

THE BIG PICTURE: Use of spectra to get electronic structure information

spec·trum: Etymology: from Latin *spectrum*= “appearance”, *specter*, from *specere*= “to look, look at”

spec·tros·co·py

1 : the process or technique of using a spectroscope or spectrometer

2 : the production and investigation of spectra

Electronic Spectroscopy (i.e., UV/vis = ultraviolet/visible): looks at **electrons**

Vibrational Spectroscopy (i.e., IR= Infrared): looks at **vibrations**

1) Describe in words or picture what is happening in electronic spectroscopy:

The energy change, measured as radiation, that results as electrons change energy states is monitored. One talks of a “ground state” at lower energy and an “excited state” at higher energy.

2) Describe in words or picture what is happening in emission vs absorption spectroscopy

In emission processes, an electron releases energy as it moves from an “excited state” at higher energy to some state at lower energy. The released energy is in the form of radiation. Atomic Line Spectra are produced from emission processes.

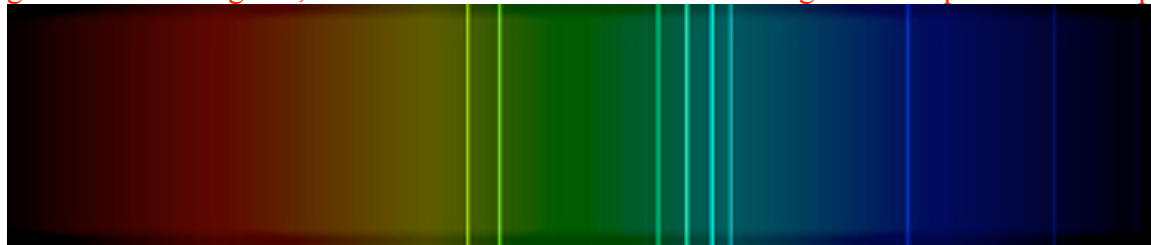
In absorption processes, an electron increase energy as it moves from a “ground state” at lower energy to an “excited state” at higher energy. The absorbed energy is in the form of radiation that is “removed” or subtracted from the source radiation (like from continuous radiation of a tungsten filament lightbulb.)

How did Cu atomic spectra look different than Na atomic spectrum?

The sodium flame viewed through the spectroscope showed one bright yellow-orange line at ~590 nm.



The copper flame viewed through the spectroscope on the other hand showed multiple and faint (barely resolved) bands in the green and blue regions, or even continuous radiation over the green-blue portion of the spectrum.

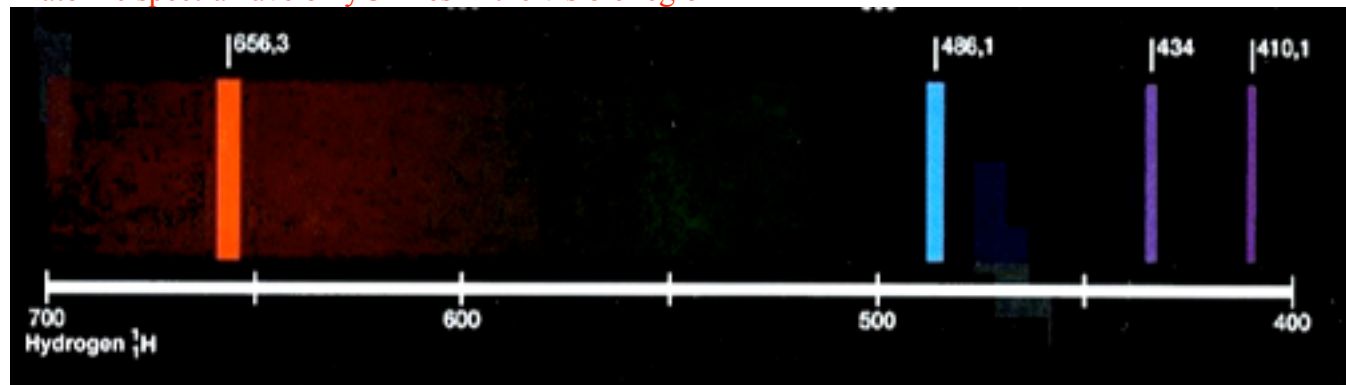


What aspect of atomic structure was deduced from atomic spectra (c.f. of hydrogen)?

