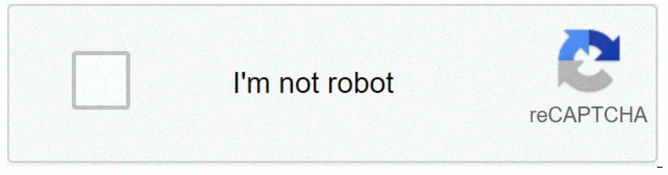

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P orbitals valence electrons

Després d'haver introduït els fonaments de l'estructura atòmica i la mecànica quàntica, podem utilitzar la nostra comprensió dels nombres quàntics per determinar com es relacionen els orbitals atòmics entre si. Això ens permet determinar quins orbitals estan ocupats per electrons en cada àtom. La disposició específica d'electrons en òrbites d'un àtom determina moltes de les propietats químiques d'aquest àtom. L'energia dels orbitals atòmics augmenta a mesura que augmenta el nombre quàntic principal, \(n\). En qualsevol àtom amb dos o més electrons, la repulsió entre els electrons fa que les energies dels subescoxells amb diferents valors de \(l\) difereixin de manera que l'energia dels orbitals augmenti dins d'una closca en l'ordre s < p < d < f. Figure \(\PageIndex{1}\) 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. The 3d orbital is higher in energy than the 4s orbital. Such overlaps continue to occur frequently as we move up the chart. Figure \(\PageIndex{1}\): Generalized energy-level diagram for atomic orbitals in an atom with two or more electrons (not to scale). 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). 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, compensant lleugerament les atraccions d'electrons-nuclis més dominants (recordem que tots els electrons tenen càrregues −1, però els nuclis tenen càrregues +Z). Aquest fenomen s'anomena blindatge i es discutirà amb més detall en la següent secció. Els electrons en òrbites que experimenten més blindatge són menys estabilitzats i, per tant, més alts en energia. Per a petites òrbites (1s a 3p), l'augment de l'energia a causa de n és més significatiu que l'augment a causa de l; no obstant això, per als orbitals més both trends are comparable and cannot be predicted simply. We will discuss methods to remember the The arrangement of electrons in the orbitals of an atom is called the electronic configuration of the atom. We describe an electron configuration with a symbol containing three pieces of information (Figure \(\PageIndex{2}\)): The number of the main quantum shell, n, The letter that designates the orbital type (the subshell, l) and A superscript number that designates the number of electrons in that particular subsell. For example, 2p4 notation (read two-p-four) indicates four electrons in a subspix p (l = 1) with a primary quantum number (n) of 2. The 3d8 notation (read three-d–eight) indicates eight electrons in the subshell d (i.e. l = 2) of the main shell for which n = 3. Figure \(\PageIndex{2}\): The diagram of an electron configuration specifies the subspix (n and value, with font symbol) and the superscript number of electrons. To determine the electron configuration for any particular atom, we can build the structures in the order of atomic numbers. Starting with hydrogen, and continuing through the periods of the periodic table, we add one proton at a time to the nucleus and an electron to the appropriate subscotch until we have described the electron configurations of all the elements. This procedure is called the Aufbau principle, of the German word Aufbau (build). Each added electron occupies the lowest available power subspix (in the order shown in figure \(\PageIndex{3}\)), subject to the limitations imposed by quantum numbers allowed in accordance with pauli's exclusion principle. Electrons enter higher energy subscoes only after lower-energy subscoes have been filled to capacity. The figure \(\PageIndex{3}\) illustrates the traditional way of remembering the filling order of atomic orbitals. Figure \(\PageIndex{3}\): The arrow leads through each subspix in the appropriate filling order for electron configurations. This graphic is simple to build. Simply make a column for all s orbits with each n shell in a separate row. Repeat for p, d and f. Be sure to include only orbitals allowed by quantum numbers (not 1p or 2d, and so on). Finally, draw diagonal lines from top to bottom as shown. Since the periodic table layout is based on electron configurations, the figure \(\PageIndex{4}\) provides an alternative method for determining electronic configuration. The filling order simply starts at hydrogen and includes each subspix as it progresses in{4} increasing the Z command. By building hydrogen, this table can be used determine the electronic configuration for any atom in the