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What is meant by effective nuclear charge

Saint Mary's College: CHEM 342 Bioinorganic Chemistry Spring 2020: Dr. Kathryn Haas Agenda ● Readings ● Worksheets ● Essays ● WiSEWIKI Figure \(\PageIndex{1}\). Effective nuclear charge in a Li atom. (CC-BY-NC-SA; Kathryn Haas) The ideal gas law is easy to remember and apply in solving problems, as long as you get the proper values a According to Coulomb's law, the attraction of an electron to a nucleus depends only on three factors: the charge of the nucleus (+Z), the charge of the electron (-1), and the distance between the two (\(r\)). Coulomb's law works well for predicting the energy of an electron in a hydrogen atom (H has only two particles: one nucleus and one electron). It also works for hydrogen-like atoms: any nucleus with exactly one electron (a He+ ion, for example, has one electron). However, Coulomb's law is insufficient for predicting the energies of electrons in multi-electron atoms and ions. Electrons within a multi-electron atom interact with the nucleus and with all other electrons. Each electron in a multi-electron atom experiences both attraction to the nucleus and repulsion from interactions with other electrons. The presence of multiple electrons decreases the nuclear attraction to some extent. Each electron in a multi-electron atom experiences a different magnitude of (and attraction to) the nuclear charge depending on what specific subshell the electron occupies. The amount of positive charge experienced by any individual electron is the effective nuclear charge (\(Z_{eff}\)). ** For example, in lithium (Li), none of the three electrons "feel" the full +3 charge from the nucleus (see Cartoon). Rather, each electron "feels" a \(Z_{eff}\) that is less than the actual Z and that depends on the electron's orbital. The actual nuclear charge in Li is +3; the 1s electrons experience a \(Z_{eff}\) =+2.69, and the 2s electron experiences a \(Z_{eff}\) = 1.28. In general, core electrons (or the electrons closest to the nucleus), "feel" a \(Z_{eff}\) that is close to, but less than, the actual nuclear charge (Z). On the other hand, outer valence electrons experience a \(Z_{eff}\) that is much less than Z. In summary: Core electrons: \(Z^* \lessapprox Z\) Valence electrons: \(Z^* \ll Z\) **You will also see \(Z_{eff}\) represented as \(Z^*\): specifically in the section in which you reviewed Periodic Trends, the symbol \(Z^*\) was used. Figure \(\PageIndex{2}\). Diagram illustrating effective nuclear charge according to Slater's rules. The \(Z_{eff}\) can be estimated using a number of different methods; probably the best known and most commonly used method is known as Slater's Rules. Slater developed a set of rules to estimate \(Z_{eff}\) depending on how many other electrons exist in the atom and on the orbital location of the electron-of-interest. These two factors are important determinants in shielding (see next section), and they are used to calculate a shielding constant (\(\sigma\)) used in Slater's formula: \[Z_{eff}=Z-\sigma\] where Z is the actual nuclear charge (the atomic number) and \(Z_{eff}\) is the effective nuclear charge. To calculate \(\sigma\), we will write out all the orbitals in an atom, separating them into "groups". Each change in shell number is a new group; s and p subshells are in the same group but d and f orbitals are their own group. You write out all the orbitals using parentheses until you get to the group of the electron-of-interest, like this: (1s)(2s,2p)(3s,3p)(3d)(4s,4p)(4d)(4f)(5s,5p) etc. **Critical: The orbitals must be written in order of increasing energy! Electrons in the same Group(): Each other electron (not counting the electron-of-interest) in the same group () as the chosen electron, contributes 0.35 to \(\sigma\). Conceptually, this means electrons in the same group shield each other 35%. Electrons in Groups() to the left: If the electron-of-interest is in a d or f subshell, every electron in groups () to the left contributes 1.00 to \(\sigma\). Conceptually, this means that d and f electrons are shielded 100% by all electrons in the same shell with a smaller value of \(l\), as well as all electrons in lower shells (\(n\)). If the electron-of-interest is in an s or p subshell, all electrons in the next lower shell (n - 1) contribute 0.85 to \(\sigma\). And all the electrons in even lower shells contribute 1.00 to \(\sigma\). Conceptually, this means that s and p electrons are shielded 85% by the electrons one shell lower, and 100% by all electrons in shells n - 2 or lower. 