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Atomic orbitals and electron configurations worksheet answers

The goal of introducing quantum numbers has been to show that the similarities in electron arrangement or electron configuration lead to similarities and differences in the properties of elements. But writing the quantum electron numbers of an element in notation defined as (2,1,-1,1-2) is time-consuming and difficult to compare for an abbreviated form to be developed. An electronic configuration lists only the first two quantum numbers, n and (ℓell), and then shows how many electrons exist in each orbital. For example, type the electronic configuration of the scandium, Sc: 1s2 2s2 2p6 3s2 3p6 4s2 3d1 . Thus, for the scandium, the 1st and 2nd electron must be in 1s orbital, the 3rd and 4th in the 2s, the 5th to the 10th in the 2p orbitals, etc. This is a memory device to remember the order of orbitals for the first two quantum numbers. Follow the arrow starting at the top right corner, when the arrow is finished go to the next arrow and start again. In Scandium, the 4s has less energy and appears before 3d (the complexity of the d orbitals leads to its higher energy), so it is written before adding 3d to the electronic configuration. But it is common to keep all quantum numbers in principle together so you can see the electronic configuration written as Sc: 1s2 2s2 2p6 3s2 3p6 4s2 3d1. Writing electron settings like this can cause difficulties in determining the element that corresponds to an electronic configuration. But if you count the number of electrons, it will be equal to the number of protons that equals the atomic number that is unique for each element. For example: Which element has the electronic configuration: 1s2 2s2 2p6 3s2 3p6 4s2 3d104s24p6 4d8 5s2 ? Counting the electrons gives 46, which is the atomic number of palladium. Here is a diagram of the first electron configurations. David's Whizzy Periodic Table is a visual way of looking at the configuration of changing electrons. Note that the 3d orbital follows the 4s on the lower line, but starting with Ga (#31) is close to orbital 3p. It is most commonly listed with the other 3 orbitals, but sometimes follows orbital 4s to indicate that the 3d orbital is lower in energy than the 4s while it is being filled. There is a great exception to the normal order of electron configuration in Cr (#24) and (#29). It turns out that the energy of the electronic configuration which is half full, 4s1 3d5 , and orbital filled, 4s1 3D10, has lower energy than the typical filling order, 4s2 3d4 and 4s2 3d9 . This pattern is followed in the 5th row with Mo (#42) and Ag (#47). Elements For completeness, some elements of block f are listed here. Neodymium, Nd, which is used in very powerful magnets, has an atomic number of 60. For 60 electrons the electronic configuration is: 1s2 2s2 2p6 3s2 3p6 4s2 3d104s24p6 4d105s25p66s24f4 For californium, Cf, with 98 electrons the electron is: 1s2 2s2 2p6 3s2 3p6 4s2 3d104s24p6 4d105s25p66s24f145d106p67s25f10 It is often necessary to see all quantum numbers in an electronic configuration, this is the purpose of the orbital diagram. In addition to listing the main quantum number, n, and the subshell, (ℓell), the orbital diagram shows all the different orientations and the gyration of each electron. The diagram shows the number of subfalls using electron boxes or lines (use three for p-orbitals, five for d-orbitals, and 7 for f-orbitals). In each box, the turning of an electron is noticed using arrows, up arrows mean 1-2 turning arrows and down means −1-2 rotate. For example, the orbital diagram of the first 18 atoms are shown below. Rules for filling orbitals The Aufbau principle states that the lower-energy orbital is filled first. Thus, electrons usually fill the lowest energy level and the simplest orbital shape first. Pauli's Exclusion Principle states that neither electron can have the same four quantum numbers. That's why each orbital has only two electrons, a spin up (1-2) and a spin down (-1-2). The Hund Rule states that orbitals of the same energy, those that differ only in their orientation, are filled with electrons with the same gyration before the second electron is added to any of the orbitals. That's why electrons rotate, ↑, in the orbital diagrams from B to N and from Al to P in the diagrams above. Here are some orbital diagrams of elements with more electrons to help you understand the rules, electron configuration, orbital diagrams, and quantum numbers. Writing the electron configuration over and over again can be tedious and shifts attention away from the outer electrons that are the most important electrons. Thus, an abbreviated form of electronic configurations was developed using the final column of the periodic table, noble gases. Any element can be abbreviated except H and He, using noble gas with fewer electrons than the