ATOMIC MODELS

BOHR ATOMIC MODEL

In 1913, Bohr asserted that electrons acted in certain orbitals around the atomic nucleus and he received the Nobel Prize in Physics in 1922 for his work on the structure of the atom.

Bohr's objections to Rutherford:

1) *According to the classical electromagnetic theory, the circular moving particle must lose its energy by continuously radiating and must slow down gradually.*
2) *Since the nucleus and electrons will attract each other, it is expected that electrons decreasing energy will collide with the nucleus by drawing a spiral.*
3) *If the electron passes from an orbital to an orbital closer to the nucleus, it emits energy. If the electron passes from an orbital to another orbital by moving away from the nucleus, it absorbs energy.*

Bohr argued that the electrons in the atom did not radiate despite the circular motion. This postulate was based on the following research which he calculated the wavelengths of the rays emitted by hydrogen atom and the results were consistent with the well-known experimental data. According to Rutherford, the atom consists of a (+) charged nucleus where almost all the mass is collected and electrons orbiting around it.

However, Rutherford's model remained insufficient in two ways:

1) According to the classical mechanics, an electron rotating around (+) the nucleus must lost energy and eventually have to fall on the nucleus.

2) There is no relation between the frequencies of the lines in the spectrum and the calculated rotational frequencies for an electron which is rotating around the nucleus.

$$mvr = n\frac{h}{2\pi}$$

Bohr cannot explain:

1. *When the spectrum of H_2 gas was examined and the spectrum lines were opened, it was seen that these lines consisted of two or more lines. This is because of the isotope effect. Bohr only used m. He should have used the reduced mass. That is, Bohr only used the mass of the electron and did not consider the nucleus.*

   $^{1}_{1}H-^{1}_{1}H\ ;\ ^{2}_{1}H-^{1}_{1}H\ ;\ ^{2}_{1}H-^{2}_{1}H$

   $$\frac{1}{\mu}=\frac{1}{m_1}+\frac{1}{m_2},\ or\ \ \mu=\frac{m_1.m_2}{m_1+m_2}$$

   μ= *reduced mass*

   m_1= *mass of the electron*

   m_2= *mass of the proton*

2. *There is objection to the concept of orbital. Bohr says only the spherical orbitals, which means that the electrons move circularly. But, other physicists say that the electron can circulate in ellipsoidal orbitals.*
3. *De Broglie and Heisenberg have objections. Bohr is thinking of the electron as a particle when creating the model. He gives the formulas accordingly. For the first time, De Broglie reveals that the electron has a wave character. De Broglie says that small particles such as electrons, neutrons and protons have a wave character.*

   The wave property of particles, whose masses are too small from the mass of the electron (9.11.10^{-31} kg), can be neglected because the wavelength is too small to be measured. However, the wave property of the electron cannot be neglected. Therefore, a quantum model is required for the electron.

BOHR HYDROGEN ATOMIC MODEL

In 1913, Niels Bohr proposed an atomic model using the line spectra of the hydrogen atom. According to Bohr, the hydrogen atom has certain energy values. The emission or absorption of an atom is possible with the electron transition from one of the energy levels to another. For example, when an electron passes from a high energy level E2 to a lower energy level E1, a photon, which its energy is equal to the difference between these two levels, is radiated. If the energy of this photon is E = hν, $\Delta E = h\nu = E_2 - E_1$

According to the classical electromagnetic theory, the electron must lose energy and fall in the nucleus.

This is in contrast to the presence of the atom with nucleus presented by Rutherford. The Bohr assumptions proposed to eliminate this contradiction are as follows:

1. *Electrons rotate at constant speed in stable circular orbitals around the nucleus. The centrifugal force on the electron during rotation and the Coulomb pulling force applied to the electron by the nucleus in the opposite direction to this are equal (Each electron can be found in circular orbitals from the nucleus only at certain distances. Each orbital has a certain energy).*

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\varepsilon_0 r^2}$$

2. *The angular momentum of the electron was quantized. n is the principal quantum number and angular momentum of electrons moving by following circular orbitals around the nucleus may take certain values.*

$$mvr = n.\frac{h}{2\pi}$$

3. *If an electron at a high energy level (*E_2*) falls to low energy level (*E_1*), ray with the energy equal to the energy difference between E1 and E2 levels spreads.*

$$\Delta E = E_2 - E_1 = h.\nu$$

Calculation of Bohr Radius (electron's distance to the nucleus, the radius of the orbitals)

Single electron systems such as H, He^{+}, Li^{2+}, Be^{3+} can be examined using the Bohr model. The electron, which follows a certain orbital, is under the influence of two opposing forces. These are the Coulomb pulling force applied to the nucleus by electrons and the centrifugal force of the electron rotating on the orbital.

