CH111 : Chemistry

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CHemistry111

3- Modules

- Physical Chemistry
- Inorganic Chemistry
- Organic Chemistry

Ground Rules: Module (1)

Attendance 80%

Continuous Evaluation

Mini Quizzes Best 4/5	4x2	= 08
Quiz	1x12	= 12
Mid-Semester Exam	1x30	= 30

Module aggregate minimum 40%

Module 1: Physical Chemistry

What Do You Get to LEARN?

- Basic Quantum Mechanics
- Atomic and Molecular Structure
- Intermolecular Forces
- Rates of Chemical Reactions
- Forces to Equilibrium

Recommended Texts (Physical Chemistry)

Physical Chemistry –I.N. Levine
Physical Chemistry – P.W. Atkins
Physical Chemistry: A Molecular Approach – McQuarrie and Simon

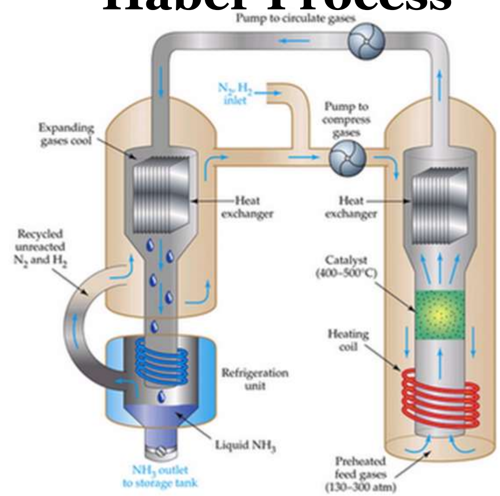
https://ocw.mit.edu/courses/5-61-physical-chemistry-fall-2017/

Why should Chemistry interest you?

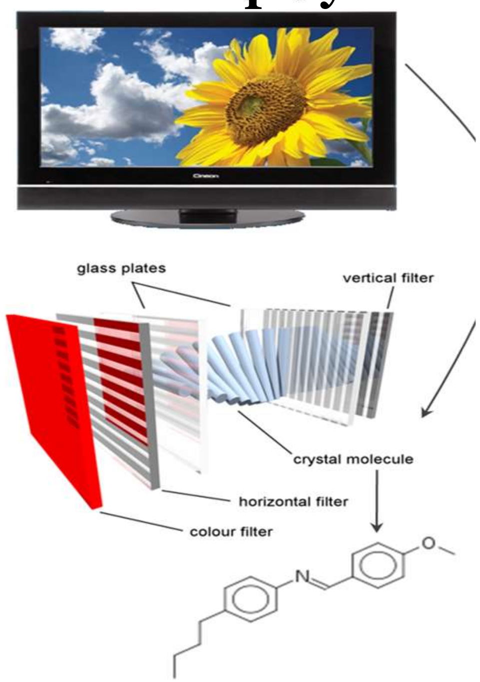
Chemistry plays major role in

1. Daily use materials:	Plastics, LCD displays
2. Medicine:	Aspirin, Vitamin supplements
3. Energy:	Li-ion Batteries, Photovoltaics
4. Atmospheric Science	Green-house gasses, Ozone depletion
5. Biotechnology	Insulin, Botox
6. Molecular electronics	Transport junctions, DNA wires

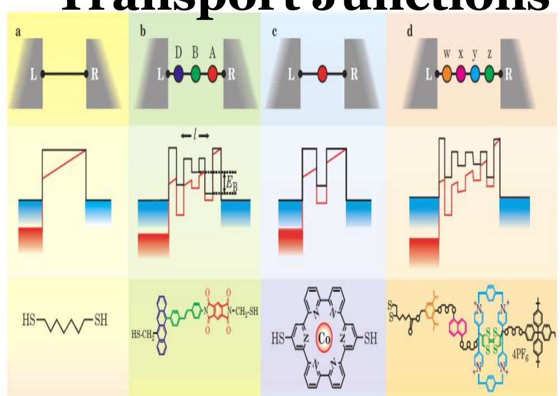
Haber Process



LCD Display



Transport Junctions



Haber Process

The Haber process remains largest chemical and economic venture. Sustains third of worlds population

Quantum theory is necessary for the understanding and the development of chemical processes and molecular devices

Classical Mechanics

Newton's Laws of Motion

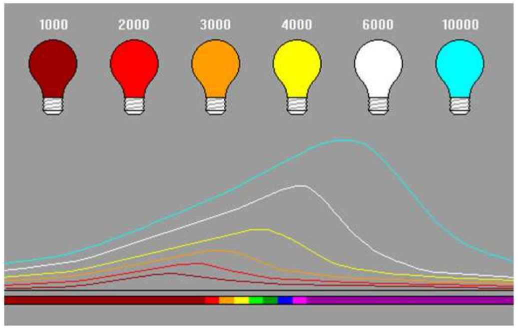
1. Every object in a state of uniform motion tends to remain in that state of motion unless an external force is applied to it.