element. For example, instead of Sc: 1s22s22p63s23p64s23d1 would be abbreviated as [Ar]4s23d1 or [Ar]3d14s2. For Ag, the abbreviation would be: [Kr]5s14d10 (see orbital diagram above), and for Os: [Xe]6s24f145d6 or [Xe]4f145d66s2. Remember that abbreviations require you to use onlyoble gases and that you use a noble gas with fewer electrons. Also, you cannot abbreviate a noble gas by using its symbol on media; i.e. Ar is [Ne]3s23p6 not [Ar]. Finally, you can still count the number of electrons to determine the element, you just start with the number of electrons in the noble gas. For exampleWhat is the element with the electronic configuration: [Xe]6s24f145d6 ? Counting electrons 54 + 2 + 14 + 6 = 76 which is the atomic number for osmium, Os. Similar properties equal. Now we can put together the first and second part of this unit, the periodic table was being developed, developed, looked at similarities in chemical and physical properties. Any theory describing the electron arrangement should be able to explain these similarities. Let's look at the electronic settings in a periodic table format again. The first column of this periodic table has a single electron in the outer s-orbital: H 1s1, Li 2s1, Na 3s1 , K 4s1. So this similarity in electrons at the external energy level should be the reason why alkaline metals are all acting the same in both their chemistry and their physical properties. Hydrogen is an exception because it is a single proton in the nucleus and a single electron that gives it totally unique properties (although at high pressure and low temperature it can act like a metal). All the way through the periodic table we see this same pattern in each column where the outermost electrons filled the subshells in a similar way. For transition metals, the outermost electrons are 4s2 electrons that surround the 3d orbital filler (the 4s is at the 4th energy level and the 3d is at the 3rd lowest energy level). As transition metals add more electrons and more protons their properties change more subtly than the earth's alkaline metals and alkaline metals, because the outermost electrons are almost always the same (remember the exceptions of Cr and Cu). The outermost electrons are so important that we give them a name: valence electrons. Valence electrons will be an important part of our discussion on binding and compound formation. Contributors At the end of this section, you can: Derive the predicted configurations of terrestrial state electrons of atoms Identify and explain exceptions to predicted electron configurations for atoms and ions Relate electron configurations to element classifications in the periodic tableHave/haviaintroduced the basics of atomic structure and quantum mechanics, we can use our understanding of quantum numbers to determine how atomic orbitals relate to each other. This allows us to determine which orbitals are occupied by electrons in each atom. The specific arrangement of electrons in an atom's orbitals determines many of the chemical properties of that atom. The energy of atomic orbitals increases as the main quantum number, n, increases. In any atom with two or more electrons, the revulsion between electrons causes the energies of subcysas with different l values to differ so that the energy of the orbitals increases within a shell in the order s< p< d< f. Figure 3.24 shows how these two trends in increasing energy relate. The orbital 1s at the bottom of the diagram is the orbital with lowest energy. The energy increases as we advance to the 2s orbitals and then 2p, 3s and 3p, showing that the value n has more influence on energy than the increasing l value for small atoms. However, this pattern is not supported for larger atoms. The 3d 3d is higher in energy than orbital 4s. Such overlaps continue to occur frequently as we advance on the chart. Figure 3.24 Generalized energy level diagram for atomic orbitals in an atom with two or more electrons (not for scalar). Electrons in successive atoms in the periodic table tend to fill low-energy orbits first. Thus, many students find it confusing that, for example, the orbitals of 5p fill up immediately after 4d, and immediately before the 6s. The order of completion is based on observed experimental results, and was confirmed by theoretical calculations. As the main quantum number, n, increases, the size of the orbital increases and the electrons spend more time further away from the nucleus. Thus, the attraction to the nucleus is weaker and the energy associated with the orbital is greater (less stabilized). But this is not the only effect we have to take into account. Within each layer, as the value of l increases, the electrons are less penetrating (meaning that there is less electron density found near the nucleus), in the order s > p > d > f. Electrons closer to the nucleus slightly repel electrons that are farther away, slightly offsetting the most dominant