

**TDC Part I
(Subsidiary)
Inorganic Chemistry**



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TOPIC: - Heisenberg uncertainty principle

Some notes on the Heisenberg uncertainty principle

The Heisenberg Uncertainty Principle relates the uncertainty Δx in the position x of a particle, to the uncertainty Δp_x in the momentum of the particle in the x direction according to

$$\Delta x \Delta p_x \geq \frac{1}{2} \hbar$$

where $\hbar = h/(2\pi)$.

The uncertainty Δx is the *standard deviation* determined from a number of different measurements of the value of x , and likewise, the uncertainty in the momentum Δp_x , is the standard deviation of the momentum p_x . The formal definition is

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \text{ and } \Delta p_x = \sqrt{\langle (p_x - \langle p_x \rangle)^2 \rangle}$$

where the $\langle \rangle$ indicate average values. We can use the equality $\Delta x \Delta p_x \approx \frac{1}{2} \hbar$ to estimate various aspects of atoms, nuclei, and other objects whose behavior is controlled by quantum mechanics.

Energetics of atoms For example, consider that the diameter of a typical atom is 1 \AA or $1 \times 10^{-10} \text{ m}$. This means electrons are trapped in 1D within objects this size. What is the typical energy scale holding electrons together in atoms and giving atoms their structure?

To answer this, let us set $\Delta x \approx 1 \times 10^{-10} \text{ m}$. In effect, we are saying that the electron is somewhere within the atom, and that is the most we know about it. Then the uncertainty in the momentum is obtained:

$$\Delta p_x \approx \frac{1}{2} \hbar / \Delta x \approx \frac{1}{2} \times \frac{1}{2\pi} \times 6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1} / 1 \times 10^{-10} \text{ m} \approx 5.27 \times 10^{-25} \text{ kg ms}^{-1}$$

Let us simply guess that the uncertainty in the momentum of the electron is in the typical range of electron momenta, $p_x \approx \Delta p_x$, and use this to calculate the kinetic energy of electrons in atoms. So $p_x = 5.27 \times 10^{-25} \text{ kg ms}^{-1}$. The kinetic energy (still in 1D) is given by

$$E_K = \frac{1}{2} m v_x^2 = \frac{p_x^2}{2m}$$

using $m = m_e$, the mass of the electron ($m_e = 9.109 \times 10^{-31} \text{ kg}$), we determine $p_x^2/(2m_e)$:

$$E_K = \frac{p_x^2}{2m_e} = (5.27 \times 10^{-25})^2 \text{ kg}^2 \text{ m}^2 \text{ s}^{-2} / 2 \times 9.109 \times 10^{-31} \text{ kg} = 1.52 \times 10^{-19} \text{ J}$$

We convert this to units that are familiar to people dealing with electrons, notably electron volts (eV). 1 eV is the energy gained by an electron when it experiences an electric field of 1 V (1 volt). The conversion is $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$, so in the case above

$$E_K = 1.52 \times 10^{-19} \text{ J} / (1.602 \times 10^{-19} \text{ J eV}^{-1}) = 0.95 \text{ eV} \approx 1 \text{ eV}$$

This is the typical energy scale for electrons in atoms !

Energetics of nucleii Lets now consider that the diameter of a typical nucleus is $\approx 10^{-15}$ m. This means protons and neutrons are trapped in 1D within objects this size. What is the typical energy scale holding nucleii together?

To answer this, we set $\Delta x = 1 \times 10^{-15}$ m. We are saying that a proton is somewhere within the nucleus, and that is the most we know about it. Then the uncertainty in the momentum is obtained:

$$\Delta p_x \approx \frac{1}{2} \hbar / \Delta x \approx \frac{1}{2} \times \frac{1}{2\pi} \times 6.626 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1} / 1 \times 10^{-15} \text{ m} \approx 5.27 \times 10^{-20} \text{ kg ms}^{-1}$$

Let us again guess that the uncertainty in the momentum of the proton is in the typical range of proton momenta, $p_x \approx \Delta p_x$, and use this to calculate the kinetic energy of electrons in atoms. So $p_x = 5.27 \times 10^{-20} \text{ kg ms}^{-1}$ and $m_p = 1.673 \times 10^{-27} \text{ kg}$. The corresponding scale of the velocity, v_x (along the x direction) is obtained from

$$v_x = p_x / m_p = 5.27 \times 10^{-20} \text{ kg m s}^{-1} / 1.673 \times 10^{-27} \text{ kg} = 3.15 \times 10^7 \text{ ms}^{-1}$$

Note that the velocity is more than 10% the speed of light, c , so we should properly use relativistic mechanics,¹ but lets just pretend that classical expressions for the energy work.

$$E_K = p_x^2 / (2m_p) = (5.27 \times 10^{-20})^2 \text{ kg}^2 \text{ m}^2 \text{ s}^{-2} / 2 \times 1.673 \times 10^{-27} \text{ kg} = 8.30 \times 10^{-13} \text{ J}$$

Converting this to eV, we have

$$E_K = 8.30 \times 10^{-13} \text{ J} / (1.602 \times 10^{-19} \text{ J eV}^{-1}) = 5.2 \times 10^6 \text{ eV} = 5.2 \text{ MeV}$$

Energies associated with the nucleus are a million times larger than energies associated with electrons!