Since the electron is constantly following up the same orbital, these two forces must be equal to each other.

$$F_{coulomb} = F_{centrifugal}$$

$$\frac{1}{4\pi\varepsilon_0} \cdot \frac{q_1 \cdot q_2}{r^2} = \frac{mv^2}{r}$$

q_1=charge of the electron
q_2=total charge of the nucleus

$$\frac{1}{4\pi\varepsilon_0} \cdot \frac{Z \cdot e^2}{r^2} = \frac{mv^2}{r} \Rightarrow \boxed{v^2 = \frac{e^2 Z}{4\pi\varepsilon_0 r m}}$$

$$mvr = n \cdot \frac{h}{2\pi} \Rightarrow v = \frac{n \cdot h}{2\pi m r} \qquad v^2 = \frac{n^2 h^2}{4\pi^2 m^2 r^2}$$

$$\frac{e^2 Z}{4\pi\varepsilon_0 r m} = \frac{n^2 h^2}{4\pi^2 m^2 r^2} \Rightarrow r = \frac{\varepsilon_0 \cdot n^2 h^2}{\pi m e^2 \cdot Z} \Rightarrow r = \frac{n^2}{Z} \cdot a_0$$

The radius of Bohr=0.0529 Å (shows 1s orbital of hydrogen)

$\varepsilon_0 = 8{,}85 \cdot 10^{-12}\ C^2/Nt \cdot m^2$
$h = 6{,}62 \cdot 10^{-34}\ J.sn$
$m = 9{,}1 \cdot 10^{-31}\ kg$
$e = 1{,}602 \cdot 10^{-19}\ C$

an electron in orbital n=1 can approach 0.529 Å to the nucleus.

Energies of Bohr Orbitals

The total energy of the electron is equal to the sum of the kinetic and potential energies.
$E_T = E_K + E_P$

$$E_k = \frac{1}{2}mv^2 \Rightarrow v^2 = \frac{e^2 Z}{4\pi\varepsilon_0 r m} \Rightarrow E_k = \frac{Z e^2}{8\pi\varepsilon_0 r}$$

$$E_p = V(-e) = -\frac{Z e^2}{4\pi\varepsilon_0 r}$$

$$E_T = E_k + E_p = \frac{Z e^2}{8\pi\varepsilon_0 r} - \frac{Z e^2}{4\pi\varepsilon_0 r} = -\frac{Z e^2}{8\pi\varepsilon_0 r} \qquad r = \frac{\varepsilon_0 n^2 h^2}{\pi m e^2 Z}$$

$$E_T = -\frac{Z e^2}{8\pi\varepsilon_0 \cdot \frac{\varepsilon_0 n^2 h^2}{\pi m e^2 Z}} = -\frac{Z^2 e^4 m}{8\varepsilon_0^2 h^2}\left(\frac{1}{n^2}\right)$$

$A = -2{,}18 \cdot 10^{-18}\ J/atom$

$_1H^0$: $Z=1$
$_2He^+$: $Z=2$
$_3Li^{2+}$: $Z=3$
$_4Be^{3+}$: $Z=4$
$_5B^{4+}$: $Z=5$
$_8O^{7+}$: $Z=8$

1 electron systems

Energy difference between energy levels (ΔE)

$$\Delta E = E_2 - E_1 = -\frac{A}{n_2^2} - \left(-\frac{A}{n_1^2}\right) = h\cdot\nu = h\cdot\frac{c}{\lambda} \Rightarrow c\cdot\bar{\nu} = \frac{A}{h}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\bar{\nu} = 10973731\ m^{-1}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

Rydberg constant

For ionization energy $E = 2{,}18 \cdot 10^{-18}\left(\frac{1}{1^2} - \frac{1}{\infty^2}\right)$