periodic table. Now we will build the terrain-state terrain-state 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 electron configuration, showing individual orbitals and electron mating arrangement. We start with a single hydrogen atom (atomic number 1), consisting of a proton and an electron. Referring to the figure \(\PageIndex{3}\) or \(\PageIndex{4}\), we hope to find the electron in orbital 1s. By convention, the value \(m_s=+\dfrac{1}{2}\) is usually filled first. The electronic configuration and orbital diagram are: Following the hydrogen is the helium of noble gas, 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, ml = 0, \(m_s=+\dfrac{1}{2}\)). The second electron also enters orbital 1s and fills this orbital. The second electron has the same quantum numbers n, l and ml, but must have the quantum number of opposite rotation, \(m_s=−\dfrac{1}{2}\). This is in keeping 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 to each box (representing two electrons in each orbital) and the arrows must point in opposite directions (representing matched twists). The electronic configuration and orbital diagram of helium are: Shell n = 1 is completely filled in a helium atom. The next atom is alkaline metallic lithium with an atomic number of 3. The first two electrons in lithium fill orbital 1 and have the same sets of four quantum numbers as the two helium electrons. The remaining electron must occupy the orbit of the next lowest energy, orbital 2s (Figure \(\PageIndex{3}\) or \(\PageIndex{4}\)). Thus, the electronic configuration and orbital lithium diagram are: An atom of the alkaline Earth metal beryle, 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 orbital 2s. A boron atom (atomic number 5) contains five electrons. The n = 1 shell is filled with two electrons and three electrons will occupy the n = 2 shell. Because any subspace can hold only two electrons, the fifth electron must occupy the next energy level, which will be a 2p orbital. There are three 2p orbitals (ml = −1, 0, +1) and the electron can occupy any of these orbital p. When we draw orbital diagrams, we include empty boxes to represent any empty orbital in the same subscover we are filling. Carbon (atomic number 6) has six electrons. Four of them fill orbits 1 and 2s. The remaining two electrons occupy the 2p subspix. Now we have the option to fill one of the 2p orbitals and match the or leave the electrons unpaved in two different orbitals, however, p. Orbitals are filled as described by the Hund rule: the lowest energy setting for an atom with electrons within a set of orbitals is that they have the maximum number of unaccompanied electrons. Thus, the two electrons in 2p carbon orbits have identical n, l, and ms quantum numbers and differ in their ml quantum number (according to Pauli's exclusion principle). The electron configuration and orbital carbon diagram are: Nitrogen (atomic number 7) fills subscoes 1 and 2 and has an electron in each of the three 2p orbits, according to the Hund rule. These three electrons have unpaved turns. Oxygen (atomic number 8) has a pair of electrons in either orbital 2p (electrons have opposite turns) and a single electron in each of the other two. Fluorine (atomic number 9) has only a 2p orbital containing an unpaved electron. All noble gas neon electrons (atomic number 10) are matched, and all orbitals of the n = 1 and n = 2 shells are filled. The configurations of electrons and orbital diagrams of these four elements are: Figure \(\PageIndex{5}\): Since the core electron shells correspond to configurations of noble gas electrons, we can abbreviated electron configurations by typing the noble gas that matches the electronic configuration of the core, along with the electrons of valencia in a condensed format. For our sodium example, the [Ne] symbol represents basic electrons, (1s22s22p6) and our abbreviated or condensed configuration is [Ne]3s1. Alkaline metallic sodium (atomic number 11) has one more electron than the neon atom. This electron must enter the lowest available power subspace, orbital 3s, giving a configuration 1s22s22p63s1. Electrons occupying the outermost shell orbitals (highest value of n) are called valencia electrons, and those that occupy the orbitals of the inner shell are called basic electrons (Figure \PageIndex5\PageIndex5). Since the core electron shells correspond to configurations of noble gas electrons, we can abbreviated electron configurations by writing