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By the end of this section, you will be able to: Derive the predicted ground state electron configurations of atoms. Identify and explain exceptions to predicted electron configurations for atoms and ions. Relate electron configurations to element classifications in the periodic table. Having introduced the basics of atomic structure and quantum mechanics, we can use our understanding of quantum numbers to determine how atomic orbitals relate to one another. This allows us to determine which orbitals are occupied by electrons in each atom. The specific arrangement of electrons in orbitals of an atom determines many of the chemical properties of that atom. The energy of atomic orbitals increases as the principal quantum number,  $n$ , increases. In any atom with two or more electrons, the repulsion between the electrons makes energies of subshells with different values of  $l$  differ so that the energy of the orbitals increases within a shell in the order  $s < p < d < f$ . Figure 10.5a depicts how these two trends in increasing energy relate. The 1s orbital at the bottom of the diagram is the orbital with electrons of lowest energy. The energy increases as we move up to the 2s and then 2p, 3s, and 3p orbitals, showing that the increasing  $n$  value has more influence on energy than the increasing  $l$  value for small atoms. However, this pattern does not hold for larger atoms with more electrons. The 3d orbital is higher in energy than the 4s orbital. Such overlaps continue to occur frequently as we move up the chart. Figure 10.5a: Generalized energy-level diagram for atomic orbitals in an atom with two or more electrons (not to scale) (credit: Chemistry (OpenStax), CC BY 4.0). Electrons in successive atoms on the periodic table tend to fill low-energy orbitals first. Thus, many students find it confusing that, for example, the 5p orbitals fill immediately after the 4d, and immediately before the 6s. The filling order is based on observed experimental results, and has been confirmed by theoretical calculations. As the principal quantum number,  $n$ , increases, the size of the orbital increases and the electrons spend more time farther from the nucleus. Thus, the attraction to the nucleus is weaker and the energy associated with the orbital is higher (less stabilized), consistent with Coulomb's Law. But this is not the only effect we have to take into account. Within each shell, as the value of  $l$  increases, the electrons are less penetrating (meaning there is less electron density found close to the nucleus), in the order  $s < p < d < f$ . Electrons that are closer to the nucleus slightly repel electrons that are farther out, offsetting the more dominant electron–nucleus attractions slightly (recall that all electrons have  $-1$  charges, but nuclei have  $+Z$  charges). This phenomenon is called shielding. Electrons in orbitals that experience more shielding are less stabilized and thus higher in energy. For small orbitals (1s through 3p), the increase in energy due to  $n$  is more significant than the increase due to  $l$ ; however, for larger orbitals the two trends are comparable and cannot be simply predicted. We will discuss methods for remembering the observed order. The arrangement of electrons in the orbitals of an atom is commonly represented using two methods: orbital diagrams and electron configurations of an atom. Both methods will be introduced in this section. It is important to apply the electron capacity rules for each type of subshell (1): electron capacity for subshell  $s$  is 2 electron capacity for subshell  $d$  is 10 electron capacity for subshell  $f$  is 14. We write an electron configuration with a symbol that contains three pieces of information (Figure 10.5b): The number of the principal energy level (shell),  $n$ , the letter that designates the orbital type (the subshell, 1), and a superscript number that designates the number of electrons in that particular subshell. For example, the notation 2p4 (read "two-p-four") indicates four electrons in a p subshell ( $l = 1$ ) with a principal quantum number ( $n$ ) of 2. The notation 3d8 (read "three-d-eight") indicates eight electrons in the d subshell ( $l = 2$ ) with a principal quantum number ( $n$ ) of 3. Figure 10.5b: Diagram of an electron configuration for hydrogen: the diagram of an electron configuration specifies the subshell ( $n$  and  $l$  value, with letter symbol) and superscript number of electrons (credit: Chemistry (OpenStax), CC BY 4.0). To determine the electron configuration (electron filling order) for any particular atom, we can "build" the structures in the order of atomic numbers. Beginning with hydrogen, and continuing across the periods of the periodic table, we add one proton at a time to the nucleus and one electron to the proper subshell until we have described the electron configurations of all the elements. This procedure is called the Aufbau principle, from the German word Aufbau ("to build up"). Each added electron occupies the subshell of lowest energy available (in the order shown in Figure 10.5a), subject to the limitations imposed by the Pauli exclusion principle. Electrons enter higher-energy subshells only after lower-energy subshells have been filled to capacity. Figure 10.5c illustrates the traditional way to remember the filling order for atomic orbitals. It is a helpful schematic to use when writing electron configurations or drawing orbital diagrams. Figure 10.5c: Using the Aufbau principle to determine appropriate filling order for electron configurations: This chart is straightforward to construct. Simply make a column for all the s orbitals with each  $n$  on a separate row. Repeat for p, d, and f. Note to only include orbitals allowed by the quantum numbers (no 1p or 2d, and so forth). Finally, draw diagonal lines from top to bottom as shown (credit: Chemistry (OpenStax), CC BY 4.0). For an introduction on how to use the Orbital Filling Diagram and