Quantum Mechanics

The hidden world of the electron

Ground state

- If all the electrons within an atom are at the lowest possible energy levels and orbitals, the atom is said to be in its ***ground state***
- this is the most stable electron configuration of the atom
- **Aufbau Principle**: “fill in the orbitals from the ground up”

Hund's Rule

- When filling an orbital set with electrons, always put one electron in each orbital in the set before placing the second electron into an orbital in the set
- Ex: each of the three p orbitals in a set of p's will get one electron before any of them get two

Orbital energy diagram

- In the hydrogen atom, all the orbitals at the same Energy level are equal in energy
  - The orbitals are "*degenerate*"
- *This is why the Bohr model works with Hydrogen*

n

Energy and energy levels in a hydrogen atom

3

___ s ___ ___ ___ p ___ ___ ___ ___ ___ d

2

___ s ___ ___ ___ p

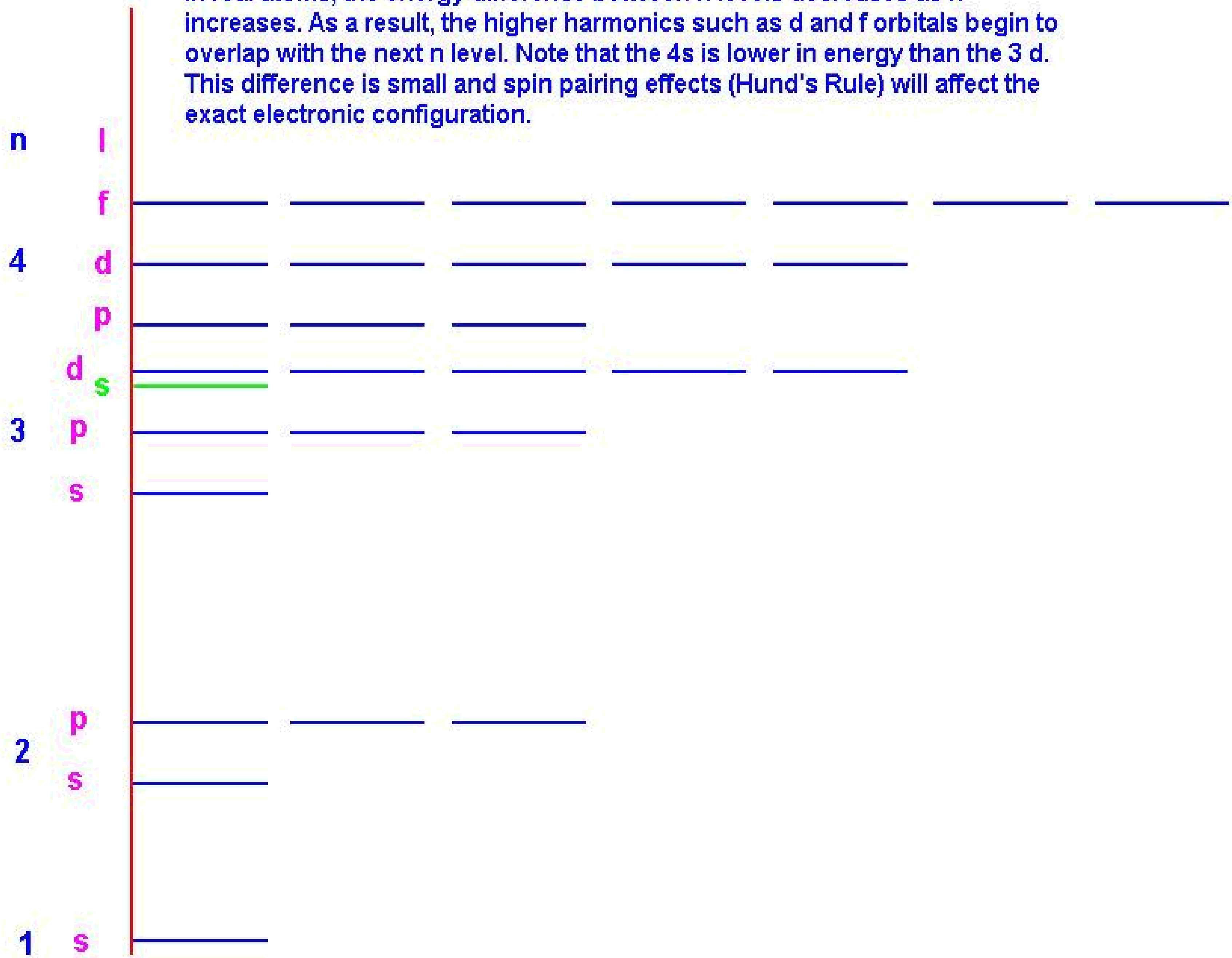
1

___ s

Orbital energy diagram

- In all other atoms, there is “orbital energy overlap” between the highest energy orbitals at one level, and the lowest energy orbitals at the next level
- ex: the 4s orbital is lower in energy than the 3d orbitals, so it fills with electrons first

In real atoms, the energy difference between n levels decreases as n increases. As a result, the higher harmonics such as d and f orbitals begin to overlap with the next n level. Note that the 4s is lower in energy than the 3 d. This difference is small and spin pairing effects (Hund's Rule) will affect the exact electronic configuration.