electron-nucleus attractions (remember that all electrons have −1 charges, but nuclei have +Z charges). This phenomenon is called shielding and will be discussed in more detail in the next section. Electrons in orbitals that experience more armor are less stabilized and therefore higher in energy. For small orbitals (1 to 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 to remember the observed order. The arrangement of electrons in the orbitals of an atom is called the electronic configuration of the atom. We describe an electronic configuration with a symbol that contains three pieces of information (Figure 3.25): The number of the main quantum layer, n, the letter that designates the orbital type (the subshell, l), and a keyfigure number that designates the number of electrons in that specific subcadifica. For example, the 2p4 notation (read two-p-four) indicates four electrons in a subshell p (l = 1) with a main quantum number (n) of 2. The 3d8 notation (read three-d-eight) indicates eight electrons in the subsaldia d (i.e., l = 2) of the main layer for which n = 3. Figure 3.25 The diagram of an electronic configuration specifies the subshell (value n and l, with letter symbol) and the number of electron scribes. To determine the electronic configuration for any particular atom, we can construct the structures in the order of atomic numbers. Starting with hydrogen, and continuing through the periodic table periods, we added a each time to the nucleus and an electron to the subshell until we have described the electronic settings of all elements. This procedure is called the Aufbau principle, of the German word Aufbau (to build). Each electron added occupies the subposition of the lowest available energy (in the order shown in Figure 3.24), subject to the limitations imposed by the quantum numbers allowed according to Pauli's exclusion principle. Electrons enter higher energy subcavas only after low-energy subbuds have been filled to capacity. Figure 3.26 illustrates the traditional way of remembering the filling order of atomic orbitals. Since the arrangement of the periodic table is based on electronic configurations, Figure 3.27 provides an alternative method for determining the electronic configuration. The filling order simply begins in hydrogen and includes each subshell as you proceed in increasing the order Z. For example, after filling the block from 3p to Air, we see that the orbital will be 4s (K, Ca), followed by orbitals 3d. Figure 3.26 This diagram depicts the energy order for atomic orbitals and is useful for obtaining early state electronic settings. Figure 3.27 This periodic table shows the electronic configuration for each sublayer. When constructing from hydrogen, this table can be used to determine the electron configuration for any atom in the periodic table. We will now construct the configuration of earth state electrons and orbital diagram for a selection of atoms in the first and second periods of the periodic table. Orbital diagrams are pictorial representations of the electronic configuration, showing the individual orbitals and the electron pairing arrangement. We start with a single hydrogen atom (atomic number 1), which consists of a proton and an electron. Referring to Figure 3.26 or Figure 3.27, we hope to find the electron in orbital 1s. By convention, the value ms=+12ms=+12 is usually filled first. The electronic configuration and orbital diagram are: Following hydrogen is the noble gaseous 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 of the electron hydrogen atom (n = 1, l = 0, ml = 0, ms=+12ms=+12). The second electron also goes to orbital 1s and fills that orbital. The second electron has the same numbers n, l, and quantum ml, but must have the opposite rotating quantum number, ms=−12.ms=−12. This is in accordance with Pauli's exclusion principle: no two electrons in the same atom can have the same set of four quantum numbers. For orbital diagrams, this means that two arrows go in each box (representing two electrons in each orbital) and the arrows must point in opposite directions (representing paired turns). The electronic configuration and diagram helium are: The shell n = 1 is completely filled into a helium atom. The next atom is alkali lithium with an atomic number of 3. The first two lithium electrons fill orbital 1s and have the same sets of four quantum numbers as the two electrons in helium. The remaining electron should occupy the orbital of the next lowest energy, orbital 2s (Figure 3.26 or Figure 3.27). Thus, the electronic configuration and orbital diagram of lithium are: An alkaline metallic beryllium atom, with an atomic number of 4, contains four protons in the nucleus and four electrons around the nucleus. The fourth electron fills the remaining space in orbital 2s. A boron atom (atomic number 5) contains five electrons. Layer n = 1 is filled with two electrons and three