

6.2: Electron Configurations - The Quantum Model and Periodic Structure

Learning Objective

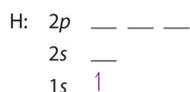
- To write the electron configuration of any element and relate its electron configuration to its position in the periodic table.

We know that each electron in an atom is described by a unique set of four quantum numbers: n , l , m_l , and m_s . Beyond their Quantum Mechanical definitions, what do these numbers actually mean, and why are they important to know in a general chemistry course?

Quantum numbers and the quantum model that derived them depict our current best understanding of what an atom actually is and how it behaves based on the energetic structure of electrons within it. The process of describing each atom's *electronic structure* consists, essentially, of beginning with hydrogen and adding one proton and one electron at a time to create the next heavier element in the table. From our theoretical understanding of the electronic structuring of electrons in each element, we will find that these electron configurations are innately related to the structure and organization of The Periodic Table.

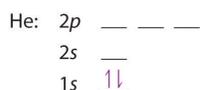
The Aufbau Principle

We construct The Periodic Table by following the *Aufbau Principle* (from German, meaning “building up”). This is the process used to build up the periodic table by adding protons one by one to the nucleus and adding the corresponding electrons to the lowest-energy orbital available without violating the Pauli exclusion principle. First we determine the number of electrons in the atom; then we add electrons one at a time to the lowest-energy orbital available *without violating the Pauli principle*. We use the orbital energy diagram of Hydrogen, recognizing that each orbital can hold two electrons, one with spin up \uparrow , corresponding to $m_s = +\frac{1}{2}$, which is arbitrarily written first, and one with spin down \downarrow , corresponding to $m_s = -\frac{1}{2}$. A filled orbital is indicated by $\uparrow\downarrow$, in which the electron spins are said to be *paired*. Here is a schematic orbital diagram for a hydrogen atom in its ground state:



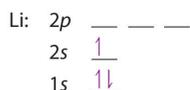
From the orbital diagram, we can write the electron configuration in an abbreviated form in which the occupied orbitals are identified by their principal quantum number n and their value of l (s , p , d , or f orbital type), with the number of electrons in the subshell indicated by a superscript. For hydrogen, therefore, the single electron is placed in the $1s$ orbital, which is the orbital lowest in energy, and the electron configuration is written as $1s^1$ and read as “one-s-one.”

A neutral helium atom, with an atomic number of 2 ($Z = 2$), has two electrons. We place one electron in the orbital that is lowest in energy, the $1s$ orbital. From the Pauli exclusion principle, we know that an orbital can contain two electrons with opposite spin, so we place the second electron in the same orbital as the first but pointing down, so that the electrons are paired. The orbital diagram for the helium atom is therefore:



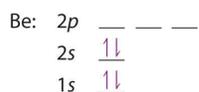
written as $1s^2$, where the superscript 2 implies the pairing of spins. Otherwise, our configuration would violate the Pauli principle. Remember that because the helium nucleus has a positive charge of +2, the $1s$ level of helium lies considerably below the $1s$ level of hydrogen, although for the purposes of building up the periodic table we do not take that into consideration. The orbital diagrams are energy ordered, the levels are in the proper energy order from bottom (most bound) to least, but the energies are not scaled.

The next element is lithium, with $Z = 3$ and three electrons in the neutral atom. We know that the $1s$ orbital can hold two of the electrons with their spins paired. The next lowest energy orbital is $2s$, so the orbital diagram for lithium is:

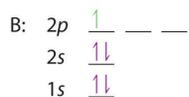


This electron configuration is written as $1s^2 2s^1$.

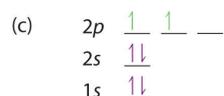
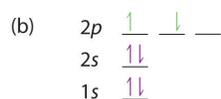
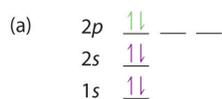
The next element is beryllium, with $Z = 4$ and four electrons. We fill both the $1s$ and $2s$ orbitals to achieve a $1s^2 2s^2$ electron configuration:



When we reach boron, with $Z = 5$ and five electrons, we must place the fifth electron in one of the $2p$ orbitals. Remember that the actual energy difference between the $2s$ and $2p$ levels is much smaller than that between the $1s$ and $2s$ levels. Because all three $2p$ orbitals are degenerate, it doesn't matter which one we select. The electron configuration of boron is $1s^2 2s^2 2p^1$:



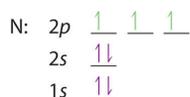
At carbon, with $Z = 6$ and six electrons, we are faced with a choice. Should the sixth electron be placed in the same $2p$ orbital that already has an electron, or should it go in one of the empty $2p$ orbitals? If it goes in an empty $2p$ orbital, will the sixth electron have its spin aligned with or be opposite to the spin of the fifth? In short, which of the following three orbital diagrams is correct for carbon, remembering that the $2p$ orbitals are degenerate?



