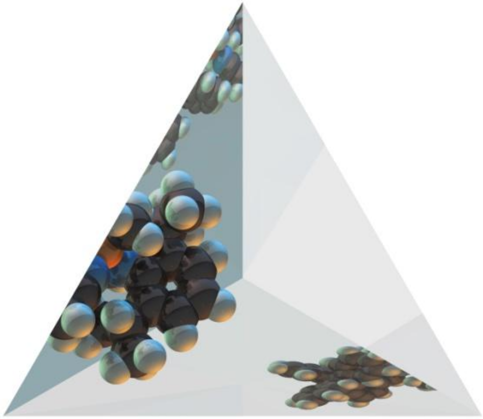


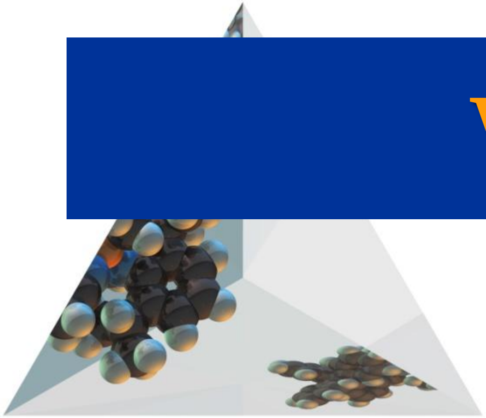
CHEMISTRY

The Central Science

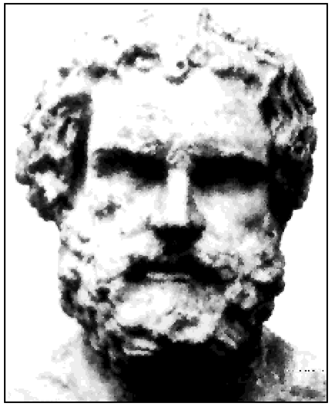
8th Edition

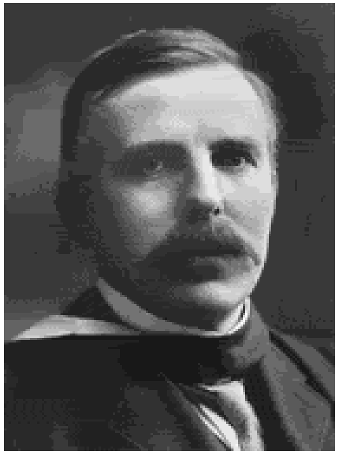
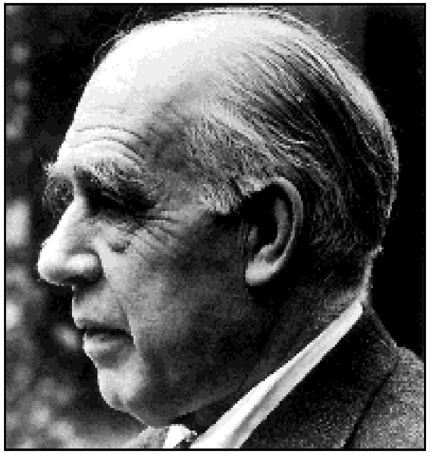
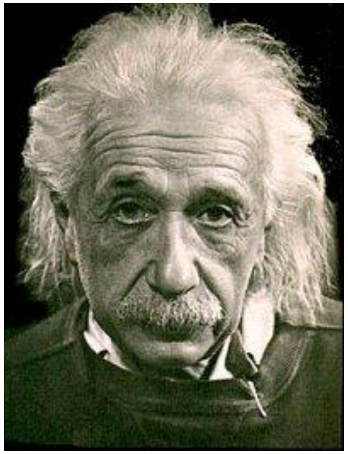
Chapter 6
Electronic Structure of Atoms

Kozet YAPSAKLI

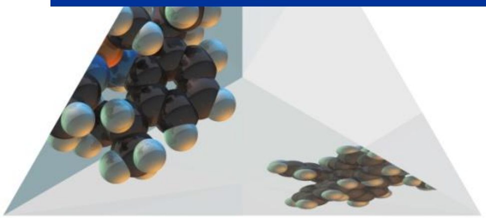


Who are these men?



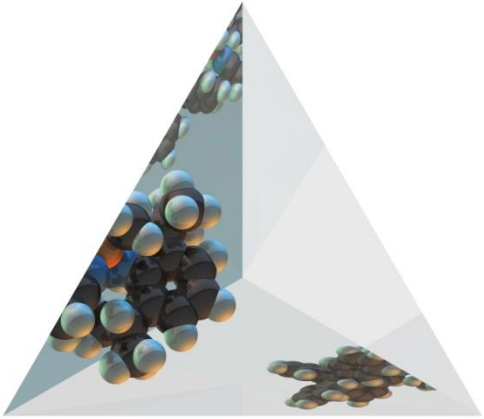






Ancient Philosophy



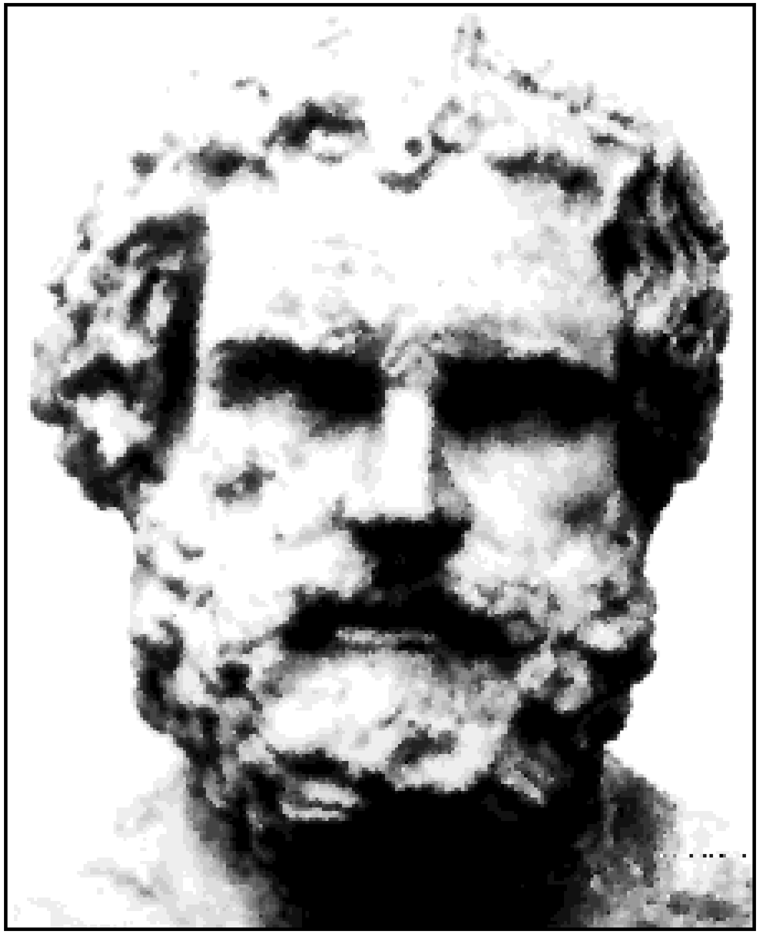
- Who: Aristotle, Democritus
- When: More than 2000 years ago
- Where: Greece
- What: Democritus believed that matter was made of small particles he named “atoms”.

  Aristotle believed in 4 elements: Earth, Air, Fire, and Water.
- Why: Aristotle and Democritus used observation and inference to explain the existence of everything.



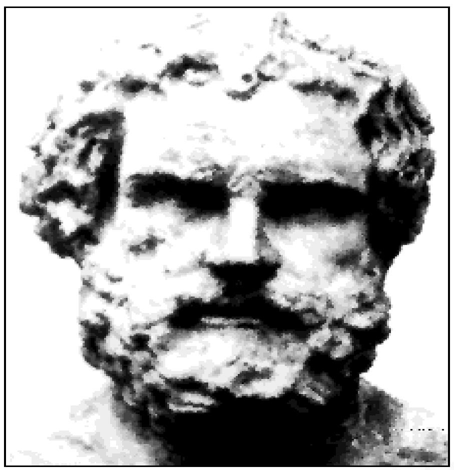
Democritus

- This is the Greek philosopher Democritus who began the search for a description of matter more than 2400 years ago.
  - He asked: Could matter be divided into smaller and smaller pieces forever, or was there a limit to the number of times a piece of matter could be divided?



