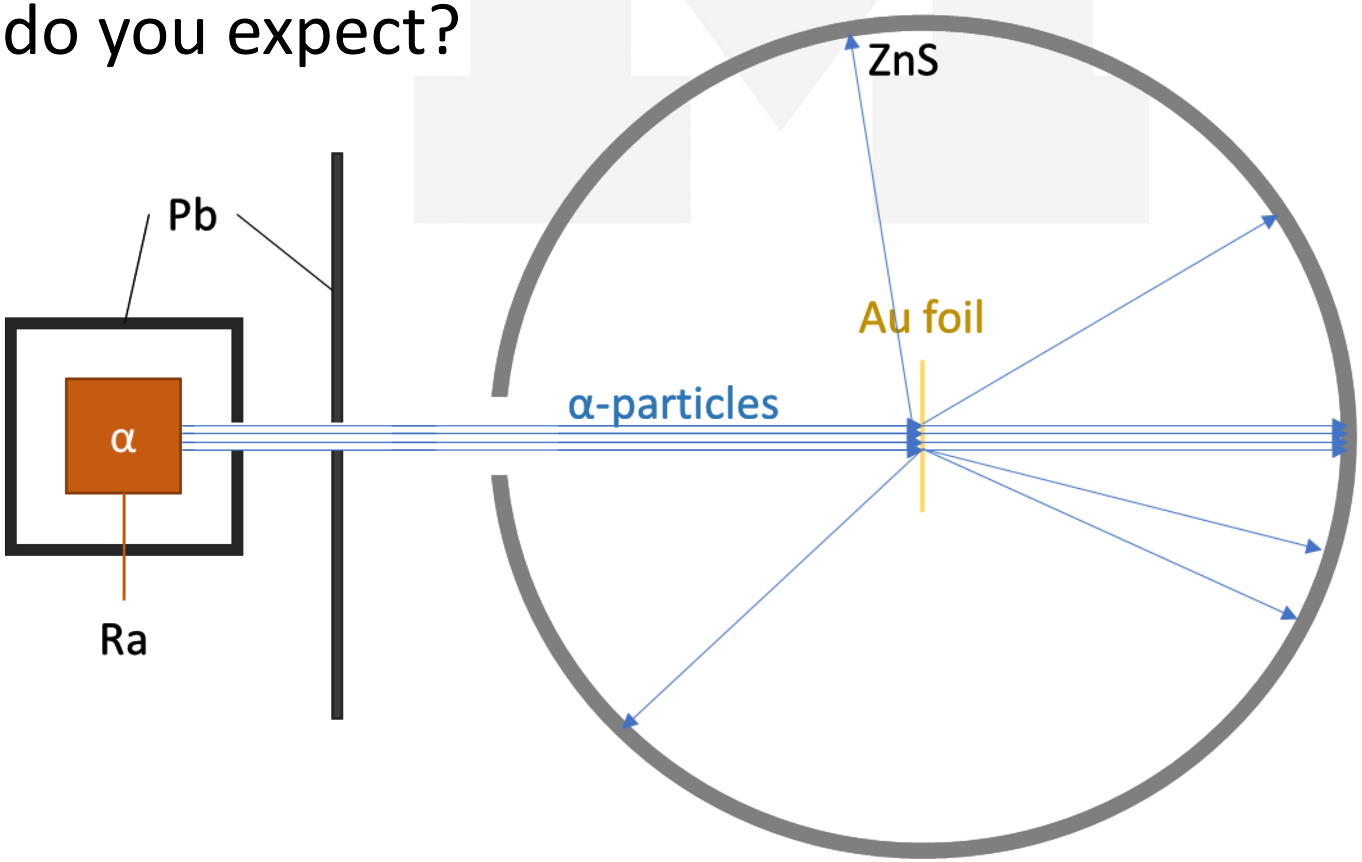


Ernest Rutherford
1911

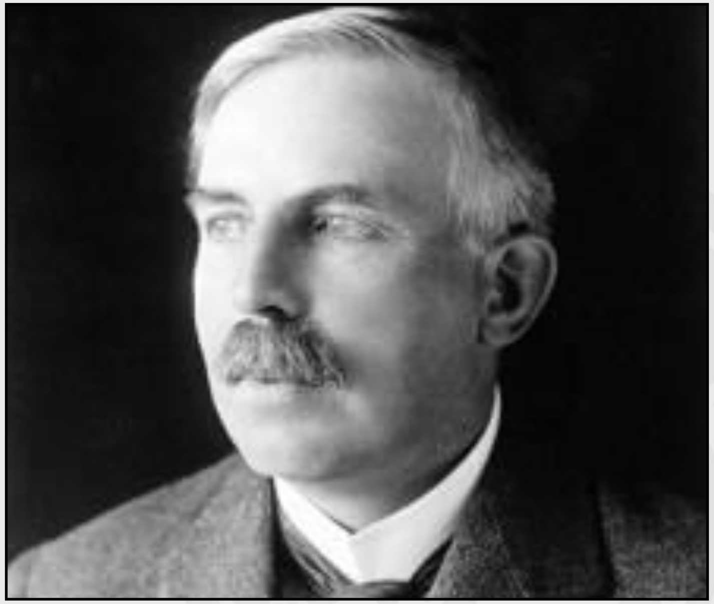
Shooting a very thin Au-foil with α-particles (He nuclei)

What was expected?

What do you expect?

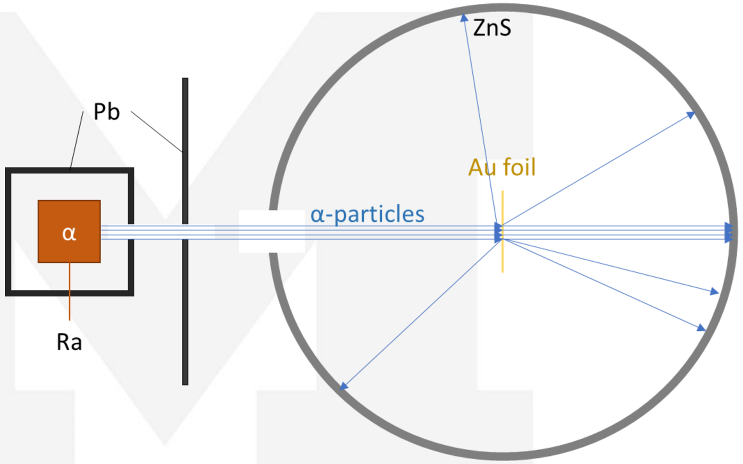


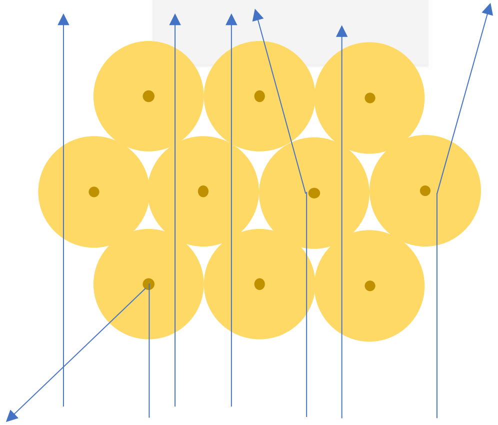
The Atomic Model



Ernest Rutherford
1911

Observation	Conclusion
Most α-particles pass through unhindered	Most of the atom is empty
Some α-particles are scattered (deflected with small angles)	The centre must be positively charged
A few α-particles are reflected	Most of the atom mass must be at its centre



