

- An e^{-1} configuration is an atom's particular distribution of e^{-1} among the available subshells and orbitals. For example, the ground state for Li is: $1s^2 2s^1$
- An orbital diagram can be used to display each orbital as a circle, and the e^{-1} 's as arrows within.

Pauli Exclusion Principle

- No two e^{-1} 's can have all four quantum numbers in common.
- So, each e^{-1} has a unique location.
- The first three quantum numbers define the shell, subshell, and orbital.
- The last quantum number, $m_s \in \{-\frac{1}{2} \text{ and } +\frac{1}{2}\}$, is for **two** e^{-1} in the same orbital, and refers to their two different (opposing) spin directions.
- An orbital can hold a maximum of two e^{-1} 's, and they will have opposing spins.
- $L = 0$ (s subshell) has only one orbital ($m_L = 0$), and holds two (2) e^{-1} 's.
- $L = 1$ (p subshell) has three orbitals ($m_L = -1, 0, \text{ and } +1$), and holds six (6) e^{-1} 's.
- $L = 2$ (d subshell) has five orbitals ($m_L = -2, -1, 0, +1, \text{ and } +2$), and holds ten (10) e^{-1} 's.
- $L = 3$ (f subshell) has seven orbitals, and holds fourteen (14) e^{-1} 's.
- See this table for the [e⁻¹ configurations of the elements](#).

Example 8.01 Electron Configurations and the Pauli Exclusion Principle

- Is $1s^3$ possible? No, because 1s would have three e^{-1} 's in one orbital, which is impossible.
- Can a 2s orbital diagram contain three e^{-1} 's? No, the maximum is two e^{-1} 's in an orbital.
- Can two e^{-1} 's be in the same 2s orbital with the same spin also? No, they must be spin-paired.
- Is $1s^2 2s^2 2p^7 3s^1$ possible? No, because the maximum amount of e^{-1} 's in 2p is six.
- Boron (B) has five e^{-1} 's. 1s and 2s are spin-paired. 2p has one e^{-1} in one of its three orbitals.
- All s subshells for Ni have two e^{-1} 's, all p subshells have six, and its 3d has eight (max is ten).

Electronic States

- The ground state is the lowest energy (E) arrangement.
The orbitals are filled in order, so that the lowest energy orbitals are filled first.
- An excited state has more energy than the ground state.
At least one e^{-1} is in a higher energy orbital for an excited state atom.

Aufbau Principle

- The e^{-1} configurations are determined by "building up" from lowest E to highest E.
- This means that the e^{-1} 's successively filling up subshells in this order:
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f
- See Figures [6.24](#) and [6.26](#) for diagrams of the filling order.
- The e^{-1} configurations can be partially abbreviated using noble gas configurations.
For example, Na's configuration can be written as $1s^2 2s^2 2p^6 3s^1$, or as $[\text{Ne}]3s^1$.
Ne's configuration is $1s^2 2s^2 2p^6$, which can be referred to as a "noble gas core".

Columns in the Periodic Table

- The pattern which follows from the Aufbau principle creates the order that is depicted in the periodic table.
- Noble gases, such as Ar and Kr, are on the far right of the table (column **VIIIA**), and they have filled s and p subshells at the end of their [electron configurations](#).
- Alkali metals (column **IA**) have one more e^{-1} than noble gases, with the last e^{-1} in an s orbital. For example, Na has $[\text{Ne}]3s^1$.
- Alkali earth metals (column **IIA**) have two e^{-1} 's in the outermost s orbital. Mg, for instance, possesses one more e^{-1} than Na. So, Mg has $[\text{Ne}]3s^2$.
- Transition metals (**B** columns in middle of table) have their outermost e^{-1} in d and s subshells. For instance, Sc has $[\text{Ar}]3d^14s^2$.
- A filled d subshell can be called a “pseudo-noble-gas core”, because the e^{-1} 's in d are not reactive when the d subshell is completely filled. For example, Ga's configuration is $[\text{Ar}]3d^{10}4s^24p^1$, and only its outer s and p subshells are reactive.
- Inner transition elements (two series at **bottom** of table) have partially filled f subshells.
- Exceptions: Cu and Cr have only one e^{-1} in s, while their d subshells are only partially filled.
- Figure [6.27](#) shows how the periodic table uses the building-up order of subshells, where an elements' outermost e^{-1} 's (that is, their **valence** e^{-1} 's) follow the Aufbau principle.