the noble gas that matches the configuration of basic electrons, along with the valencia electrons in a condensed format. For our sodium example, the [Ne] symbol represents basic electrons, (1s22s22p6) and our abbreviated or condensed configuration is [Ne]3s1. Figure \(\PageIndex{5}\): An abbreviated electronic configuration (right) replaces the basic electrons with the noble gas symbol whose configuration matches the main electronic configuration of the other item. Similarly, the abbreviated configuration of lithium can be represented as [He]2s1, where [He] represents the configuration of the helium atom, which is to that of the lithium-filled inner shell. Writing the configurations in this way emphasizes the similarity of the lithium and sodium. Both atoms, found in the alkaline metal family, have only one electron in a valencia shell out of a set filled with inner shells. \[\ce{Li:[He]}\,2s^1\\\ce{Na:[Ne]}\,3s^1\] Alkaline Earth metal magnesium (atomic number 12), with its 12 electrons in a configuration [Ne]3s2, is analogous to its family berile, [He]2s2. Both atoms have a full subselling outside their filled inner shells. Aluminium (atomic number 13), with 13 electrons and electron configuration [Ne]3s23p1, is analogous to its family member boron, [He]2s22p1. The configurations of silicon electrons (14 electrons), phosphorus (15 electrons), sulfur (16 electrons), chlorine (17 electrons) and argon (18 electrons) are analogous in the electron configurations of their outer shells to their corresponding members of the carbon family, nitrogen, oxygen, fluorine, and neon respectively, except that the main quantum number of the outer shell of the heaviest elements has increased by one to n = 3. The figure \(\PageIndex{6}\) shows the lowest energy, or state of the ground, the configuration of electrons for these elements, as well as that of the atoms of each of the known elements. Figure \(\PageIndex{6}\): This version of the periodic table shows the electronic configuration of the outer shell of each item. Note that in each group, the settings are often similar. When we reach the next element of the periodic table, the alkaline metal potassium (atomic number 19), we could expect us to start adding electrons to the 3D subcar. However, all available chemical and physical evidence indicates that potassium is such as lithium and sodium, and that the next electron is not added to the 3D level, but added to level 4 (Figure \(\PageIndex{3}\) or \(\PageIndex{4}\)). As discussed above, the 3D orbit without radial nodes is higher in energy because it is less penetrating and more protected from the nucleus than the 4, which has three radial nodes. Therefore, potassium has an electronic configuration of [Ar]4s1. Therefore, potassium corresponds to Li and Na in their configuration of the valencia shell. The following electron is added to complete subscoix 4s and calcium has an electronic configuration of [Ar]4s2. This gives calcium an outer shell electronic configuration corresponding to that of beryleum and magnesium. From the transition metal scandal (atomic number 21), additional electrons are successively added to the 3D subspix. This subspix is filled at 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 orbital ds that have a combined capacity of 10 electrons). The 4p subsellation is filled below. Note that for three series of items, scandium (Sc) through copper (Cu), yttrium (Y) through silver (Ag), and lutetium (Lu) through gold (Au), a total of 10 d electrons are successively in the shell (n – 1) next to the shell n to carry this shell (n – 1) from 8 to 18 electrons. For two series, lanthanum (La) through lutetium (Lu) and actinium (Ac) through lawrencium (Lr), 14 f electrons (l = 3, 2l + 1 = 7 ml values; therefore, seven orbitals with a combined capacity of 14 electrons) are added successively to the shell (n – 2) to carry this 18-electron shell to a total of 32 electrons. Example \(\PageIndex{1}\): Quantum numbers and electron configurations What is the electronic configuration and orbital diagram for a phosphorus atom? What are the four quantum numbers of the last added electron? Solution The atomic number of phosphorus is 15. Thus, a phosphorus atom contains 15 electrons. The order of filling energy levels is 1s, 2s, 2p, 3s, 3p, 4s, . . . The 15 electrons of the phosphorus atom will fill up to 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 could be –1, 0 or +1. The three orbital p are, so