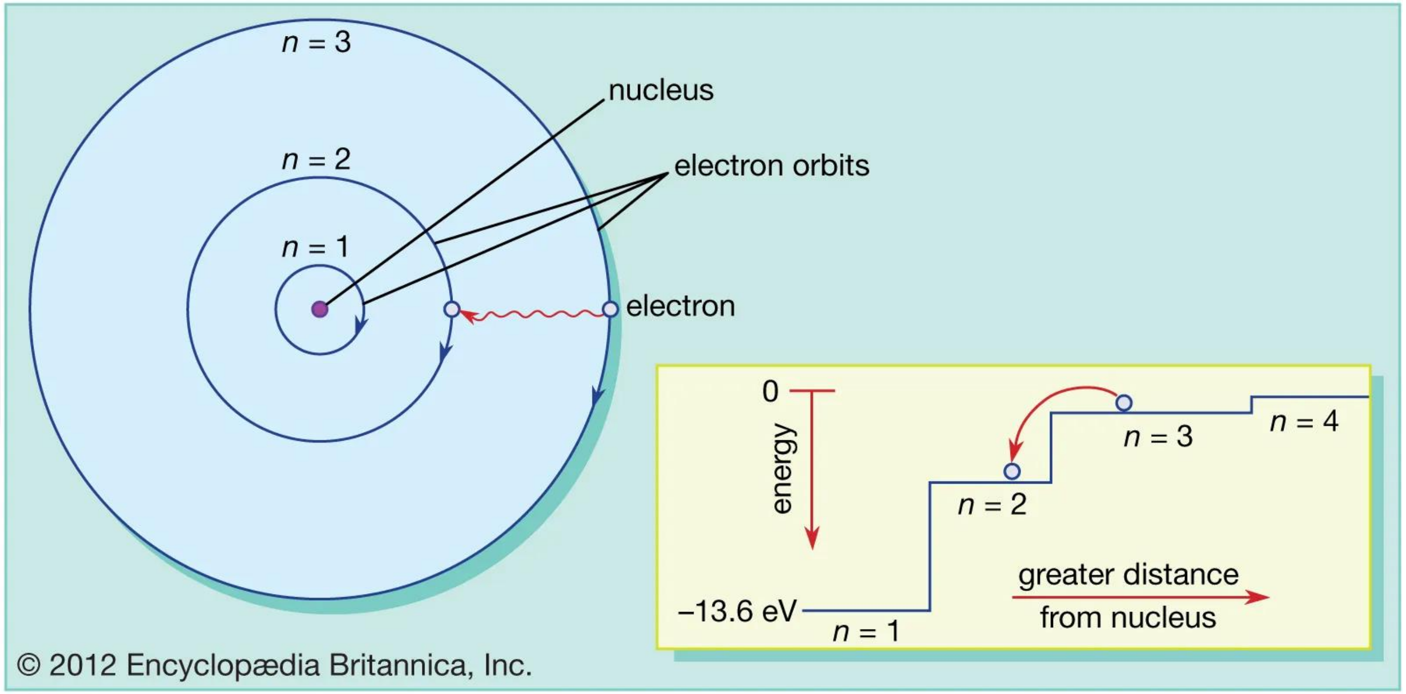


Atoms have a tiny, positively charged core (nucleus). Electrons surround the nucleus on circular orbits of arbitrary radii.

The Atomic Model

The radii of electronic orbits around the nucleus are not arbitrary. Instead, there is a set of allowed values.

Niels Bohr
1913
Student of E. Rutherford



https://www.atomicheritage.org/article/niels-bohr-announces-discovery-fission
https://www.britannica.com/science/Bohr-model

The Atomic Nucleus

The nucleus of an atom contains two particles:

- Protons, each of which has a charge of +e (“one unit of positive charge”)
- Neutrons

The number of protons in the nucleus is different for each element and is called the atomic number, Z.

The total charge on an atomic nucleus of atomic number Z is +Ze and, for the atoms to be electrically neutral, there must be Z electrons around it.

The Electrons

The nucleus of atom was understood, therefore attention turned to what the electrons were doing.

At the time, scientists studied both **light** and **electrons**.

It was necessary to link the two together because as it turned out they were related.

Light: Wave or Particle? Why not Both?

