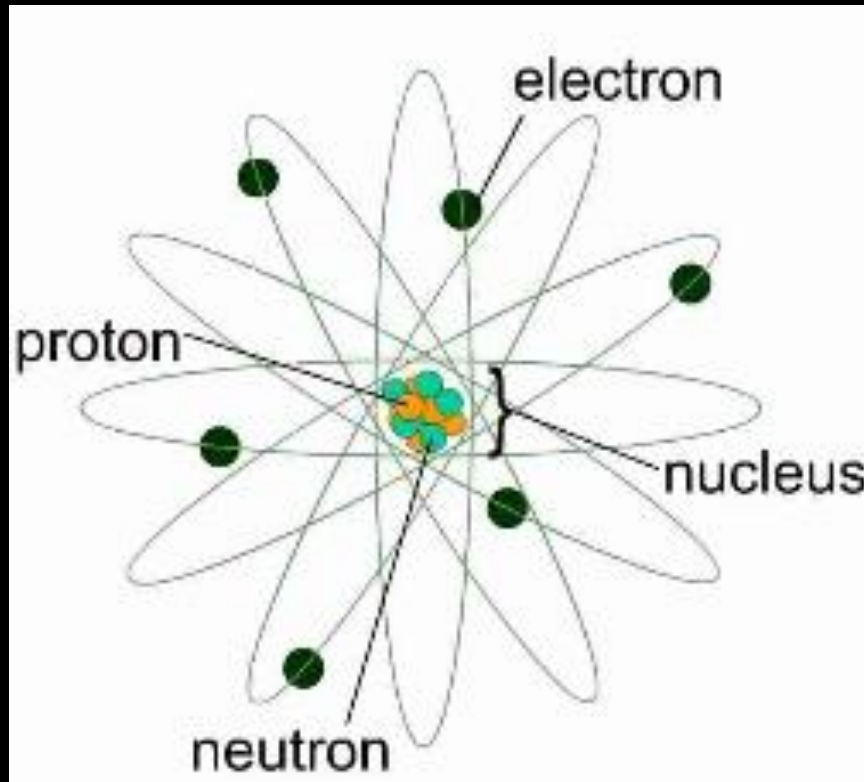




QUANTUM CHEMISTRY

REMEMBER THE ATOM...



- Protons have a charge of +1 and a mass of 1.
- Neutrons have no charge and a mass of 1. Protons and neutrons make up the nucleus.
- Electrons have a charge of -1 and a mass of $1/1837$. They are found around the nucleus, confined to specific regions of space known as orbitals.

ENERGY LEVEL

- Orbitals are 3-dimensional regions of space around a nucleus in which electrons are likely to be found.
- Bohr's discovery of the energy levels was later refined and is now known as the principle quantum number or shell.
- These energy levels (or shells) are assigned whole numbers (1, 2, 3, 4...).
- The term energy level reminds us that this simply describes the average energy of electrons found within that shell.
- The main categories of orbitals correspond to the various energy levels around the nucleus, which the electrons can occupy.

ORBITS AND ORBITALS

- Orbits refer to specific *paths* around an object, like the orbit of the Earth around the Sun.
- Orbitals refer to *regions* of space.
- Electrons **do NOT** travel in orbits, but rather are located in orbitals.
- Rutherford established that electrons are located around the nucleus, and Bohr determined that they travel in paths in various levels
- The chemists and physicists who developed quantum mechanics (also called wave mechanics) established that electrons are located in orbitals; they also found that the electrons are governed by several other quantum numbers

NUMBER OF ORBITALS

- The maximum number of orbitals that can be in each energy level is given by the formula:

$$\# \text{ orbitals} = n^2$$

where n = energy level

- The maximum number of electrons that can be in each energy level is given by the formula:

$$e = 2n^2$$

where e = electrons

n = energy level

ENERGY LEVELS, ORBITALS AND ELECTRONS

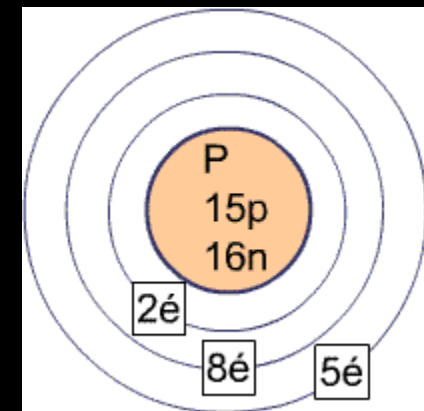
Energy Level (n)	Number of orbitals (n^2)	Number of electrons ($2n^2$)
1	$n^2=1$	2
2	$n^2=4$	8
3	$n^2=9$	18
4	$n^2=16$	32
...

