

X-Ray Crystallography

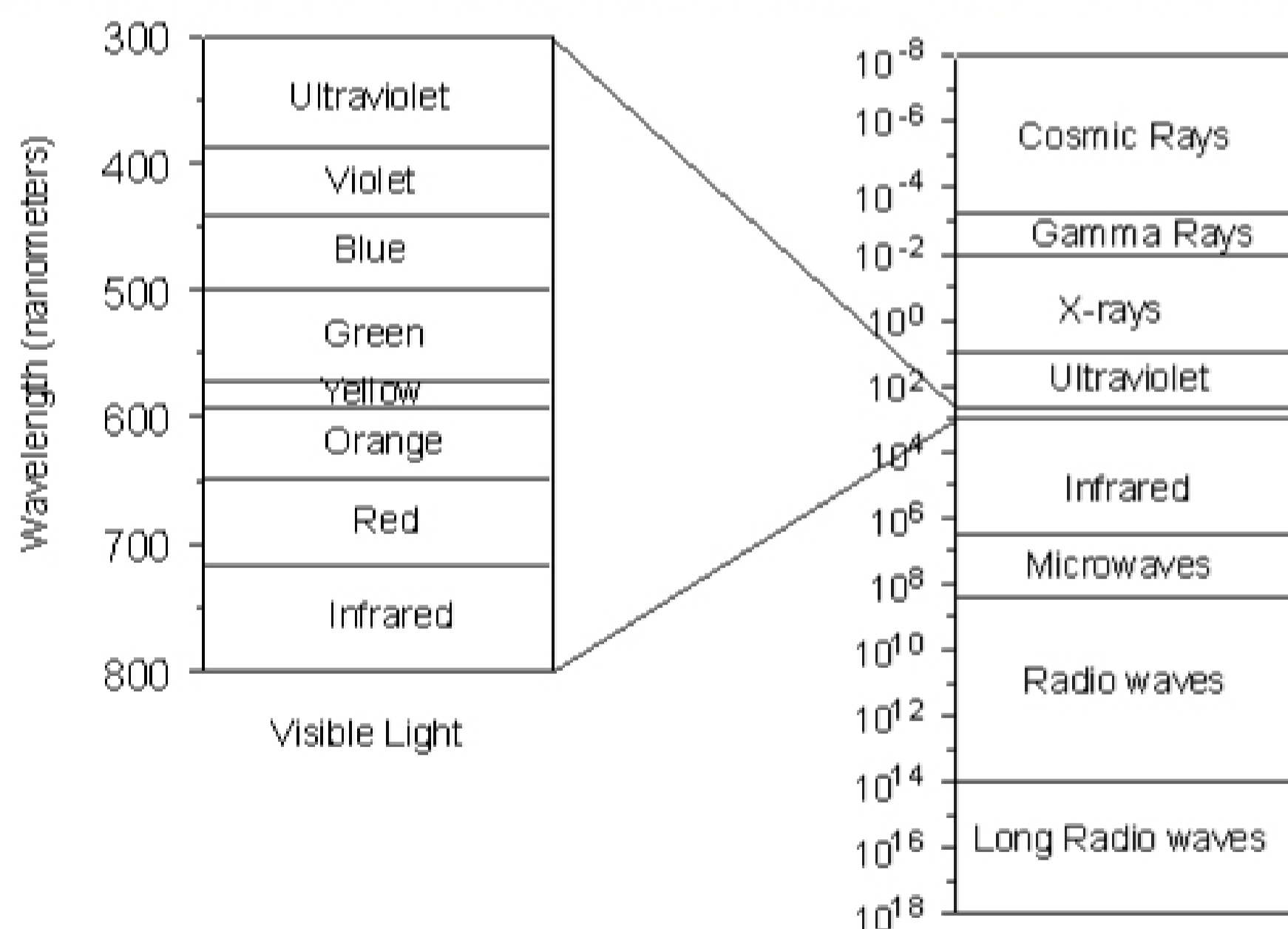
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Prior to the discovery of X-rays by Conrad Roentgen in 1895, crystallographers had deduced that crystals are made of an orderly arrangement of atoms and could infer something about this orderly arrangement from measurements of the angles between crystal faces. The discovery of X-rays gave crystallographers a powerful tool that could "see inside" of crystals and allow for detailed determination of crystal structures and unit cell size. Here we discuss the application of X-rays, not so much in terms of how they are used to determine crystal structure, but how they can be used to identify minerals.

