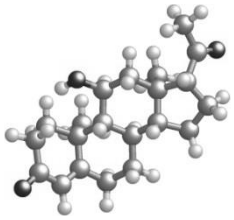

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Atomic Orbital Theory – Concepts: Evidence and Models

Learning Outcomes

Students should be able to:

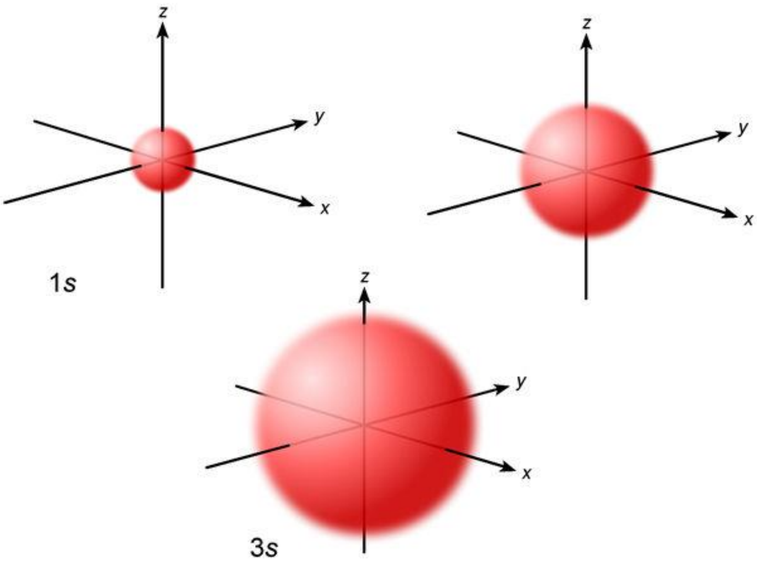
- State the electronic configuration of an atom of any one of the first thirty elements using atomic orbital theory.
- Assign electrons to the orbital schematic of an atom based upon the *Aufbau Principle*, *Hund's Rule of Maximum Multiplicity* and *Pauli's Exclusion Principle*.

Essential Understandings

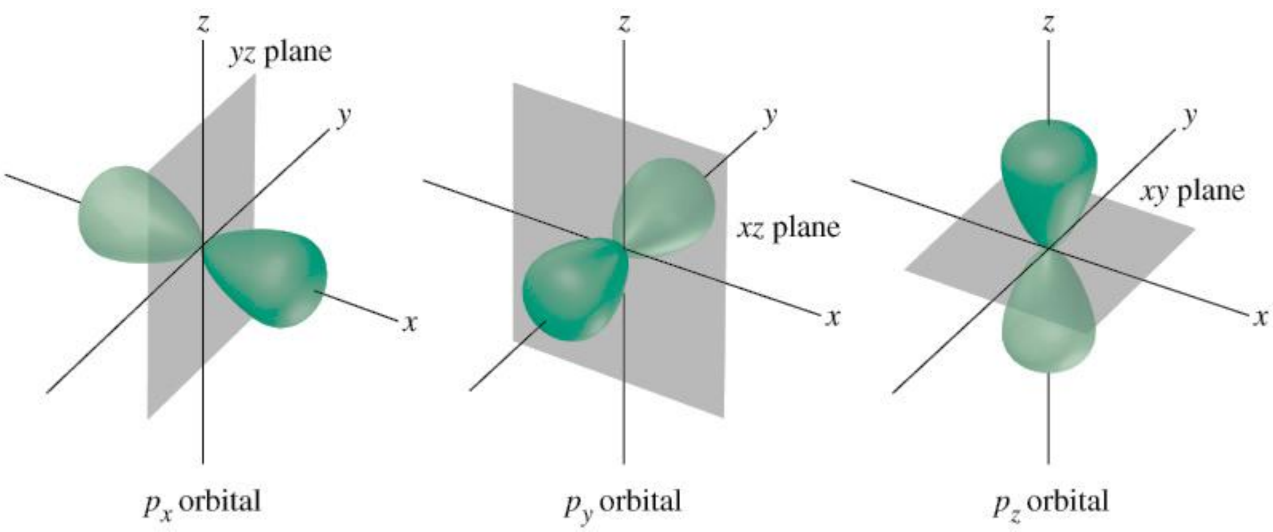
- In 1924, Louis De Broglie made the bold suggestion that electrons might behave as waves instead of just behaving as particles. Erwin Schrödinger and Paul Dirac built on this idea and formulated the now famous *Schrodinger's Wave Equation* which describes how electrons – behaving as waves – orbit the nucleus of the atom.
- If electrons are treated as waves and their behaviour is modelled mathematically, the result is a series of three dimensional shapes or *orbitals*.
- An orbital is the *volume* of space around the nucleus of the atom in which there is a 95% probability of locating an electron.
- An atomic orbital can hold a maximum number of two electrons.
- The location of an electron in an atom (*i.e.* which atomic orbital it belongs to) is given by four electronic quantum numbers.
    1. n is the principle quantum number. It describes the principle quantum shell that the electron occupies.
    2. l is the sub-shell within the principle quantum shell that the electron occupies, *e.g.* *s*-orbitals, *p*-orbitals and *d*-orbitals.
    3. m is the orbital in the sub-shell that the electron occupies, *e.g.* *p*-orbitals are always arranged in groups of three, so if an electron occupies a *p*-orbital, this electronic quantum number states exactly which one, the p_x-orbital, p_y-orbital or the p_z-orbital.