electrons will occupy n = 2 layer. As any subshell can contain only two electrons, the fifth electron must occupy the next energy level, which will be an orbital of 2p. There are three degenerate 2p orbitals (ml = −1, 0, +1) and the electron can occupy any of these orbitals p. When designing orbital diagrams, we include empty boxes to represent any empty orbitals in the same subshell we are filling. Carbon (atomic number 6) has six electrons. Four of them fill orbitals 1 and 2s. The other two electrons occupy the 2p sublayer. Now we have the option of filling one of the 2p orbitals and pairing the electrons or leaving the unpaid electrons in two different but degenerate orbitals. Orbitals are filled as described by the Hund rule: the lowest energy setting for an atom with electrons within a set of degenerate orbitals is that having the maximum number of undamaged electrons. Thus, the two electrons in the 2p carbon orbitals have identical quantum numbers n, l and ms and differ in their quantum number ml (according to Pauli's exclusion principle). The electronic configuration and orbital diagram for carbon are: Nitrogen (atomic number 7) fills subwalks 1s and 2s and has one electron in each of the three 2p orbitals, according to hund's rule. These three electrons have unpaid spins. Oxygen (atomic number 8) has a pair of electrons in any of the 2p orbitals (electrons have opposite gyrations) and a single electron in each of the other two. Fluoride (atomic number 9) has only a 2p orbital containing an unsresnated electron. All electrons of the neon noble gas (atomic number 10) are paired, and all orbitals in n = 1 and n = 2 shells are filled. The electronic configurations and orbital diagrams of these four elements are: Alkaline metallic sodium (atomic number 11) has one electron more than the neon atom. This electron should go to the subshell of the lowest available energy, the orbital 3s, giving a configuration of 1s22s22p63s1. The electrons that occupy the orbital of the outermost layer (higher value of n) are called valence electrons, and those that occupy the orbitals of the inner shell are electron-nucleus electron-electron-nucleus 3.28). Since the electronic shells of the nucleus correspond to noble configurations of gas electrons, we can abbreviate electron settings by writing the noble gas that corresponds to the electron core configuration, along with the valence electrons in a condensed format. For our sodium example, the symbol [Ne] represents central electrons (1s22s22p6) and our abbreviated or condensed configuration is [Ne]3s1. Figure 3.28 An abbreviated electronic core configuration (right) replaces the electrons of the nucleus with the noble gas symbol whose configuration corresponds to the electron core configuration of the other element. Similarly, the abbreviated lithium configuration can be represented as [He]2s1, where [l] represents the configuration of the helium atom, which is identical to that of the lithium-filled inner layer. Writing settings in this way emphasizes the similarity of lithium and sodium settings. Both atoms, which are in the alkaline metal family, have only one electron in a valence subhult out of a set full of internal shells. Li [He 12s1Na: [Ne 3s1Li: [He 12s1Na: [Ne 3s1. Alkaline Metallic Magnesium (atomic number 12), with its 12 electrons in a configuration [Ne]3s2, is analogous to its beryllium family member, [He]2s2. Both atoms have a full subhult out of their full inner shells. Aluminum (atomic number 13), with 13 electrons and the electronic configuration [Ne]3s23p1, is analogous to its boron family member, [He]2s22p1. The electronic configurations of silicon (14 electrons), phosphorus (15 electrons), sulfur (16 electrons), chlorine (17 electrons) and argon (18 electrons) are analogous in the electronic configurations of their outer shells to the carbon of their corresponding members of the family, nitrogen, oxygen, fluoride and neon, respectively, except that the main quantum number of the outer layer of the heaviest elements increased from one to n = 3. Figure 3.29 shows the smallest configuration of energy, or terrestrial state, of electrons for these elements, as well as for atoms of each of the known elements. Figure 3.29 This version of the periodic table shows the electronic configuration of the outer layer of each element. Note that down in each group, the configuration is often similar. When we get to the next element in the periodic table, alkaline metallic potassium (atomic number 19), we can expect us to start adding electrons to the subcadidic 3d. However, all available chemical and physical evidence indicates that potassium is like lithium and sodium, and that the next electron is not added to the 3d level, but is instead added to the 4s level (Figure 3.29). As discussed earlier, the orbital 3d without radial nodules is larger in energy because it is less penetrating and more protected