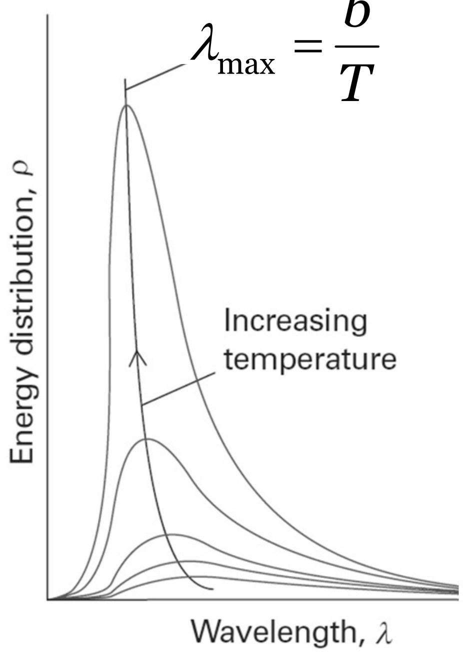
2. The relationship between an object's mass m, its acceleration a, and the applied force F is F = ma. The direction of the force vector is the same as the direction of the acceleration vector

3. For every action there is an equal and opposite reaction.

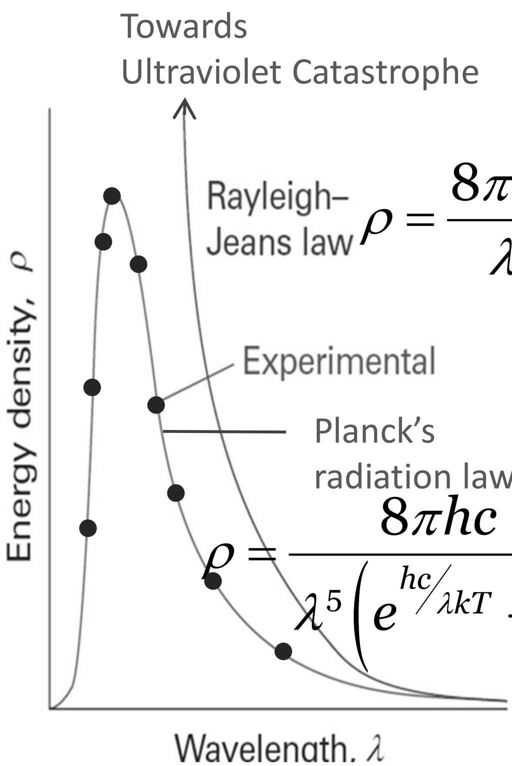
Black-Body Radiation; Beginnings of Quantum Theory

Hot objects glow





$$\lambda_{max} = \frac{b}{T}$$



$$\rho = \frac{8\pi kT}{\lambda^4}$$

$$\rho = \frac{8\pi hc}{\lambda^5\left(e^{hc/\lambda kT} - 1\right)}$$

Rayleigh-Jeans law was based on equipartitioning of energy

Planck's hypothesis
The permitted values of energies are integral multiples of frequencies
$E = nh\nu = nhc/\lambda$ $n = 0,1,2,\ldots$

Value of 'h' (6.626×10^{-34} J s) was determined by fitting the experimental curve to the Planck's radiation law

Planck did not believe in the quantum theory and struggled to avoid quantum theory and make its influence as small as possible

Heat Capacities of Solids

Element	Gram heat capacity J deg⁻¹ g⁻¹	Atomic weight	Molar heat capacity J deg⁻¹ mol⁻¹
Bi	0.120	212.8	25.64
Au	0.125	198.9	24.79
Pt	0.133	188.6	25.04
Sn	0.215	117.6	25.30
Zn	0.388	64.5	25.01
Ga	0.382	64.5	24.60
Cu	0.397	63.31	25.14
Ni	0.433	59.0	25.56
Fe	0.460	54.27	24.98
Ca	0.627	39.36	24.67
S	0.787	32.19	25.30

