

Atomic Structure and Periodic Trends

Introduction to Electronic Structure

- Electrons are responsible for most properties of an element.
- The arrangement and energy levels of the electrons as they move around the nucleus determine these properties.
- In this lecture we will be learning about the rules that determine the energy levels of electrons and the regions of space occupied by the electrons
- In a later lecture we will consider how these characteristic of the electrons determine the chemistry of the elements.

Electronic Orbitals

- When electrons are held near the nucleus they are arranged in electronic orbitals.
- Though called orbitals, electrons do not move around the nucleus the way planets orbit around the sun.
- They occupy space in a manner that can be described by Quantum Mechanics, which is a part of physics that is concerned with subatomic particles.

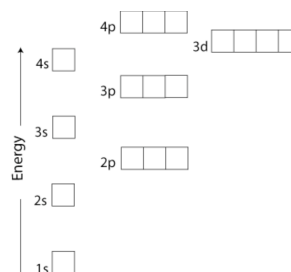
Quantum Mechanics and Chemistry

- Though a branch of physics, quantum mechanics and how it can be used to explain and predict the electronic structure of elements and compounds
- Electrons occupy specific energy levels, and principally exist in a particular arrangement around atoms, these properties determine how elements interact and the types of bonds they form and how compounds made of them behave.

The Electron Game

- There are multiple orbitals around a nucleus.
- One can argue that orbitals exist even when electrons are not in them.
- When electrons are placed around a nucleus, when one orbital, additional electrons are placed in the next highest energy orbital.

A Preview of an Orbital Diagram



3.6 Electronic Structure of Atoms

Quantum mechanical model of atomic structure:

- ▶ The electrons in an atom are grouped around the nucleus into shells, roughly like the layers in an onion.
- ▶ The farther a shell is from the nucleus, the larger it is, the more electrons it can hold, and the higher the energies of those electrons.
- ▶ The smallest shell closest to the nucleus is labeled shell 1, the next one is shell 2, and so on.

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Not Quite an Onion

Images from <http://www.uwgb.edu/dutchs/PETROLOGY/WhatElmsLookLike.HTM>

1 or 2 electrons

9 or 10 electrons

- ▶ Within the shells, electrons are further grouped into subshells of four different types, identified as s , p , d , and f in order of increasing energy.
- ▶ A shell has a number of subshells equal to its shell number.
- ▶ The first shell has only an s subshell; the second shell has an s and a p subshell; the third shell has an s , a p , and a d subshell, and so on.

Shell number:	1	2	3	4
Subshell designation:	s	s, p	s, p, d	s, p, d, f

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- ▶ Within each subshell, electrons are further grouped into orbitals, regions of space within an atom where the specific electrons are more likely to be found.
- ▶ The number of orbitals within a subshell increases as the odd numbers.
- ▶ An s subshell has 1 orbital, a p has 3, a d has 5, and so on.

Shell number:	1	2	3	4
Subshell designation:	s	s, p	s, p, d	s, p, d, f
Number of orbitals:	1	1, 3	1, 3, 5	1, 3, 5, 7

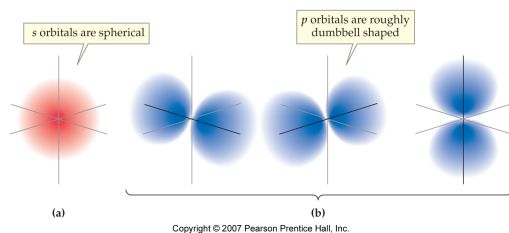
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Different orbitals have different shapes. Orbitals in s subshells are spherical (a), while orbitals in p subshells are roughly dumbbell shaped (b).



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- ▶ Any orbital can hold a maximum of 2 electrons.
- ▶ The first shell has one $1s$ orbital and holds 2 electrons.
- ▶ The second shell can hold 8 electrons, 2 in a $2s$ orbital, and 6 in three $2p$ orbitals.
- ▶ The third shell can hold 18 electrons, 2 in a $3s$ orbital, 6 in three $3p$ orbitals, and 10 in five $3d$ orbitals, and so on.

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The overall electron distribution within an atom is summarized in Table 3.2 below.

TABLE 3.2 Electron Distribution in Atoms

SHELL NUMBER:	1	2	3	4
Subshell designation:	s	s, p	s, p, d	s, p, d, f
Number of orbitals:	1	1, 3	1, 3, 5	1, 3, 5, 7
Number of electrons:	2	2, 6	2, 6, 10	2, 6, 10, 14
Total electron capacity:	2	8	18	32

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3.7 Electron Configurations

Electron Configuration: The exact arrangement of electrons in atom's shells and subshells. Rules to predict electron configuration:

1. Electrons occupy the lowest energy orbitals available first.
2. Each orbital can hold only two electrons, which must be of opposite spin.
3. If two or more orbitals have the same energy, each orbital gets one electron before any orbital gets two.

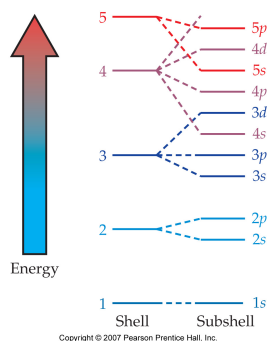
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Order of orbital energy levels:

- ▶ Electrons fill orbitals from the lowest-energy orbitals upward.
- ▶ Lower numbered shells fill before higher numbered shells at first.
- ▶ Some overlap in energy levels occurs starting with shell 3 and 4.



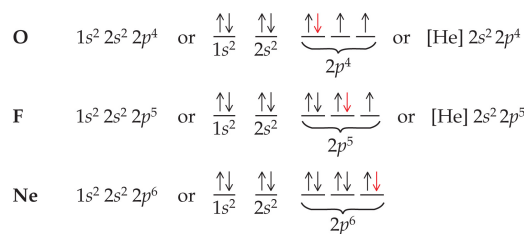
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These are the electron configurations for O - Ne



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3.8 Electron Configuration and the Periodic table

Valence shell: Outermost, highest energy shell of an atom.

Valence electrons: An electron in an outermost shell of an atom. These electrons are loosely held, they are most important in determining an element's properties.

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- ▶ The periodic table can be divided into four regions or blocks, of elements according to the subshells that are last to fill, *s*, *p*, *d*, or *f*.
- ▶ Beginning at the top left corner of the periodic table, the first row contains only two elements, H and He. The 1*s* subshell is being filled here.
- ▶ The second row begins with two *s*-block elements (Li and Be) and continues with six *p*-block elements (B through Ne), so electrons fill the next available *s* orbital (2*s*) and then the first available *p* orbitals (2*p*).

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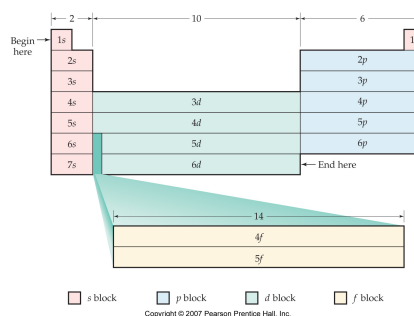
- ▶ The third row is similar to the second row, so the 3*s* and 3*p* orbitals are filled next.
- ▶ The fourth row again starts with two *s*-block elements (K and Ca) but is then followed by ten *d*-block elements (Sc through Zn) and six *p*-block elements (Ga through Kr). Thus, the order of orbital filling is 4*s* followed by the first available *d* orbitals (3*d*) followed by 4*p*.
- ▶ Continuing through successive rows of the periodic table provides a visual method to recall the entire filling order.

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Visual method to recall the order of orbital filling.



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