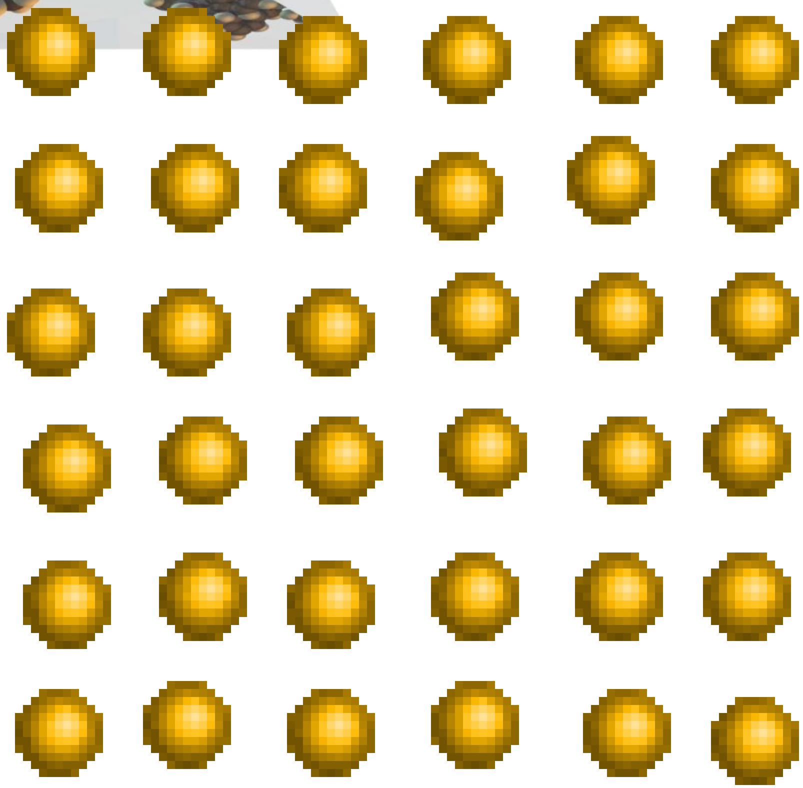
400 BC

Atomos

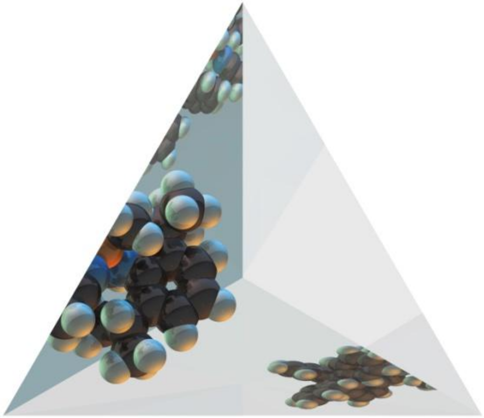


- His theory: Matter could not be divided into smaller and smaller pieces forever, eventually the smallest possible piece would be obtained.
- He named the smallest piece of matter “atomos,” meaning “not to be cut.”

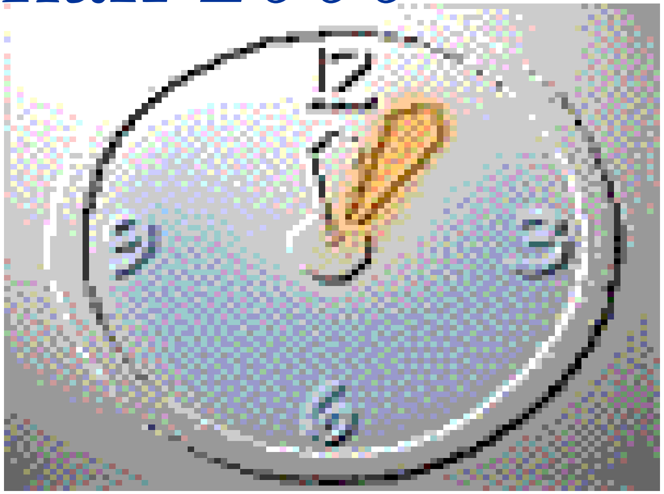
Atomos



- To Democritus, atoms were small, hard particles that were all made of the same material but were different shapes and sizes.
- Atoms were infinite in number, always moving and capable of joining together.



This theory was ignored and forgotten for more than *2000* years!

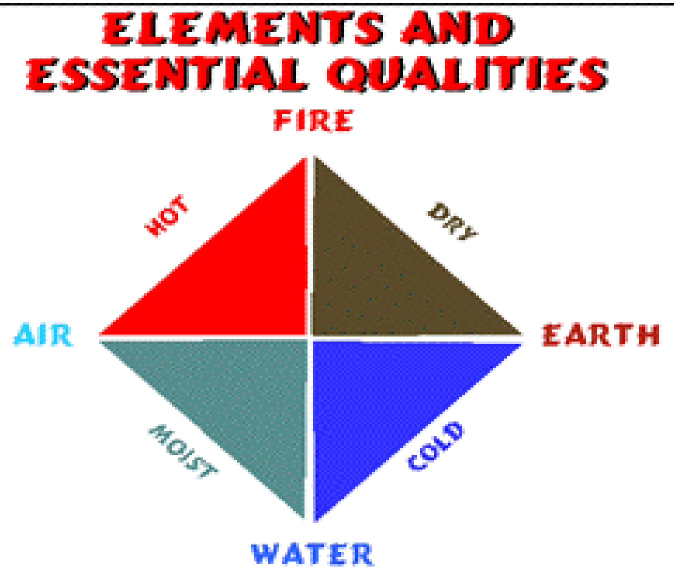


New Theory?

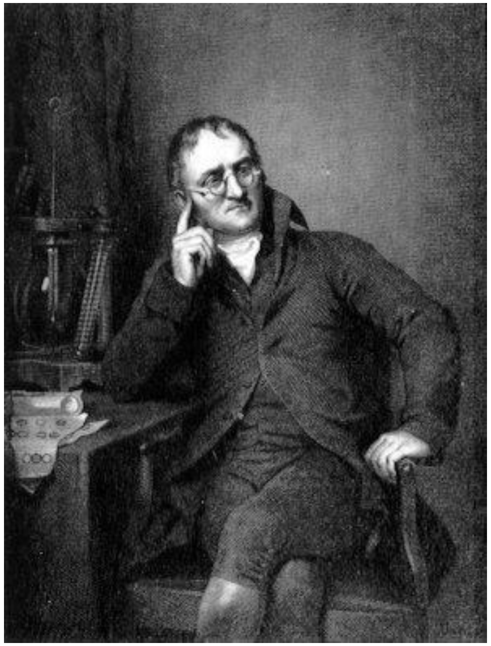
- The eminent philosophers of the time, Aristotle and Plato, had a more respected, (and ultimately wrong) theory.

Aristotle and Plato favored the *earth, fire, air and water* approach to the nature of matter. The elements, while distinguished from each other, are also related by four qualities. These qualities are dry, moist, hot, and cold.

- Each element possesses two qualities, of which one predominates, and each element is linked to two other elements by the quality they possess in common.
  - Fire is hot and dry with heat predominating.
  - Air is hot and moist with moisture predominating.
  - Water is moist and cold with cold predominating.
  - Earth is cold and dry with dryness predominating.



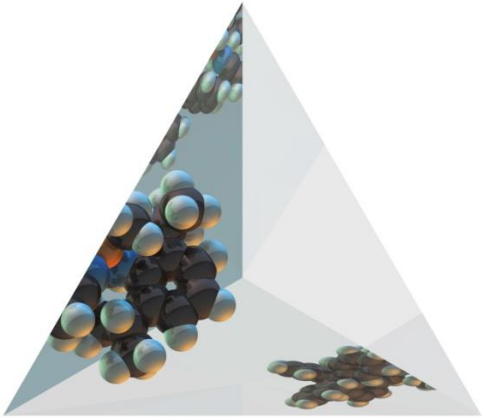
Particle Theory



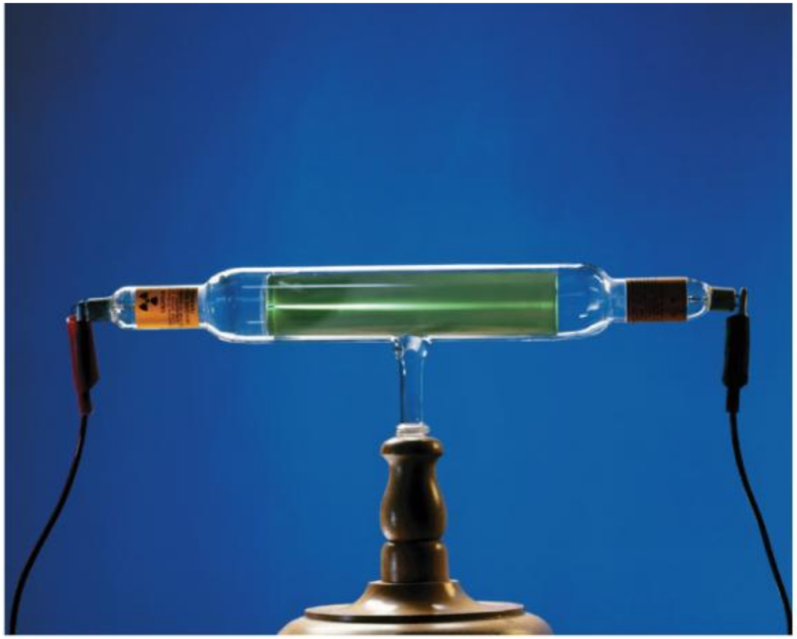
- Who: John Dalton
- When: 1808
- Where: England
- What: Described atoms as tiny particles that could not be divided. Each element was made of its own kind of atom.
- Why: Building on the ideas of Democritus in ancient Greece.

