

Understanding the electronic structure of atoms. And how electrons move in that structure.





Up to the Nuclear Age

A Brief History of Atomic Theory

Greeks were the first to suggest that matter is made up of atoms

Early chemists performed experiments

Their experiments led to Dalton's Atomic Theory

Limitations of Dalton's model led to the Thompson and Rutherford models of the atom.

While these models work reasonably well their limitatons have led to more modern theories as to the nature of the atom.



The Quantum Atom



Ch05

E-M Radiation & Waves

- Wave nature & structure
- E-M Radiation
- The planetary model of the atom.
 - Energy Quanta
 - Line Spectra
 - Bohr's Atom
- The quantum atom
 - New Math & Uncertainty
 - Thinking of Electrons as Waves
 - Orbitals
 - The modern atom
- Electron-Electron Interactions
 - Electron Spin
 - Schrödinger Equation
 - Orbital Energies



charg

- Orbital Splitting
 - Shielding & Penetration
- Sub-level overlap
- Orbital Diagrams
 - Order of Sub-Levels
- Ground State Filling
 - Auf Bau Principle
 - Hund's Rule
 - Pauli Exclusion Principle
- Electron Configuration
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 - Core Electrons
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 - Compact notation
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What is a wave?

- Energy can be transmitted by particles or waves.
 - We can apply energy to an object, transfer the object to another location, and recover the energy at the new location.
 - The energy is transmitted by matter moving through empty space.
 - Example: Toss a baseball across the road and hit a window. The energy of the toss get's transmitted to the window.
 - We can apply energy to a media. The energy creates a disturbance. The disturbance moves through the media. The disturbance imparts energy at the other end.
 - The energy is transmitted without matter moving through space.
 - It's transmitted by a disturbance moving through a media.
 - Example: Sing a high note and crack a window with it. The energy of the disturbance get's transmitted to the window.
 - The energy of the singing disturbs the air. The air does not cross the road. The disturbance within the air crosses the road.
 - Disturbances in matter are well described by a mathematical concept called a wave.







Quantifying Waves

- Waves can be defined structurally by their amplitude and wavelength.
- The wave transmission can be defined by speed, and frequency.
- Amplitude (A) is the height of a wave. It is sometimes measured from peak to peak and other times measured peak to midpoint. It can be negative or positive.
- Intensity (I) is proportional to amplitude squared, intensity is always positive.
- Wavelength (λ) is length of a wave, trough to through or peak to peak.
- Speed (s) is how fast waves move.
- Frequency (v) is how many waves pass a fixed point in one second
 -- frequency is measured in 1/s or s⁻¹ also called Hertz (Hz).









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Radiant Energy

λ = Wavelength

- Waves can be transmitted through different media.
 - Ocean waves are disturbances in the ocean water.
 - Sound waves are disturbances in air molecules.
- ► E-M Fields
 - Magnetic fields are empty space in which a magnetic particle feels a force (the space around a magnet for example).
 - Electric fields are empty space in which charged particles feel a force (like the space around a proton or electron).
 - There are protons and electrons everywhere.
 - There are electric fields everywhere.
 - Electric fields create magnetic fields (and vice versa)
 - We are surrounded by electromagnetic fields.
- E-M waves are disturbances in E-M fields.
 - E-M waves are radiant energy.
 - Unlike ocean waves or sounds waves, the media contains no matter – only energy.
 - There are different types of radiant energy:
 - Light
 - X-Rays
 - Microwaves
 - Radio Waves



Radiant Energy

- All Radiant Energy moves at the speed of light (c) in a vacuum.
 - Radiant energy moves at exactly 299,792,458 m/s (don't memorize)
 - We generally use the measurement 3.00 x 10⁸ m/s instead of the exact value.
- If all e-m waves move at the same speed:
 - those with higher frequency must have shorter wavelength.
 - those with lower frequency must have longer wavelength.

 $c = \lambda v$

• The speed of e-m radiation in a vacuum is 3.00 x 10⁸ m/s

 $c = 3.00 \times 10^8 \,\mathrm{m/s}$

(a measurement)

- Visible light is just a small part of the e-m spectrum.
- Visible light has wavelengths of 400 nm (blue) to 750 nm (red)







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Energy Quanta

- Max Planck and later Albert Einstein explored how electromagnetic radiation is absorbed and released from matter.
- Their observations about black body radiation and the photoelectric effect demonstrated that matter only absorbed or emitted electromagnetic radiation in bursts.
- That this energy is always some multiple of 6.626 × 10⁻³⁴ J-s, Planck's Constant (h) times the frequency of the light carrying it.
- Max Planck called this smallest unit of radiant energy a quanta.





