Orbital box diagram

Electron orbital diagrams and written configurations tell you which orbitals are filled and which are partially filled for any atom. The number of valence electrons impacts on their chemical properties, and the specific ordering and properties of the orbitals are important in physics, so many students have to get to grips with the basics. Electron configurations have the format: 1s 2 2s 2 2p 6. Electron configurations are expressed through a notation that looks like this: 1s 2 2s 2 2p 1. Learn the three main parts of this notation to understand how it works. The second letter tells you the value of l, the angular momentum quantum number. Remember that s orbitals contain a maximum of two electrons, p orbitals a maximum of six, d a maximum of 10 and f a maximum of See Resources for a diagram showing the filling order. This electron is the valence electron. Identify an element from the notation by simply counting the electrons and finding the element with a matching atomic number. Writing out every single orbital for heavier elements is tedious, so physicists often use a shorthand notation. This works by using the noble gases in the far right column of the periodic table as a starting point and adding the final orbitals onto them. So scandium has the same configuration as argon, except with electrons in two extra orbitals. The shorthand form is therefore:. Orbital diagrams are like the configuration notation just introduced, except with the spins of electrons indicated. The exclusion principle states that no two electrons can share the same four quantum numbers, which basically results in pairs of states containing electrons with opposite spins. This means that when writing orbital diagrams for partially full shells, fill in all of the up-spin electrons before adding any down-spin electrons. The electrons are represented by the arrows, which also indicate their spins, and the notation on the left is standard electron configuration notation. Note that the higher-energy orbitals are at the top of the diagram. They consist of the symbol for the element in the center, surrounded by dots indicating the number of valence electrons. For example, carbon has four valence electrons and the symbol C, so it is represented as:. When electrons are shared between two atoms in covalent bonding , the atoms share the dot in the diagram in the same way. This makes the approach very useful for understanding chemical bonding. Lee Johnson is a freelance writer and science enthusiast, with a passion for distilling complex concepts into simple, digestible language. He's written about science for several websites including eHow UK and WiseGeek, mainly covering physics and astronomy. He was also a science blogger for Elements Behavioral Health's blog network for five years. He studied physics at the Open University and graduated in These rules are easy to work with, so the notation for the configuration of scandium is:. You can use this with any elements apart from hydrogen and helium. This example shows how orbital diagrams work, using argon as an example:. About the Author. Copyright Leaf Group Ltd. 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. This section includes worked examples, a glossary, and practice problems. The energy of atomic orbitals increases as the principal quantum number, n, increases. The 1 s orbital at the bottom of the diagram is the orbital with electrons of lowest energy. The energy increases as we move up to the 2 s and then 2 p , 3 s , and 3 p 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. For example, the 3 d orbital is higher in energy than the 4s orbital. Such overlaps continue to occur frequently as we move up the chart. 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 5 p orbitals fill immediately after the 4 d , and immediately before the 6 s . 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. But this is not the only effect we have to take into account. This phenomenon is called shielding and will be discussed in more detail in the next section. Electrons in orbitals that experience more shielding are less stabilized and thus higher in energy. For small orbitals 1 s through 3 p , 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. The arrangement of electrons in the orbitals of an atom is called the electron configuration of the atom. We describe an electron configuration with a symbol that contains three pieces of information Figure 2 : 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. Each added electron occupies the subshell of lowest energy available in the order shown in Figure 1 , subject to the limitations imposed by

the allowed quantum numbers according to the Pauli exclusion principle. Electrons enter higher-energy subshells only after lower-energy subshells have been filled to capacity. Figure 3 illustrates the traditional way to remember the filling order for atomic orbitals. Since the arrangement of the periodic table is based on the electron configurations, Figure 4 provides an alternative 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 3 p block up to Ar, we see the orbital will be 4 s K, Ca , followed by the 3 d orbitals. 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. Orbital diagrams are pictorial representations of the electron configuration, showing the individual orbitals and the pairing arrangement of electrons. We start with a single hydrogen atom atomic number 1 , which consists of one proton and one electron. Referring to Figure 3 or Figure 4 , we would expect to find the electron in the 1 s orbital. The electron configuration and the orbital diagram are:. Following hydrogen is the noble gas helium, which has an atomic number of 2. The helium atom contains two protons and two electrons. The second electron also goes into the 1 s orbital and fills that orbital. This is in accord 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:. The next atom is the alkali metal lithium with an atomic number of 3. The first two electrons in lithium fill the 1 s orbital and have the same sets of four quantum numbers as the two electrons in helium. The remaining electron must occupy the orbital of next lowest energy, the 2 s orbital Figure 3 or Figure 4. Thus, the electron configuration and orbital diagram of lithium are:. 