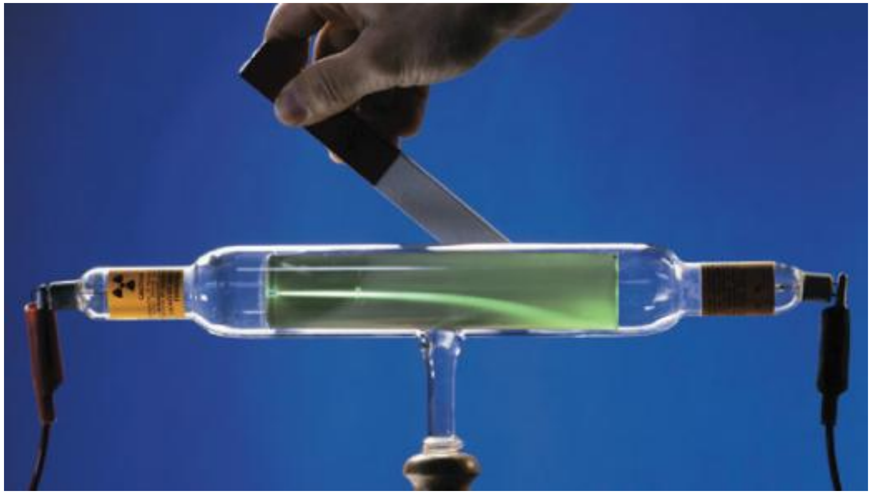
Discovery of Electrons

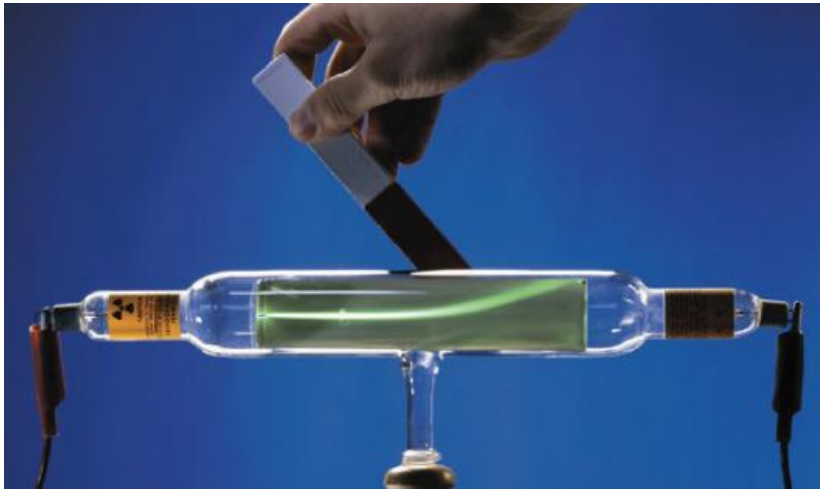
- Who: J. J. Thompson
- When: 1897
- Where: England
- What: Thompson discovered that electrons were smaller particles of an atom and were negatively charged.
- Why: Thompson knew atoms were neutrally charged, but couldn’t find the positive particle.



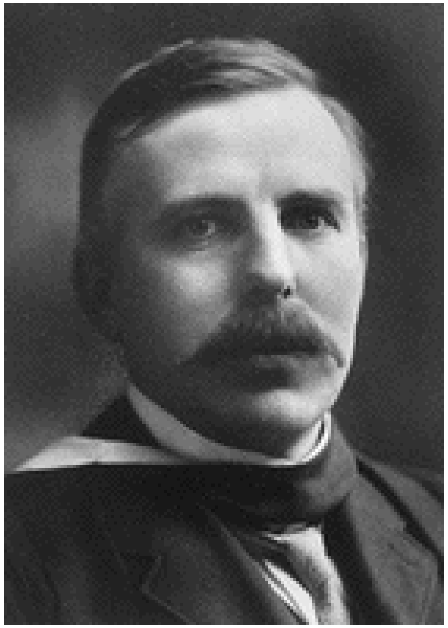
Cathode Ray Tube







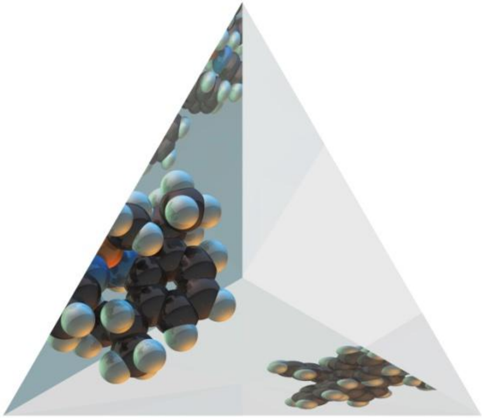
Atomic Structure I



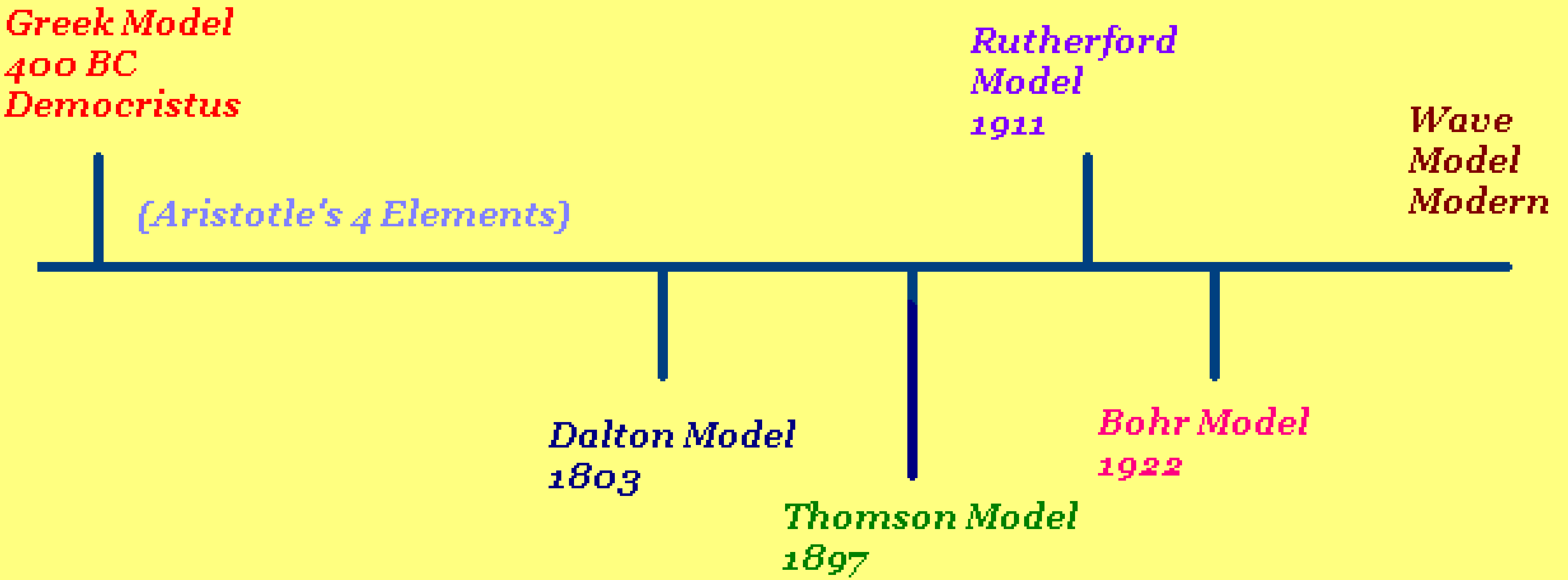
- Who: Ernest Rutherford
- When: 1911
- Where: England
- What: Conducted an experiment to isolate the positive particles in an atom. Decided that the atoms were mostly empty space, but had a dense central core.
- Why: He knew that atoms had positive and negative particles, but could not decide how they were arranged.

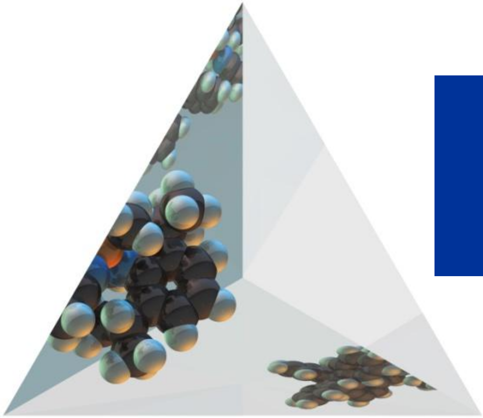
Atomic Structure II

- Who: Niels Bohr
- When: 1913
- Where: England
- What: Proposed that electrons traveled in fixed paths around the nucleus. Scientists still use the Bohr model to show the number of electrons in each orbit around the nucleus.
- Why: Bohr was trying to show why the negative electrons were not sucked into the nucleus.



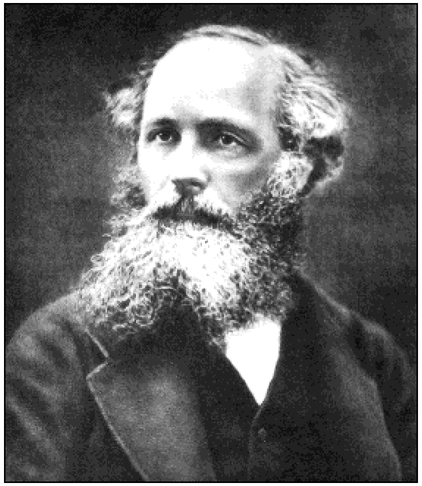
Timeline of Atomic Theory





Scientist

- James Maxwell (1831-1879) - Scottish
- Max Planck (1858-1947) - German - 1918 Nobel Prize
- Albert Einstein (1879-1955) - German - 1921 Nobel Prize
- Niels Bohr (1885-1962) - Danish - 1922 Nobel Prize
- Louis de Broglie (1892-1987) - French - 1929 Nobel Prize
- Erwin Schrödinger (1887-1961) - Austrian - 1933 Nobel Prize
- Werner Heisenberg (1901-1976) - German - 1932 Nobel Prize
- Wolfgang Pauli (1900-1958) - Austrian - 1945 Nobel Prize
- Friedrich Hund (1896 - 1997) - German