Waves didn't explain all our observations of light:

Four non-classical experiments with LIGHT

1. Ultraviolet catastrophe
   Why don't atoms vibrate faster? Hints at a particle nature of light.

2. Light emission spectrum
   Why don't electrons vibrate faster and make all the colors of the rainbow?

3. Is it a particle or is it a wave?
   Experiments prove both to be true.

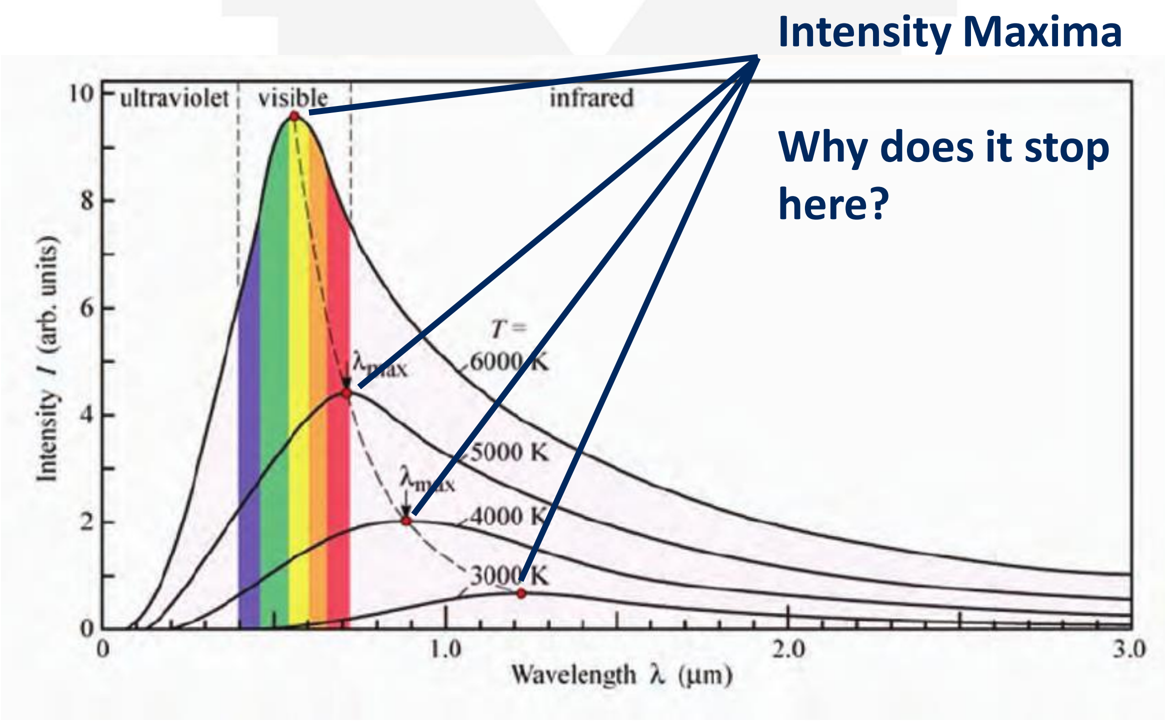
4. Einstein's photoelectric effect

Ultraviolet Catastrophe

Electromagnetic radiation emitted by a heated black body caused one of the greatest revolutions that has ever occurred in science.

At high temperatures an object begins to glow—the phenomenon of incandescence. As the object is heated to higher temperatures it glows more brightly, and the colour of light it gives off changes from red through orange and yellow towards white.

The problem is the curve should be linear, going straight UP, not dying away in UV!



The "hot object" is known as a black body (even though it might be glowing white hot!).

Stefan-Boltzmann Law

Describes the exponential-like behaviour of black-body objects.

$$Total\ intensity = constant \cdot T^4$$

The total intensity of radiation emitted increases as the fourth power of the temperature.

A body at 1000 K emits 120 times more energy than a body at 300 K.