Example

Consider the phosphorus atom.

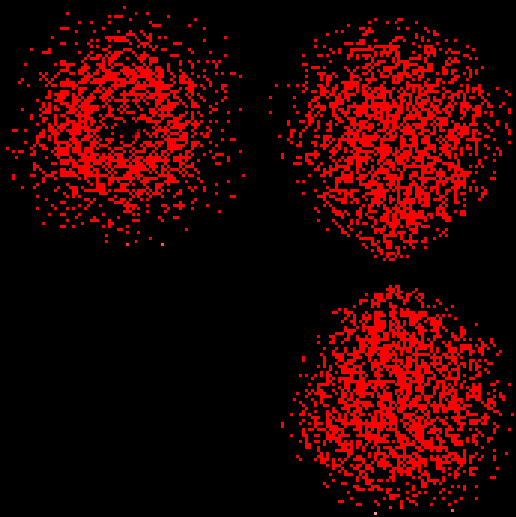
Its atomic number of 15, so it has 15 electrons and 15 protons.

Its atomic mass is 31, which means that it has $31-15=16$ neutrons.

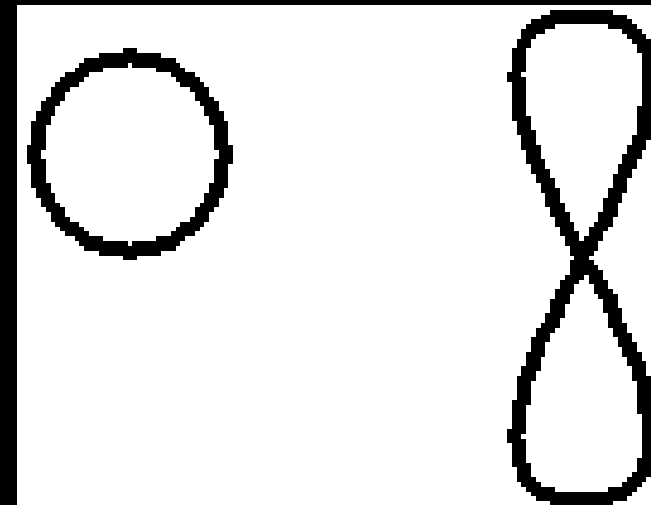


HEISENBERG'S UNCERTAINTY PRINCIPLE

- In 1926, Werner Heisenberg (1901-1976) formulated **Heisenberg's uncertainty principle**
 - an electron's location and velocity around an atom's nucleus at a given time cannot both be determined precisely. A cloud of probability is used to represent where the electrons are most likely to be found.



To simplify you can represent the orbitals with lines instead of the “speckled” areas.



QUANTUM NUMBERS

- **Quantum Numbers**
- Each electron orbital of the atom may be described by a set of four quantum numbers. They give the position with respect to the nucleus, the shape of the orbital, its special orientation and the spin of the electron in the orbital.
- **Principal quantum number (n)**
- Refers to the average distance of the orbital from the nucleus. They are the energy levels or shells.
- **Secondary quantum number (azimuthal quantum number) (l)**
- Refers to the shape of the orbital. It is also referred to as the angular momentum quantum number. This number controls the number of subshells within a particular energy level.

SPIN AND PAULI EXCLUSION PRINCIPLE

- **Magnetic quantum number (m_l)**
- Refers to the number of special orientations of orbitals in space.
- **Spin quantum number (m_s)**
- Describes the spin in either of two possible directions. Each orbital can be filled by only two electrons, each with an opposite spin.
- The main significance of electron spin is explained by the postulate of Wolfgang Pauli (1900-1958). It states that in a given atom, no 2 electrons can occupy the same quantum state (therefore they cannot have the same set of 4 quantum numbers (n , l , m_l and m_s)). This is referred to as the **Pauli exclusion principle**.

n	l	Orbital designation	m_l	# of orbitals	# electrons per orbital	# electrons per energy level
1	0	1s	0	1	2	2
2	0	2s	0	1	2	8
	1	2p	-1,0,+1	3	6	
3	0	3s	0	1	2	18
	1	3p	-1,0,+1	3	6	
	2	3d	-2,-1,0,+1,+2	5	10	
4	0	4s	0	1	2	32
	1	4p	-1,0,+1	3	6	
	2	4d	-2,-1,0,+1,+2	5	10	
	3	4f	-3,-2,-1,0,+1,+2,+3	7	14	

PAGES...