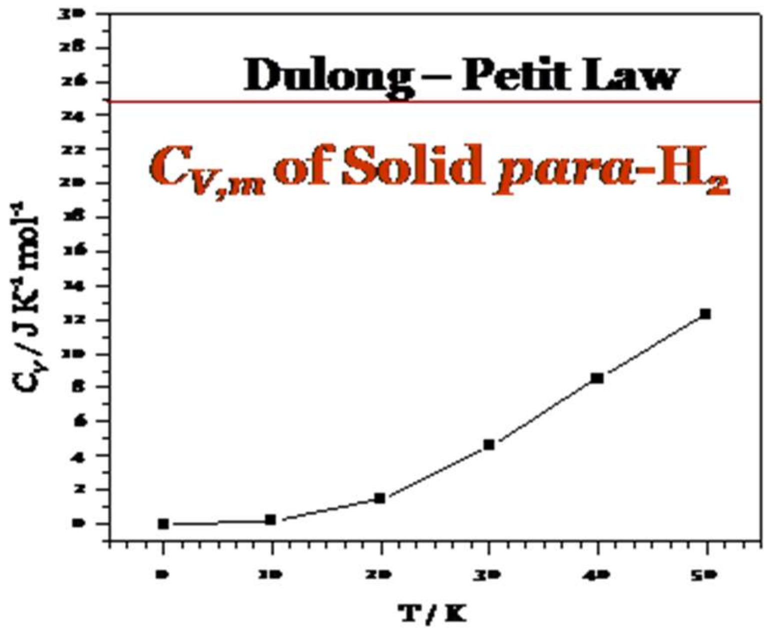
$$Um = 3N_A kT = 3RT$$

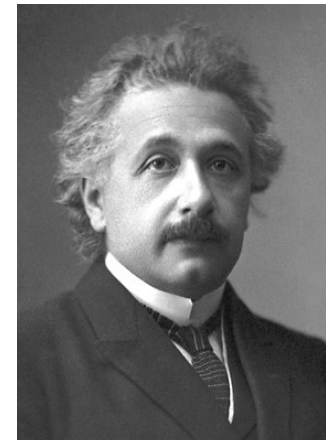
$$C_{V,m} = \left(\frac{\partial U_m}{\partial T}\right)_V = 3R \approx 25kJmol^{-1}$$