4. s is the spin quantum number. For electrons to occupy exactly the same orbital, they must spin in opposite directions. This electronic quantum number states whether an electron has a spin of +½ or –½.

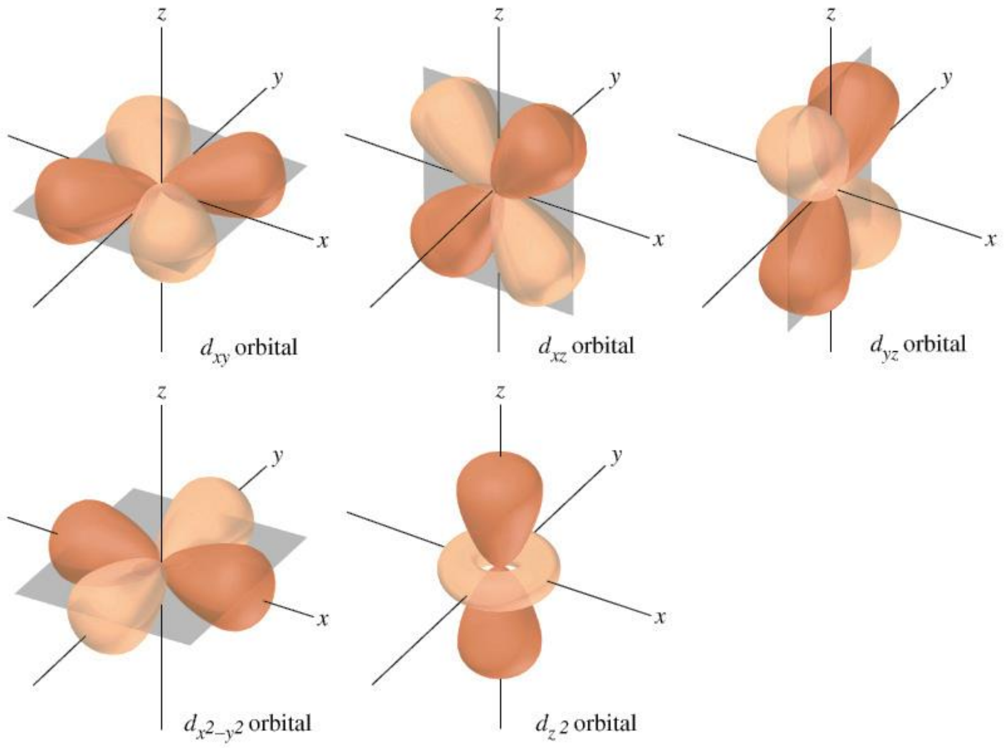
- Different numerical values for the various electronic quantum numbers give rise to orbitals with different shapes and different properties.
- *s-orbitals* are *spherical* and exist *individually*. The diagram below shows the shapes of the 1s, 2s and 3s-orbitals.