- Copy out the figure 3.14 into your notes (page 177)
- Page 179 Questions 1-10

IMPORTANT TO REMEMBER

- the energy levels start at 1 and increase as whole numbers
- the maximum value of l in an energy level(n) is up to $(n-1)$
- each orbital is allowed to have a maximum of 2 electrons of opposite spin
- the combined effect of these quantum numbers give rise to both the number of orbitals in a certain energy level (shell 2 has 4), but also the number of subshells within an energy level (shell 2 has 2s and 2p) and also the number of orbitals within each subshell (2p contains 3 orbitals).

HUND'S RULE OF MULTIPLICITY

- When there is more than one orbital at a given energy level (3 p or 5 d) the electrons spread out and remain unpaired if possible. Then, the electrons will begin to pair up as electrons are added to the orbitals.
- This is known as **Hund's rule of maximum multiplicity**.
 - It states that *electrons line up in degenerate orbitals (orbitals of the same energy), one to each orbital, with parallel spins, before pairing occurs*. This was developed by Friedrich Hund (1896-1997) in 1925.
 - This rule is also referred to as the "bus seat rule", since it is similar to the way transit bus passengers will prefer to sit alone and only sit with another stranger once all double seats are occupied with a person.

ELECTRON CONFIGURATION

- The notion that represents the arrangement of electrons around the atom's nucleus is called electron configuration.
- Orbitals with different l values are usually known by the following labels, which are derived from early terms for different families of spectroscopic (spectral) lines before quantum mechanics was developed:

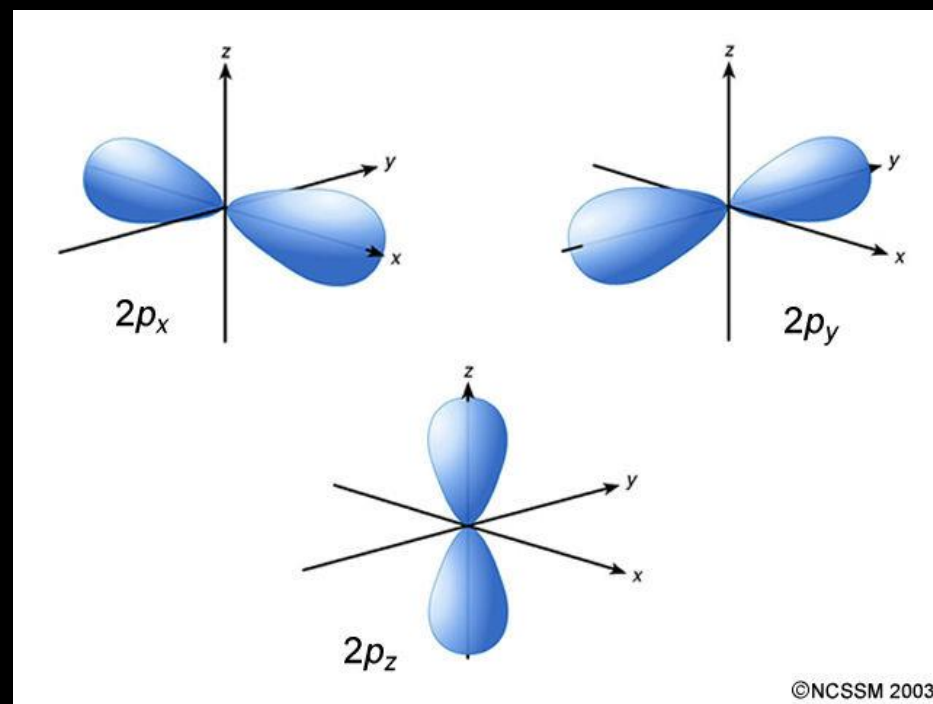
Value of l	0	1	2	3	4
Letter Used	s	p	d	f	g
Name	Sharp	Principle	Diffuse	Fundamental	Just alpha after 'f'!

ELECTRON CONFIGURATION

- Electron configuration is expressed as:
 - $1s^22s^22p^3$
 - the red coefficients (1,2,2) correspond to the energy levels
 - the white letters (s,s,p) correspond to the orbitals
 - the blue exponents correspond to the number of electrons in that orbital
- To read this... one s two, two s two, two p three

THINGS TO THINK ON...

- the maximum number of electrons per orbital is 2
- BUT!! there are 6 possible “p” electrons per energy level
- Therefore there must be 3 different “p” orbitals.
- These orbitals are p_x , p_y and p_z . These orbitals are identical in nature and shape; they only differ in their special orientation along the x, y and z axes in 3-dimensional space.