any of these ml values is correct. For unpaved electrons, the convention assigns the value of \(+\dfrac{1}{2}\) for the centrifugation quantum number; therefore, \(m_s=+\dfrac{1}{2}\). Exercise \(\PageIndex{1}\) Identify the atoms of the given electron configurations: [Ar]4s23d5 [Kr]5s24d105p6 Replying to Mn Answer b Xe The periodic table can be a powerful tool for predicting the electronic configuration of an item. However, we find exceptions to the orbital filling order shown in figure \(\PageIndex{3}\) or \(\PageIndex{4}\). For example, the electron configurations of the transition metal chromium (Cr; atomic number 24) and copper (Cu; atomic number 29), among others, are not what we expected. In general, these exceptions involve subscoes 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 the half-filled and completely full subscoes apparently represent preferred stability conditions. This stability is such that an electron changes from 4 to 3D orbital to get the additional stability of a half-filled 3D subscotch (in Cr) or a full 3D subscoix (in Cu). Other exceptions also occur. For example, niobium (Nb, atomic number 41) is expected to have the electronic configuration [Kr]5s24d3. Experimentally, we note that its configuration of earth-state electrons is actually [Kr]5s14d4. We can rationalize this observation by saying that the repulsions of electrons and electrons experienced by mating electrons in the orbit of the 5 are greater than the energy gap between orbital 5s and 4d. There is no simple method to predict exceptions for atoms where the magnitude of repulsions between is greater than small energy differences between subscos. As described above, the periodic table atoms based on increasing the atomic number so that elements with the same chemical properties are repeated periodically. When their electron configurations are added to the table (Figure \(\PageIndex{6}\)), we also see a periodic recurrence of similar electron configurations in the outer shells of these elements. Because they are in the outer shells of an atom, valencia electrons play the most important role in chemical reactions. Outer electrons have the highest energy of electrons in an atom and are more easily lost or shared than basic electrons. Valencia electrons are also the determining factor in some physical properties of the elements. Elements of a single group (or column) have the same number of valencia electrons; Lithium alkaline metals and sodium have only one valencia electron, berylelic and magnesium alkaline terrestrial metals have two, and fluorine and chlorine haligens each have seven valencia electrons. The similarity in the chemical properties between elements of the same group occurs because they have the same number of valencia electrons. It is the loss, gain or exchange of valencia electrons that defines how the elements react. It is important to remember that the periodic table was developed on the basis of the chemical behavior of the elements, long before there was any idea of their atomic structure. Now we can understand why the periodic table has the arrangement it has— the layout puts elements against the same number of valencia electrons in the same group. This layout is emphasized in the figure \(\PageIndex{6}\), which shows in the form of a periodic table the electronic configuration of the last subspix that will fill the beginning of Aufbau. The color sections of the figure \(\PageIndex{6}\) show the three categories of elements classified by orbitals that are filled: main group elements, transition, and internal transition. These classifications determine which orbitals are counted in the valencia shell, or higher energy level orbitals of an atom. The main elements of the group (sometimes called representative elements) are those in which the last added electron enters an orbital s or p in the outer most external shell, which is shown in blue and red in the figure \(\PageIndex{6}\). This category includes all non-metallic elements, as well as many metals and intermediate semi-metallic elements. The valencia electrons for the main elements of the group are those with the highest level n. For example, gallium (Ga, atomic number 31) has the electronic configuration [Ar]4s23d104p1, containing three valencia electrons (underlined). Fully filled orbitals count as a nucleus, not valencia, electrons. Transition elements or transition metals. These are elements in which the last added electron enters