Example 8.02 Configuration for Ge ($Z=32$) using the Aufbau principle

- The subshells are filled up through 4s and 3d, while 4p has the two remaining e^{-1} 's.
- So, filling all the lower subshells completely, we get: $1s^22s^22p^63s^23p^63d^{10}4s^24p^2$.
- Note the superscripted numbers add up to 32, which is the total number of e^{-1} 's.

Example 8.03 Configurations for outer e^{-1} 's of I ($Z=53$) and Ti ($Z=22$)

- I (iodine) is the fifth element in the **5p** block on the table.
So, 5p has **five** e^{-1} 's, and all of the subshells with less energy than 5p are full.
This gives us the complete configuration as $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^5$, which can be abbreviated as $[\text{Kr}]4d^{10}5s^25p^5$.
- Ti (titanium) is the second element in the **3d** block on the table.
So, 3d has **two** e^{-1} 's, and all of the subshells with less energy than 3d are full.
This gives us: $1s^22s^22p^63s^23p^63d^24s^2$, which can be abbreviated as $[\text{Ar}]3d^24s^2$.

Hund's Rule

- The [lowest energy arrangement](#) within a single subshell puts one e^{-1} in each of the **separate orbitals**, with each e^{-1} having the same spin direction, before pairing two e^{-1} 's in any one same orbital with opposing spins.
- Each orbital in a subshell is filled halfway with one e^{-1} in each orbital, before any of the orbitals in the subshell can have a second e^{-1} .

Example 8.04 Arrangement of e^{-1} 's in 3d Subshell for Iron Atom according to Hund's Rule

- Fe ($Z = 26$) is in the 3d block of the periodic table (which has ten elements from Sc to Zn).
- The subshells through 4s are completely filled using the first twenty e^{-1} 's.
- That leaves six e^{-1} 's to partially fill 3d. Since 3d has five orbitals, only one orbital needs to be spin-paired, and the remaining four orbitals get one unpaired e^{-1} each.

Magnetism

- Magnetic attraction is caused by unpaired e^{-1} 's, that is an orbital with only one e^{-1} .
- Two spin-paired e^{-1} 's in the same orbital will cancel each other's magnetic field.
- There are three general categories for substances' magnetic behaviors.
- Ferromagnetic is a strong, permanent field due to cooperative (aligned) spins in many atoms. It is named after iron, which has four unpaired d electrons as in Example 8.04 above.
- Paramagnetic is a weak attraction due to only one or two unpaired e^{-1} 's. $\text{Na}_{(g)}$ is paramagnetic and it has one unpaired e^{-1} with $[\text{Ne}]3s^1$.
- Diamagnetic substances are not attracted to magnetic fields at all, and are even slightly repelled by the fields. This happens when there are no unpaired e^{-1} 's. For example, $\text{Hg}_{(L)}$, is diamagnetic because it is at end of the 5d block, where 6s, 4f, and 5d are all full.

Periodic Law

- When elements are arranged by their atomic number (Z), their physical and chemical properties vary periodically.
- That is, we can put the elements in rows, so that elements in the same column have similar behavior.