EXAMPLE CARBON

- Carbon would have the electronic structure:
 - $1s^2 2s^2 2p_x^1 2p_y^1$ since it has 6 electrons total.
 - Any 2 of the 3 types of “p” orbitals could be used in the expression,
 - For convenience start with “ p_x ” then “ p_y ” and then use “ p_z ”.
 - So, even though the electronic configuration of carbon is actually $1s^2 2s^2 2p_x^1 2p_y^1$, it is normally written $1s^2 2s^2 2p^2$ for simplicity.
- To determine the total number of electrons in an element's electron configuration, you add all of the exponents in its electron configuration. Carbon has the electron configuration $1s^2 2s^2 2p^2$, therefore it has $2+2+2=6$ electrons.

AUFBAU PRINCIPLE

- German for 'building up'
- Created by Niels Bohr and Wolfgang Pauli
- The **Aufbau principle** gives the order in which orbitals are filled in successive elements, with lowest energy first. (This does not always make logical numeral sense...)

Electronic Structure

Work through this tutorial in sequence,
or go directly to the section required using the links below.
Use the 'home' button (to right) to return to this screen.

[Energy levels within atoms: sub-levels and orbitals](#)

[Filling energy levels with electrons](#)

[Electronic configuration notation](#)

[Ionisation](#)

[Credits](#)