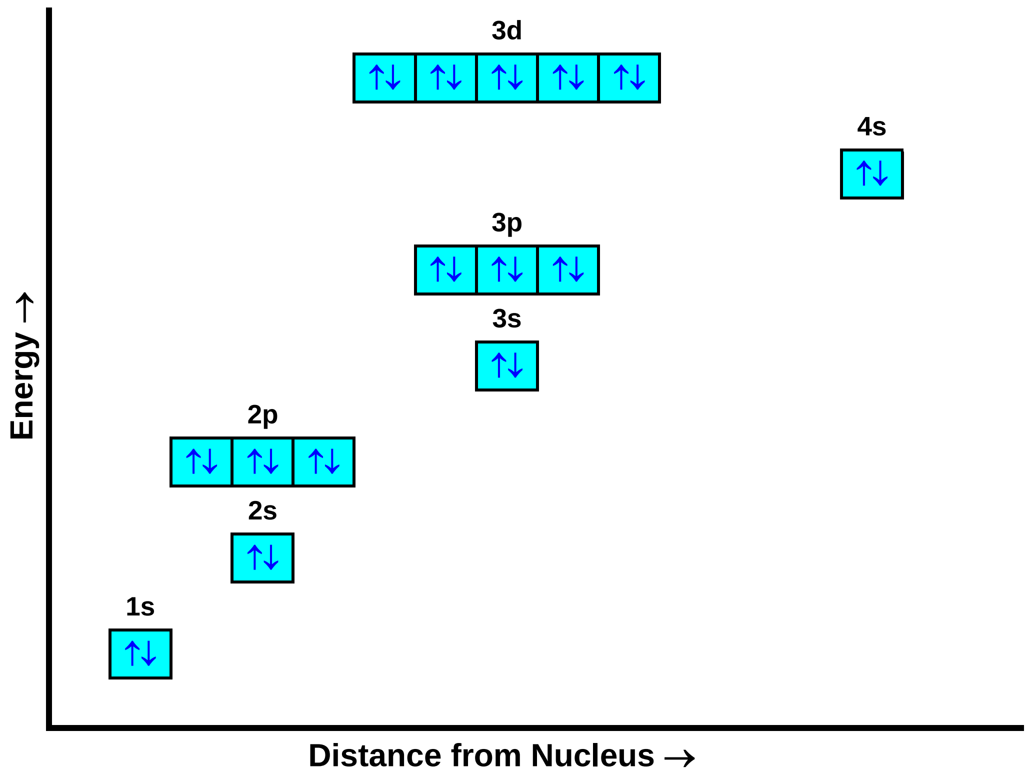
- *p-orbitals* have an *hourglass* shape and exist in *groups of three*, arranged at right-angles to each other. The diagram below shows the shapes and arrangements of three different *p*-orbitals. **Note**: For clarity, the three different *p*-orbitals have been drawn separately. In reality, it is assumed that they are all superimposed on top of each other.



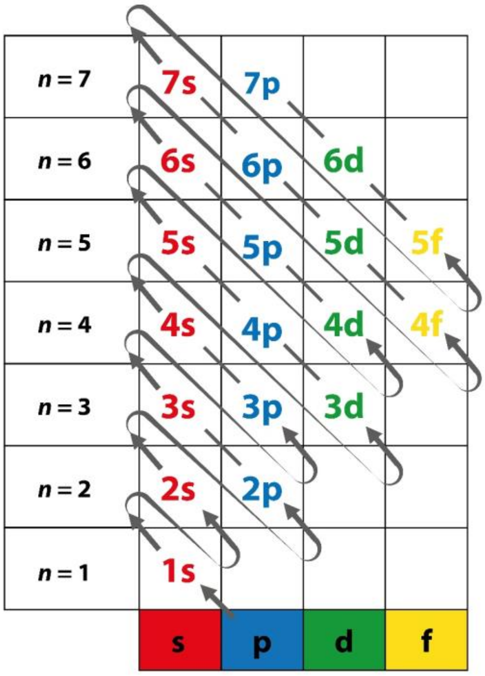
- *d-orbitals* have a variety of *complex* three-dimensional shapes and exist in *groups of five*. The diagram below shows the shapes and arrangements of five different *d*-orbitals. **Note**: For clarity, the five different *d*-orbitals have been drawn separately. In reality, it is assumed that they are all superimposed on top of each other.



- The diagram below shows the distribution of *s*-, *p*- and *d*-orbitals in terms of their energy and physical distance from the nucleus of the atom.



- The diagram below shows the order in which atomic orbitals fill-up with electrons.



<u>Rules for Filling Atomic Orbitals</u>

1. **Heisenberg's Uncertainty Principle**: *It is not possible to determine both the position and the momentum of an electron at the same time*. This gives rise to the idea that an electron's position in an atom is *uncertain*, and therefore scientists can only identify where there is the *highest probability* of finding an electron – which is how the atomic orbital is defined.
2. **The Aufbau Principle**: *Electrons fill-up atomic orbitals from the lowest energy to the highest energy*. Left undisturbed, objects will tend to their lowest possible energy.
3. **Pauli's Exclusion Principle**: *No two electrons within the same atom can have the same four quantum numbers*. Every electron in the same atom must have a unique combination of quantum numbers. Electrons in the same orbital must spin in opposite directions. In atomic orbital diagrams, the spin quantum number is represented by an arrow (↑ or ↓). Two arrows pointing in opposite directions represent two electrons with opposite spin (↑ and ↓).
4. **Hund's Rule of Maximum Multiplicity**: *When placed in atomic orbitals of equal energy, electrons will remain unpaired*. Electrons carry a charge of –1. There will be an electrostatic force of repulsion between electrons in the same orbital. Placing electrons in different atomic orbitals of the same energy will reduce the electrostatic force of repulsion between the electrons and make the system more stable.

- Each principle quantum shell is divided into one or more sub-shells.
- There are four sub-shells, arranged in increasing energy *s* → *p* → *d* → *f*. Each sub-shell holds a different number of electrons.