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 fourth electron fills the remaining space in the 2 s orbital. An atom of boron atomic number 5 contains five electrons. Because any s subshell can contain only two electrons, the fifth electron must occupy the next energy level, which will be a 2p orbital. When drawing orbital diagrams, we include empty boxes to depict any empty orbitals in the same subshell that we are filling. Carbon atomic number 6 has six electrons. Four of them fill the 1 s and 2 s orbitals. The remaining two electrons occupy the 2 p subshell. We now have a choice of filling one of the 2 p orbitals and pairing the electrons or of leaving the electrons unpaired in two different, but degenerate, p orbitals. Placing the electrons in different orbitals and with parallel spins tends to keep the electrons in different regions of space, thus minimizing their Coulomb repulsion and lowering the energy. Thus, the two electrons in the carbon 2 p orbitals have identical n , l , and m s quantum numbers and differ in their m l quantum number in accord with the Pauli exclusion principle. The electron configuration and orbital diagram for carbon are:. These three electrons have unpaired spins. Oxygen atomic number 8 has a pair of electrons in any one of the 2 p orbitals the electrons have opposite spins and a single electron in each of the other two. Fluorine atomic number 9 has only one 2 p orbital containing an unpaired electron. The electron configurations and orbital diagrams of these four elements are:. The alkali metal sodium atomic number 11 has one more electron than the neon atom. This electron must go into the lowest-energy subshell available, the 3 s orbital, giving a 1 s 2 2 s 2 2 p 6 3 s 1 configuration. The electrons occupying the outermost shell orbital s highest value of n are called valence electrons , and those occupying the inner shell orbitals are called core electrons Figure 5. Since the core electron shells correspond to noble gas electron configurations, we can abbreviate electron configurations by writing the noble gas that matches the core electron configuration, along with the valence electrons in a condensed format. For our sodium example, the symbol [Ne] represents core electrons 1 s 2 2 s 2 2 p 6 and our abbreviated or condensed configuration is [Ne]3 s 1. Similarly, the abbreviated configuration of lithium can be represented as [He]2 s 1 , where [He] represents the configuration of the helium atom, which is identical to that of the filled inner shell of lithium. Writing the configurations in this way emphasizes the similarity of the configurations of lithium and sodium. Both atoms, which are in the alkali metal family, have only one electron in a valence s subshell outside a filled set of inner shells. The alkaline earth metal magnesium atomic number 12 , with its 12 electrons in a [Ne]3 s 2 configuration, is analogous to its family member beryllium, [He]2 s 2. Both atoms have a filled s subshell outside their filled inner shells. Aluminum atomic number 13 , with 13 electrons and the electron configuration [Ne]3 s 2 3 p 1 , is analogous to its family member boron, [He]2 s 2 2 p 1. Figure 6 shows the lowest energy, or ground-state, electron configuration for the valence electrons of these elements as well as that for atoms of each of the known elements. When we come to the next element in the periodic table, the alkali metal potassium atomic number 19 , we might expect that we would begin to add electrons to the 3 d subshell. 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 3 d level but is, instead, added to the 4 s level Figure 6. As discussed previously, the 3 d orbital with no radial nodes is higher in energy because it is less penetrating and more shielded from the nucleus than the 4 s , which has three radial nodes. Thus, potassium has an electron configuration of [Ar]4 s 1. Hence, potassium corresponds to Li and Na in its valence shell configuration. The next electron is added to complete the 4 s subshell and calcium has an electron configuration of [Ar]4 s 2. This gives calcium an outer-shell electron configuration corresponding to that of beryllium and magnesium. Beginning with the transition metal scandium atomic number 21 , additional electrons are added successively to the 3 d subshell. The 4 p subshell fills next. Note that for three series of elements, 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 the n shell to bring that n − 1 shell from 8 to 18 electrons. Quantum Numbers and Electron Configurations What is the electron configuration and orbital diagram for a phosphorus atom? What are the four quantum numbers for the last electron added? Solution The atomic number of phosphorus is Thus, a phosphorus atom contains 15 electrons. The 15 electrons of the phosphorus atom will fill up to the 3 p orbital, which will contain three electrons:. The last electron added is a 3 p electron. The three p orbitals are degenerate, so any of these m l values is correct. Check Your Learning Identify the atoms from the electron configurations given:. The periodic table can be a powerful tool in predicting the electron configuration of an element. However, we do find exceptions to the order of filling of orbitals