Nevertheless, we still need to know something about X-rays, how they are generated, and how they interact with crystalline solids.

X-rays and the Production of X-rays

X-rays are electromagnetic radiation with wavelengths between about 0.02 \AA and 100 \AA ($1 \text{ \AA} = 10^{-10}$ meters). They are part of the electromagnetic spectrum that includes wavelengths of electromagnetic radiation called visible light which our eyes are sensitive to (different wavelengths of visible light appear to us as different colors). Because X-rays have wavelengths similar to the size of atoms, they are useful to explore within crystals.



The energy of X-rays, like all electromagnetic radiation, is inversely proportional to their wavelength as given by the Einstein equation:

$$E = h\nu = hc/\lambda$$

where E = energy

h = Planck's constant, 6.62517×10^{-27} erg·sec

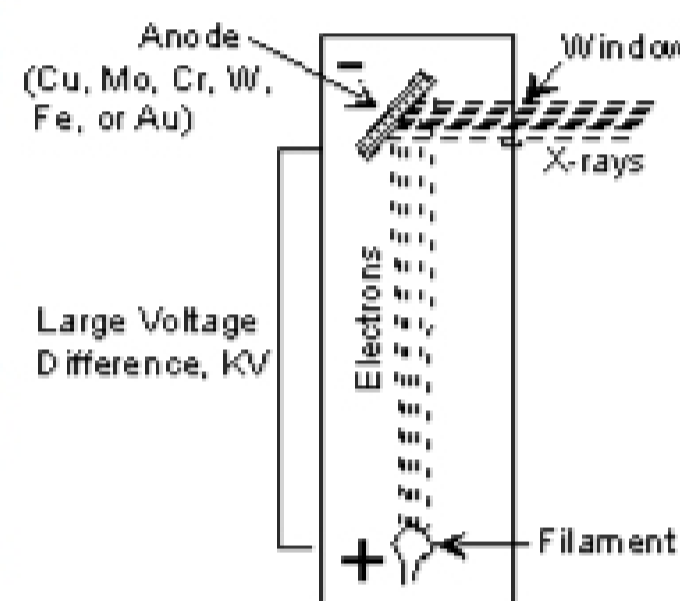
ν = frequency

c = velocity of light = 2.99793×10^{10} cm/sec

λ = wavelength

Thus, since X-rays have a smaller wavelength than visible light, they have higher energy. With their higher energy, X-rays can penetrate matter more easily than can visible light. Their ability to penetrate matter depends on the density of the matter, and thus X-rays provide a powerful tool in medicine for mapping internal structures of the human body (bones have higher density than tissue, and thus are harder for X-rays to penetrate, fractures in bones have a different density than the bone, thus fractures can be seen in X-ray pictures).

X-rays are produced in a device called an *X-ray tube*. Such a tube is illustrated here. It consists of an evacuated chamber with a tungsten filament at one end of the tube, called the cathode, and a metal target at the other end, called an anode. Electrical current is run through the tungsten filament, causing it to glow and emit electrons. A large voltage difference (measured in kilovolts) is placed between the cathode and the anode, causing the electrons to move at high velocity from the filament to the anode target. Upon striking the atoms in the target, the electrons dislodge inner shell electrons resulting in outer shell electrons having to jump to a lower energy shell to replace the dislodged electrons. These electronic transitions results in the generation of X-rays. The X-rays then move through a window in the X-ray tube and can be used to provide information on the internal arrangement of atoms in crystals or the structure of internal body parts.