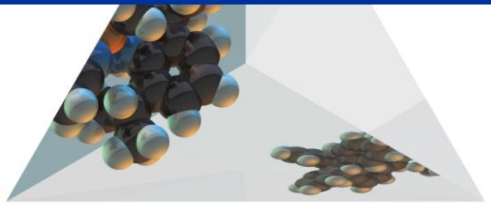


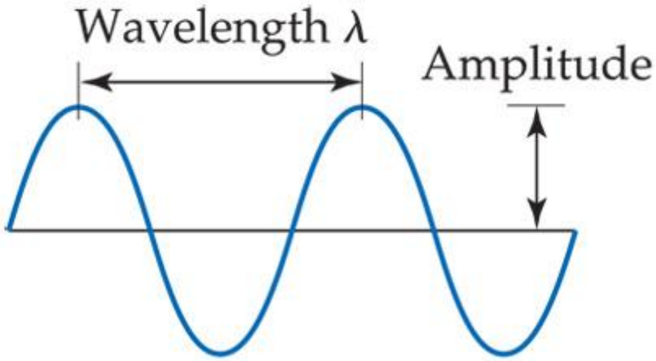
James Clerk Maxwell

- developed a mathematical theory that describes all forms of radiation.
- formulated a set of equations expressing the basic laws of ***electricity*** and ***magnetism*** and developed the Maxwell distribution in the kinetic theory of gases.
- The ***speed*** of a wave, *c*, is given by its frequency multiplied by its wavelength:

$$c = \nu\lambda$$

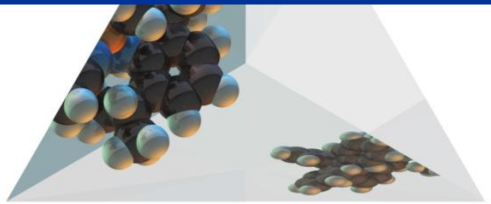
Waves

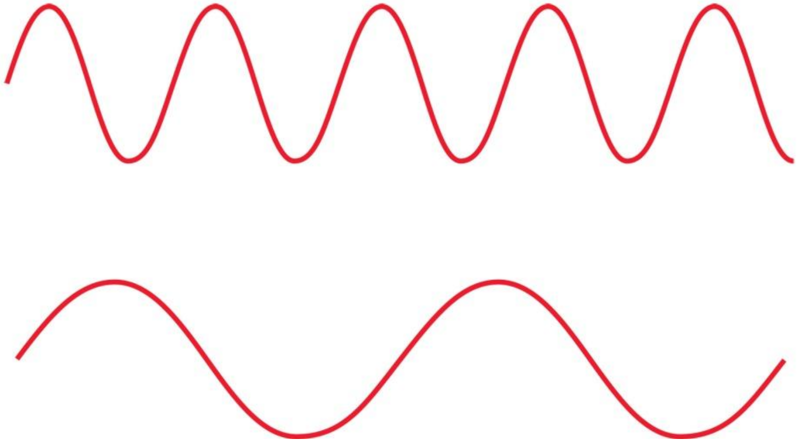




- To understand the electronic structure of atoms, one must understand the nature of electromagnetic radiation.
- The distance between corresponding points on adjacent waves is the wavelength (λ).

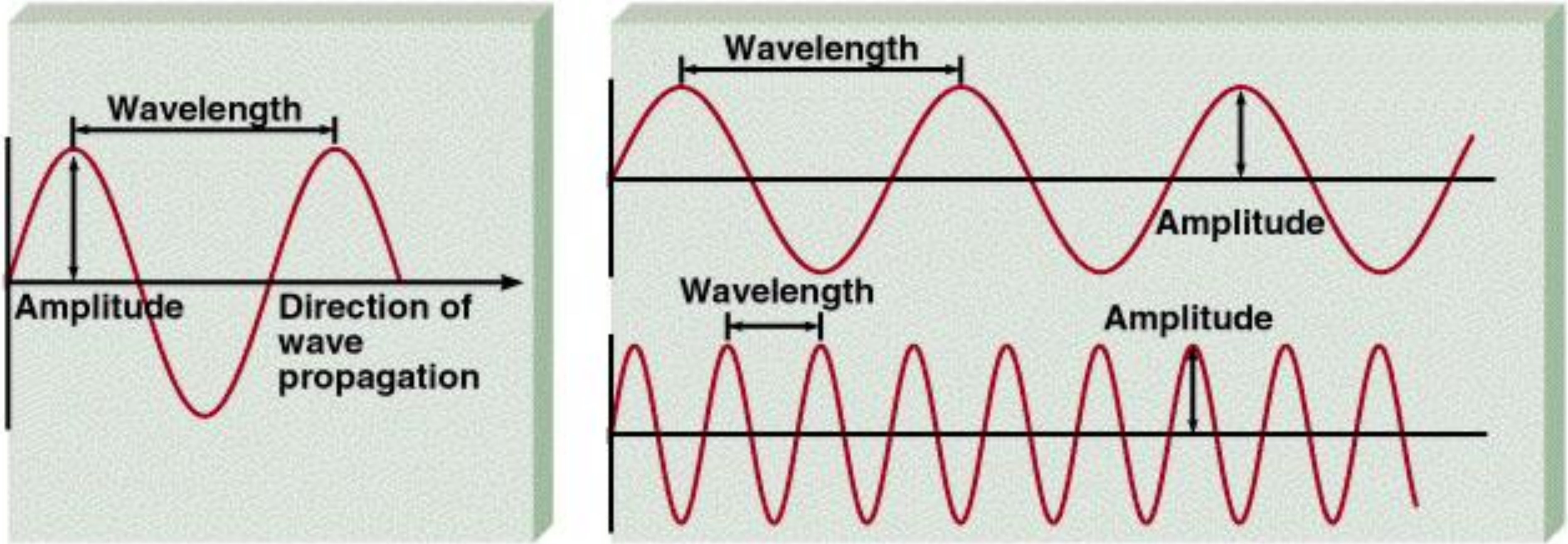
Waves





- The number of waves passing a given point per unit of time is the frequency (ν).
- For waves traveling at the same velocity, the longer the wavelength, the smaller the frequency.

Wavelength and Amplitude



(a) (b)