from the nucleus than the 4s, which has three radial nodules. Thus, potassium has electronic configuration of [Ar]4s1. Therefore, potassium corresponds to and Na in its valence shell configuration. The next electron is added to complete the subcals and calcium has an electronic configuration of [Ar]4s2. This gives calcium an external layer electron configuration corresponding to beryllium and magnesium. Starting with the transition metal scandium (atomic number 21), additional electrons are added successively to the subcad. This subshell is filled to its capacity with 10 electrons (remember that for l = 2 [d orbitals], there are 2l + 1 = 5 ml values, which means that there are five d orbitals that have a combined capacity of 10 electrons). The 4p subsalada fills up next. Note that for three series of elements, the scandium (Sc) through copper (Cu), yttrium (Y) through silver (Ag) and lutetium (Lu) through gold (Au), a total of 10 d electrons are successively added to the (n − 1) shell next to shell n to bring this (n − 1) shell of 8 to 18 electrons. For two series, lanthanum (La) through lutetium (Lu) and actinium (Ac) values through lawrencium (Lr), 14 f electrons (l = 3, 2l + 1 = 7 ml of values; thus, seven orbitals with a combined capacity of 14 electrons) are successively added to the (n − 2) shell to bring this shell of 18 electrons to a total of 32 electrons. Quantum Numbers and Electronic Configurations What is the electronic configuration and orbital diagram of a phosphorus atom? What are the four quantum numbers for the last electron added? Solution The atomic number of phosphorus is 15. Thus, a phosphorus atom contains 15 electrons. The filling order of the energy levels is 1s, 2s, 2p, 3s, 3p, 4s, . The 15 electrons of the phosphorus atom will fill up to the orbital 3p, which will contain three electrons: The last electron added is a 3p electron. Therefore, n = 3 and for an orbital type p, l = 1. The ml value can be −1, 0, or +1. The three p orbitals are degenerate, so any of these ml values are correct. For unchecked electrons, the convention assigns the value of +12+12 to the quantum number of spin; so, ms=+12.ms=+12. Check your learning Identify atoms from the given electronic settings: (a) [Ar]4s23d5 (b) [Kr]5s24d105p6 The periodic table can be a powerful tool in predicting the electronic configuration of an element. However, we find exceptions to the order of filling orbitals that are shown in Figure 3.26 or Figure 3.27. For example, the electronic configurations (shown in Figure 3.29) of transition metals chromium (Cr; atomic number 24) and copper (Cu; atomic number 29), among others, are not the ones we expected. In general, such exceptions involve subcysas with very similar energy, and small effects can lead to changes in the order of completion. In the case of Cr e, we found that semi-filled and completely filled subcysapparently represent preferential stability. This stability is such that an electron changes from 4s to 3d 3d to get the extra stability of a semi-filled 3d subdigging (in Cr) or a filled 3d subcadia (in Cu). Other exceptions also occur. For example, the niobium (Nb, atomic number 41) is expected to have the electronic configuration [Kr]5s24d3. Experimentally, we observed that its configuration of terrestrial state electrons is actually [Kr]5s14d4. We can rationalize this observation by saying that the electron-electron repulsions experienced by the pairing of electrons in orbital 5s are larger than the energy gap between orbitals 5s and 4d. There is no simple method to predict exceptions for atoms where the magnitude of repulsions between electrons is greater than the small energy differences between subwalks. As described earlier, the periodic table organizes atoms based on the increase in atomic number so that elements with the same chemical properties periodically reuse. When your electronic settings are added to the table (Figure 3.29), we also see a periodic recurrence of similar electron configurations in the outer layers of these elements. Because they are in the outer layers of an atom, valence electrons play the most important role in chemical reactions. External electrons have the highest energy of electrons in an atom and are more easily lost or shared than nucleus electrons. Valence electrons are also the determining factor in some physical properties of the elements. Elements of any group (or column) have the same number of valence electrons; the alkaline metals of lithium and sodium each have only one valence electron, the alkaline metals of beryllium and magnesium each have two, and the halogens fluoride and chlorine each have seven valence electrons. The similarity in the chemical properties between the elements of the same group occurs because they have the same number of valence electrons. It is the loss, gain or sharing of valence electrons that defines how elements react. It is important