Energy Quanta

- Light is not matter. It has no mass.
- But if we think of radiant energy as a stream of particles, many problems of how energy interacts with matter are simpler.
- We call these imaginary light particles photons. Photons don't exist. They're just a trick to describe particle like behavior of light.
- Planck and Einstein created a new field of study based on the hypothesis of quanta and photons. One that provided tremendous new insights into the nature of matter.
- Quantum Mechanics explained many things about chemistry that Classical Mechanics could not.







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At high temperatures or voltages, pure elements in the gaseous state emit light of different colors.

There is something special about this light.



When you pass light through a prism, it bends the path of higher frequency light more than lower frequency light. It creates a smooth rainbow spectrum.

When the light of heated pure elements is passed through a prism or diffraction grating a line spectrum results. You get something that looks more like a computer readout than a rainbow.

This demonstrates that only a few frequencies of light were in the original beam.

Line spectra of Hydrogen Gas Each element has a different unique set of spectral emissions that distinguish it from the other elements.

EMISSION (LINE) SPECTRA





- Niels Bohr started with Rutherford's model that electrons float around a heavy positively charged nucleus.
- He postulated that much the same way planets orbit the sun in only orbits of a fixed distance, that electrons are also constrained to orbits of a fixed distance from the nucleus.
 - There are reasons why planets must maintain those fixed orbits, those reasons don't apply to negatively charged electrons orbiting a positive nucleus.
 - Bohr knew his hypothesis had this hole in it.
 - But even incomplete hypothesis can move knowledge forward.





- Bohr suggested that if electrons move in fixed orbits, then an atom could emit e-m radiation when an electron falls from a higher orbit to a lower one.
- And the burst of energy would always be the difference in energy between what it took to keep the electron in those respective orbits.
- This would explain why energy was released in these fixed bursts.





• The line spectra would indicate all the possible transitions that specific element element was capable of.



- Bohr suggested that when an electron falls from a higher orbit to a lower energy orbit, it emits a photon.
- The color of that light depends on the wavelength, which depends on the energy difference between the two levels.
- With this model, only photons of with energy that equals the difference between levels can be emitted.
- This would explain why only discrete colors are seen in the line spectra.
- The Nobel Prize in Physics 1922 was awarded to Niels Bohr "for his services in the investigation of the structure of atoms and of the radiation emanating from them".



n = 3

n = 2

n = 1





Nucleus

Energy



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Louis de Broglie & Matter Waves

- Einstein had shown us it was sometimes useful to treat energy as if it was matter.
- He showed us that if we treated light like a particle, it could explain the photo-electric effect.
- A math student (still in graduate school) asked the question, would there be any advantages to treating matter as if it were energy?
- Louis de Broglie created a mathematical structure for coming up with the "wavelength" of physical objects and invited us to apply wave mechanics to matter.
- For most objects, this turns out to be valid but not very interesting.
- For very small objects, like electrons, it turns out to be amazing.
- Louis de Broglie developed the equation for representing particles as waves:

 $\lambda = \frac{h}{p} = \frac{h}{mv} \sqrt{1 - \frac{v^2}{c^2}} \qquad \qquad \mbox{do not} \\ \mbox{memorize this} \end{cases}$

- de Broglie was a brilliant mathematician who received a nobel prize for work he did as a student. Think Google.
- When applied to electrons, matter waves unlocked a new model of atomic behavior.
- The Nobel Prize in Physics 1929 was awarded to Louis de Broglie "for his discovery of the wave nature of electrons".







Heisenberg & Uncertainty

- The biggest problem with exploring the Bohr model was it was based on classical mechanics.
- ▶ It treated subatomic particles, like particles bits of matter.
- Starting with de Broglie's matter wave equation, Werner Heisenberg showed that there was an inherent uncertainty in our knowledge of both the position and velocity of a particle.

$$\Delta x \times m \Delta v \ge \frac{h}{4\pi} \qquad \qquad \frac{h}{4\pi} = 5.27 \times 10^{-35}$$
$$\Delta x \times \Delta v \ge \frac{h}{m_e \times 4\pi} = 5.79 \times 10^{-5}$$

- Electrons move at a speed of about 5 x 10⁶ m/s. If we could determine that speed to within 1% (an uncertainty of 5 x 10⁴ m/s), the uncertainty in position would be a nanometer (10⁻⁹ m).
- The diameter of a hydrogen atom is around 10 nanometers (1.06 x 10⁻¹⁰ m).
- Heisenberg showed that classical mechanics could not even be used to demonstrate an electron remains in an atom, much less in some specific orbit within the atom.
- Werner Karl Heisenberg showed us we would have to abandon classical mechanics if we wanted to understand the atom.
- The Nobel Prize in Physics 1932 was awarded to Werner Heisenberg "for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen".