Components of an Electromagnetic Wave

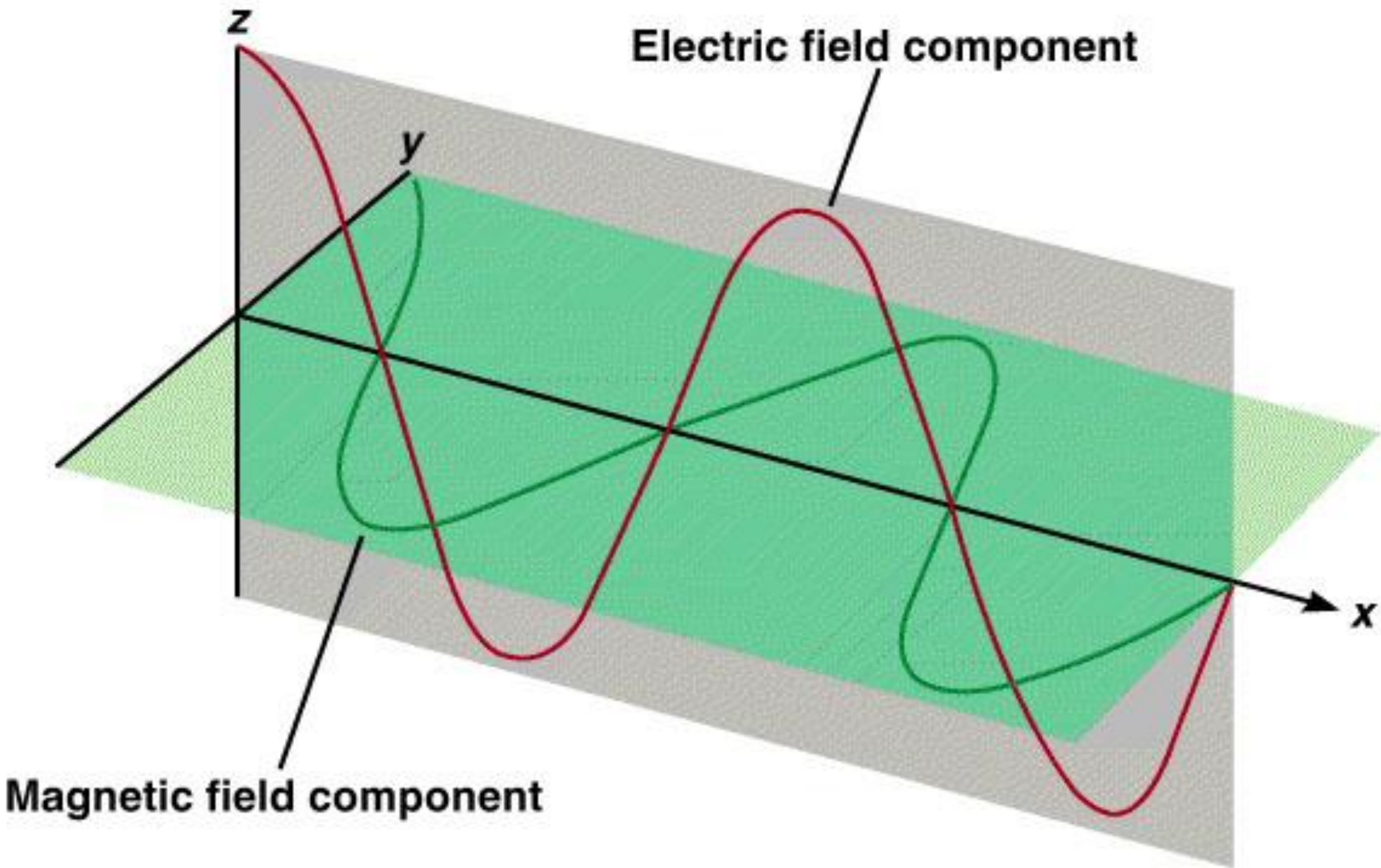
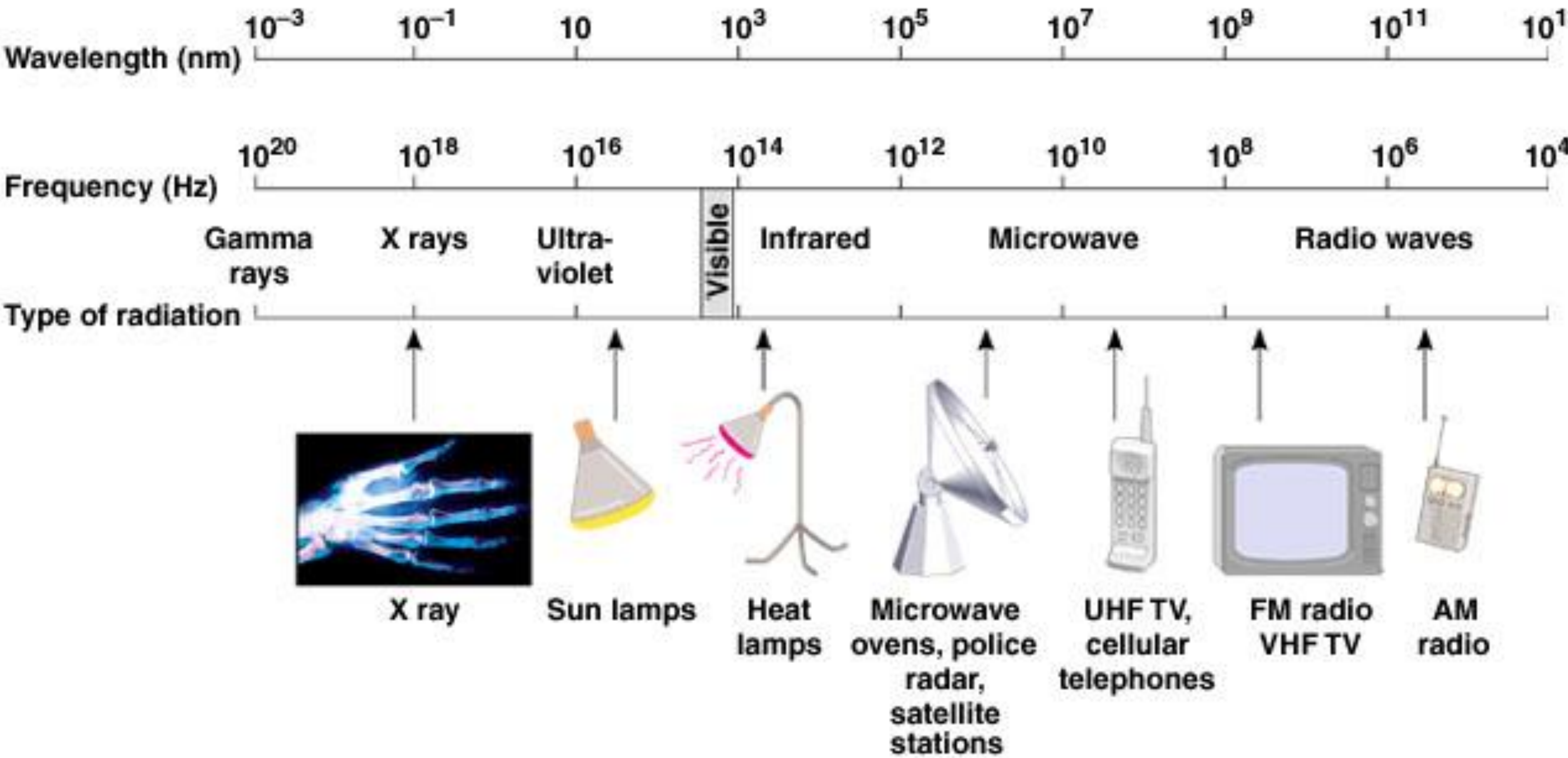


Fig. 7.4a

Electromagnetic Radiation



(a)

Uses of Radiation

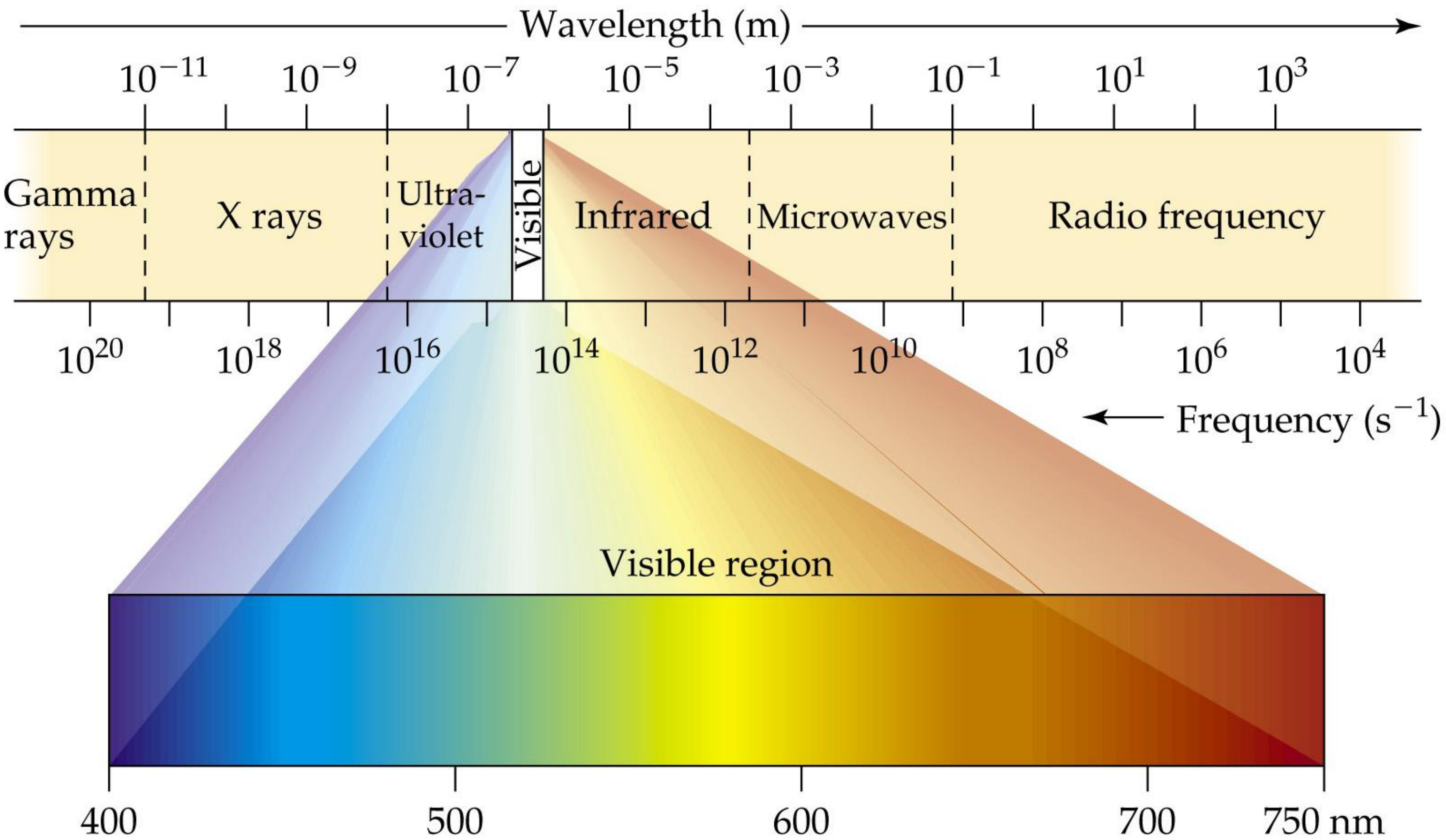
- radio waves - communication, MRI; nuclear rotation
- microwaves - cooking, energy transmission, radar; molecular rotation
- infrared - heat lamps, burglar alarms, night scopes, heat sensing missiles; atomic vibrations
- visible light - vision; electronic transitions
- ultraviolet - sunburn, bacterial sterilization; electronic transitions
- X-rays - medical imaging; diffracted by solids
- γ rays - nuclear radiation

Fig. 7.4b

Visible Light Range

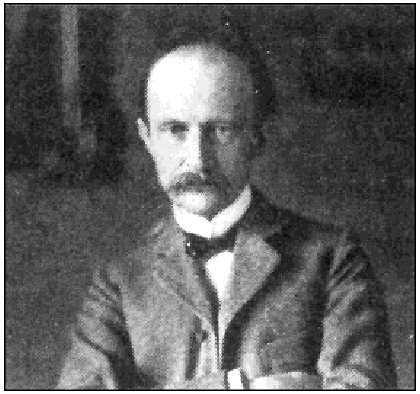
(b)

The Wave Nature of Light



visible radiation has wavelengths btw 400 nm (violet) and 750 nm (red).