1s —

2p —

2s —

1s —

3d —————

--	--	--	--	--

3p ———

--	--	--

3s —

--

2p ———

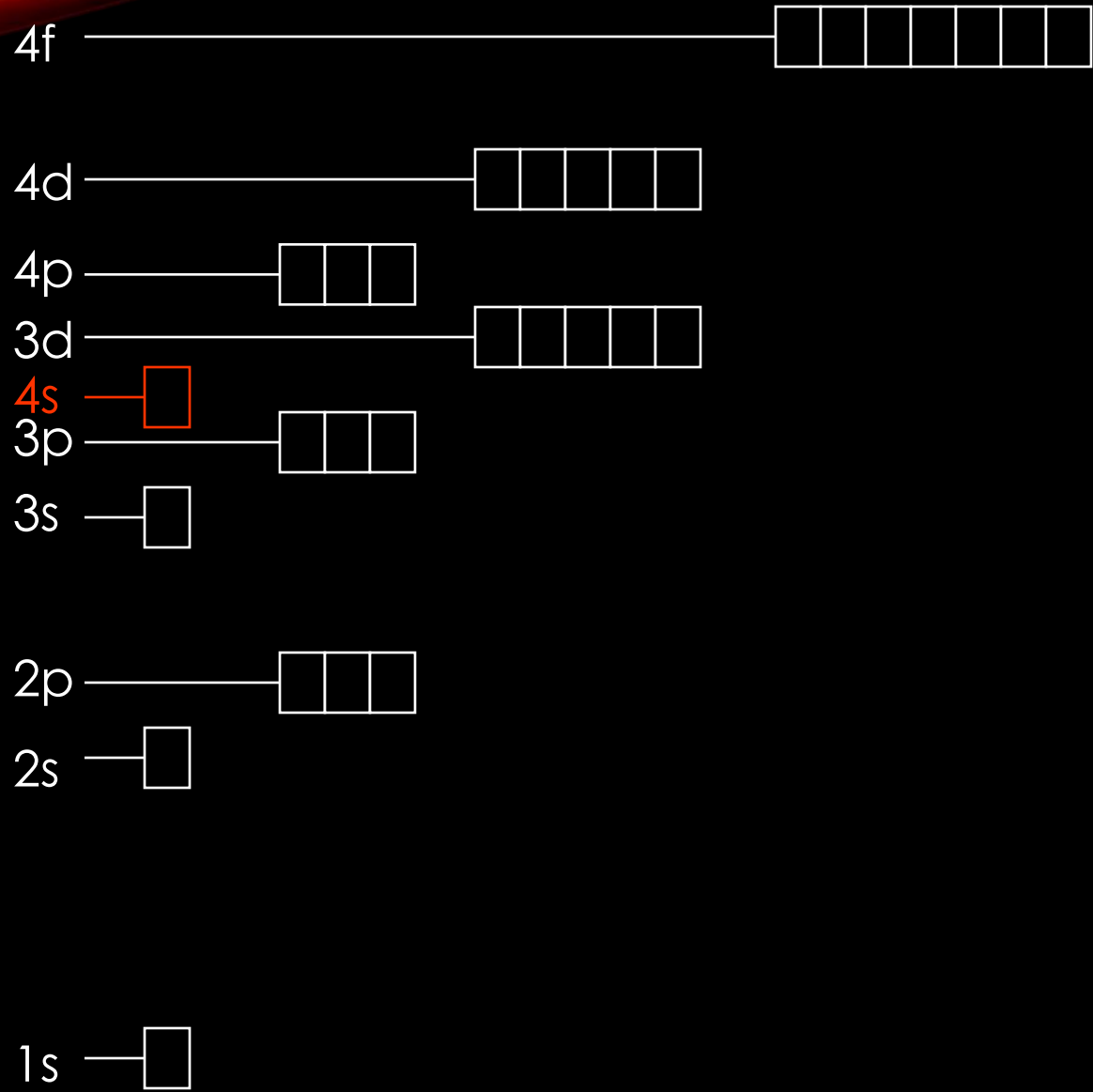
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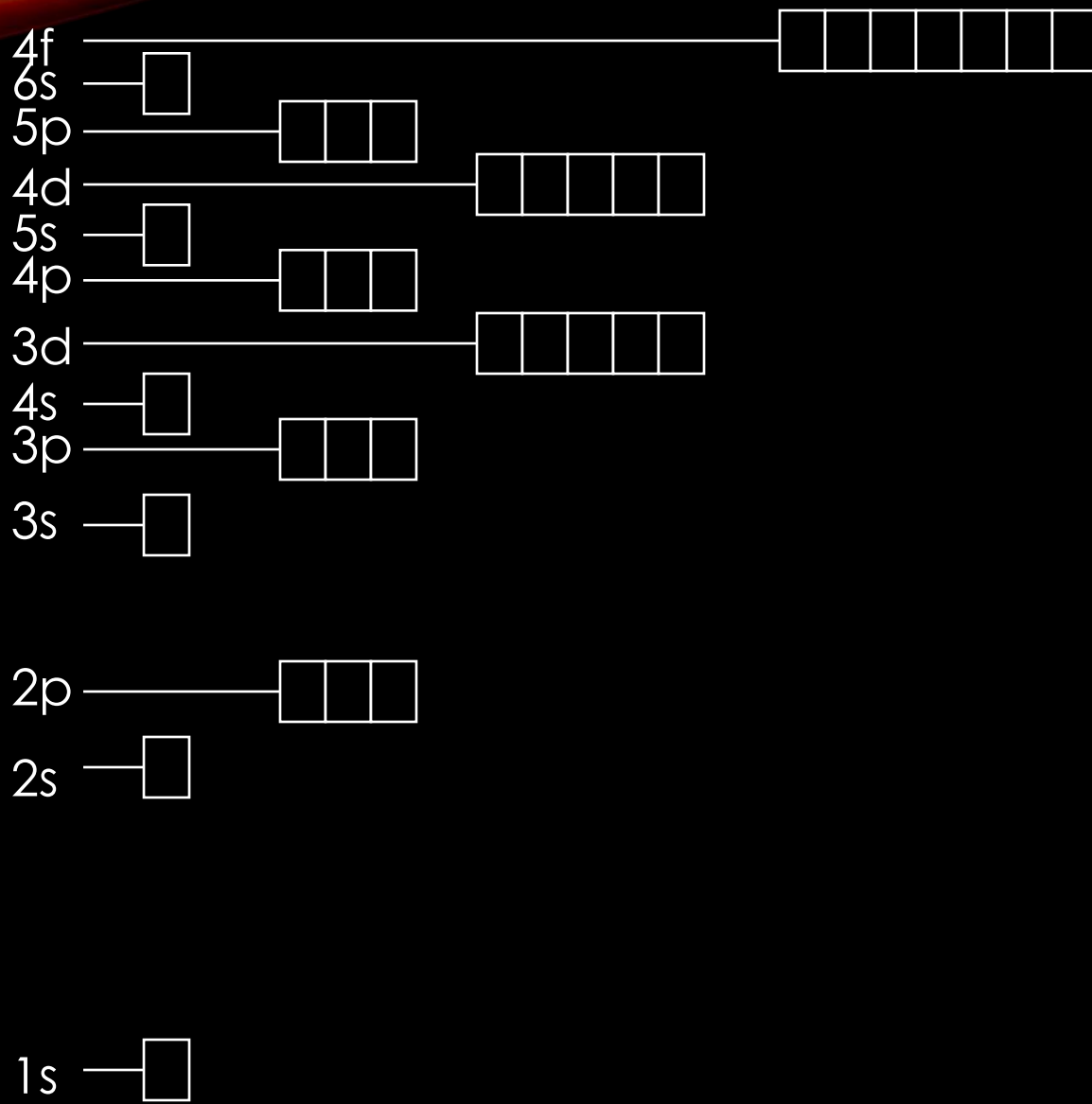
2s —

