Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- The fifth lecture -

Stage 4

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Chapter 3

(Origin of quantum theory)

((The origin Quantum Theory))

The relationship of energy radiated by materials is one of the issues that scientists were interested in, as at the end of the 18th century scientists accepted Newton's theory.

(Visible color change, which is a component of fine particles)

But at the beginning of the 17th century Thomas provided an introduction to wave theory, and at the end of the century Schrodenker discovered X-rays, then the phenomenon of radiation activity by Birkel, and then the discovery of the electron by Thompson until the emergence of electromagnetic radiation results by maxwell, thus making it clear to scientists that the general laws of nature are

1) Newton's laws of mechanics.
2) Laws of maxwell Electromagnetic Theory

Newton's laws are used to calculate celestial bodies as well as the movement of machines, but McQuill developed a general theoryfor the treatment of electromagnetic radiation after the discoveries of scientists(Faraday,Amber, Nolte, Colom) so some experiments and phenomena that led to the emergence of quantum theory are briefly addressed:

1. Black-body radiation
2. Photoelelctric effect photoelelctric effect
3. Atomic Spectra

1)Black-body radiation

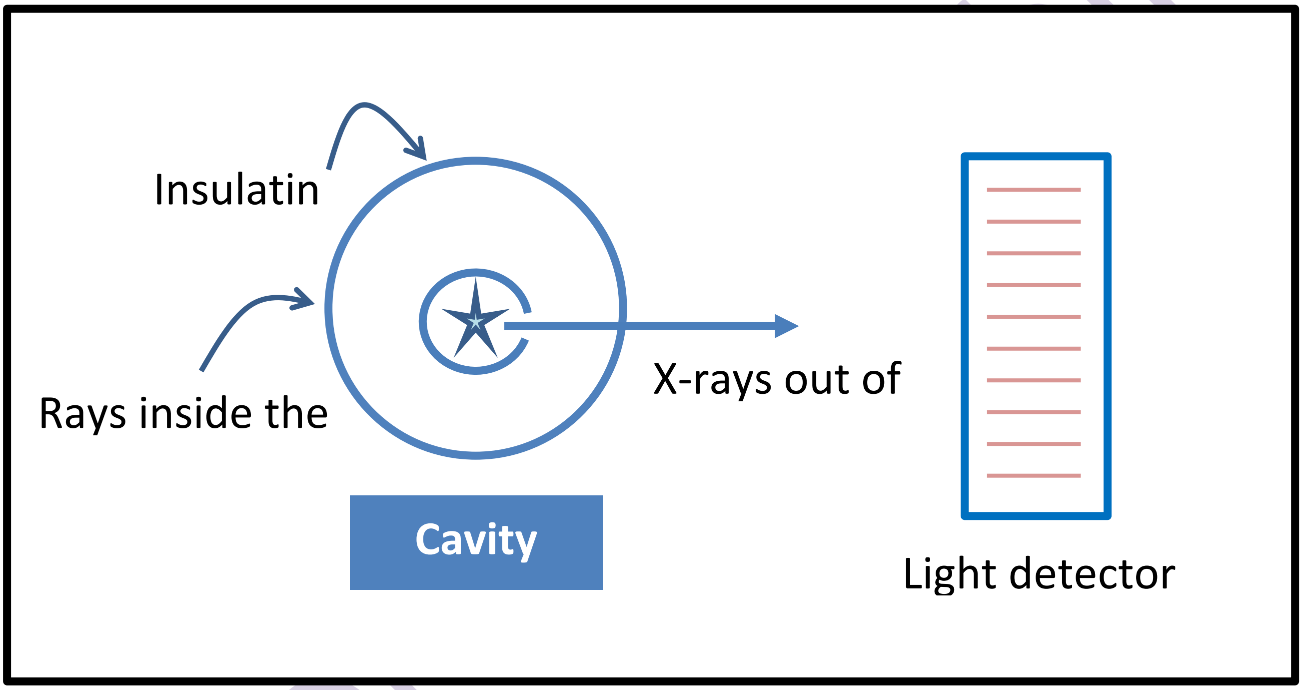
It is an ideal system that absorbs all the rays falling on it (it is also an ideal radiator when it is a source of radiation)and can be represented practically by a narrow opening and the least cavity gap or hollow object.