an orbital d. Valencia electrons (those added after the last configuration of noble gas) in these elements include ns and (n – 1) d electrons. Electrons. the official IUPAC definition of transition elements specifies those with partially filled orbitals. Thus, elements with full orbitals (Zn, Cd, Hg, as well as Cu, Ag and Au in figure \(\PageIndex{6}\)) are not technically transitional elements. However, the term is frequently used to refer to the entire block d (color yellow in figure \(\PageIndex{6}\)), and we will adopt this use in this textbook. The interior transition elements are metallic elements in which the last added electron occupies an orbital f. They are shown in green in the figure \(\PageIndex{6}\). The valencia shells of the interior transition elements consist of the (n – 2)f, the (n – 1)d, and the subshells. There are two series of inner transition: The Lanthanide Series: Lanthanide (La) through Lutetium (Lu) The Actinide Series: Actinide (Ac) via Lawrencium (Lr) Lanthanum and Actinium, due to their similarities to the other members of the series, are included and used to name the series, even though they are We have seen that ions form when atoms gain or lose electrons. A positively charged cation (ion) is formed when one or more electrons are removed from a parent atom. For the main elements of the group, the electrons that were last added are the first electrons removed. For transition metals and inner transition metals, however, electrons in orbit s are easier to remove than d or f electrons, so that higher electrons ns are lost, and then electrons (n – 1) d or (n – 2)f electrons are removed. An anion (negatively charged ion) is formed when one or more electrons are added to a parent atom. The added electrons fill the order predicted by the Aufbau principle. Example \(\PageIndex{2}\): Prediction of Ion electron configurations What is the electronic configuration and orbital diagram of: Solution First, type the electronic configuration for each primary atom. We have chosen to show the full, non-abbreviated configurations to provide more practice to students who want it, but the list of basic abbreviated electron configurations is also acceptable. Then determine if an electron is won or lost. Remember that electrons load negatively, so ions with a positive charge have lost an electron. For the main elements of the group, the latest orbital gains or lose the electron. For transition metals, the last orbital s loses an electron before orbits d. Na: 1s22s22p63s1. Sodium cation loses an electron, so Na+: 1s22s22p63s1 = Na+: 1s22s22p6. Modify your reservation or put in English. The phosphorus triad gains three electrons, so P3−: 1s22s22p63s23p6. Al: 1s22s22p63s23p1. Aluminium indication loses two electrons 1s22s22p63s23p1 = Al2+: 1s22s22p63s1. Faith: 1s22s22p63s23p64s23d6. Iron(II) loses two electrons and, since it is a transition metal, are removed from orbital 4s Fe2+: 1s22s22p63s23p64s23d6 = 1s22s22p63s23p63d6. Sm: Sm: The samarian trication loses three electrons. The first two will be lost from orbital 6s, and the last will be removed from orbit 4f. Sm3+: 1s22s22p63s23p64s23d104p65s24d105p66s24f6 = 1s22p63s23p64s23d104p65s24d105p64f5. Exercise \(\PageIndex{2}\) Which ion with a load of +2 has the electronic configuration 1s22s2p63s23p63d104s24p64d5? Which charge +3 does this setting have? Respond to a Tc2+ b Ru3 + Relative energy of subschokes determines the order in which atomic orbits are filled (1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, and so on). Configurations of electrons and orbital diagrams can be determined by applying the Pauli exclusion principle (no two electrons can have the same set of four quantum numbers) and the Hund rule (whenever possible, electrons retain unpaved turns in degenerate orbitals). Electrons in the outerst orbitals, called valencia electrons, are responsible for most of the chemical behavior of the elements. In the periodic table, elements with analog configurations of valencia electrons usually occur within the same group. There are a few exceptions to the planned filling order, especially when half full or full orbitals can be formed. The periodic table can be divided into three categories based on the orbital in which the last electron is added: main elements of the group (orbitals s and p), transition elements (d orbitals) and elements of inner transition (f orbital). orbitals).

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