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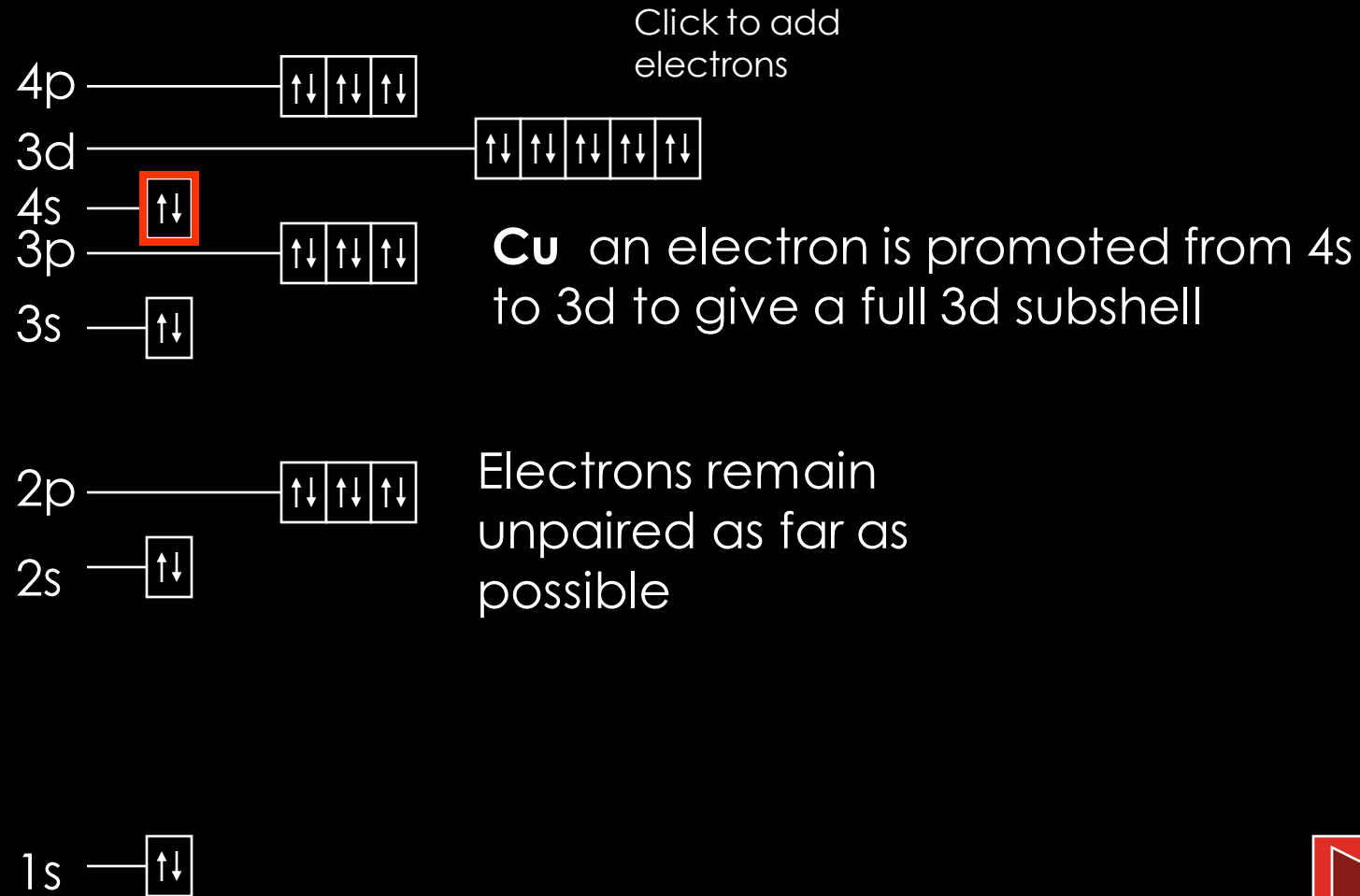
1s —