Aufbau's principle to write electron configurations watch Using the Electron Configuration Chart (3min 32s) Video Source: Breslyn, W. (2013, November 12). Using the electron configuration chart [Video]. YouTube. Electron Configuration Arrangement using the Periodic Table Since the arrangement of the periodic table is based on the electron configurations, the periodic table can be converted to an electron configuration table to map out electron filling order. Figure 10.5d illustrates this method for determining the electron configuration. The filling order simply begins at hydrogen and includes each subshell as you proceed in increasing  $Z$  order. For example, after filling the 3p block up to Argon (Ar), we see the next orbital to be filled with electrons will be 4s (for potassium (K) and calcium (Ca)), followed by the 3d orbitals. Figure 10.5d: Using the periodic table to predict electron configurations or orbital diagrams, remember the number of electrons increases by one as the atomic number increases by one. For an introduction on how to use the periodic table to write electron configurations, watch Writing Electron Configurations Using Only the Periodic Table (4min 51s) Video Source: Breslyn, W. (2013, November 13). Writing electron configurations using only the periodic table [Video]. YouTube. Writing Electron Configuration and Orbital Diagrams of Elements We will now construct the ground-state electron configuration and orbital diagram for a selection of atoms in the first and second periods of the periodic table. You can use the orbital filling diagram or your periodic table as tools to determine correct filling order. Orbital diagrams are pictorial representations of the electron configuration, showing the individual orbitals and the pairing arrangement of electrons. Boxes are drawn to represent each orbital (which can only contain zero, one, or two electrons). The orbitals'  $n$  and  $l$  value are written under the box. Small arrows are used to indicate electrons. If two electrons share the same orbital, the first is drawn pointing in the up direction and the other in the down direction; this illustrates that the two electrons have opposite spins. When reading orbital diagrams, you may notice two different versions of arrows drawn: a full arrow head or "half" arrow head. Either is appropriate to use when drawing orbital diagrams, as both represent an electron. In this textbook, orbital diagrams will use both options interchangeably in examples, exercises, and answers. We start with a single hydrogen atom (atomic number 1), which consists of one proton and one electron. Referring to Figure 10.5c or Figure 10.5d, we would expect to find the electron in the 1s orbital. By convention, the  $[\text{latextm} s = +\text{frac}(1\{2\})\{2\}]\text{[latext]}$  value is usually filled first. The symbol for hydrogen, its electron configuration, and its orbital diagram, respectively, are: Figure 10.5c: Electron configuration and orbital diagram for hydrogen (credit: Chemistry (OpenStax), CC BY 4.0). Following hydrogen is the noble gas helium, which has an atomic number of 2. The helium atom contains two protons and two electrons. The first electron has the same four quantum numbers as the hydrogen atom electron ( $n = 1, l = 0, m = 0, [\text{latextm} s = +\text{frac}(1\{2\})\{2\}]\text{[latext]}$ ). The second electron also goes into the 1s orbital and fills that orbital. The second electron has the same  $n$ ,  $l$ , and  $m$  quantum numbers, but must have the opposite spin quantum number,  $[\text{latextm} s = -\text{frac}(1\{2\})\{2\}]\text{[latext]}$ . This is in accordance with the Pauli exclusion principle: No two electrons in the same atom can have the same set of four quantum numbers. For orbital diagrams, this means two arrows go in each box (representing two electrons in each orbital) and the arrows must point in opposite directions (representing paired spins). The electron configuration and orbital diagram of helium are: Figure 10.5c: Electron configuration and orbital diagram for helium (credit: Chemistry (OpenStax), CC BY 4.0). When filling electrons into higher-energy subshells, the arrows must point in opposite directions (representing paired spins). The electron configuration and orbital diagram of helium are: Figure 10.5c: Electron configuration and orbital diagram for helium (credit: Chemistry (OpenStax), CC BY 4.0). The n = 1 shell is completely filled in a helium atom. The next atom is the alkali metal lithium, with an atomic number of 3, which means it has three electrons to fill. The first two electrons in lithium fill the 1s orbital and have the same set of four quantum numbers as the two electrons in helium. The remaining electron must occupy the orbital of next lowest energy, the 2s orbital (Figure 10.5c or Figure 10.5d). Thus, the electron configuration and orbital diagram of lithium are: Figure 10.5c: Electron configuration and orbital diagram for lithium (credit: Chemistry (OpenStax), CC BY 4.0). An atom of the alkaline earth metal beryllium, with an atomic number of 4, contains four protons in the nucleus and four electrons surrounding the nucleus. The 1s orbital is filled with two electrons and three electrons will occupy the 2s orbital. Figure 10.5c: Electron configuration and orbital diagram for beryllium (credit: Chemistry (OpenStax), CC BY 4.0). An atom of boron (atomic number 5) contains five electrons. The  $n = 1$  shell is filled with two electrons and three electrons will occupy the 2s orbital. The fourth electron fills the remaining space in the 2s orbital. Figure 10.5c: Electron configuration and orbital diagram for beryllium (credit: Chemistry (OpenStax), CC BY 4.0). Thus, the electron configuration and orbital diagram of lithium are: Figure 10.5c: Electron configuration and orbital diagram for lithium (credit: Chemistry (OpenStax), CC BY 4.0). The n = 1 shell is filled with two electrons and three electrons will occupy the 2s orbital. 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