Therefore, when a particular particle is heated, the resulting radiation spectrum has a wide range of frequencies, i.e. when hot objects emit radiation at different wavelengths where:

a)In hot gases give linear spectra.
b)Hot solids give continuous spectra.
c)Irritable molecules give packages called package spectrum.

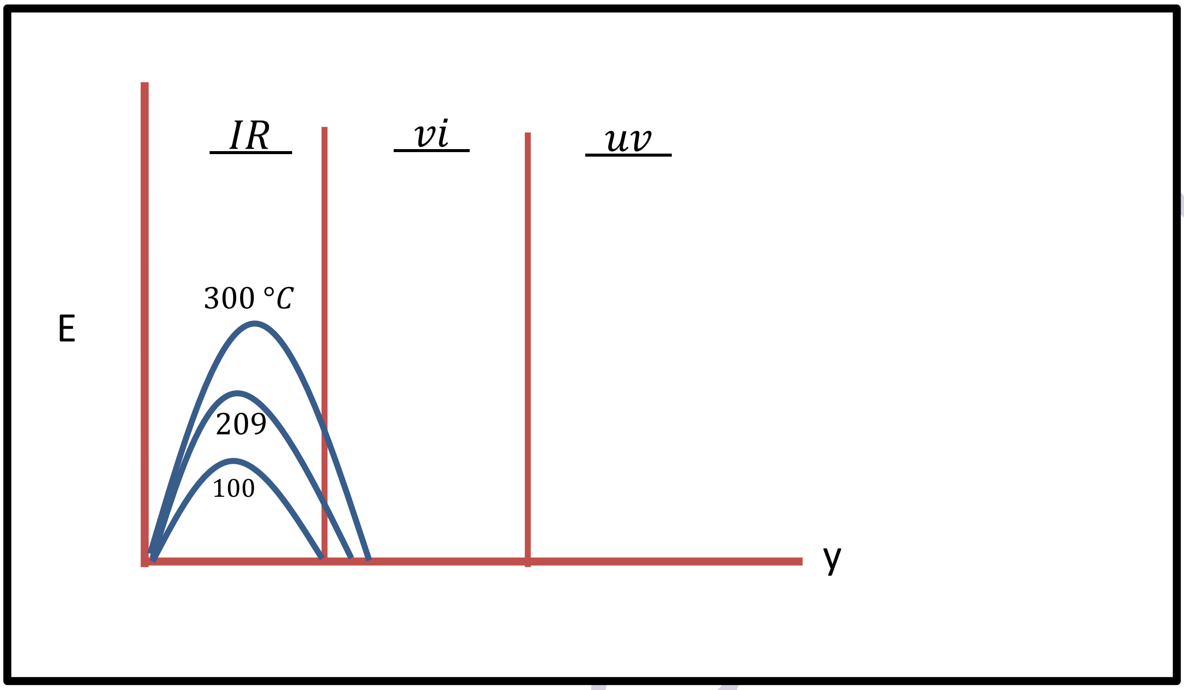
So these studies need a black particle that absorbs all the rays falling on it and no black particle has this characteristic.

So a cavity gap with a insulating wall was used in the ocean which contains a small hole as in shape



The energy coming out of the hole is calculated only so the space heats up inside the gap and thus emits radiation where radiation is a bundle of different frequencies and the bodies differ in their absorption of radiation and this is the result of different frequencies and this is done with different temperatures.   It can be observed through color change so the color of radiation varies as a result of different frequency so the device can measure energy for each frequency

Thus, the spectral distribution curve of black body radiation energy can be drawn.



So when 100 ℃ curves show a value with little red radiation, the energy is not evenly distributed on all frequencies.