Because of electron-electron repulsions, it is more favorable energetically for an electron to be in an unoccupied orbital than in one that is already occupied; hence we can eliminate choice (a). Similarly, experiments have shown that choice (b) is slightly higher in energy (less stable) than choice (c) because electrons in degenerate orbitals prefer to line up with their spins parallel; thus, we can eliminate choice (b).

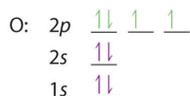
Choice (c) illustrates **Hund's rule** (named after the German physicist Friedrich H. Hund, 1896–1997), which today says that the lowest-energy electron configuration for an atom is the one that has the maximum number of electrons with parallel spins in degenerate orbitals. By Hund's rule, the electron configuration of carbon, which is $1s^2 2s^2 2p^2$, is understood to correspond to the orbital diagram shown in c. Experimentally, it is found that the ground state of a neutral carbon atom does indeed contain two unpaired electrons.

When we get to nitrogen ($Z = 7$, with seven electrons), Hund's rule tells us that the lowest-energy arrangement is:

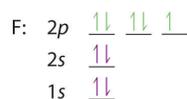


with three unpaired electrons. The electron configuration of nitrogen is thus $1s^2 2s^2 2p^3$.

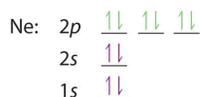
At oxygen, with $Z = 8$ and eight electrons, we have no choice. One electron must be paired with another in one of the $2p$ orbitals, which gives us two unpaired electrons and a $1s^2 2s^2 2p^4$ electron configuration. Because all the $2p$ orbitals are degenerate, it doesn't matter which one has the pair of electrons.



Similarly, fluorine has the electron configuration $1s^2 2s^2 2p^5$:



When we reach neon, with $Z = 10$, we have filled the $2p$ subshell, giving a $1s^2 2s^2 2p^6$ electron configuration:



Notice that for neon, as for helium, all the orbitals through the $2p$ level are completely filled. This fact is very important in dictating both the chemical reactivity and the bonding of helium and neon, as you will see.

Valence Electrons

As we continue through the periodic table in this way, writing the electron configurations of larger and larger atoms, it becomes tedious to keep copying the configurations of the filled inner orbitals. In practice, chemists simplify the notation by using a bracketed noble gas symbol to represent the configuration of the noble gas from the preceding row because all the orbitals in a noble gas are filled. For example, [Ne] represents the $1s^2 2s^2 2p^6$ electron configuration of neon ($Z = 10$), so the electron configuration of sodium, with $Z = 11$, which is $1s^2 2s^2 2p^6 3s^1$, is written as [Ne] $3s^1$:

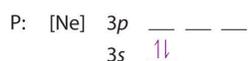
Neon	$Z = 10$	$1s^2 2s^2 2p^6$
Sodium	$Z = 11$	$1s^2 2s^2 2p^6 3s^1 = [\text{Ne}]3s^1$

Because electrons in filled inner orbitals are closer to the nucleus and more tightly bound to it, they are rarely involved in chemical reactions. This means that the chemistry of an atom depends mostly on the electrons in its outermost shell, which are called the **valence electrons**. The simplified notation allows us to see the valence-electron configuration more easily. Using this notation to compare the electron configurations of sodium and lithium, we have:

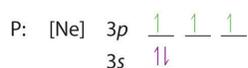
Sodium	$1s^2 2s^2 2p^6 3s^1 = [\text{Ne}]3s^1$
Lithium	$1s^2 2s^1 = [\text{He}]2s^1$

It is readily apparent that both sodium and lithium have one s electron in their valence shell. We would therefore predict that sodium and lithium have very similar chemistry, which is indeed the case.

As we continue to build the eight elements of period 3, the $3s$ and $3p$ orbitals are filled, one electron at a time. This row concludes with the noble gas argon, which has the electron configuration [Ne] $3s^2 3p^6$, corresponding to a filled valence shell.



Hund's rule tells us that the remaining three electrons will occupy the degenerate $3p$ orbitals separately but with their spins aligned:



The electron configuration is [Ne] $3s^2 3p^3$.