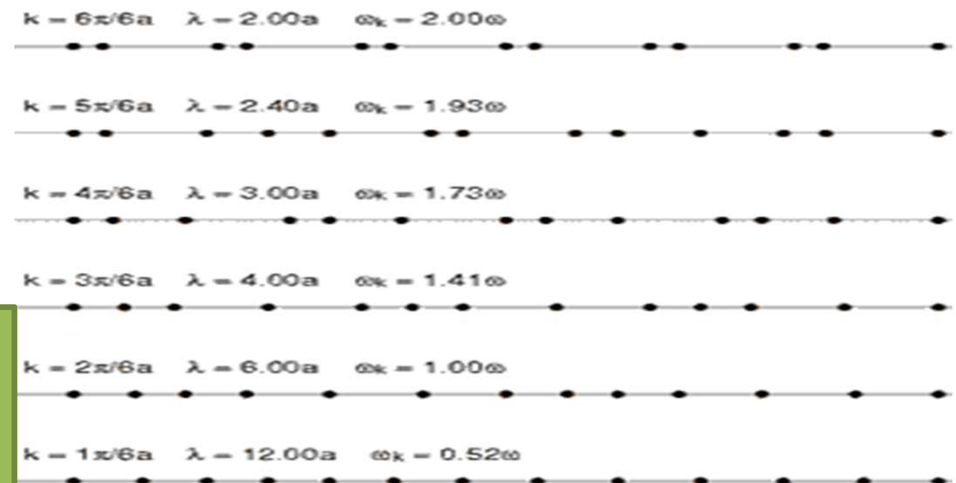
Dulong – Petit Law

The molar heat capacity of all solids have nearly same value of ~25 kJ

Heat Capacities of Solids







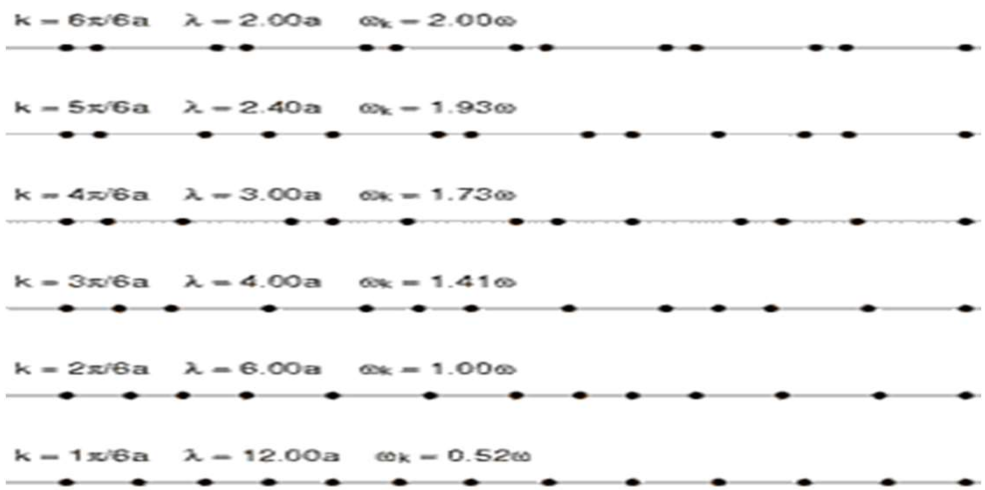
Einstein formula

Einstein considered the oscillations of atoms in the crystal about its equilibrium position with a single frequency ‘ν’ and invoked the Planck’s hypothesis that these vibrations have quantized energies ***nhν***

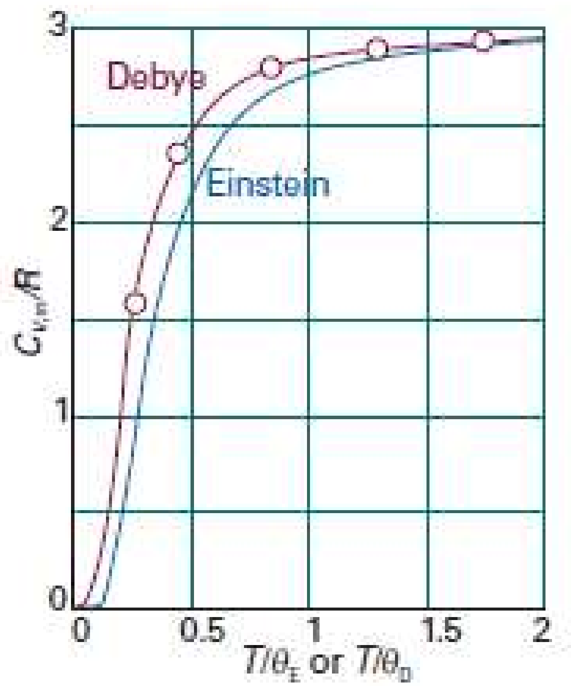
$$C_{V,m} = 3R\left(\frac{\theta_E}{T}\right)^2 \left(\frac{e^{\theta_E/2T}}{e^{\theta_E/T} - 1}\right)^2 ; \theta_E = \frac{h\nu}{k}$$

$$U_m = \frac{3N_A h\nu}{e^{h\nu/kT} - 1}$$

Heat Capacities of Solids



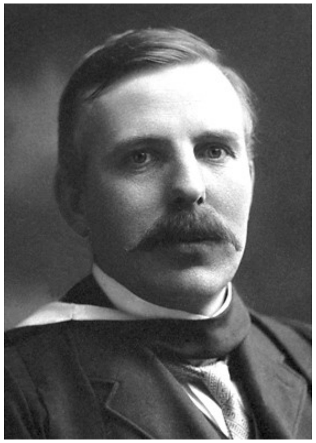
$$C_{V,m} = 3R\left(\frac{\theta_D}{T}\right)^3 \int_o^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\,dx; \theta_D = \frac{h\nu_D}{k}$$