The point represents the highest value at 200 curves with a value that gives the highest energy towards higher frequencies as well as observe the large value and see thecolor clearly at <u>300.</u>

Attempts to explain the phenomenon of black body radiation

1. The hypothesis or principle of equal energy assessment

principle of equipration energy

The energy of any particle body is KT.

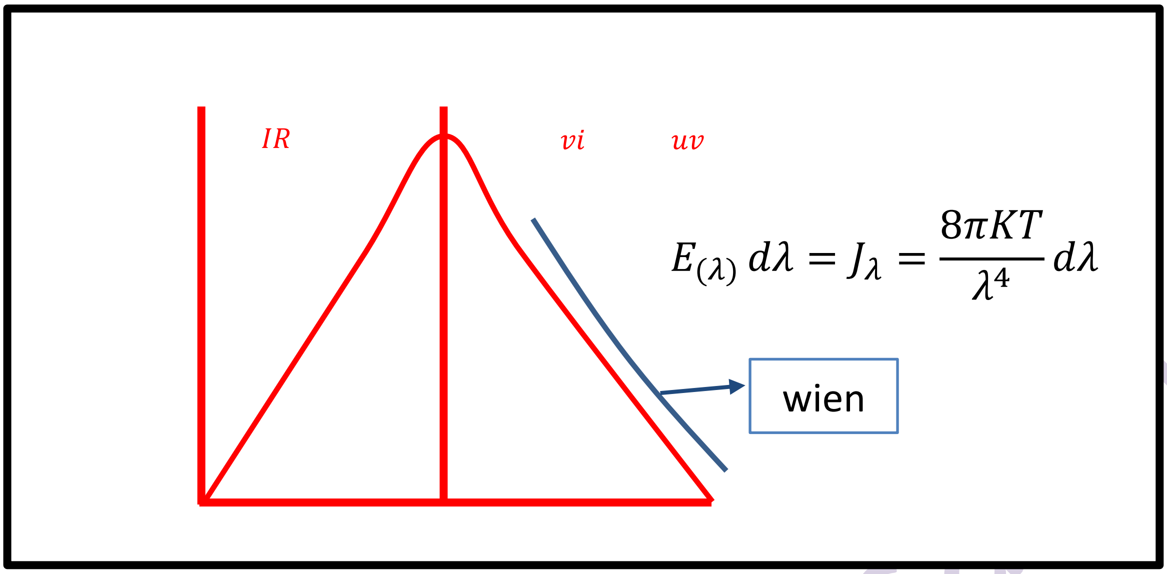
K: Boltzman Constant = 1.38*10-23

T:Absolute thermal grade.

So this hypothesis assumes energy is evenly distributed half KT by kinetic energy and half KT in latent energy so when applied to this form it is possible not to contain frequency and curve is to draw energy versus frequency so this principle is a failure.

2. Try wien (Finn)

Finn noted that the energy emitted by a hot body consists of a continuous spectra continuous spectrum where wavelengths change by changing the heat reaction as in the form:



So at low temperatures, radiation has low energy (higher wavelength) in the infrared region.

However, radiation energy (frequency increases) increases with temperature.

That is, the frequencies of radiation emitted are displaced to higher values as the temperature increases, so the Finn Law of Displacement is called wien displacement law.

$$\lambda_{max} T = Constant = 2.9\ nm$$

It is also clear from the change in the color of a piece of iron when raising the temperature of red, then orange, then yellow and then white.

So Finn's relationship to displacement changes energy for a range of frequencies:

$$E\gamma\, d\gamma = \frac{8\pi k\, B\, y^3}{C^3} \cdot e^{-Byr} dy$$

Constant Boltzman k

Fixed Finn B

$$B = \frac{h}{k} \Longrightarrow \frac{6.63 * 10^{-34}}{1.38 * 10^{-23}} = 4.8 * 10^{-11}$$

The world was able to derive the spectral distribution of black body energy, which was consistent with high frequencies and failed in the low frequency area.