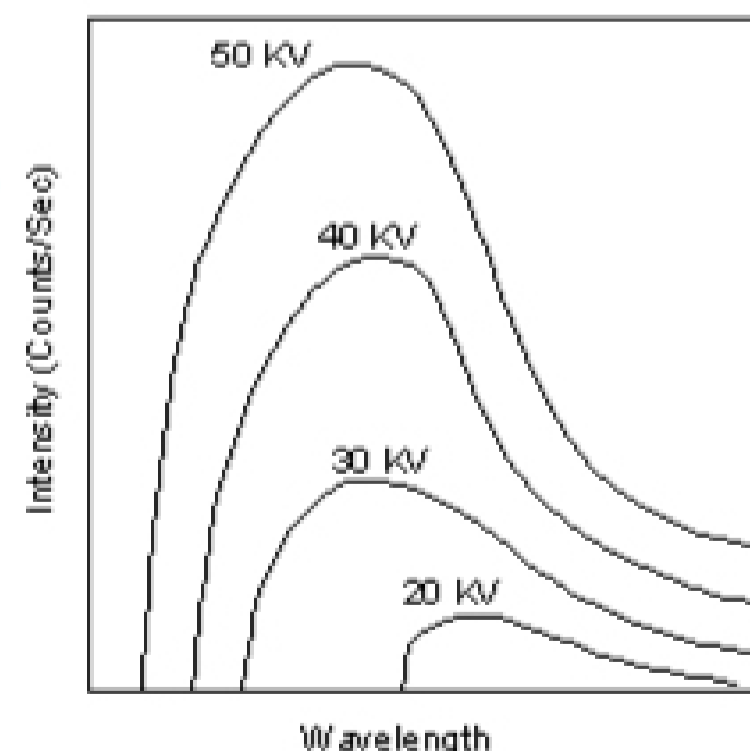


Continuous and Characteristic X-ray Spectra

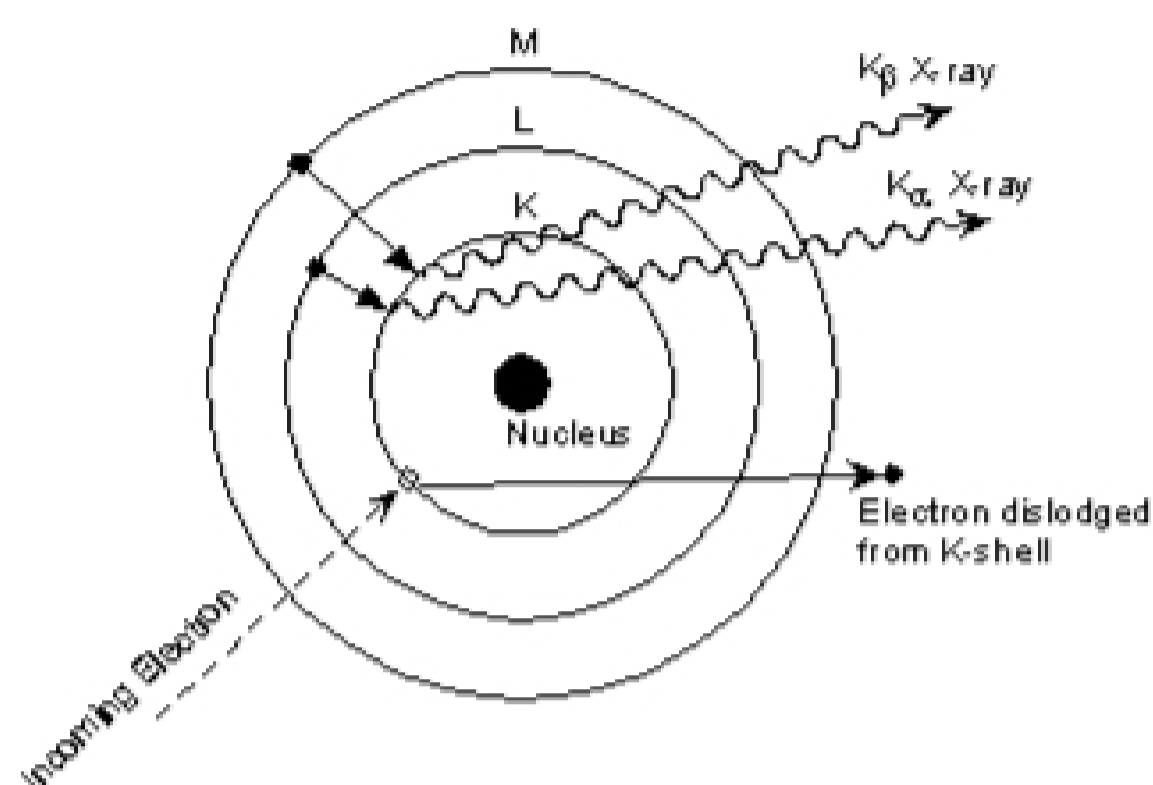
When the target material of the X-ray tube is bombarded with electrons accelerated from the cathode filament, two types of X-ray spectra are produced. The first is called the **continuous spectra**.