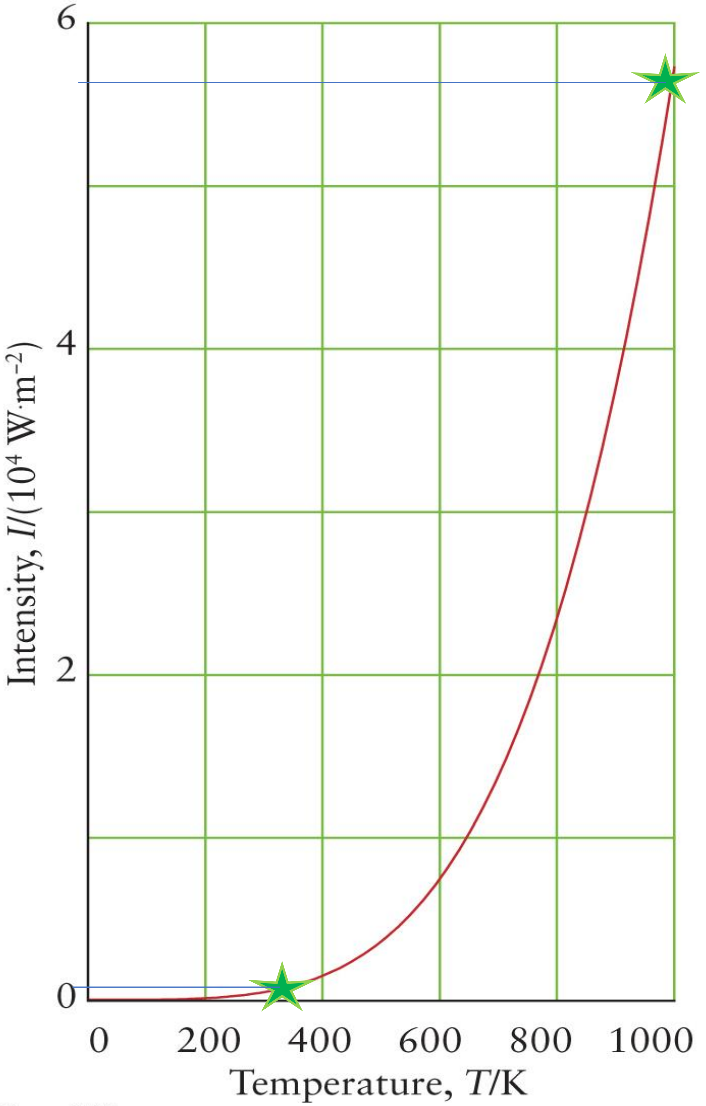


Figure 1B.2
Atkins, *Chemical Principles: The Quest for Insight*, 7e

Wien's Law

Shows that a maxima existed in black-body radiation.