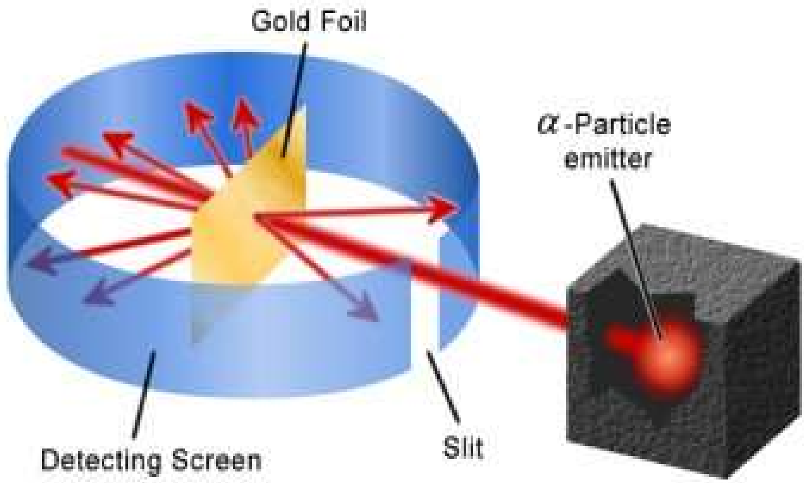


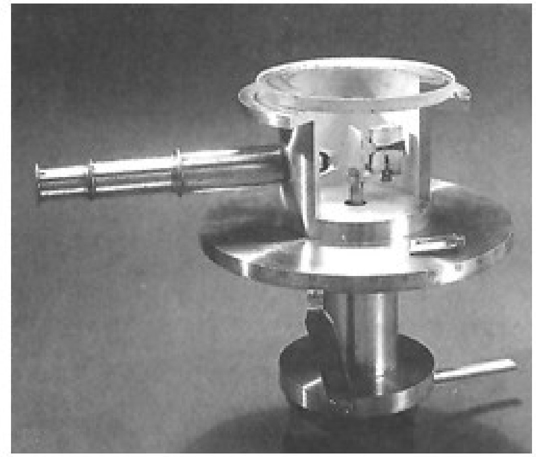
Debye formula

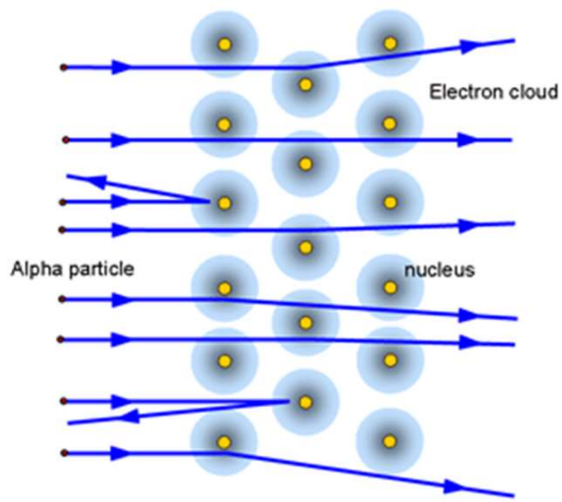
Averaging of all the frequencies ν_D

Rutherford Model of Atom



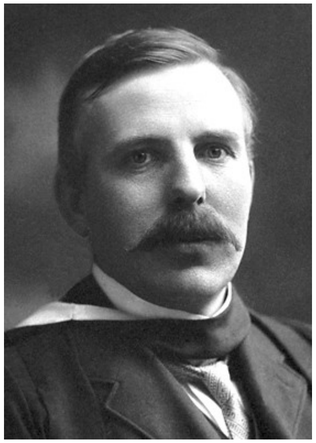


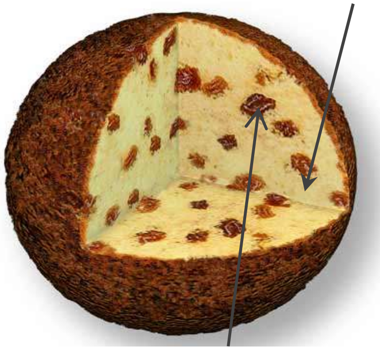




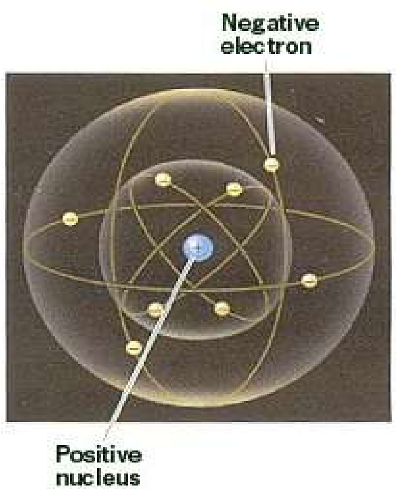
Alpha particles were (He^{2+}) bombarded on a 0.00004 cm (few hundreds of atoms) thick gold foil and most of the alpha particles were not deflected