3.Stefan 1879 (Stefan Equation)

Stefan derived an equation through painting and was named after Stefan's equation, where he found Wallace's fourth energy relationship to the thermal degree through a constant amount called Stefan's tits.
$(\sigma = 5.6 * 10^{-8}\, J.m^2\, T^{-4}\, s^{-1})$

This law states: -

* (The rate of energy emission from a hot object is directly proportional to the fourth ace of absolute thermal degree)**

$$E = \sigma T^4$$

This attempt could not explain low energy at high frequencies and thus failed to explain the stratification of radiation.

4. Try Riley - Rayleigh Jeans

Scientists Riley and Jeans incorporated Stefan's law into one law (the intensity of thermal radiation from a hot object is consistent with both the absolute thermal degree and the frequency of radiation emitted).

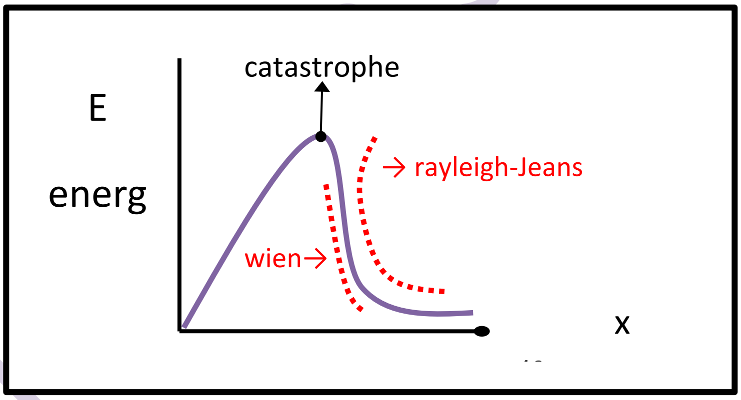
Electromagnetic radiation is an electrical oscillator and each oscillator can take any value from energy and these oscillators are all affected at the same time when powered up to high frequencies can be affected by low energy and depending on the following relationship

$$Ey \, . dy = \frac{8\pi KT \, y^2}{C^3} dy$$

Therefore, when this was applied, it was found to be correct at low frequencies (high wavelengths), the IRarea.

As we approach the uv area, the calculated energy increases and approaches the end (approaching the danger zone) and no body has infinity energy.

This equation matches the results in low frequencies (IR) and according to this formula, the energy increases as it approaches the high frequencies until it reaches the infinity. This is not true in practice, so we reach the so-called ultraviolet catastrophe



5. Plank Distribution Law

Planck assumed that harmonic oscillator harmonic oscillator oscillator

Does not continuously emit or absorb energy, but in specific quantities called quantum punches, i.e. energy

$$E = h\gamma \longrightarrow (1)$$

To see how many patterns in the size unit have frequencies $(\gamma + \Delta\gamma)$

So the frequency range pattern according to Planck's relationship is

$$N_A = \frac{8\pi\gamma^2}{C^3} dy \longrightarrow (2)$$

According to Boltzman's law,

$$N_A = N_o e^{-E/KT} \longrightarrow (3)$$

N_{A}: - The number of oscillators that have its capacity $E = h\gamma$

N_{o}: - Number of oscillators in the case of minimum energy

So the total number of oscillators

$$N = N_o + N_1 + N_2 + \cdots \longrightarrow (4)$$

The equation (4) can be written in Boltzman format

$$N = N_0 + N_\circ e^{-h\gamma/KT} + N.e^{-2h\gamma/KT} + \cdots \longrightarrow (5)$$

And you write a shortcut.

$$N = N_o \sum_{n=0}^{n=\infty} e^{-nh\gamma/KT} \longrightarrow (6)$$

Thus, the total energy of all oscillators can be calculated from the $E\gamma$ product of the collection of power multipliers in the number of oscillators and by the following relationship:

$$E\gamma = \sum_{n=0}^{n=\infty} N_A \; En \;\longrightarrow (7)$$

$$\left.\begin{aligned} N_A &= \frac{8\pi\gamma^2}{c^3} dy \\ En &= \frac{h\,\gamma\, e^{-h\gamma/KT}}{i - e^{-h\gamma/KT}} \end{aligned}\right\} \longrightarrow (8)$$

$$E\gamma = \frac{8\pi h\gamma^3}{c^3} \cdot \frac{e^{-h\gamma/KT}}{1 - e^{-h\gamma/KT}}$$

Planck
Distribution Act

Planck's spectroscopic distribution law, which corresponds to the results of black body radiation at low and high frequencies.