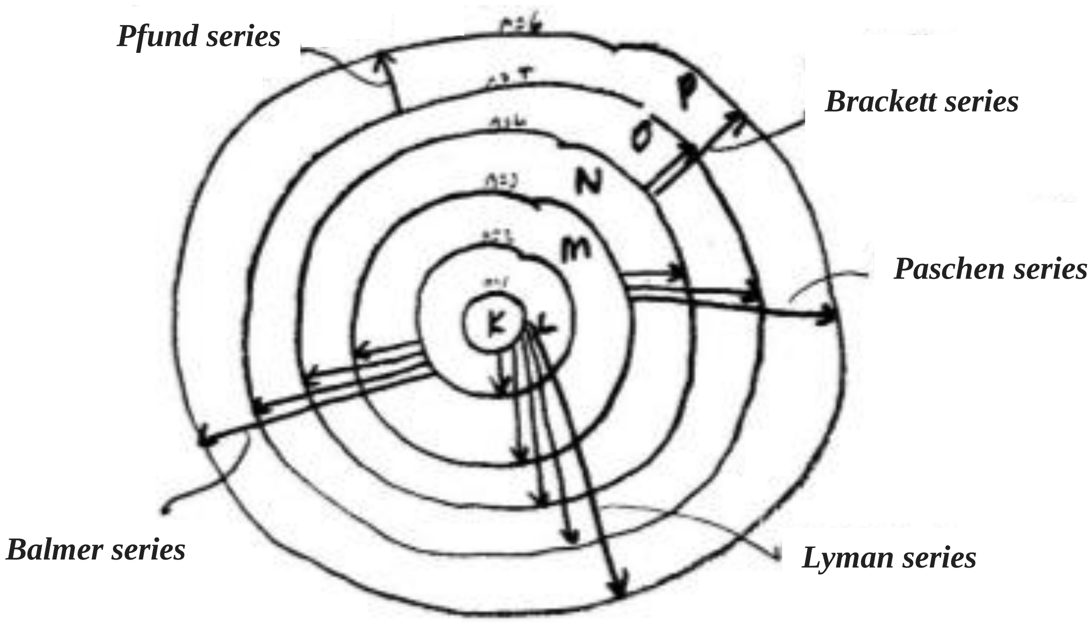
$1\ eV = 1\ J$
$1\ J = 10^7\ erg$
$1\ eV = 23{,}06\ kcal/mol$
$1\ cal = 4{,}184\ J$

$$2{,}18\times10^{-18}\ J/atom\ (6{,}022\times10^{23}\ atom/mol) = 2{,}18\times10^{-18}\times 6{,}022\times10^{23}\ J/mol = 1312\ kJ/mol.$$

For multi-electron atoms, in the Bohr energy equation, Z is replaced by Z. Because there is screening.*

$$E_T = -\frac{m Z^{*2} e^4}{8\varepsilon_0^2 n^2 h^2}$$

Bohr theory explains the atomic spectrum of hydrogen. By changing the n_1 and n_2 values in the equation, the series corresponding to the different spectrum lines are obtained (Lyman, Balmer, ...).



When an atom makes an emulsion it gives the line spectrum. Absorption of an atom equals the emulsion. It is a fingerprint for an atom.

The dark radiation and the luminous radiation of hydrogen are the same.

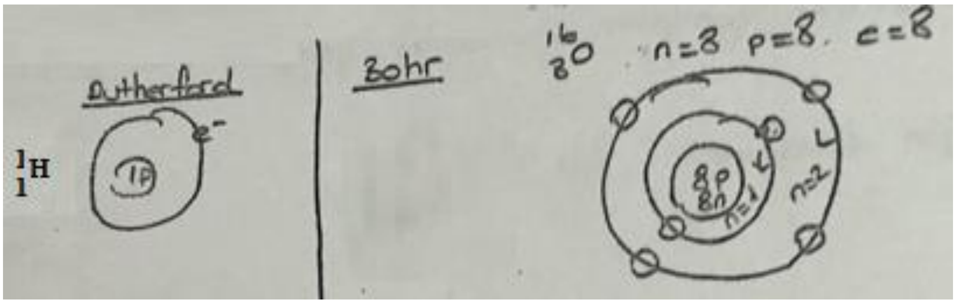
The energy of the layers closest to the nucleus is larger than the others.

$$\nu = \frac{1}{x} = Ry\left(\frac{1}{{n_1}^2} - \frac{1}{{n_2}^2}\right) = \frac{A\,(Z*)^2}{h.c}\left(\frac{1}{{n_1}^2} - \frac{1}{{n_2}^2}\right)$$