Dimitri Mendeleev's Periodic Table

- Mendeleev showed that elements can be arranged, so that elements in the same column have similar chemical and physical properties, and show trends.
- We can see these trends in this [1871 periodic table](#).
- For example, metals in the same column usually have the same oxide formula, such as Na_2O and K_2O and Cs_2O for IA, as well as MgO , CaO , and BaO for IIA.
- The table allowed Mendeleev to predict properties of elements that had not yet been discovered. He started with blanks in the table, where an undiscovered element should belong. Then, he interpolated the trends for known elements to predict atomic weight, oxide formula, and melting/boiling points of then-unknown elements.
- For instance, he accurately predicted properties of gallium, which was discovered soon after his table was published. He had called the element eka-aluminum because it fits directly below Al on his table.
- His predictions based on the table were again found to be accurate with the later discoveries of scandium (eka-boron) and germanium (eka-silicon).

Atomic Radii

- The atomic radius, or the relative size of the atom, is determined by the principle quantum number (n) and effective nuclear charge of its outermost e^{-1} 's.
- Effective nuclear charge is the nucleus' actual positive charge minus the effect of shielding by the inner e^{-1} 's.
- So, the positive charge felt by an e^{-1} is actually less than the total charge of the nucleus.
- The total charge of the nucleus increases left to right as Z increases.
- Shielding is relatively constant across a row (same period or shell), but increases when going down a column in the table (more shells).
- As we go across a row, charge increases with Z , but shielding is approximately constant. So, effective nuclear charge (attraction between nucleus and the e^{-1}) increases across a row, and the observed trend is that the size decreases left to right.
- As we go down a column, Z increases (more protons), but so does shielding (more shells). The change in shielding is slightly larger. So, effective nuclear charge decreases slightly down a column. Size increases with n , as shells are added, going down a column.
- The overall results are two general size trends:
 - 1) Atoms get smaller going across a row, left to right.
Atoms in same row have same n (and shielding effect).
But, Z (and effective nuclear charge) increases across the row.
 - 2) Atoms get bigger going down a column.
Here, n (or number of shells) is increasing.
The effective nuclear charge decreases slightly.

Example 8.05 Atomic Radii for P (phosphorus), O (oxygen), and S (sulfur)

- S is directly below O. $S > O$ because atoms become larger going down a column.
- P is directly to the left of S. $P > S$ because atoms become smaller going left to right.
- The complete sequence is $P > S > O$.

Ionization Energy ([IE](#))

- The 1st IE is the energy input required ($\Delta E > 0$) to remove the outermost e^{-1} .
- The 2nd IE is the energy needed to remove the next e^{-1} , after the first e^{-1} has already been removed.
- An e^{-1} is easiest to remove (**low IE**) when the result is a **stable ion**.
Column IA has s^1 and loses one e^{-1} easily.
Li ($1s^2 2s^1$), for instance, has a very low 1st IE and becomes a very stable ion, Li^{+1} ($1s^2$).
 $Li_{(g)} \rightarrow Li^{+1}_{(g)} + 1e^{-1} \quad IE_1 = \Delta H^0 = + 520.2 \text{ kJ/mol}$
- An e^{-1} is difficult to remove (**high IE**) when the result is **destabilizing**.
Column VIIIA has $s^2 p^6$, and is already stable without losing an e^{-1} .
So, Ne ($1s^2 2s^2 2p^6$) has a high 1st IE and becomes a very unstable ion, Ne^{+1} ($1s^2 2s^2 2p^5$).
 $Ne_{(g)} \rightarrow Ne^{+1}_{(g)} + 1e^{-1} \quad IE_1 = \Delta H^0 = + 2080.7 \text{ kJ/mol}$
- Also, Li has a very high 2nd IE, because Li^{+1} ($1s^2$) is very stable while Li^{+2} ($1s^1$) is not.
 $Li^{+1}_{(g)} \rightarrow Li^{+2}_{(g)} + 1e^{-1} \quad IE_2 = \Delta H^0 = + 7298.1 \text{ kJ/mol}$
- Larger atomic radius has lower IE, so IE decreases going down a column.
This decrease can be seen with column IA elements (Li, Na, K, Rb, and Cs).
- [This table](#) shows that the 1st IE increases across row 2, as nuclear charge increases.
The table also shows that IE becomes much larger once all valence e^{-1} 's have been removed (just to the right of the blue line).