All electromagnetic radiation travels at the same velocity $c = \nu\lambda$



Max Karl Ludwig Planck

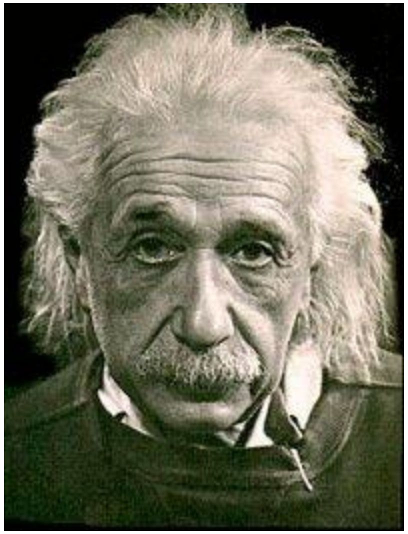
- He is considered to be the founder of quantum theory.
- explained how things give off electromagnetic radiation when they are heated.
- A quantum is the smallest amount of energy that can be absorbed or emitted as electromagnetic radiation.
- The relationship between energy and frequency is

$$E = h\nu \qquad E = h \cdot \nu = \frac{h \cdot c}{\lambda}$$

where h is Planck's constant (6.626 × 10-34 J.s).

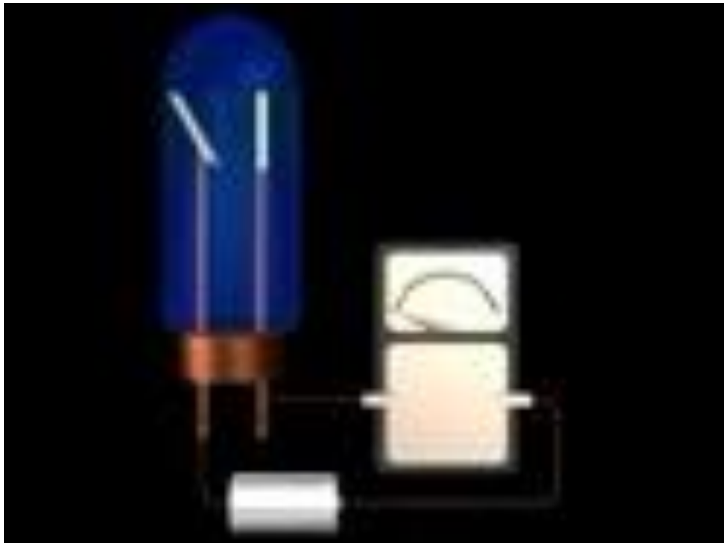
The Nature of Energy

- The wave nature of light does not explain how an object can glow when its temperature increases.
- Max Planck explained it by assuming that energy comes in packets called quanta.



Albert Einstein

Photoelectric effect demonstrates the particle nature of light.

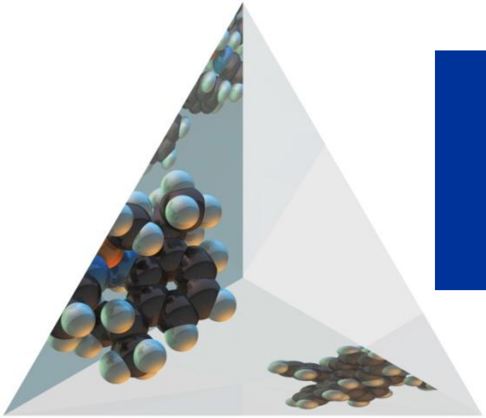


No e^- observed until the threshold frequency is reached.

Number of e^- ejected does NOT depend on frequency,

it depends on light intensity.

Einstein assumed that light traveled in energy packets called *photons*

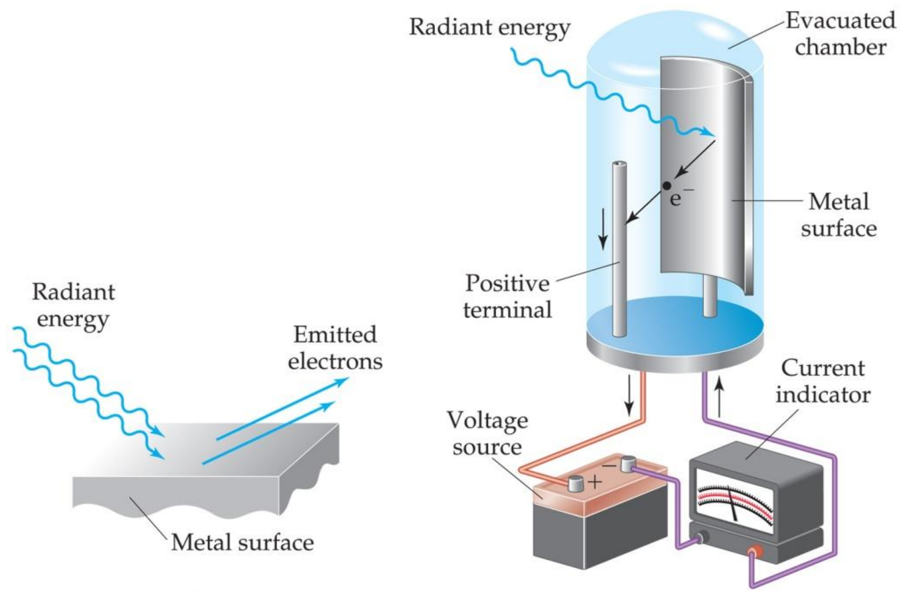


The Nature of Energy

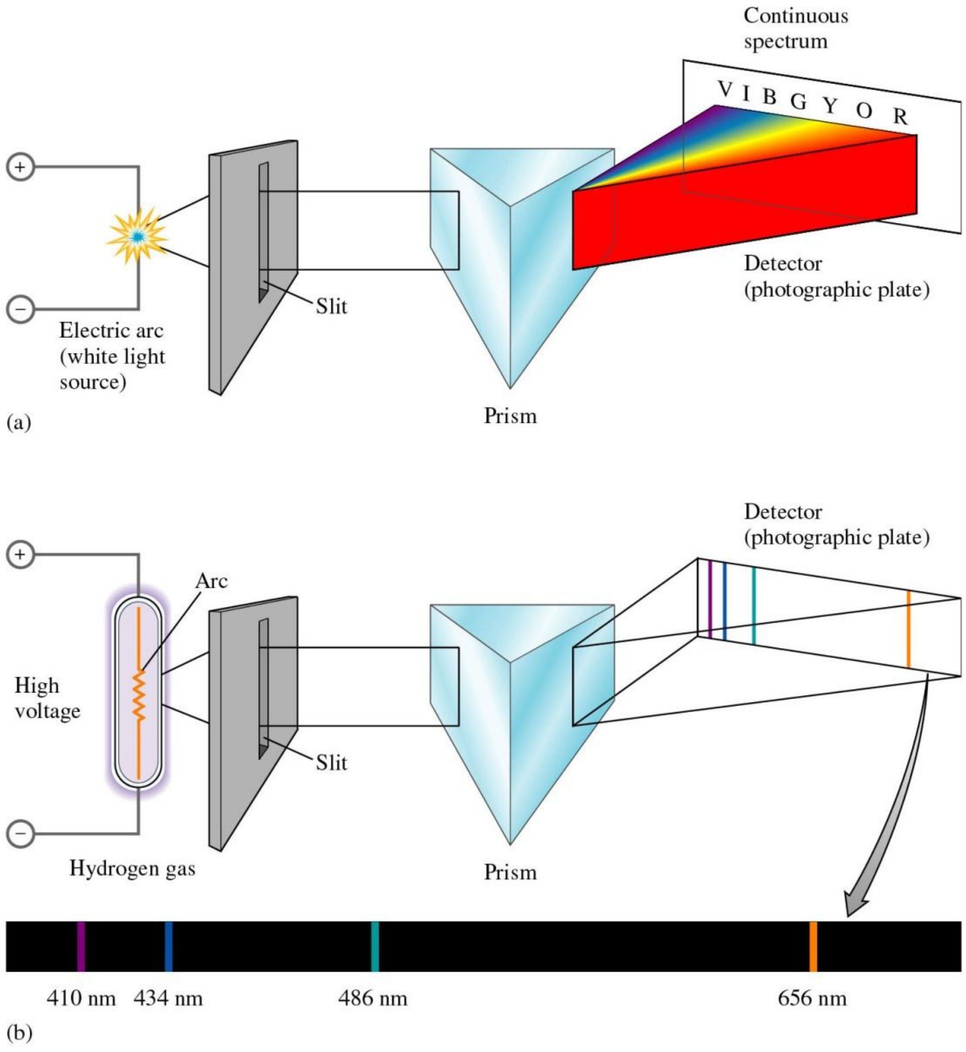
- Einstein used this assumption to explain the photoelectric effect.
- He concluded that energy is proportional to frequency:

$$E = h\nu$$

where *h* is Planck’s constant, 6.63×10^{-34} J-s.