The continuous spectra consists of a range of wavelengths of X-rays with minimum wavelength and intensity (measured in counts per second) dependent on the target material and the voltage across the X-ray tube. The minimum wavelength decreases and the intensity increases as voltage increases.

The second type of spectra, called the *characteristic spectra*, is produced at high voltage as a result of specific electronic transitions that take place within individual atoms of the target material.

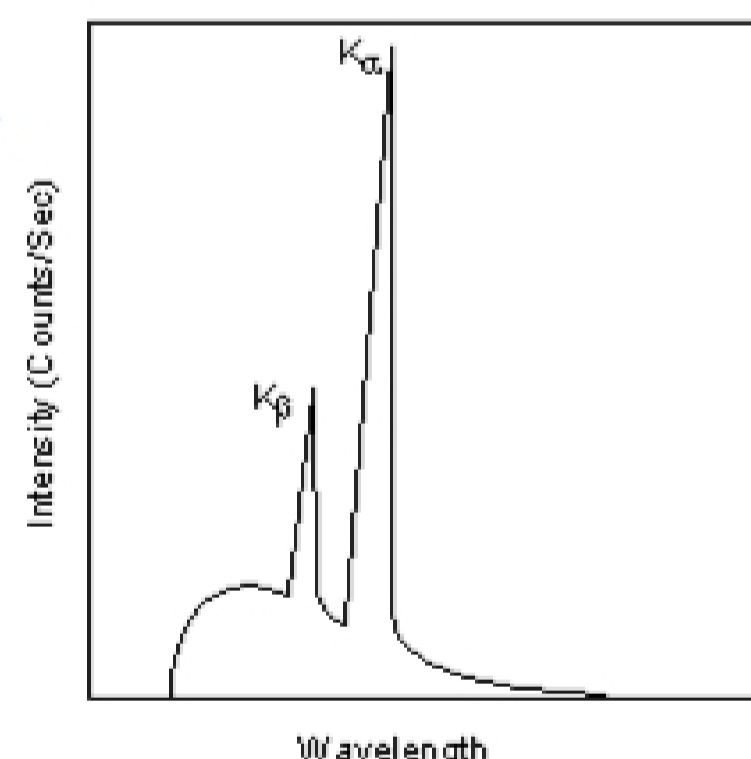


This is easiest to see using the simple Bohr model of the atom. In such a model, the nucleus of the atom containing the protons and neutrons is surrounded by shells of electrons. The innermost shell, called the K-shell, is surrounded by the L- and M-shells. When the energy of the electrons accelerated toward the target becomes high enough to dislodge K-shell electrons, electrons from the L- and M-shells move in to take the place of those dislodged.



Each of these electronic transitions produces an X-ray with a wavelength that depends on the exact structure of the atom being bombarded. A transition from the L-shell to the K-shell produces a K_α X-ray, while the transition from an M-shell to the K-shell produces a K_β X-ray.

These characteristic X-rays have a much higher intensity than those produced by the continuous spectra, with K_α X-rays having higher intensity than K_β X-rays. The important point here is that the wavelength of these characteristic x-rays is different for each atom in the periodic table (of course only those elements with higher atomic number have L- and M-shell electrons that can undergo transitions to produce X-rays). A filter is generally used to filter out the lower intensity K_β X-rays.



For commonly used target materials in X-ray tubes, the X-rays have the following well-known experimentally determined wavelengths:

Element	K _α Wavelength (λ) Å
Mo	0.7107
Cu	1.5418
Co	1.7902
Fe	1.9373
Cr	2.2909