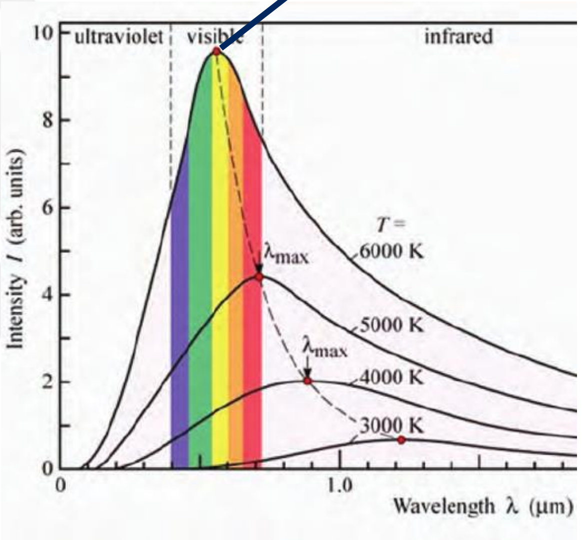
$$T \cdot \lambda_{max} = constant$$

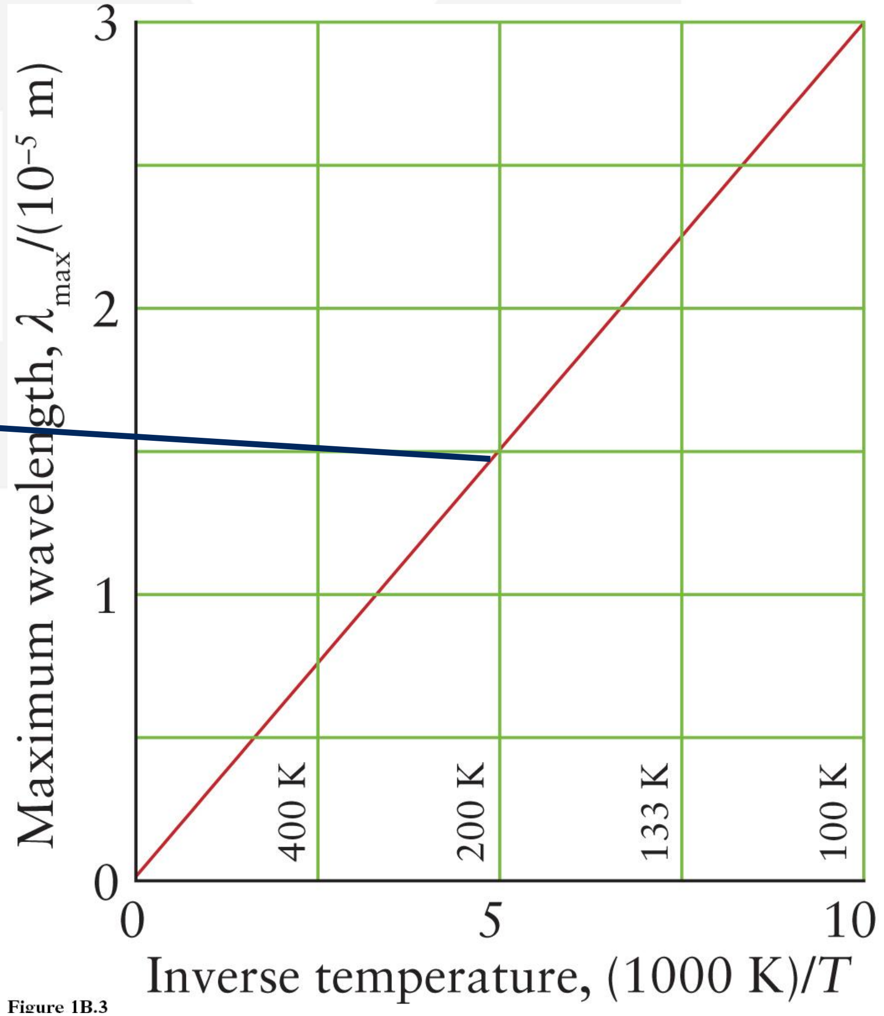
Inverse Relationship:

as T ↑, λ_{max} ↓

Often used by astronomers to measure a star's surface temperature.

Intensity Maxima



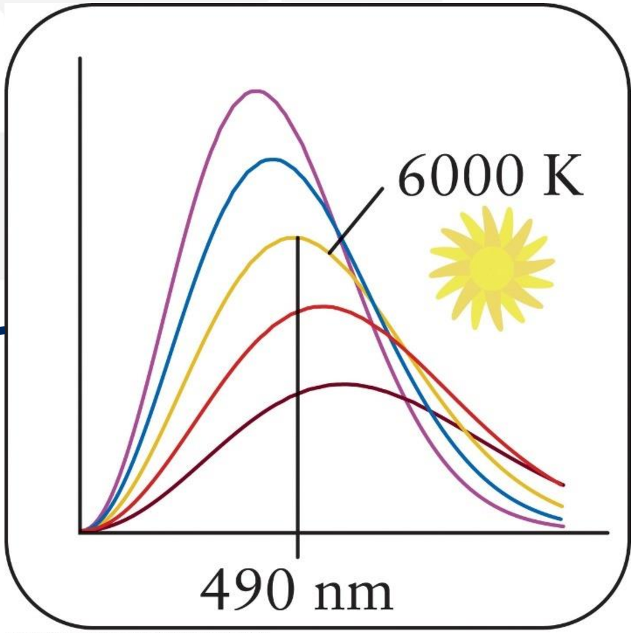


Side Quest: How Hot is the Sun?