The general order in which orbitals are filled is depicted below. Subshells corresponding to each value of n are written from left to right on successive horizontal lines, where each row represents a row in the periodic table. The order in which the orbitals are filled is indicated by the diagonal lines running from the upper right to the lower left. Accordingly, the $4s$ orbital is filled prior to the $3d$ orbital because of shielding and penetration effects. Consequently, the electron configuration of potassium, which begins the fourth period, is [Ar] $4s^1$, and the configuration of calcium is [Ar] $4s^2$. Five $3d$ orbitals are filled by the next 10 elements, the transition metals, followed by three $4p$ orbitals. Notice that the last member of this row is the noble gas krypton ($Z = 36$), [Ar] $4s^2 3d^{10} 4p^6 = [\text{Kr}]$, which has filled $4s$, $3d$, and $4p$ orbitals. The fifth row of the periodic table is essentially the same as the fourth, except that the $5s$, $4d$, and $5p$ orbitals are filled sequentially.

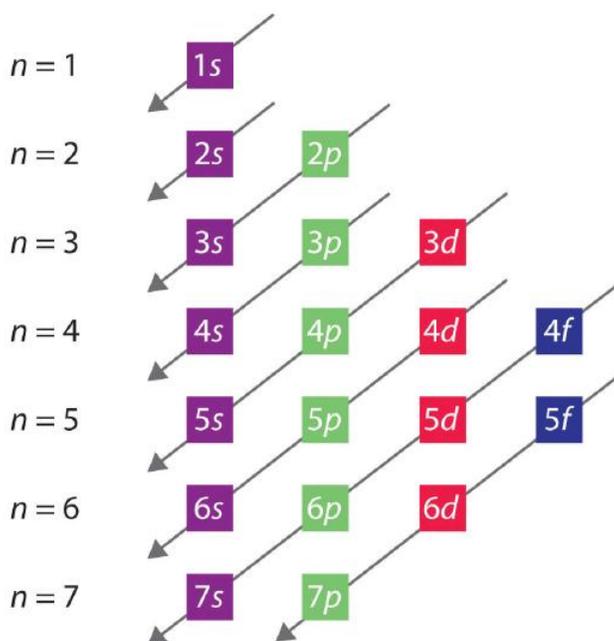


Figure 1: Predicting the Order in Which Orbitals Are Filled in Multielectron Atoms If you write the subshells for each value of the principal quantum number on successive lines, the observed order in which they are filled is indicated by a series of diagonal lines running from the upper right to the lower left.

The sixth row of the periodic table will be different from the preceding two because the $4f$ orbitals, which can hold 14 electrons, are filled between the $6s$ and the $5d$ orbitals. The elements that contain $4f$ orbitals in their valence shell are the lanthanides. When the $6p$ orbitals are finally filled, we have reached the next (and last known) noble gas, radon ($Z = 86$), $[\text{Xe}]6s^2 4f^{14} 5d^{10} 6p^6 = [\text{Rn}]$. In the last row, the $5f$ orbitals are filled between the $7s$ and the $6d$ orbitals, which gives the 14 actinide elements. Because the large number of protons makes their nuclei unstable, all the actinides are radioactive.

Note that the Aufbau Principle has some exceptions. By definition, orbitals are most stable when they are either full or half-full. Thus, in some cases where valency is very near a stable configuration, the actual electron configuration of the element differs from what is predicted by Aufbau.

Blocks in the Periodic Table

The electron configurations of the elements explain the otherwise peculiar shape of the periodic table. Although the table was originally organized on the basis of physical and chemical similarities between the elements within groups, these similarities are ultimately attributable to orbital energy levels and the Pauli principle, which cause the individual subshells to be filled in a particular order. As a result, the periodic table can be divided into “blocks” corresponding to the type of subshell that is being filled, as illustrated in Figure 2.3.3. For example, the two columns on the left, known as the s block, consist of elements in which the ns orbitals are being filled. The six columns on the right, elements in which the np orbitals are being filled, constitute the p block. In between are the 10 columns of the d block, elements in which the $(n - 1)d$ orbitals are being filled. At the bottom lie the 14 columns of the f block, elements in which the $(n - 2)f$ orbitals are being filled. Because two electrons can be accommodated per orbital, the number of columns in each block is the same as the maximum electron capacity of the subshell: 2 for ns , 6 for np , 10 for $(n - 1)d$, and 14 for $(n - 2)f$. Within each column, each element has the same valence electron configuration—for example, ns^1 (group 1) or $ns^2 np^1$ (group 13). As you will see, this is reflected in important similarities in the chemical reactivity and the bonding for the elements in each column.