1) *If n_1=1 and n_2=2,3,4,5,… Lyman series, ends at K, UV region.*
2) *If n_1=2 and n_2=3,4,5,6,… Balmer series, ends at L, Visible region.*
3) *If n_1=3 and n_2=4,5,6,7,… Phashen series, ends at M, IR region.*
4) *If n_1=4 and n_2=5,6,7,8,… Bracket series, ends at N, IR region.*
5) *If n_1=5 and n_2=6,7,8,9,… Pfund series, ends at O, IR region.*
6) *If n_1=6 and n_2=7,8,9,10,… Humpheries series, ends at P, IR region.*

Developments after the Bohr Atomic Model

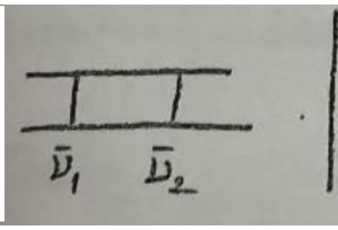
The only common side of the Rutherford atomic model with the Bohr atomic model is the drawing at $_1{}^1H$.



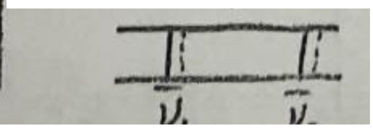
QUESTION: *Why has not the spectrum of hydrogen the only one line? Why didn't the Bohr atomic model explain this?*

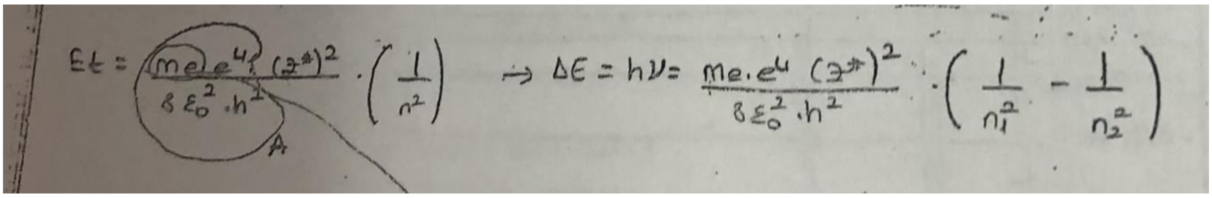
Because there are isotopes of hydrogen. Bohr saw these isotopes overlapping. Therefore, he said a single line. However, it was observed that this spectrum had more lines with developing devices.

The spectrum drawn by Bohr



The spectrum after Bohr

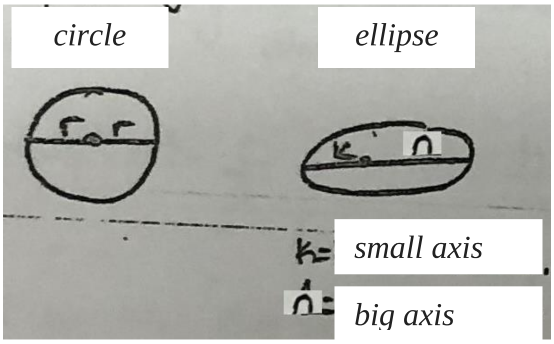


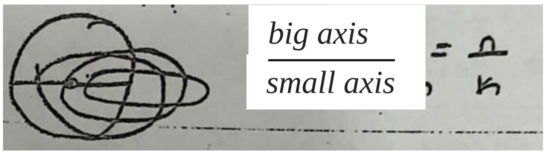


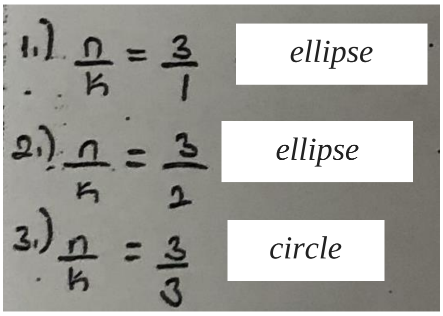
All of the values here are ''A''. The value is constant for $_1{}^1H$. But, since the isotopes of hydrogen are present, the m_e is calculated for each $_1H$ atom. It is calculated with reduced mass. The event here is the isotope effect.

Orbital

Orbital is a space volume with the greatest probability of the presence of the electron.







k=n (circle)

According to the Bohr atomic model, n=1 is either a circle or a sphere. An orbital for Bohr's layer K can then be considered. For layer L, when n=2, two orbitals can be considered. One is the circle (2/2) and the other one (2/1) is ellipse. For layer L, when n=3, it can be considered 1 circle (3/3) and 2 ellipses (3/2 and 3/1).