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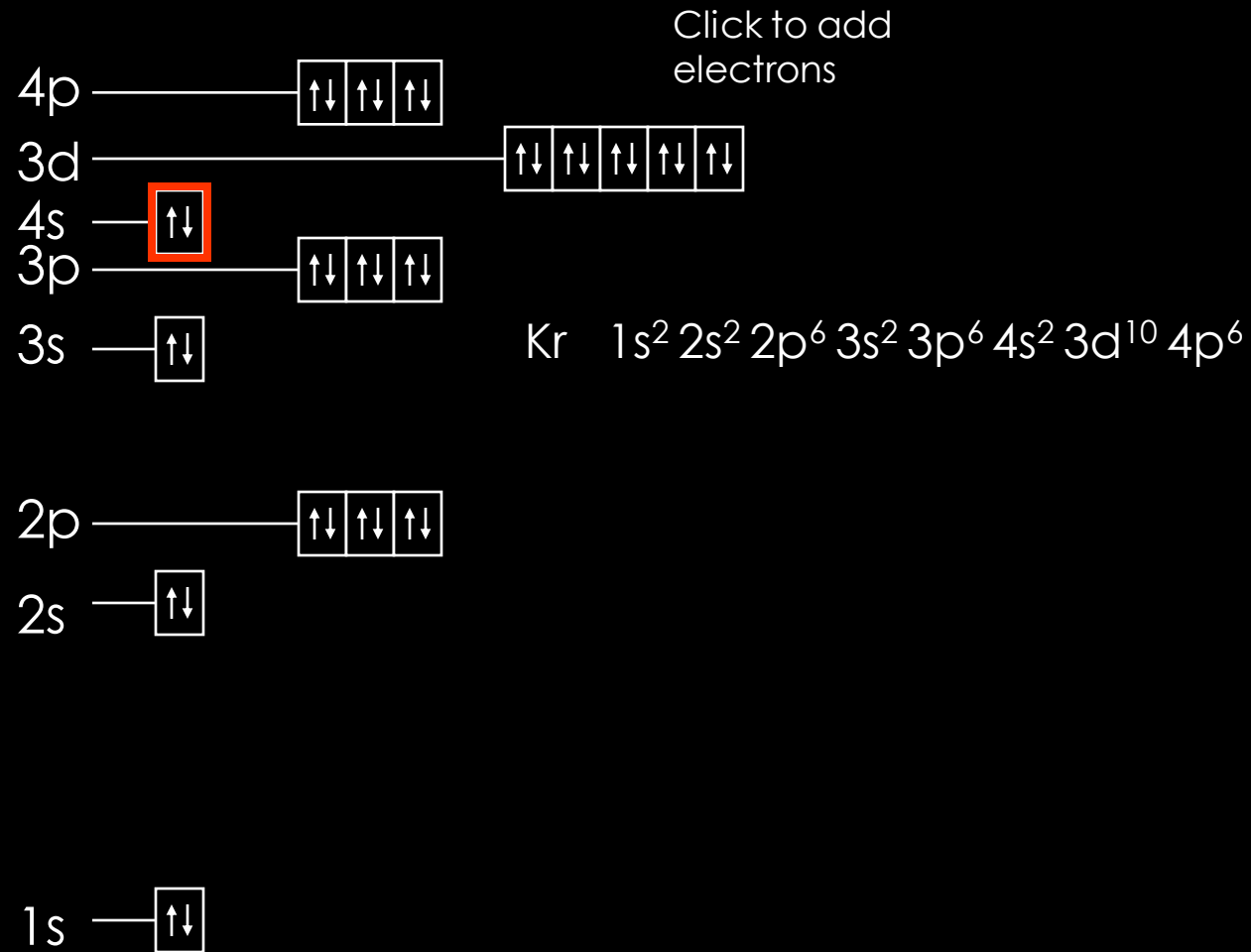




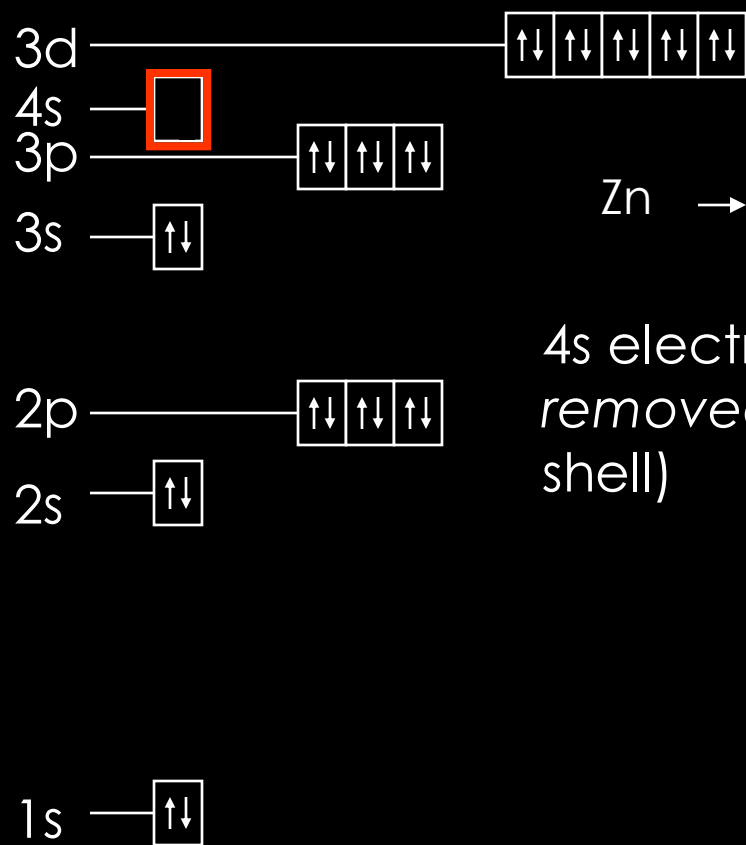
Electrons fill the lowest available energy level