1s electrons: \(\sigma\) of a 1s electron is just (\sigma=0.3\), no matter the element. Example \(\PageIndex{1}\): Fluorine, Neon, and Sodium What is the \(Z_{eff}\) experienced by the valence electrons in the three isoelectronic species: fluorine anion (F-), neutral neon atom (Ne), and sodium cation (Na+)? Solution Each species has 10 electrons, and the number of core electrons is 2 (10 total electrons - 8 valence), but the effective nuclear charge varies because each has a different atomic number (Z). The approximate \(Z_{eff}\) can be found with Slater's Rules. For all of these species, we would calculate the same sigma value: Calculating \(\sigma\): (1s)(2s,2p), \(\sigma = 2(0.85) + 7(0.35) = 1.7 + 2.45 = 4.15 \) Fluorine anion: \(Z_{eff}=9-\sigma = 9 - 4.15 = 4.85\) Neon atom: \(Z_{eff}=10-\sigma = 10 - 4.15 = 5.85\) Sodium Cation: \(Z_{eff}=11-\sigma = 11 - 4.15 = 6.85\) So, the sodium cation has the greatest effective nuclear charge. Exercise \(\PageIndex{1}\) Calculate Zeff for a 3d-electron in a zinc (Zn) atom. Answer Write out the relevant orbitals: (1s)(2s,2p)(3s,3p)(3d) (4s) Notice that although 4s is fully occupied, we don't include it because in Zn, 4s is higher in energy than 3d, and is thus to the right of the d electrons we are looking at. The electron-of-interest is in 3d, so the other nine electrons in 3d each contribute 0.35 to the value of S. The other 18 electrons each contribute 1 to the value of S. \(S=18(1)+9(0.35)=21.15\) \(Z_{eff}=30-21.15=8.85\) So, although the nuclear charge of Zn is 30, the 3d electrons only experience a \(Z_eff \approx 8.85\)! Slater's rules are a set of simple rules for predicting \(\sigma\) and \(Z_{eff}\) based on empirical evidence from quantum mechanical calculations. In other words, the \(Z_{eff}\) calculated from Slater's rules are approximate values. The values considered to be the most accurate are derived from quantum mechanical calculations directly. You can find these values in a nice chart on the Wikipedia article of Effective Nuclear Charge. I've recreated the chart in Figure \(\PageIndex{3}\) for convenience: Figure \(\PageIndex{3}\). This chart shows \(Z_{eff}\) values calculated by Clementi et. al. in 1963 and 1967 that are consistent with SCF Calculations. This chart was created using data from the Wikipedia article on Effective Nuclear Charge. When valence electrons experience less nuclear charge than core electrons, different electrons experiencing different magnitudes of attraction to the nucleus. A modified form of Coulomb's Law is written below, where \(e\) is the charge of an electron, \(Z_{eff}\) is the effective nuclear charge experienced by that electron, and \(r\) is the radius (distance of the electron from the nucleus). \[F_{eff}=k \dfrac{Z_{eff}e^2}{r^2}\] This formula would suggest that if we can estimate \(Z_{eff}\), then we can predict the attractive force experienced by, and the energy of, an electron in a multi-electron atom, like Li. The attraction of the nucleus to valence electrons determines the atomic or ionic size, ionization energy, electron affinity, and electronegativity. The stronger the attraction, and the stronger \(Z_{eff}\), the closer the electrons are pulled toward the nucleus. This in turn results in a smaller size, higher ionization energy, higher electron affinity, and stronger electronegativity. Close inspection of Figure \(\PageIndex{3}\) and analysis of Slater's rules indicate that there are some predictable trends in \(Z_{eff}\). The data from Figure \(\PageIndex{3}\) is plotted below in Figure \(\PageIndex{4}\) to provide a visual aid to the discussion below. Figure \(\PageIndex{4}\): The \(Z_{eff}\) values for electrons in each subshell of the first 54 elements (H to Xe) are plotted. Each subshell is plotted as a different series (see legend) and the valence shell is highlighted by a solid black line with open circles. (CC-BY-NC-SA; Kathryn Haas) The \(Z_{eff}\) for electrons in a given shell and subshell generally increases as atomic number increases; this trend holds true going across the periodic table and down the periodic table. Convince yourself that this is true for any subshell by examining Figure \(\PageIndex{4}\). Do you notice any exceptions to this general trend? Inspection of figure \(\PageIndex{4}\) should confirm for you that the \(Z_{eff}\) increases as Z increases for electrons in any subshell (like the 1s subshell for example, which is plotted above as a red line with square points). You can see this trend as the positive slope in each series. There is one obvious exception in Period 5 in elements 39 (Y) to 41 (Nb; the \(Z_{eff}\) of 4s actually decreases across these three elements as atomic number increases. There is also an exception between Y and Zr in the 3d subshell, and