Pauli exclusion principle

- No two electrons within the atom can have exactly the same energy
- Each individual orbital can contain at most two electrons
  - –they must have “opposite spin”

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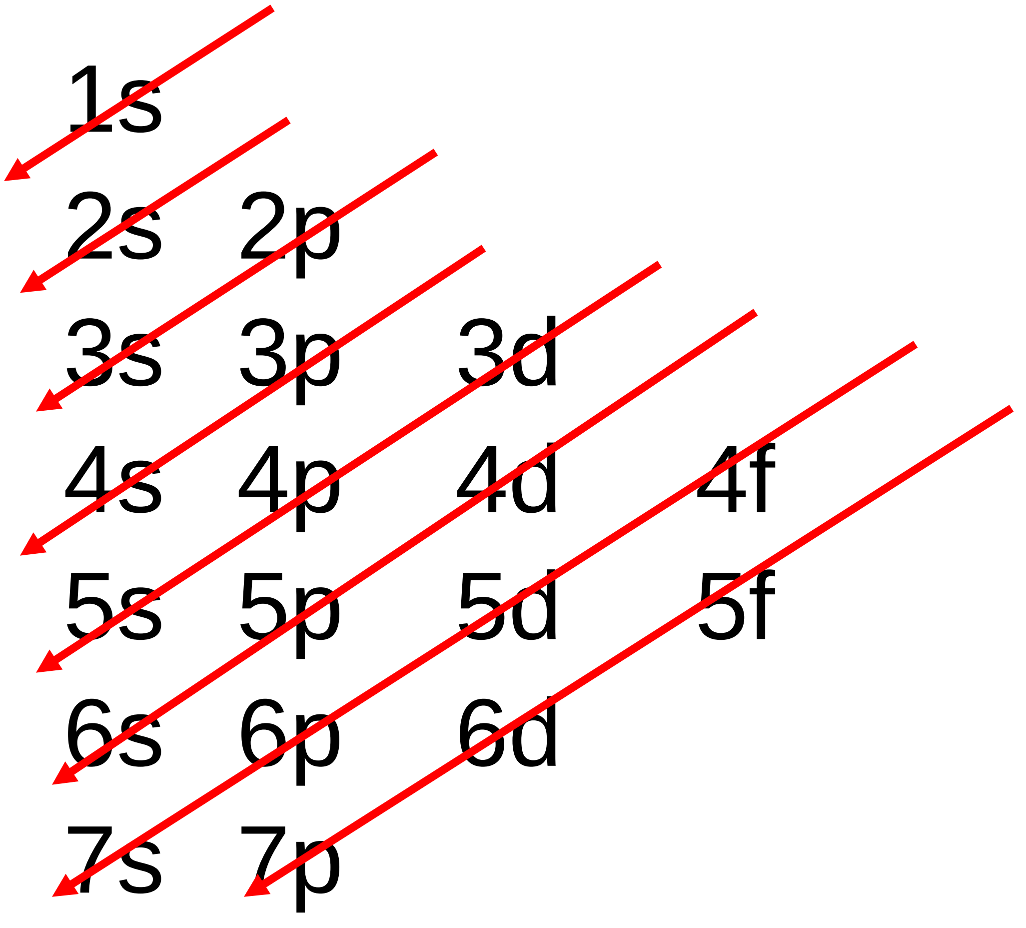
Aufbau order of filling



Order of filling

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p

Periodic table structure

- The actual structure of the periodic table reflects our current theory of quantum mechanics and atomic structure
- atoms of like structure are arranges into “blocks”

Periodic Table - Electronic Structure

Note that He has been moved next to H

s block | d block | p block

n																		
1	H	He																
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Unq	Unp	Unh												

Lanthanides	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Actinides	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

f block

Periodic table structure

- For the s and p block elements:

  The <u>energy level</u> is the <u>same</u> as the <u>period</u> on the periodic table

Periodic table structure

- due to orbital energy overlap, the d block is one energy level lower than the period it is in, and the f orbital block is two energy levels lower than the period it is in.