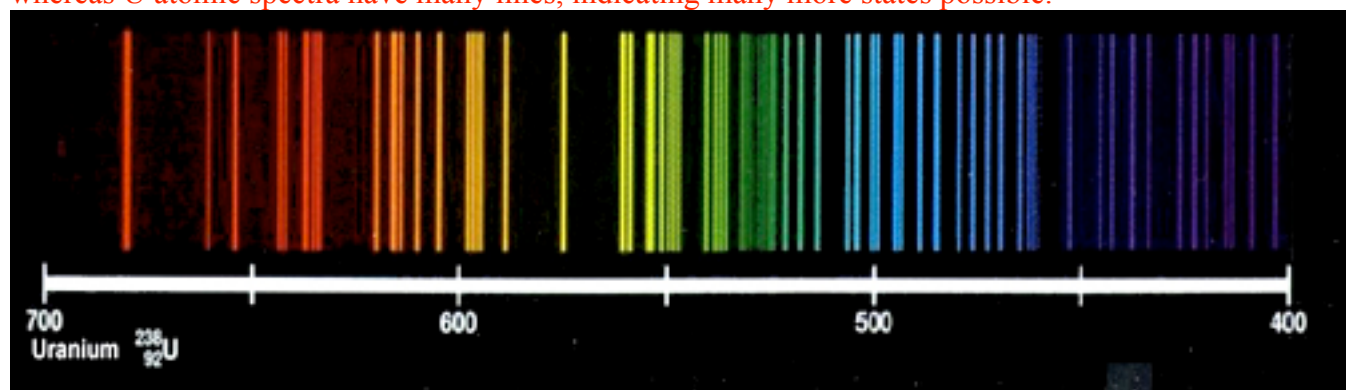
The quantized nature of electron states. That is, only certain lines corresponding to light of certain energies were observed, not a continuous spectrum of all energies. This corresponded to the quantized energies of the electron “orbitals”.

How is H different from Uranium?

H atomic spectra have only 3 lines in the visible region



whereas U atomic spectra have many lines, indicating many more states possible.



Now, it becomes useful to think about the relationship of wavelength to energy:

Calculations:

wavelength to frequency: use $c = \lambda \nu$

frequency units used in spectroscopy are: s^{-1} , Hz, cm^{-1}

energy: use $E = h \nu$

energy units used in spectroscopy are: cm^{-1} , eV

differences between energy levels: use $E = h \nu$ and $E = h (c / \lambda)$

Convert	λ (nm)	to	ν (s^{-1})	to	E (J)	transition
Lyman	121 nm		$2.48 \times 10^{15} s^{-1}$		$1.635 \times 10^{-18} J$ or 989kJ/mol	$n=2 \rightarrow n=1$
Balmer	486		$6.18 \times 10^{14} s^{-1}$		$4.09 \times 10^{-19} J$ or 246kJ/mol	$n=4 \rightarrow n=2$
Paschen	1093		$2.74 \times 10^{14} s^{-1}$		$1.82 \times 10^{-19} J$ or 109kJ/mol	$n=5 \rightarrow n=3$

What is the significance of Lyman series in UV, Balmer series in the visible and Paschen series in the infrared for H atomic structure?

The Lyman series is in the ultraviolet region (~100-300 nm), the Balmer series is in the visible region at longer wavelengths (400-800) and the Paschen series is at still longer wavelengths in the infrared region >1000 nm. This seems to indicate that as the quantized energies of higher energy states (excited states) get closer and closer together.

Where is the one electron in an H atom? (most of the time)

It is at the lowest energy, $n=1$ level.