The maximum intensity of solar radiation occurs at 490 nm. What is the temperature of the surface of the Sun?

$$T \cdot \lambda_{max} = constant$$

$$\mathrm{T} = \frac{2.9 \times 10^{-3}\ \mathrm{m} \cdot \mathrm{K}}{4.90 \times 10^{-7}\ \mathrm{m}} = 5.9 \times 10^{3}\ \mathrm{K}$$



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That is, the surface temperature of the Sun is about 6000 K.

Ultraviolet Catastrophe

Classical Mechanics

Simple harmonic motion:

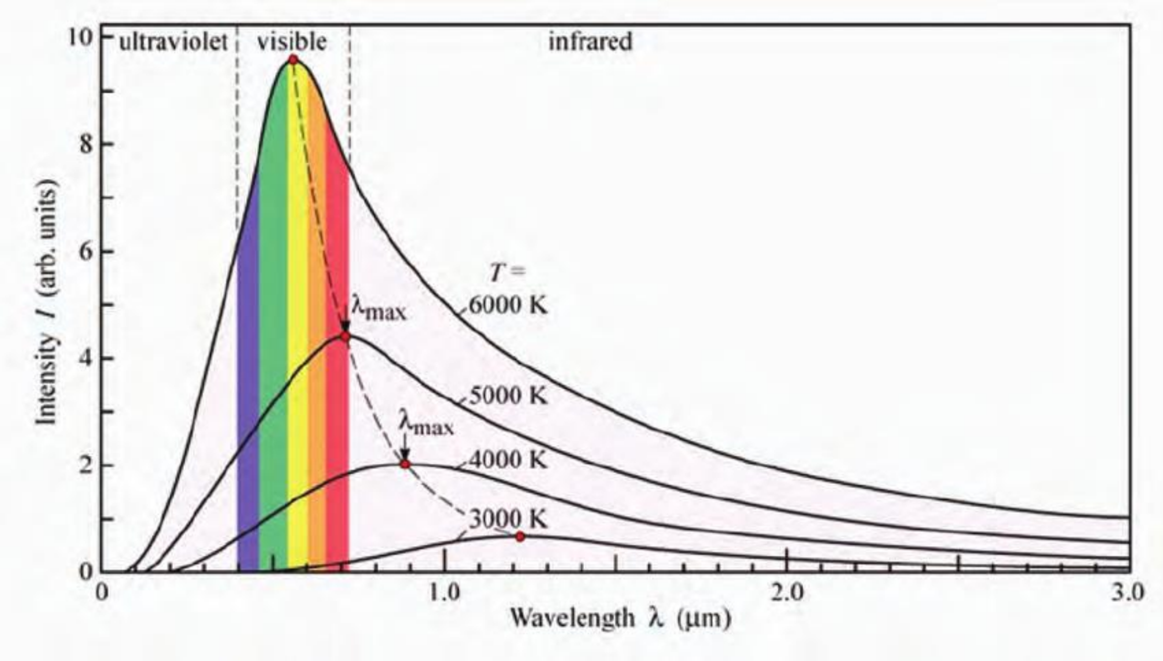
$$F = -kx$$

F: force constant

k: spring constant

x: distance the object oscillates

Classical mechanics did not match with experimental observations when heating objects, hence the **ultraviolet catastrophe**: oscillating atoms, which oscillate rapidly, should emit intense ultraviolet and even gamma radiation!