Periodic Table - Electronic Structure

Note that He has been moved next to H

n	s block		d block										p block					
1	H	He																
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Unq	Unp	Unh												

f block														
Lanthanides	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Actinides	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Electron configurations

- Shorthand method of indicating where the electrons are in an atom
- Follows the order of filling, but removes the necessity of drawing out the orbital energy diagram

Electron configurations

- H - 1 electron

$1s^1$

- He - 2 electrons

$1s^2$

- Li - 3 electrons

$1s^2\ 2s^1$

- Be - 4 electrons

$1s^2\ 2s^2$

- B - 5 electrons

$1s^2\ 2s^2\ 2p^1$

- C - 6 electrons

$1s^2\ 2s^2\ 2p^2$

Electron configurations

- N - 7 electrons

$1s^2\ 2s^2\ 2p^3$

- O - 8 electrons

$1s^2\ 2s^2\ 2p^4$

- F - 9 electrons

$1s^2\ 2s^2\ 2p^5$

- Ne - 10 electrons

$1s^2\ 2s^2\ 2p^6$

- Na - 11 electrons

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

- Mg - 12 electrons

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

Electron configurations

- What about the transition metals?
- All are filling the d orbitals, which means there is some orbital energy overlap
- $ns^2(n-1)d^x$

Electron configurations

- Examples:
- Sc - 21 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^1$

- Fe - 26 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

Electron configurations

- Zn - 30 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}$

- Ga - 31 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$

- Kr - 36 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

Shell or kernel notation

- Notice: the order of filling “starts over” after each noble gas
- example: Kr

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

- now, consider Rb, with one more electron:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^1$

Shell or kernel notation

- Because the configuration for Rb is basically the same as Kr, with one additional electron added, there is a “shorthand” notation

☹ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^1$

☺ $[Kr]5s^1$

Shell or kernel notation

Table 5.5 Electron Configurations for Elements 11–18

Element	Atomic Number	Complete Electron Configuration	Electron Configuration Using Noble Gas
Sodium	11	$1s^22s^22p^63s^1$	$[Ne]3s^1$
Magnesium	12	$1s^22s^22p^63s^2$	$[Ne]3s^2$
Aluminum	13	$1s^22s^22p^63s^23p^1$	$[Ne]3s^23p^1$
Silicon	14	$1s^22s^22p^63s^23p^2$	$[Ne]3s^23p^2$
Phosphorus	15	$1s^22s^22p^63s^23p^3$	$[Ne]3s^23p^3$
Sulfur	16	$1s^22s^22p^63s^23p^4$	$[Ne]3s^23p^4$
Chlorine	17	$1s^22s^22p^63s^23p^5$	$[Ne]3s^23p^5$
Argon	18	$1s^22s^22p^63s^23p^6$	$[Ne]3s^23p^6$ or [Ar]

Which electrons “matter” the most?

- All types of chemical bonds involve electrons
- Valence electrons, the electrons in the *outermost occupied* ***energy level*** of an atom, are usually the electrons involved in bonding

- The representative elements have the same number of valence electrons as their family number in the American system
  - Example: Mg, column 2A, 2 valence electrons

- The transition metals all have two valence electrons

  $ns^2(n-1)d^x$

How many valence electrons?

- Zn - 30 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}$

- Ga - 31 electrons

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$

- Kr - 36 electrons

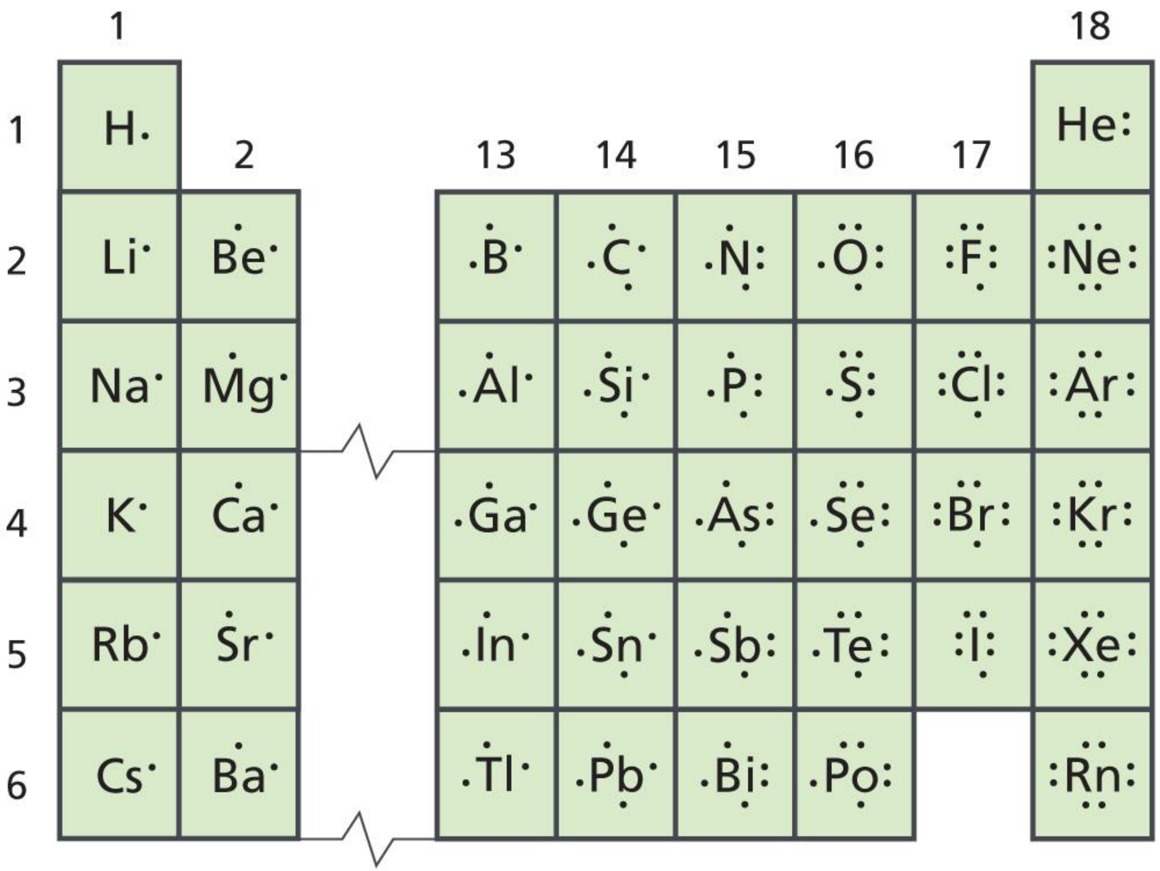
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