to remember that the periodic table was developed based on the chemical behavior of the elements, well before any idea of their atomic structure was available. Now we can understand why the periodic table has the arrangement it has—the arrangement places elements whose atoms have the same number of valence electrons in the same group. This arrangement is emphasized in Figure 3.29, which shows in a periodic table the electronic configuration of the last subshell to be filled by the Aufbau principle. The colored sections in Figure 3.29 show the three categories of elements classified by orbitals being filled: transition, transition, and internal transition elements. These classifications determine which orbitals are counted in the valence shell, or higher energy level orbitals of an atom. The main elements of the group (called representative elements) are those in which the last electron added enters an orbital s or p in the outermost shown in blue and red in Figure 3.29. This category includes all non-metallic elements as well as many metals and metalloides. The valence electrons for the main group elements are those with the highest n level. For example, the thrium (Ga, atomic number 31) has the electronic configuration [Ar]4s23d104p1, which contains three valence electrons (underscores). Fully filled d orbitals count as nucleus, not valence, electrons. Transition elements or transition metals. These are metallic elements in which the last added electron enters an orbital d. Valence electrons (those added after the last noble gas configuration) in these elements include electrons ns and (n − 1) d. The official definition of The IUPAC of transition elements specifies those with partially filled d orbitals. Thus, the elements with completely filled orbitals (Zn, Cd, Hg, as well as Ag and Au in Figure 3.29) are not elements of technical transition. However, the term is often used to refer to the entire block d (colored yellow in Figure 3.29), and we will adopt this use in this textbook. Interior transition elements are metallic elements in which the last added electron occupies an orbital f. They are shown in green in Figure 3.29. The valence shells of the internal transition elements consist of (n - 2)f, (n - 1)d and subbuds ns. There are two series of interior transition: The lanthanida series: lanthanida (La) through lutetium (Lu) The actinide series: actinide (Ac) through lawrencium (Lr) Lanthanum and actinium, because of their similarities with the other members of the series, are included and used to name the series, even if they are transition metals without f electrons. Ions are formed when atoms gain or lose electrons. The swimming ion (positively charged ion) forms when one or more electrons are removed from a parent atom. For the main group elements, the electrons that were added last are the first electrons removed. For transition metals and internal transition metals, however, electrons in orbital s are easier to remove than electrons d or f, and so the higher ns electrons are lost, and then the (n − 1)d or (n − 2)f electrons are removed. An anion (negatively charged ion) forms when one or more electrons are added to a parent atom. The added electrons fill the order predicted by the Aufbau principle. Predict ing electronic ion settingsWhat is the electronic configuration of (a) Na+ (b) P3− (c) Al2+ (d) Fe2+ Solution (e) Sm3+ First, write the electronic configuration for each parent atom. We chose to show the complete and non-abbreviated settings to provide more practice for students who want it, but listing the abbreviated electronic settings of the nucleus is also acceptable. Then whether an electron is gained or lost. Remember electrons are charged negatively, so ions with a positive charge have have an electron. For the elements of the main group, the last orbital gains or loses the electron. For transition metals, the last orbital s loses an electron before orbitals d, to Na: 1s22s2p63s1. The sodium casing loses an electron, then Na+: 1s22s22p63s1 = Na+. 1s22s22p6. (b) P: 1s22s22p63s23p3. The titanium phosphorus gains three electrons, then P3−: 1s22s22p63s23p6. (c) Al: 1s22s22p63s23p1. Aluminum indicatio loses two electrons. Al2+: 1s22s22p63s23p1 = Al2+. 1s22s22p63s1. (d) Fe: 1s22s22p63s23p64s23d6. Iron(l) loses two electrons and, because it is a transition metal, they are removed from the Fe2+ orbital: 1s22s22p63s23p64s23d6 = 1s22s22p63s23p63d6. (e) Sm: 1s22s22p63s23p64s23d104p65s24d105p66s24f6. Trication samarium loses three electrons. The first two will be lost from orbital 6s, and the latter is removed from orbital 4f. SM3+: 1s22s22p63s23p64s23d104p65s24d105p66s24f6 = 1s22p63s23p64s23d104p65s24d105p64f5. Check your learning Which ion with a +2 charge has the electronic configuration 1s22s2p63s23p63d104s24p64d5? Which ion with a +3 payload has this setting? Configuration?

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