Erwin Schrödinger

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
- The Nobel Prize in Physics 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac "for the discovery of new productive forms of atomic theory."
- Schrödinger produced the quantum model of the atom.



 $\Psi(n,l,m_l,m_s)$



The Schrödinger Equation: Allowed Orbits

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
- His model was based on de Broglie's mathematics.
- We won't explore the the mathematical details of that model, we'll represent it as the symbol psi (ψ) .
- The first consequence of looking at electrons as waves rather than particles was to explain why only certain energy levels existed.
- Only certain energies create stable, standing waves, in a jump rope.
- Only certain energies create stable orbitals in an atom.









The Schrödinger Equation: Orbitals

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
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- A second consequence of looking at at electrons as waves rather than particles, means we abandon the idea of particles following a predictable path.
- Instead we describe electron motion as probability field, denser where the particle is more likely to be, sparse where it is less likely to be.





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- Instead we describe electron motion as probability field, denser where the particle is more likely to be, sparse where it is less likely to be.
- As n increases, the size of the orbital increases.
- Larger orbitals encompass smaller ones.
 - n=1 orbitals are inside
 - ▶ n=2 orbitals are inside
 - n=3 orbitals etc





Possible

electron

orbits

- Erwin Schrödinger produced a model of the Bohr atom that described electrons not as particles, but as waves.
- A third consequence of looking at at electrons as waves rather than particles is it explains orbital splitting and sub-levels.
- The solution to the wave equations shows us there are multiple places for electrons at each level, there are sub-levels.
- They are described as the s, p, d, and f sub-levels.
- Their are n² sub-levels at each level n.
 - One at n=1; four at n=2; nine at n=3; sixteen at n=4, and so on.
- The probability field for each orbital looks different.





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31

 $|n = \infty$

30

20

2p

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Ω

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Number of sublevels

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orbital

 $f_{z^3} - \frac{3}{2}zr^2$ orbital

 $f_{y(x^2-z^2)}$ orbital

The probability field for each orbital looks different.



Atomic Shape & Orbital Size

- At any given energy level n, the sum of all the orbitals approximates a sphere.
- This is why we draw atoms as spheres.





 All orbitals of a given type are identical in shape, but larger in size depending on the value of n.











n = 11s
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Electron Spin

- > The Bohr Model predicts the line spectra of hydrogen perfectly.
- It's predictions for sodium or any multi-electron atom are close, but a little off.
- If we look closely at the line spectra of multi-electron atoms, we find lines split into two.
- Electrons are found to have a property called spin.
- Spin can be thought of as rotation relative to a magnetic pole.
 - Spin can be demonstrated by applying a magnetic fields, which increases electron splitting.
- There are only two kinds of spin, spin up (\uparrow) and spin down (\downarrow) .







- Electrons with opposite spin have a small repulsion, they avoid each other but the repulsion is small enough that two electrons can occupy a single orbital.
- Electrons with the same spin have a huge repulsion, two electrons with the same spin do not occupy the same orbital.
- We say electrons are paired if they occupy the same orbital with opposite spin.
- We say an electrons is unpaired if it occupies an orbital by itself.

- The Schrödinger equation $\Psi()$ describes the stable orbitals which can contain electrons inside the atom.
 - Think of them as buckets in which you can put electrons.
- The equation takes four variables which define the orbital.
 - n = 1, 2, 3, 4... (describes the size)
 - $l = 0 \dots n-1$ (describes the shape we also uses letters s,p,d,f)
 - m_l = -l... 0... +l (describes the orientation)
 - $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$ (describes the spin of the electron)







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Electron Shielding & Penetration



- In a multi-electron atom, each electron sees a different nuclear charge.
- Electrons farther away from the nucleus, see a reduced nuclear charge.
 - Electrons between the outer electron and the nucleus cancel out part of the nuclear charge.
 - An electron on the outer shell is held with a smaller charge.
 - The charge it sees is called the effective nuclear charge.
 - The electron has more energy than it would have if it were held more tightly by the atom.
 - This effect is called electron shielding.

$$E = \frac{1}{4\pi\varepsilon_0} \times \frac{q_1 q_2}{r}$$



Electron Shielding & Penetration



- In a multi-electron atom, each electron sees a different nuclear charge.
- If the electron moves closer to the nucleus, electron shielding is reduced.
- The electron is said to have penetrated the electron shell that is causing the shielding.
- The electron now sees a greater effective nuclear charge than it saw in it's previous position.
- Electron shielding & penetration is one reason why the Bohr model does not provide the correct energy levels for multi-electron atoms.