Electronic configuration in shorthand nomenclature



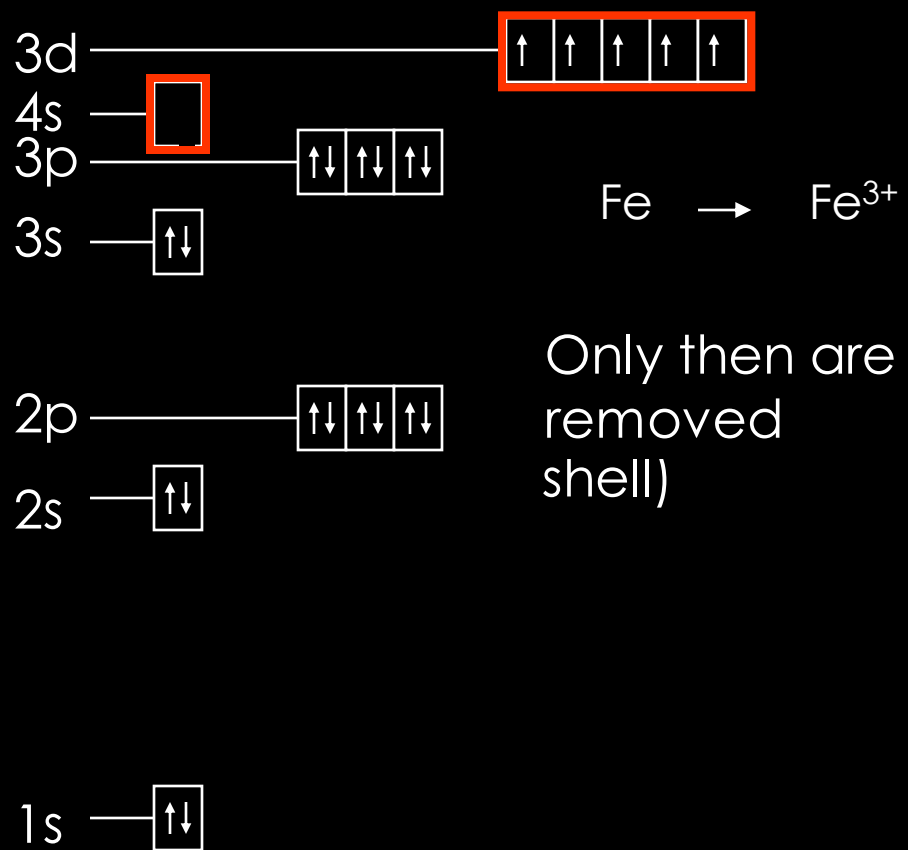
Ionisation



4s electrons (outer shell) are removed before 3d (inner shell)



Ionisation





Created by Dave Tandy
Solihull Sixth Form College

FILLING ORDER

1s

2s 2p

3s 3p 3d

4s 4p 4d 4f

5s 5p 5d 5f

6s 6p 6d

7s 7p

8s

TRY THESE...

- What is the electron configuration of $_{13}\text{Al}$
 - $1s^22s^22p^63s^23p^1$
- What is the electron configuration of $_{20}\text{Ca}$
 - $1s^22s^22p^63s^23p^64s^2$
- The electron configuration of $1s^22s^22p^63s^23p^64s^23d^1$ is what element?
 - $_{21}\text{Sc}$

ASSIGNMENT

- Please go to <http://learninghood.ca> for your assignment.
- Submit to your work to the dropbox in the virtual classroom and an answer key will open up for you.
- You **MUST** assess your own work and do a self reflection paragraph and resubmit this to the same dropbox.