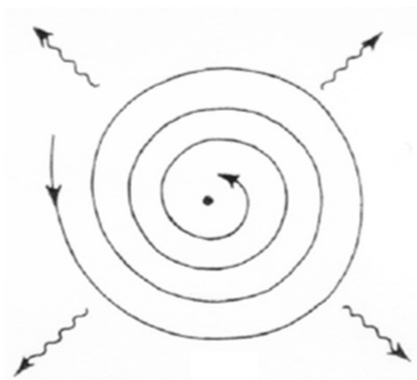
Rutherford Model of Atom





Thompson's model of atom is incorrect. Cannot explain Rutherford's experimental results

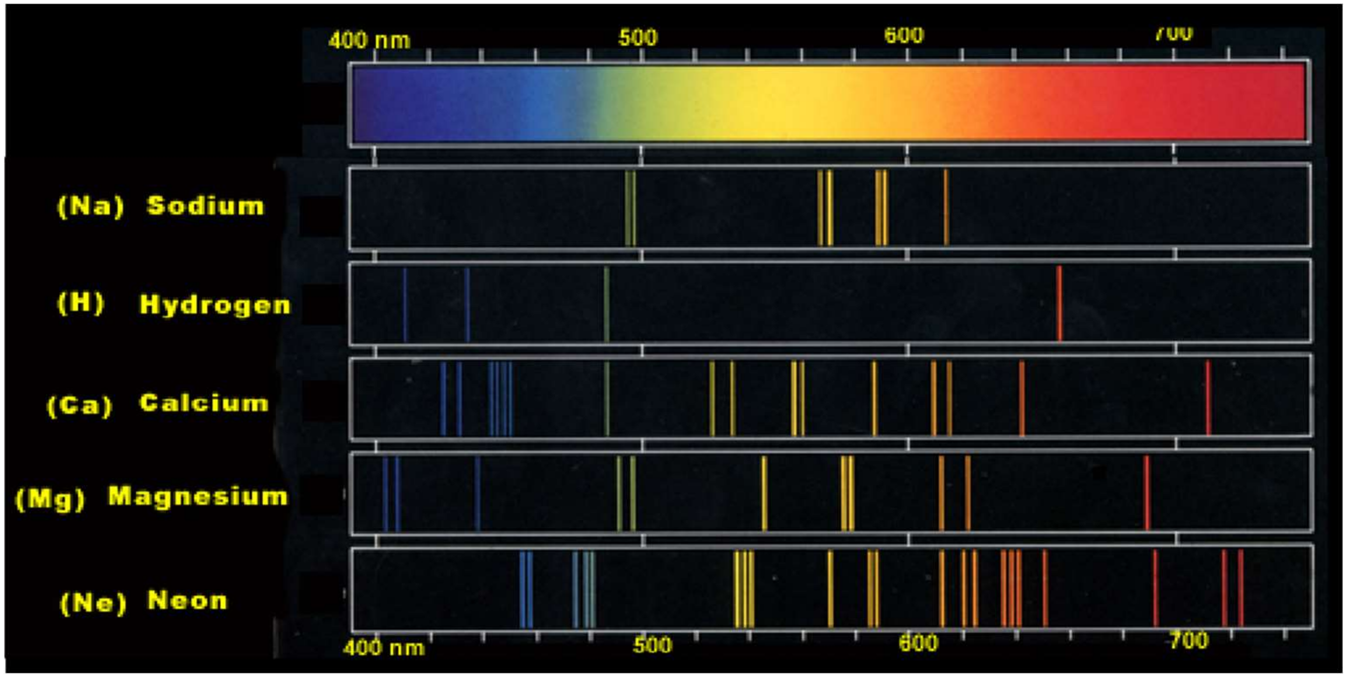




Planetary model of atoms with central positively charged nucleus and electrons going around

Classical electrodynamics predicts that such an arrangement emits radiation continuously and is unstable

Atomic Spectra



Balmer Series

410.1 nm
434.0 nm
486.1 nm
656.2 nm

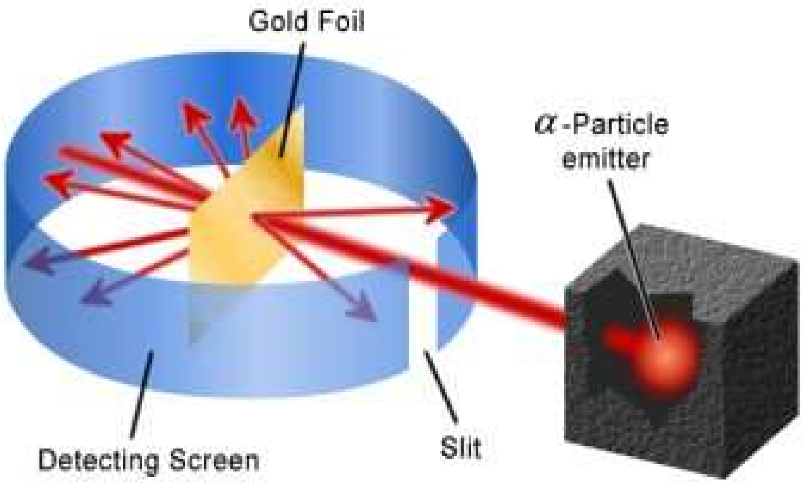
$$\frac{1}{\lambda} = R_\infty \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