Orbital Splitting

- The Bohr Model predicts the line spectra of hydrogen perfectly.
- It's predictions for sodium or any multi-electron atom are close, but a little off.
- One of the consequence of the wave mechanic analysis of the atom, is the existence of sub-levels (s, p, d, f, etc).
- When we put more than one electron into an atom, electron interactions cause the sub-levels to split.
- This corresponds to complexity we see in the line spectra of many electron atoms.
- With a primary level, the sub-levels have increasing energy according to the sequence s, p, d, f.
- All orbitals of the same sub-level are degenerate. Degenerate means having the same energy.



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Orbital Diagrams

- Orbital diagrams order the position of orbitals according to increasing energy.
- Electrons can and do populate these orbitals in endless combinations.
- Changing the configuration of electrons in an atom, changes it's chemical properties. Like a computer program.
- Many important chemical reactions are initiated by exciting electrons from one configuration to another.
- We call the lowest energy electron configuration of an atom it's ground state. It's the rest state of the atom.
- There are rules that will help you locate the ground state of any neutral atom or ion.



Orbital Diagrams

- The periodic table is a useful tool for drawing orbital diagrams.
 - It helps you find the number of electrons for any given atom.
 - Each period will tell you the n value of the box.
 - Each block of the periodic table will tell you l value.



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- Rules for filling orbitals to create the ground state configuration:
 - Rule #1 Aufbau Principle:
 - Fill each sub-level, before beginning to fill the next (there are some exceptions, but this works for most atoms).
 - ▶ Rule #2 "Hund's Rule":
 - > Place one electron in each degenerate sub-shell before "double booking" a second electron.
 - > Unpaired electrons in the same orbital have lower energy if their spins are aligned.
 - Rule #3 "Pauli Exclusion Principle":
 - Double book if you have to before going to the next sub-level.
 - A maximum of two electrons can be placed in any orbital.
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 - Fill each sub-level, before beginning to fill the next (there are some exceptions, but this works for most atoms).
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Electron Configuration

- Electron Shells
 - Valence Electrons
 - Core Electrons
- Electron Configuration notation
 - Compact notation
- Lewis Symbols
- Quantum Numbers
 - Describing Electron Positions







- The principle quantum number corresponds to the shell:
 - All sub-levels that share that number are part of that shell.
 - The shell with the greatest quantum number is valence shell.
 - The valence shell is the outermost layer of the atom.
 - Other atoms interact with the valence shell.
 - There are always 1-8 electrons in the valence shell.
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- Each occupied sub-shell is listed in order of increasing energy.
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Electron Configuration Notation



- Electron Configuration notation is a compact description of the electron distribution in an orbital diagram.
- Each occupied sub-shell is listed in order of increasing energy.
- A superscript denotes the number of electrons in that sub-shell.
- Compact electron configuration replaces most of the core electrons with the corresponding nobel gas symbol.







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- Lewis notation is how we described the connectivity of all covalent compounds (molecules).
- It's how we show the difference between compounds that have the same composition (molecular formula).
- Lewis notation starts with understanding the Lewis symbols for each atom or ion.
- Symbols that communicate the valence structure of the electronic configuration of those particles.







H:O:H





- The electrons involved in bonding are called valence electrons.
- Valence electrons are found in the incomplete, outermost shell of an atom. The valence shell.
- As a pictorial understanding of where the electrons are in an atom, we represent the electrons as dots around the symbol for the element.
- The number of valence electrons available for bonding are indicated by unpaired dots.
- We generally place the electrons on four sides of a square around the element's symbol.



• These symbols are called Lewis symbols or Lewis electron-dot symbols.

•• Be •Be• We won't discriminate between ground state and excited states in Lewis structures. If you're asked for the Lewis structure anyone of these is fine.