shown in Figure 3 and Figure 4. For instance, the electron configurations shown in Figure 6 of the transition metals chromium Cr; atomic number 24 and copper Cu; atomic number 29 , among others, are not those we would expect. In general, such exceptions involve subshells with very similar energy, and small effects can lead to changes in the order of filling. In the case of Cr and Cu, we find that half-filled and completely filled subshells apparently represent conditions of preferred stability. This stability is such that an electron shifts from the 4 s into the 3 d orbital to gain the extra stability of a half-filled 3 d subshell in Cr or a filled 3 d subshell in Cu. Other exceptions also occur. For example, niobium Nb, atomic number 41 is predicted to have the electron configuration [Kr]5 s 2 4 d 3. Experimentally, we observe that its ground-state electron configuration is actually [Kr]5 s 1 4 d 4. We can rationalize this observation by saying that the electron–electron repulsions experienced by pairing the electrons in the 5 s orbital are larger than the gap in energy between the 5 s and 4 d orbitals. There is no simple method to predict the exceptions for atoms where the magnitude of the repulsions between electrons is greater than the small differences in energy between subshells. The relative energy of the subshells determine the order in which atomic orbitals are filled 1 s , 2 s , 2 p , 3 s , 3 p , 4 s , 3 d , 4 p , and so on. Electrons in the outermost orbitals are called valence electrons. In the periodic table, elements with analogous valence electron configurations usually occur within the same group column. There are some exceptions to the predicted filling order, particularly when half-filled or completely filled orbitals can be formed. Your email address will not be published. Skip to content Introduction 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. Write an electron configuration for an atom. Orbital Energies and Electron Configurations of Atoms Apply the Aufbau principle to rationalize the structure of the periodic table. Li: [He]2 s 1. Example 1 Quantum Numbers and Electron Configurations What is the electron configuration and orbital diagram for a phosphorus atom? The 15 electrons of the phosphorus atom will fill up to the 3 p orbital, which will contain three electrons: The last electron added is a 3 p electron. Explain your answer. Cobalt−60 and iodine− are radioactive isotopes commonly used in nuclear medicine. How many protons, neutrons, and electrons are in atoms of these isotopes? Write the complete electron configuration for each isotope. Which atom would be expected to have a half-filled 4 s subshell? Which atom would be expected to have a half-filled 6 p subshell? Which of the following has two unpaired electrons? B K Bi Although both b and c are correct, e encompasses both and is the best answer. Share This Book Share on Twitter. Leave a Reply Cancel reply Your email address will not be published. An orbital diagram, or orbital box diagram, is a way of representing the electron configuration of an atom. Arrows or half arrows are used to represent the electrons occupying the orbitals. A maximum of 2 arrows can be drawn in each box because a maximum of 2 electrons can occupy an orbital. When 2 arrows occupy the same box we refer to the electrons as paired, and we must apply the Pauli Exclusion Principle so that these arrows face in opposite directions one "spin up", one "spin down". The paired electrons are said to have antiparallel spin. One arrow is positioned in each box according to Hund's Rule which tells us to maximise the number of unpaired electrons in orbitals of the same subshell, and; to give those electrons the same "spin" parallel spin. For

atoms of " d block " elements, in Period 4 for example, the crowding of the 4s and 3d orbitals results in the application of Hund's Rule to all these orbitals. Please do not block ads on this website. You should already be familiar with the Bohr Model of the Atom which states that electrons exist in discrete energy levels or electron shells. The principal quantum number , n, tells us the energy level or electron shell that the electron is found in. We can use this to write the simple electron configuration of an atom just by noting how many electrons are occupying each energy level or shell. You should also be aware that each energy level or shell is further divided into energy sub-levels or sub-shells. Using this information, and the Aufbau Principle , we can write an electron configuration using subshells or sublevels, filling each sublevel in the following order. Each sublevel subshell is divided up into a set of orbitals. The number of orbitals is given by n 2. Furthermore, each orbital has a particular shape. Another quantum number, the azimuthal quantum number l tells us the shape of the orbital that the electron is occupying. Another quantum number, the magnetic quantum number , m l , tells us the orientation of the orbital in space:. All of this information together allows us to draw a set of boxes to represent the orbitals of each energy level shell. We can build up a set of boxes to represent the energy level shells and orbitals for the atoms of each element in each period of the periodic table:. Period 2, the 1s orbital of 1 st energy level K shell , as well as an s orbital and 3 p orbitals in the 2 nd energy level L shell :. Period 3, the 1s orbital of 1 st energy level K shell , as well as an s orbital and 3 p orbitals in the 2 nd energy level L shell and the s and p orbitals of the 3 rd energy level M shell :. Period 4, the 3d orbitals become available to the " d-block elements " or transition metals straight after the " s-block" elements. We will keep orbitals of the same energy