Principle Quantum Shell (*n*)	Sub-shell (*l*)	Maximum number of electrons
1	1*s*	2
2	2*s*, 2*p*	8
3	3*s*, 3*p*, 3*d*	18
4	4*s*, 4*p*, 4*d*, 4*f*	32

Orbital	Shape	Occurrence
s-orbital (sharp)	Spherical	**1** in every principle level
p-orbital (principle)	Dumb Bell / Hour Glass	**3** in every principle level from **2** onwards
d-orbital (diffuse)	Complex and Various	**5** in every principle level from **3** onwards.
f-orbital (fundamental)	Complex and Various	**7** in every principle level from **4** onwards

<u>Electron Configurations of the First Thirty Chemical Elements</u>

Use the information that has been provided to complete the electronic configurations given below. Some of the electronic configurations have already been completed to help guide you **Note:** Electrons are represented by arrows, ↑ and ↓ to reflect their opposite spin.

Hydrogen Atom – H – Atomic Number 1

1s	**2s**	**2p**			**3s**	**3p**			**3d**					**4s**

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Helium Atom – He – Atomic Number 2

1s	**2s**	**2p**			**3s**	**3p**			**3d**					**4s**

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Lithium Atom – Li – Atomic Number 3

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Beryllium Atom – Be – Atomic Number 4

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Boron Atom – B – Atomic Number 5

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Carbon Atom – C – Atomic Number 6

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Nitrogen Atom – N – Atomic Number 7

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑	↑	↑										

Lower Energy Higher Energy

- Written as: $1s^2 2s^2 2p^3$

Oxygen Atom – O – Atomic Number 8

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Fluorine Atom – F – Atomic Number 9

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Neon Atom – Ne – Atomic Number 10

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Sodium Atom – Na – Atomic Number 11

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Magnesium Atom – Mg – Atomic Number 12

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Aluminium Atom – A*l* – Atomic Number 13

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Silicon Atom – Si – Atomic Number 14

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Phosphorus Atom – P – Atomic Number 15

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Sulfur Atom – S – Atomic Number 16

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Chlorine Atom – C*l* – Atomic Number 17

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ………………………………………………………………………………………..

Argon Atom – Ar – Atomic Number 18

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Potassium Atom – K – Atomic Number 19

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

  - **Note:** The 4s sub-shell is occupied before the 3d sub-shell because, although 4s is further from the nucleus than 3d, 4s is *lower in energy* than 3d (Aufbau Principle).

Calcium Atom – Ca – Atomic Number 20

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Scandium Atom – Sc – Atomic Number 21

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑					↑↓

Lower Energy Higher Energy

- Written as: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$ or $[Ar]3d^1 4s^2$

Titanium Atom – Ti – Atomic Number 22

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Vanadium Atom – V – Atomic Number 23

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Chromium Atom – Cr – Atomic Number 24

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑	↑	↑

Lower Energy Higher Energy

- Written as: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$ or $[Ar]3d^5 4s^1$

- **Note:** Sub-shells that are half-filled or completely filled are inherently stable.

Manganese Atom – Mn – Atomic Number 25

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Iron Atom – Fe – Atomic Number 26

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Cobalt Atom – Co – Atomic Number 27

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Nickel Atom – Ni – Atomic Number 28

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Copper Atom – Cu – Atomic Number 29

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

- **Note:** Sub-shells that are half-filled or completely filled are inherently stable.

Zinc Atom – Zn – Atomic Number 30

1s	2s	2p			3s	3p			3d					4s
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

Lower Energy Higher Energy

- Written as: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$ or $[Ar]3d^{10}4s^2$

Electronic Configurations of Ions

Nitride Ion – N^{3-}

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Chloride Ion – Cl^-

1s	2s	2p			3s	3p			3d					4s

Lower Energy Higher Energy

- Written as: ……………………………………………………………………………………..

Magnesium Ion – Mg^{2+}

1s	2s	2p			3s	3p			3d					4s

Lower Energy — Higher Energy

- Written as: ……………………………………………………………………………………………..

Chromium(III) Ion – Cr^{3+}

1s	2s	2p			3s	3p			3d					4s

Lower Energy — Higher Energy

- Written as: ……………………………………………………………………………………………..

Iron(III) Ion – Fe^{3+}

1s	2s	2p			3s	3p			3d					4s

Lower Energy — Higher Energy

- Written as: ……………………………………………………………………………………………..

- **Note:** When atoms of the transition metals react to form ions, electrons from the 4s orbital are the first to be removed.

- Scan the QR Code below to view the answers to this assignment.

http://www.chemist.sg/chemical_bonding/notes_atomic_structure/advanced_notes_atomic_structure_ans.pdf