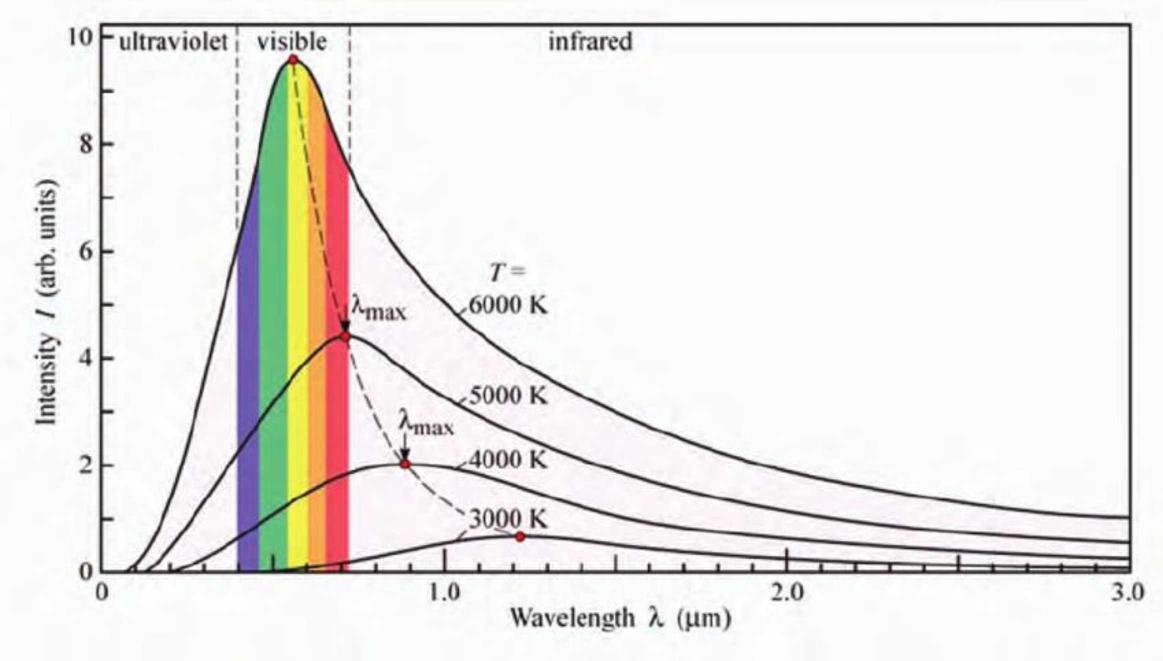


https://nevillesphantasticphysicsphun.home.blog/2020/06/04/the-ultraviolet-catastrophe/

Ultraviolet Catastrophe

Classical (Newtonian) mechanics treats all objects, such as energy and heat, as having a **continuous** quantity, for example, an infinite number of energy units, oscillations, or vibrations.

This is clearly not the case with atomic vibrations which does not exhibit Classical behavior.



https://nevillesphantasticphysicsphun.home.blog/2020/06/04/the-ultraviolet-catastrophe/

Short Quiz

The fundamental importance of the ultraviolet catastrophe is that it:

A. Proved that adding an infinite amount of energy did not produce shorter and shorter wavelengths of light

B. Proved that no matter how hot an object, it could only emit light up to a limit, and not beyond the UV frequency

C. Proved that light could not be treated as a continuous spectrum

D. All of the above

Wave and Particle

Planck hypothesizes that oscillations start at a particular minimum energy level.

To make oscillations occur at higher energies requires a specific or minimum amount of energy or "**packet**" sometimes called quanta; this idea hints at the particle nature of electrons!

The UV catastrophe helped scientist understand that small things, typically thought as a wave, could also behave as a **particle**.

$$E = h \cdot \nu$$

$\boldsymbol{h}$ **= 6.626×10^{-34} J·s**

Planck's constant

Wave and Particle

Next, we look **emission spectra**, a true **particle** experiment!

This will help tell us explain “where” the electron is.