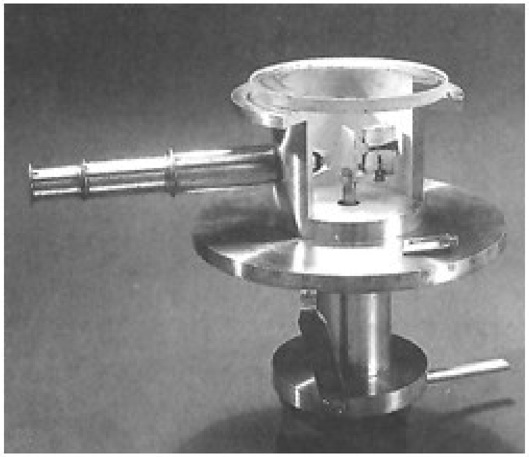
$$R_\infty = 1.09678 \times 10^7 \, m^{-1}$$

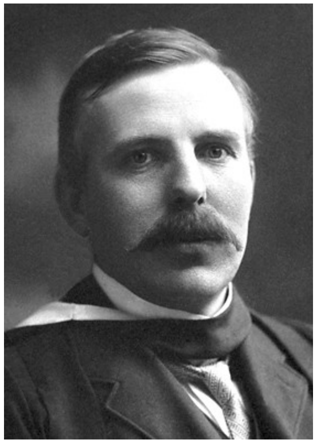
The Rydberg-Ritz Combination Principle states that the spectral lines of any element include frequencies that are either the sum or the difference of the frequencies of two other lines.

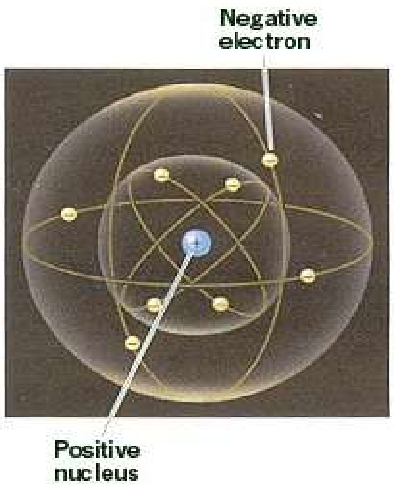
"R_∞ is the most accurately measured fundamental physical constant"