- Lewis dot structures are used to represent the valence electrons
  - each dot represents a valence electron
  - no more than 8 dots total
  - no more than 2 dots on a side
  - example = Mg: Na·

Think about it…

- What would be true about the dot structure for any atom in the same group or family
  - Ex: any halogen? Any group 5B element?
- Every element in the same vertical column would be expected to have the identical dot structure.
  - Ex: all group 5A elements have 5 valence electrons, and have 5 dots

Lewis dot structures of representative elements



The Octet Rule

- In bonding situations, atoms of representative elements will tend to *gain*, *lose*, or *share* electrons until they achieve an ns^2np^6 valence configuration
- This results in 8 valence electrons
- The noble gases start with 8 valence electrons

Electron Configuration of Ions

Na $\Rightarrow$ $1s^2 2s^2 2p^6 3s^1$

- will tend to lose it's one valence e- to gain ns^2np^6 configuration
- $Na^+ \Rightarrow 1s^2 2s^2 2p^6$

S $\Rightarrow$ $1s^2 2s^2 2p^6 3s^2 3p^4$

- will tend to gain 2 e- to gain ns^2np^6 configuration
- $S^{2-} \Rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6$

Electrons and magnetism

- Electrons behave like tiny magnets
  - Any moving electric charge induces a magnetic field
- Paired electrons, with opposite spins, “cancel out” each other
- Unpaired electrons can lead to observable magnetic properties

paramagnetic

- A substance that is attracted to a magnetic field
- The result of <u>unpaired electrons</u>

Na: $[Ne]3s^1$ 3s ↑

O: $1s^2 2s^2 2p^4$ 2s ↑↓ 2p ↑↓ ↑ ↑

Fe: $[Ar]4s^2 3d^6$ 4s ↑↓ 3d ↑↓ ↑ ↑ ↑ ↑

diamagnetic

- A substance that is not attracted to a magnetic field
- All electrons are paired
- Opposite spins cancel out each electron's magnetic field
- Zn: [Ar]$4s^2 3d^{10}$

4s ↑↓   3d ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

Electron Configuration - excited state

Na$\Rightarrow$ $1s^2 2s^2 2p^6 3s^1$

– If it absorbs energy, one or more electrons will be promoted to a higher, *unoccupied* orbital

Ex: Na$\Rightarrow$ $1s^2 2s^1 2p^6 3s^1 3p^1$

You can spot the configuration for an excited state atom by noticing **unfilled orbital sets** at **lower energy levels**

Inner transition elements

- All place one electron in a “d” orbital before beginning to fill the “f” orbitals
- *This is <u>only true for elements in the f-block</u>*
- All other elements follow the 6s - 4f - 5d or 7s - 5f - 6d order of filling as expected

Electron configurations

Inner transition exception examples

- Ba [Xe] $6s^2$
- La   [Xe] $6s^2\ 5d^1$
- Ce [Xe] $6s^2\ 5d^1\ 4f^1$
- Lu [Xe] $6s^2\ 5d^1\ 4f^{14}$
- Hf [Xe] $6s^2\ 4f^{14}\ 5d^2$