Note the Pattern

Because each orbital can have a maximum of 2 electrons, there are 2 columns in the *s* block, 6 columns in the *p* block, 10 columns in the *d* block, and 14 columns in the *f* block.

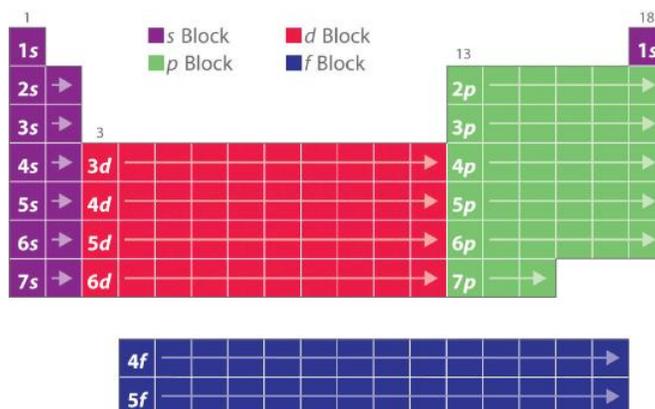


Figure 2: The Periodic Table, Showing How the Elements Are Grouped According to the Kind of Subshell (*s*, *p*, *d*, *f*) Being Filled with Electrons in the Valence Shell of Each Element

There is an alternate form, which integrates the *f* orbitals into the main table

This alternate form of the periodic table shows the *f* orbitals (lanthanides and actinides) integrated into the main table between the *s* and *d* blocks. The elements are arranged in a grid with atomic numbers 1 through 118.

Figure 3: An Alternate Form of the Periodic Table This wide form of the periodic table shows how the *4f/5f* orbitals fit between the *6s/7s* and *5d/6d* orbitals

Hydrogen and helium are placed somewhat arbitrarily. Although hydrogen is not an alkali metal, its $1s^1$ electron configuration suggests a similarity to lithium ($[\text{He}]2s^1$) and the other elements in the first column. Although helium, with a filled ns^2 subshell, should be similar chemically to other elements with an ns^2 electron configuration, the closed principal shell dominates its chemistry making it unreactive like the other noble gases, justifying its placement above neon on the right. In [Chapter 3](#), we will examine how electron configurations affect the properties and reactivity of the elements.

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

Figure 4: Electron Configurations of the Elements

The electron configurations of elements indicated in red are exceptions due to the added stability associated with half-filled and filled subshells. The electron configurations of the elements indicated in blue are also anomalous, but the reasons for the observed configurations are more complex. For elements after No, the electron configurations are tentative.

Exercises

1. Use the periodic table to predict the valence electron configuration of all the elements of group 2 (beryllium, magnesium, calcium, strontium, barium, and radium).

Given: series of elements

Asked for: valence electron configurations

Strategy:

- Identify the block in the periodic table to which the group 2 elements belong. Locate the nearest noble gas preceding each element and identify the principal quantum number of the valence shell of each element.
- Write the valence electron configuration of each element by first indicating the filled inner shells using the symbol for the nearest preceding noble gas and then listing the principal quantum number of its valence shell, its valence orbitals, and the number of valence electrons in each orbital as superscripts.

Solution:

The group 2 elements are in the s block of the periodic table, and as group 2 elements, they all have two valence electrons. Beginning with beryllium, we see that its nearest preceding noble gas is helium and that the principal quantum number of its valence shell is $n = 2$.

Thus beryllium has an $[\text{He}]s^2$ electron configuration. The next element down, magnesium, is expected to have exactly the same arrangement of electrons in the $n = 3$ principal shell: $[\text{Ne}]s^2$. By extrapolation, we expect all the group 2 elements to have an ns^2 electron configuration.

2. Use the periodic table to predict the characteristic valence electron configuration of the halogens in group 17.

Answer: All have an ns^2np^5 electron configuration, one electron short of a noble gas electron configuration. (Note that the heavier halogens also have filled $(n - 1)d^{10}$ subshells, as well as an $(n - 2)f^{14}$ subshell for Rn; these do not, however, affect their chemistry in any significant way.

3. A set of four quantum numbers specifies each wave function. What information is given by each quantum number? How does this information relate to the periodic table?

4. The periodic table is divided into blocks. Identify each block and explain the principle behind the divisions. Why does the p-block contain 6 total columns?

5. Propose an explanation as to why the noble gases are inert.

Key Takeaway

- The arrangement of atoms in the periodic table arises from the lowest energy arrangement of electrons in the valence shell.

This page was originally authored by Joshua Halpern, Scott Sinex and Scott Johnson with modifications/edits made by Camille Kaslan.

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