Example 8.06 Trends in [IE Values](#) for Ne, Cl, and F

- Cl is directly below F. $Cl < F$ because IE decreases going down a column.
- F is to the left of Ne. $F < Ne$ because IE increases going across a row.
- The complete sequence for IE is $Cl < F < Ne$.

Electron Affinity ([EA](#))

- The absolute value of a negative EA is the energy output that occurs when an e^{-1} is added.
- Generally, EA is negative ($\Delta E < 0$) because the e^{-1} is attracted to (and bonds with) the nucleus, so that energy is released.
- A higher output energy for EA results when a stable ion is created.
Atoms in column VIIA become $s^2 p^6$ (very stable) when an e^{-1} is added.
F, Cl, Br, and I have large, negative EA values and easily become -1 ions.
For instance, F ($1s^2 2s^2 2p^5$) becomes a very stable ion, F^{-1} ($1s^2 2s^2 2p^6$).
 $F_{(g)} + 1e^{-1} \rightarrow F^{-1}_{(g)} \quad EA = \Delta H^0 = - 322 \text{ kJ/mol}$
- Atoms in IA become s^2 (moderately stable with s filled).
So, their EA's values are small, but still negative.
For instance, Li ($1s^2 2s^1$) becomes a moderately stable ion, Li^{-1} ($1s^2 2s^2$).
 $Li_{(g)} + 1e^{-1} \rightarrow Li^{-1}_{(g)} \quad EA = \Delta H^0 = - 60 \text{ kJ/mol}$
- Atoms in IIA become $s^2 p^1$ (unstable). So, their EA's are actually positive.
For instance, Be ($1s^2 2s^2$) becomes a very unstable ion, Be^{-1} ($1s^2 2s^2 2p^1$).
 $Be_{(g)} + 1e^{-1} \rightarrow Be^{-1}_{(g)} \quad EA = \Delta H^0 = + 240 \text{ kJ/mol (calculated value)}$

Periodicity of Main Group Elements

- H Hydrogen is unlike the rest of column IA because $n = 1$ has only one orbital ($1s^1$). Shell $n = 1$ is filled by only two e^{-1} 's. So, H_2 is a molecular gas, and not a solid metal. Although H usually becomes +1 (a proton), it can become -1 (hydride ion) as well.
- I A These elements lose one e^{-1} easily. They react with H_2O to create $H_{2(g)}$ and OH^{-1} . The oxides are basic, and have the formula R_2O , such as Na_2O .
- II A These elements lose two e^{-1} easily. They are somewhat less reactive than IA, but some will react with H_2O . The oxides are basic, and have the formula RO , such as MgO .
- III A The trend going down the column is from metalloid (B) at the top, to metal (Al, Ga, In, and Tl) at the bottom. The oxide formulas are R_2O_3 . B_2O_3 is acidic, while Al_2O_3 and Ga_2O_3 are amphoteric (can be either acid or base).
- IV A At the top of the table, there is a nonmetal (C). In the middle, there are metalloids (Si and Ge). At the bottom, there are metals (Sn and Pb). The oxides are molecular, and their formulas are RO_2 (except for PbO). CO_2 , SiO_2 , and GeO_2 are acidic, while SnO_2 and PbO_2 are amphoteric.
- V A N and P are nonmetals, As and Sb are metalloids, and Bi is a metal. N_2 is a molecular gas, while the other elements are solids.
- VI A The chalcogens consist of a nonmetal gas (O_2), two nonmetal solids (S and Se), a metalloid (Te), and a metal (Po). Their oxides range from acidic to amphoteric.
- VII A Halogens are all nonmetals that form diatomic molecules. F_2 and Cl_2 are gases, Br_2 is liquid, and I_2 is solid. Their oxides are acidic and unstable.
- VIII A Noble gases, such as Ne, have s^2p^6 (filled subshells) and are not reactive.