 $1s^{2}2s^{2}$

4 electrons 2 valence electrons

ground state

excited state



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 $ls^2 2s^2 2p^l$

5 electrons3 valence electrons



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6 electrons4 valence electrons



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 $1s^{2}2s^{2}2p^{3}$

7 electrons5 valence electrons



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 $1s^2 2s^2 2p^6 2s^2 2p^3$

15 electrons5 valence electrons



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³⁵ electrons7 valence electrons

| | | | | | | | | NY CALL | Constants (| | | | | | | 1 | | |
|---|---------------|-----------------|-----------|----------------|-----------------------|-----------------|----------------|-----------------------|----------------|------------------|----------------|-----------------------|-----------------------|-----------------------|-----------------|------------------------|------------------------|------------------|
| | 1A 1 | - | | | | | | | | | | | | | | | | 8A 18 |
| 1 | 1 H | 2A 2 | | | | | | | | | | | 3A 13 | 4A 14 | 5A 15 | 6A 16 | 7A 17 | 2 He |
| 2 | 3 Li | 4 Be | | | | | | | | | | | 5 B | 6 C | 7 N | 8 0 | 9 F | 10 Ne |
| 3 | 11 Na | 12 Mg | 3B 3 | 4B 4 | 5B 5 | 6B 6 | 7B 7 | 8 | 8B 9 | 10 | 1B 11 | 2B 12 | 13 Al | 14 Si | 15 P | 16 S | 17 Cl | 18 A1 |
| 4 | 19 K | 20 Ca | 21 Sc | 22 Ti | 23 V | 24 Cr | 25 Mn | 26 Fe | 27 Co | 28 Ni | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | 35 Br | 36 K i |
| 5 | 37 Rb | 38 Sr | 39 Y | 40 Zr | 41 Nb | 42 Mo | 43 Tc | 44 Ru | 45 Rh | 46 Pd | 47 Ag | 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te | 53 I | 54 Xe |
| 6 | 55 Cs | 56 Ba | 71 Lu | 72 Hf | 73 Ta | 74 W | 75 Re | 76 Os | 77 Ir | 78 Pt | 79 Au | 80 Hg | 81 Tl | 82 Pb | 83 Bi | 84 Po | 85 At | 86 Rr |
| 7 | 87 Fr | 88 Ra | 103 Lr | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Ds | 111 Rg | 112 | 113 | 114 | 115 | 116 | | 118 |
| | | Metal | s | 57 La 89 | 58 Ce 90 | 59 Pr 91 | 60 Nd 92 | 61 Pm 93 | 62 Sm 94 | 63 Eu 95 | 64 Gd 96 | 65 Tb 97 | 66 Dy 98 | 67 Ho 99 | 68 Er 100 | 69 Tm 101 | 70 Yb 102 | |
| | | Nonn | netals | Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No | |

| Element | Electron Configuration | Lewis Symbol |
|---------|-------------------------------|--------------|
| Li | [He]2 <i>s</i> ¹ | Li• |
| Be | [He]2 <i>s</i> ² | ·Be· |
| В | $[He]2s^22p^1$ | ٠ġ٠ |
| С | $[He]2s^22p^2$ | ٠Ċ٠ |
| Ν | $[He]2s^22p^3$ | ٠Ņ: |
| 0 | $[He]2s^22p^4$ | :Ģ: |
| F | $[He]2s^22p^5$ | ٠Ë٠ |
| Ne | $[He]2s^22p^6$ | :Ne: |
| Na | $[Ne]3s^1$ | Na• |
| Mg | [Ne]3 <i>s</i> ² | ·Mg· |
| Al | $[Ne]3s^23p^1$ | ٠Ål٠ |
| Si | $[Ne]3s^23p^2$ | ·Si· |
| Р | $[Ne]3s^23p^3$ | . <u>P</u> : |
| S | $[Ne]3s^23p^4$ | :ș: |
| Cl | $[Ne]3s^23p^5$ | ·Ċŀ |
| Ar | $[Ne]3s^23p^6$ | :Är: |

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$n = 2; 1 = 1; m_1 = -1; m_s = +\frac{1}{2}$

The position of any electron position can be described by four numbers.

- n is the principle quantum number, it corresponds to the shell.
- l is the angular quantum number, it corresponds to the sub-shell.
 - l < n eg, if n =3 l = 0, 1, or 2</pre>
 - ▶ 0 = s; 1 = p; 2 = d; 3 = f
- mi is the magnetic quantum number, it's used to differentiate degenerate sub-shells.
 - m_l has values that run from -l ... +l; eg if l=3 m_l = -2, -1, 0, 1, 2
- m_s is the spin quantum number, it's either +1/2 (spin up) or -1/2 (spin down)





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$n = 3; 1 = 2; m_1 = +1; m_s = -\frac{1}{2}$

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 $n = 4; l = 1; m_l = 0; m_s = -\frac{1}{2}$

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Questions?