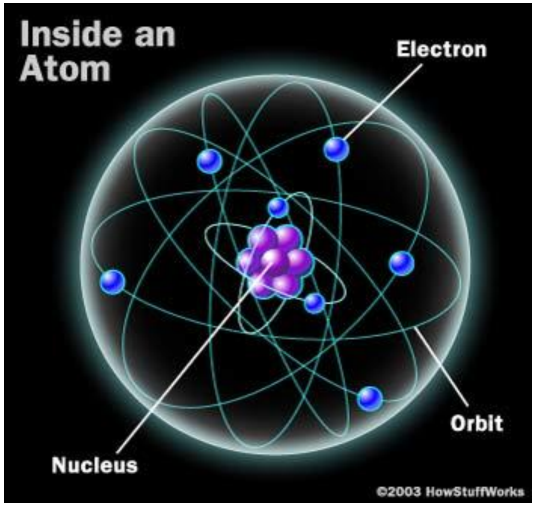
Emission spectrum of H



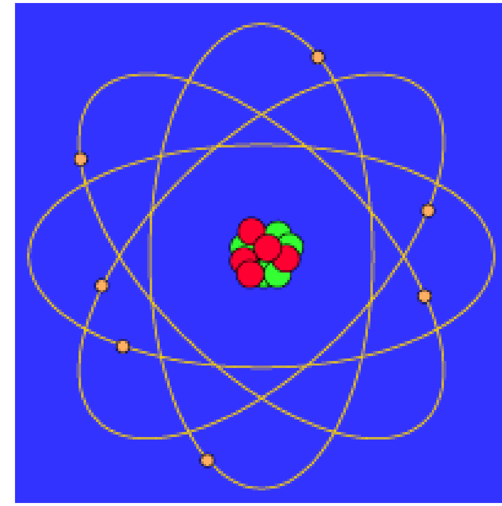
Light Bulb

Hydrogen Lamp

Quantized, not continuous

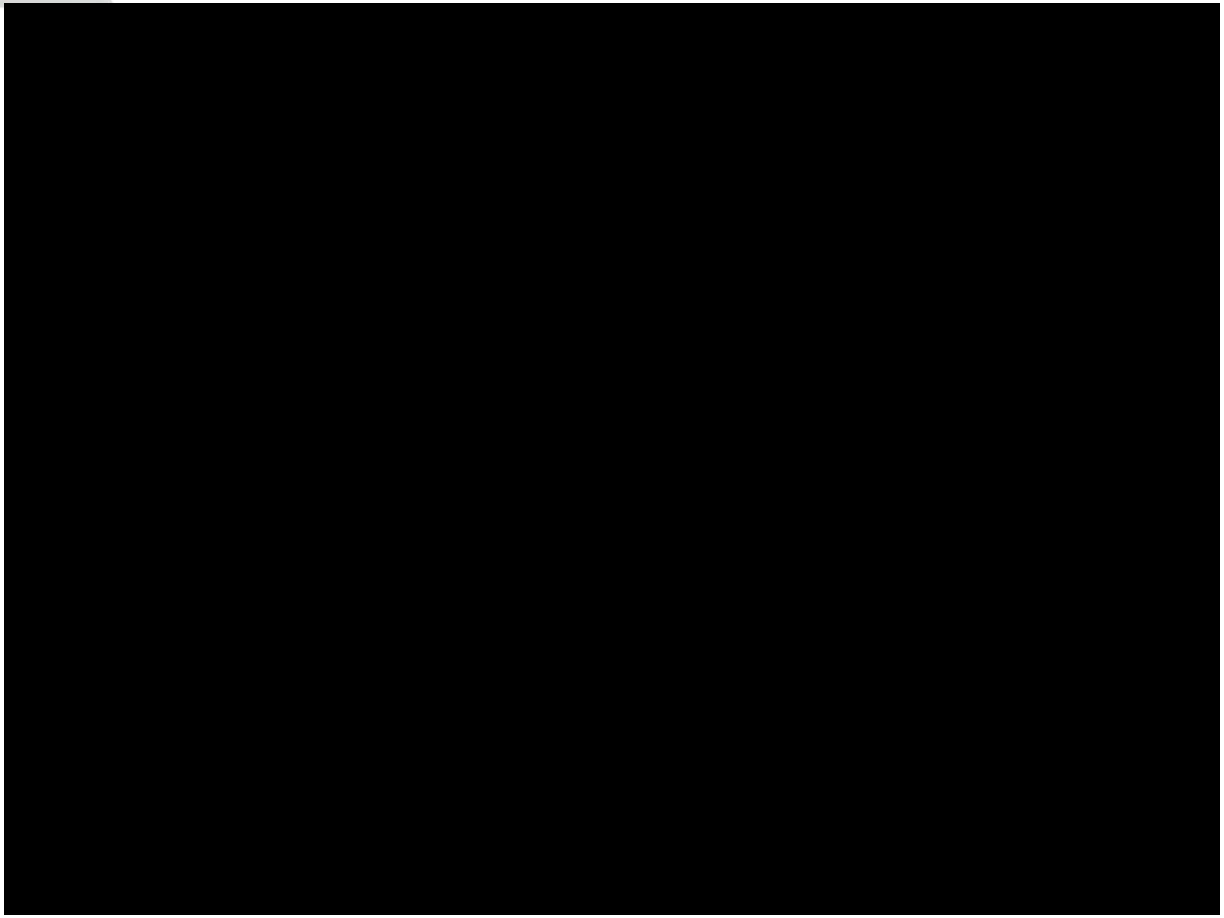


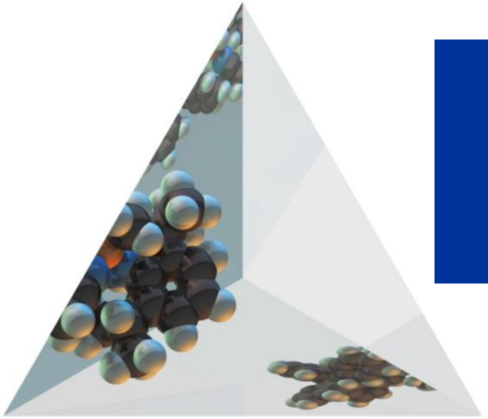
Niels Bohr



- Provided the first connection btw Planck and Einstein.
- Bohr's Model of Hydrogen
  - The electron moves in a circular orbit around the nucleus.
- moving an electron from a high n to a lower n is and exothermic process; energy is released…
  - This energy release is observed as light.

$$\text{Energy of the } n^{th} \text{ level} = E_n = -\frac{Rhc}{n^2}$$



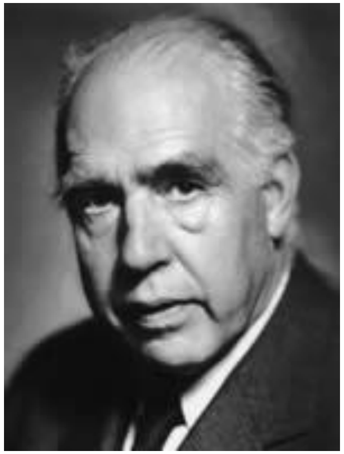


Bohr Model

Bohr Model

- The first orbit in the Bohr model has n = 1, is closest to the nucleus, and has negative energy.
- The furthest orbit in the Bohr model has n close to infinity and corresponds to zero energy.
- Electrons in the Bohr model can only move between orbits by absorbing and emitting energy in quanta ($h\nu$).
- The amount of energy absorbed or emitted on movement between states is given by

$$\Delta E = E_f - E_i = h\nu$$



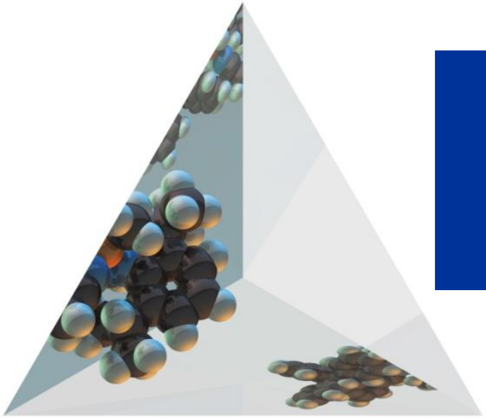
Bohr Model

Bohr Model

- We can show that

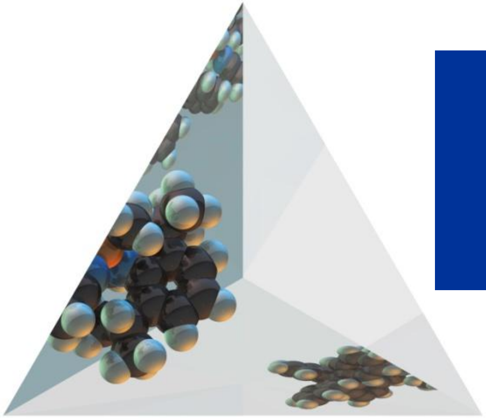
$$\Delta E = h\nu = \frac{hc}{\lambda} = \left(-2.18\times10^{-18}\ \mathrm{J}\right)\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

- When $n_i > n_f$, energy is emitted.
- When $n_f > n_i$, energy is absorbed



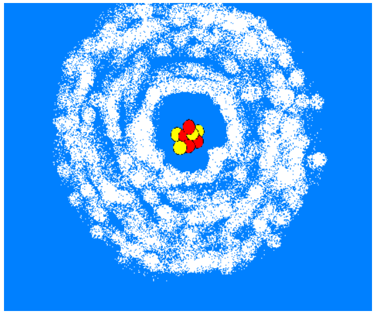
Wave Model

- **Bohr Model** does ***not*** work for multi-electron atoms
- Could ***not*** account for the intensities or the fine structure of the spectral lines (for example, in magnetic fields).
- Today's atomic model is based on the principles of wave mechanics.
- According to the theory of wave mechanics, electrons do not move about an atom in a definite path, like the planets around the sun.



Modern Atomic Model

- It is impossible to determine the exact location of an electron. The probable location of an electron is based on how much energy the electron has.
- According to the modern atomic model, at atom has a small positively charged nucleus surrounded by a large region in which there are enough electrons to make an atom neutral.