level together, but remember that electrons will occupy the 4s orbital before the 3d orbitals in accordance with the Aufbau Principle :. In order to build up an orbital diagram for an atom of each element, we will need to place electrons into the boxes we have drawn. The first thing we need to remember is that an orbital can hold a maximum of 2 electrons: that is, an orbital can hold 0 electrons, 1 electron or 2 electrons. But, the Pauli Exclusion Principle tells us that no two atoms in a given atom can be exactly the same, if we already have an electron in the 1s orbital, then there must be something different about the second electron we place in the same orbital. In orbital diagrams we represent these two different states for each electron as two different arrows:. If 2 arrows or half arrows are paired occupy the same box then they must face in opposite directions they are said to have antiparallel spin. The following diagram illustrates correct pairs of electrons in an orbital box, and incorrect pairs of electrons in an orbital box:. But before we start pairing electrons up in orbitals, we need to position electrons in accordance with Hund's Rule: electrons in a given subshell tend to remain unpaired with parallel spins. This means that if we have 3 electrons to place into a p-subshell a set of 3 p orbitals , we put 1 arrow in each of the 3 boxes BEFORE we start placing 2 electrons in any of the boxes. Each of these three arrows must be the same, for example, all "up spin" parallel spin. The diagram below shows correct and incorrect allocations of 3 electrons to the p orbital boxes of the p subshell:. Nitrogen is a period 2 element, and is a p-block element, therefore: The 1 st energy level is full: 1s 2 In the 2 nd energy level the s orbital is full, 2s 2 and there are 3 electrons in the p orbitals, 2p 3. So we draw the required orbital boxes for the orbital diagram using the Aufbau Principle to get the correct order for filling the boxes:. Now we need to place the second arrow to represent the second electron. We must complete the s subshell before we can begin the next energy level, so the second arrow is placed in the same 1s box. Because 2 arrows will occupy the same box, we apply the Pauli Exclusion Principle so that these two arrows face the opposite way antiparallel spin :. The fourth arrow goes in the same 2s box because we need to complete the s orbital of the second energy level before moving on to the p orbitals of the second energy level: We apply the Pauli Exclusion Principle so that these arrows face in opposite directions antiparallel spin. The fifth arrow must go in a p orbital of the second energy level say, the 2p x orbital :. Now the sixth arrow WILL NOT pair up with the previous arrow because there are 2 other orbitals available in this sublevel, so, we use Hund's Rule to place this arrow in the next p orbital say the 2p y box AND both arrows must face the same direction have parallel spin :. The seventh arrow the final arrow will not pair up with either of the previous 2 arrows because there is still an empty p orbital available in the second energy level. We apply Hund's Rule again so that this arrow is positioned in the last available p orbital 2p z and facing the same direction as the other two arrows parallel spin. The completed orbital diagram for an atom of nitrogen is therefore given below:. In the following sections we present the orbital diagrams for atoms of the first 36 elements of the Periodic Table. Before you look at the next section, why don't you try to draw the orbital diagrams for the atoms in each Period first, then compare your orbital diagrams with the orbital diagrams below. If your orbital diagram is not the same as the one given below, read through the explanation and try again. Play the game now! The Aufbau Principle tells us that

there are 3 p orbitals making up the p-subshell. Five electrons occupy the three 4p orbitals Apply the Pauli Exclusion Principle so that one electron of the pair is defined as "spin up" and the other as "spin down". Now we add six electrons to the p orbitals of the fourth energy level remember there are 3 p orbitals making up the p-subshell Each of the three 4p orbitals must be occupied by a pair of electrons. Take the test now! Question 1: The ground state electronic configuration for an atom of oxygen is 1s 2 2s 2 2p 4. Draw the orbital diagram to represent O What is the question asking you to do? Draw the orbital diagram for O What data information have you been given in the question? Extract the data from the question:. What is the relationship between what you know and what you need to find out? Maximise unpaired electrons in the orbitals of a subshell before pairing

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up electrons. Work through the steps to draw the orbital diagram for O then o 2- a Draw orbital box diagram for O: 1s 2 2s 2 2p 4 i Apply Hund's Rule :. A pair of electrons in 1 of the p orbitals, the other 2 p orbitals occupied by single electrons. Pairs of electrons in 1s, 2s, and one of the 2p orbitals have antiparallel spin. Maximise unpaired electrons in the orbitals of a subshell before pairing up electrons All electrons will be paired. Is your answer plausible? An atom of oxygen has 8 electrons. O 2- is isoelectronic with an atom of neon Electronic configuration of Ne shells : 2,8 Electronic configuration of Ne subshells : 1s 2 2s 2 2p 6 Electronic configuration of Ne orbital notation : 1s 2 2s 2 2p x 2 2p y 2 2p z 2 Orbital diagram for an atom of Ne in ground state:. Since the orbital diagram for an atom of Ne agrees with the orbital diagram for O 2- , we are confident that our answer is plausible. Do you know this? Do you understand this? Can you apply this? Take the exam now!