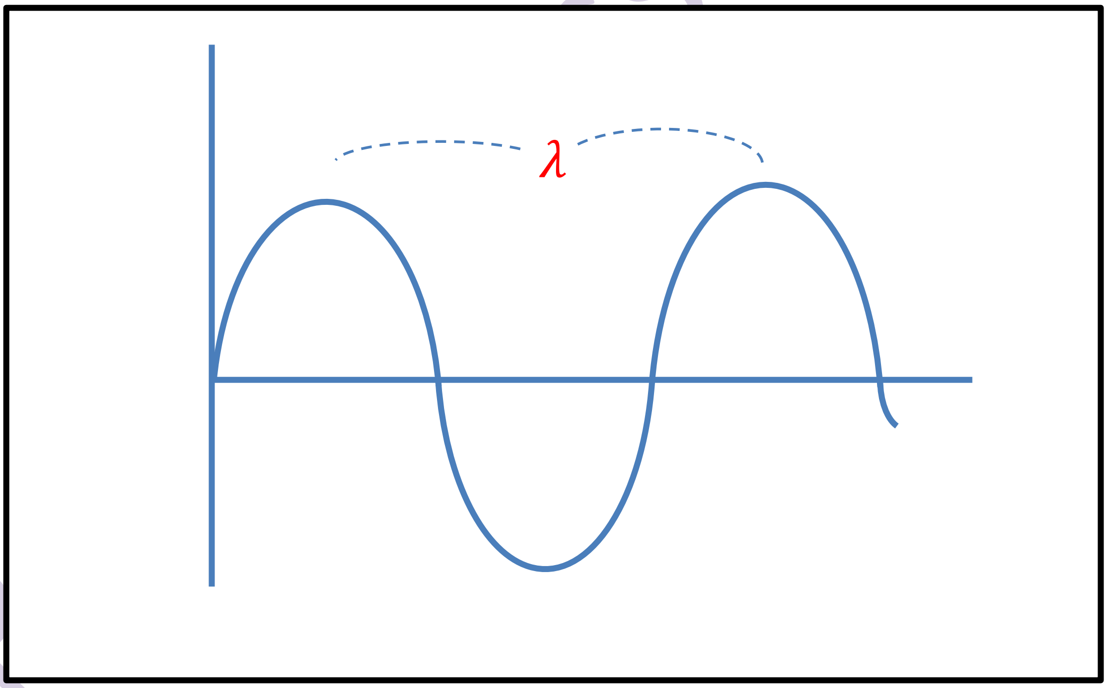
But Planck proved that the oscillator's energy is unstable, proportional to the frequency, $E = h\gamma$where the oscillator's energy is the multiples of this magnitude.

Anyenergy equals:

$$E = nh\gamma \qquad n = 0,1,2,3, \ldots$$

Electro magnetic electro-radiation

It is one of the images of energy. Any means of energy transmission in vacuum and does not need a medium to move and thus consists of an electrical magnetic vector in the case of perpendicular changes periodically and flows in a direction called the direction of the wave rays as in the form



Electromagnetic radiation must therefore possess all waveform qualities:

1)Frequency: - frequency γ - the number of cycles per second.

$$\gamma = \frac{c}{\lambda} reluctance$$

2)Wave length:- is the necessary distance for one cycle and expressed (no,nm).

$$\lambda = \frac{c}{\gamma}$$

3)Wave number number:- Number of courses per cm

$$\bar{\gamma} = \frac{1}{\lambda} = \frac{\gamma}{c}$$

So the oscillator's energy can be calculated from the relationship.

$E = hc\bar{\gamma}$ (Derivation)