Wave Behavior of Matter
Louis de Broglie

- de Broglie (1924) proposed that all moving objects have wave properties.
- Light has both wave & particle properties
- For light: $E = h\nu = hc / \lambda$
- $E = mc^2$ (Einstein) Therefore, $mc = h / \lambda$

for particles (mass) x (velocity) = h / λ

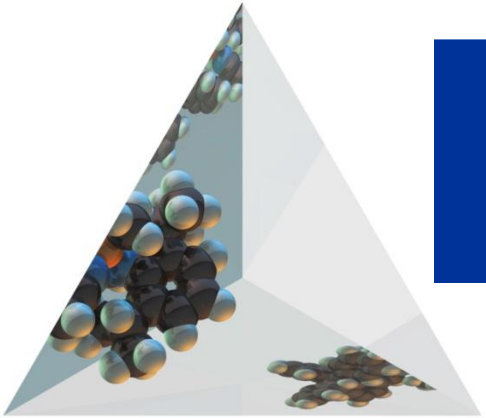
- The momentum, *mv*, is a particle property, whereas λ is a wave property.

Wave Behavior of Matter

The Uncertainty Principle

- **Heisenberg's Uncertainty Principle** : we ***cannot*** determine the exact position, direct motion, and speed of subatomic particles simultaneously.

- At best ***Erwin Schrödinger*** describe the position and velocity of an electron by a probability distribution, which is given by ψ^2



Quantum Mechanics and Atomic Orbitals

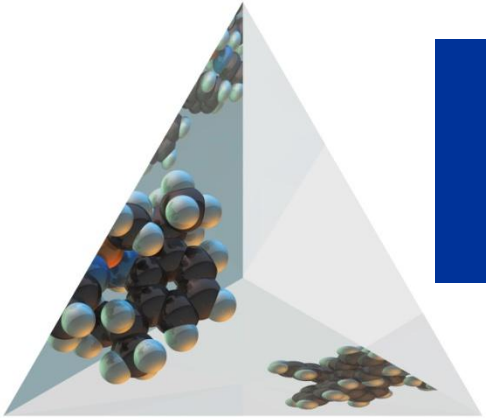
Orbitals and Quantum Numbers

- If we solve the Schrödinger equation, we get wave functions and energies for the wave functions.

  We call wave functions *orbitals*. (ψ)

- Schrödinger's equation requires 3 quantum numbers:

1. ***Principal Quantum Number, n.*** This is the same as Bohr's *n*. As *n* becomes larger, the atom becomes larger and the electron is further from the nucleus.

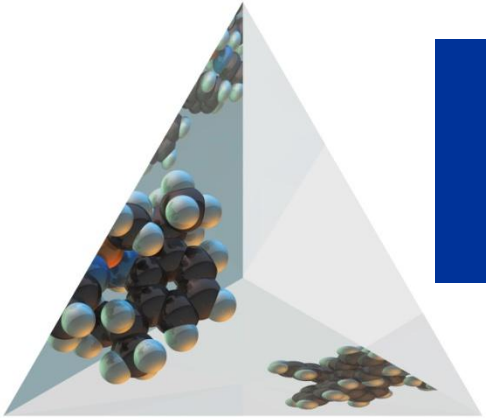


Quantum Mechanics and Atomic Orbitals

Orbitals and Quantum Numbers

2. ***Azimuthal Quantum Number, l*** This quantum number depends on the value of n. The values of *l* begin at 0 and increase to (*n* - 1). We usually use letters for *l* (*s*, *p*, *d* and *f* for *l* = 0, 1, 2, and 3). Usually we refer to the *s*, *p*, *d* and *f*-orbitals.

3. ***Magnetic Quantum Number, m_l*** This quantum number depends on *l*. The magnetic quantum number has integral values between -*l* and +*l*. Magnetic quantum numbers give the 3D orientation of each orbital.



Quantum Mechanics and Atomic Orbitals

Orbitals and Quantum Numbers

TABLE 6.2 Relationship Among Values of n, l, and m_l Through $n = 4$

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1*s*	0	1	1
2	0	2*s*	0	1	
	1	2*p*	1, 0, −1	3	4
3	0	3*s*	0	1	
	1	3*p*	1, 0, −1	3	
	2	3*d*	2, 1, 0, −1, −2	5	9
4	0	4*s*	0	1	
	1	4*p*	1, 0, −1	3	
	2	4*d*	2, 1, 0, −1, −2	5	
	3	4*f*	3, 2, 1, 0, −1, −2, −3	7	16

As *n* increases, note that the spacing between energy levels becomes smaller.

Many-Electron Atoms

Pauli Exclusion Principle

- **Pauli's Exclusions Principle**: No two electrons in the same atom can have exactly the same energy.
  - Therefore, two electrons in the same orbital must have opposite spins.

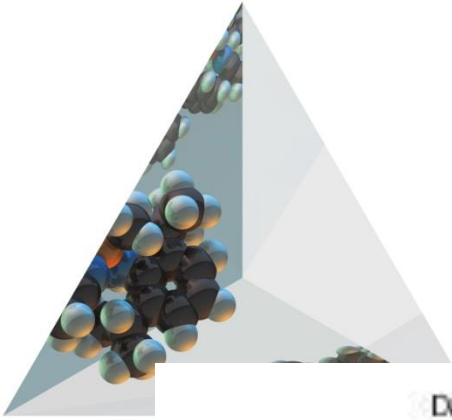
$4p^5$

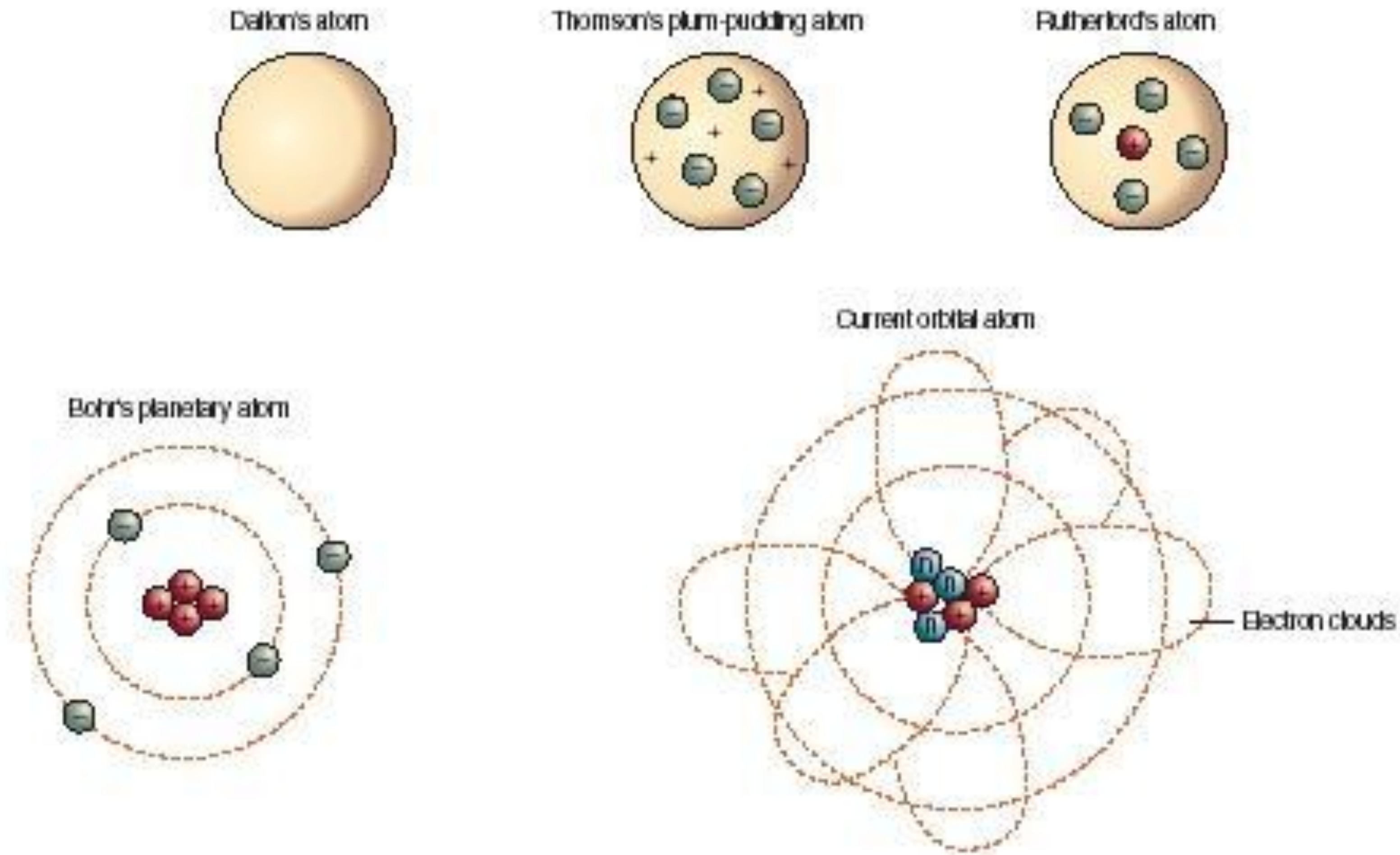
- **Distribution of all electrons in an atom, consist of**
  - **Number shows the energy level.**
  - **Letter shows the type of orbital.**
  - **Superscript shows the number of electrons in those orbitals.**

Electron Configurations

Hund's Rule

- Electron configurations tells us in which orbitals the electrons for an element are located.
- Three rules:
  - electrons fill orbitals starting with lowest *n* and moving upwards;
  - no two electrons can fill one orbital with the same spin (**Pauli**)
  - electrons fill each orbital singly before any orbital gets a second electron (**Hund's rule**).




Dalton's atom
Thomson's plum-pudding atom
Rutherford's atom
Bohr's planetary atom
Current orbital atom
Electron clouds