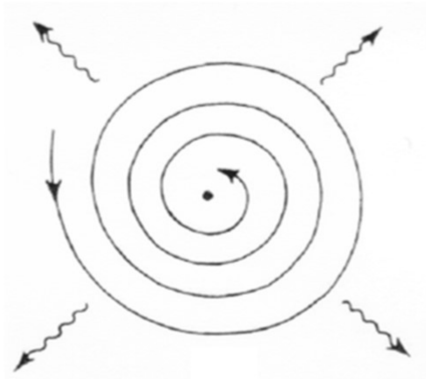
Rutherford Model of Atom







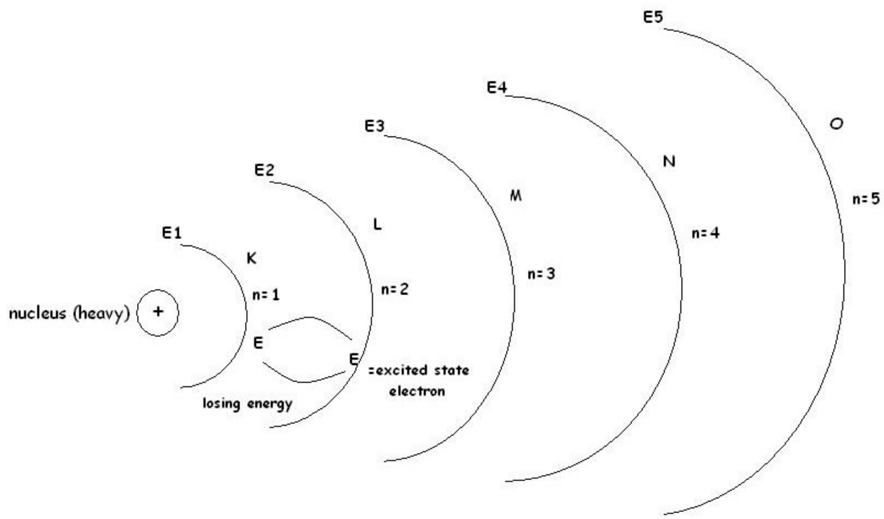




Planetary model of atoms with central positively charged nucleus and electrons going around

Classical electrodynamics predicts that such an arrangement emits radiation continuously and is unstable

Bohr Phenomenological Model of Atom



Electrons rotate in circular orbits around a central (massive) nucleus, and obeys the laws of classical mechanics.

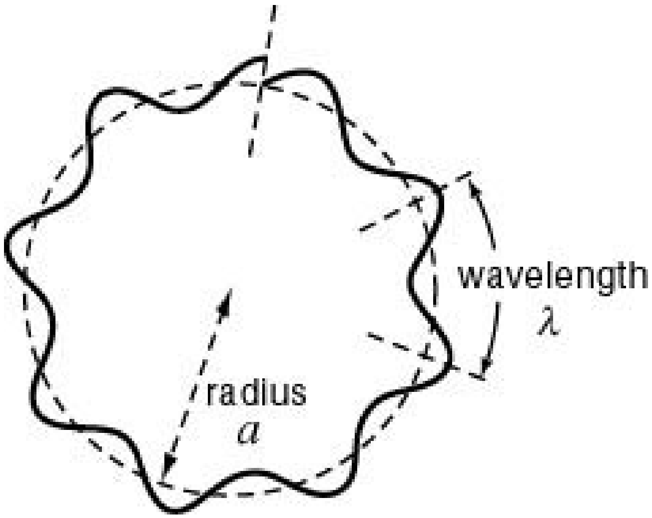
Allowed orbits are those for which the electron's angular momentum equals an integral multiple of $h/2\pi$ *i.e.* $m_e v r = nh/2\pi$

Energy of H-atom can only take certain discrete values: "Stationary States"

The Atom in a stationary state does not emit electromagnetic radiation

When an atom makes a transition from one stationary state of energy E_a to another of energy E_b, it emits or absorbs a photon of light: $E_a - E_b = h\nu$

Bohr Model of Atom



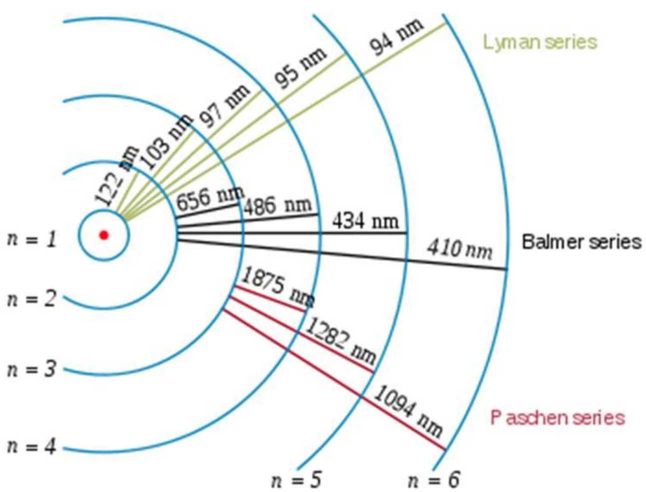
Angular momentum quantized

$$mvr = \frac{nh}{2\pi} \qquad \text{n=1,2,3,...}$$

$$(2\pi r = n\lambda\ )$$

Energy expression

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2} . \frac{1}{n^2}$$



Spectral lines

$$\Delta E = \frac{m_e e^4}{8\varepsilon^2 h^2}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = h\nu \qquad n_i, n_f = 1, 2, 3, \ldots$$

Explains Rydberg formula

$$R_\infty = \frac{m_e e^4}{8\varepsilon^2 h^2} = 1.09678 \text{ x } 10^{-2}\,\text{nm}^{-1}$$

Ionization potential of H atom 13.6 eV

Bohr Model of Atom

The Bohr model is a primitive model of the hydrogen atom. As a theory, it can be derived as a first-order approximation of the hydrogen atom using the broader and much more accurate quantum mechanics