between Tc and Ru in the 5s subshell. It is useful to understand trends in valence \(Z_{eff}\) because the valence \(Z_{eff}\) determines atomic/ionic properties and chemical reactivity. The trends in the valence \(Z_{eff}\) are not simple because as atomic number increases, the valence shell and/or subshell also changes. The valence \(Z_{eff}\) is indicated in Figure \(\PageIndex{4}\) as a black line with open circles. Down the table: As we go down a column of the periodic table, the valence \(Z_{eff}\) increases. This is a simple trend because type of subshell is consistent and there is an increase only in shell and in atomic number, Z. This trend is best illustrated by inspection of Figure \(\PageIndex{3}\). Across the table: the trend depends on shell and subshell. Periods 1-3 (s and p only): As we go across the table in periods 1-3, the shell stays constant as Z increases and subshell changes from s to p. In these periods, there is a gradual increase in valence \(Z_{eff}\) as we move across any of the first three periods. Periods 4 and 5 (s, p, and d): Now we have some more complex trends because valence subshell and shell are changing as we increase in atomic number. Notice that the valence \(Z_{eff}\) generally increases going across a period as long as subshell isn't changing; the exception is within the 4d subshell (elements 39-44 or Y-Ru). In general, going from \((n)s\) subshell to \((n-1)d\) subshell, there a relatively large increase in valence \(Z_{eff}\). And in going from \((n-1)d\) subshell to \((n)p\) subshell, there is a relatively large decrease in \(Z_{eff}\). From one period to another: From Figure \(\PageIndex{4}\), we can see that as we increase Z by one proton, going from one period to the next, there is a relatively large decrease in \(Z_{eff}\) (from Ne to Na, for example). This is because as Z increases by a small interval, the shell number increases, and so the electrons in the valence shell are much farther from the nucleus and are more shielded by all the electrons in the lower shell numbers. Exercise \(\PageIndex{2}\) 1. Compare trends in \(Z_{eff}\) and atomic size. Explain how and why atomic size depends on \(Z_{eff}\). 2. Compare trends in \(Z_{eff}\) and ionization energy. Explain how and why ionization energy depends on \(Z_{eff}\). Answer 1. As \(Z_{eff}\) increases, the valence electrons are pulled in tighter to the nucleus resulting in a small radius for atoms. 2. As \(Z_{eff}\) increases, the distance between the valence electrons and the nucleus decreases. This creates a stronger force holding the valence electrons, and thus requires a higher ionization energy to remove a valence electron. Contributors Calculate effective nuclear charges experienced by valence electrons. The shielding effect describes the balance between the pull of the protons on valence electrons and the repulsion forces from inner electrons. The shielding effect explains why valence-shell electrons are more easily removed from the atom. The effect also explains atomic size. The more shielding, the further the valence shell can spread out and the bigger atoms will be. The effective nuclear charge is the net positive charge experienced by valence electrons. It can be approximated by the equation: Zeff = Z – S, where Z is the atomic number and S is the number of shielding electrons. Electrons in an atom can shield each other from the pull of the nucleus. This effect, called the shielding effect, describes the decrease in attraction between an electron and the nucleus in any atom with more than one electron shell. The more electron shells there are, the greater the shielding effect experienced by the outermost electrons. In hydrogen-like atoms, which have just one electron, the net force on the electron is as large as the electric attraction from the nucleus. However, when more electrons are involved, each electron (in the n-shell) feels not only the electromagnetic attraction from the positive nucleus but also repulsion forces from other electrons in shells from 1 to n-1. This causes the net electrostatic force on electrons in outer shells to be significantly smaller in magnitude. Therefore, these electrons are not as strongly bound as electrons closer to the nucleus. The shielding effect explains why valence shell electrons are more easily removed from the atom. The nucleus can pull the valence shell in tighter when the attraction is strong and less tight when the attraction is weakened. The more shielding that occurs, the further the valence shell can spread out. As a result, atoms will be larger. Example: Why is cesium bigger than elemental sodium? Solution: The element sodium has the electron configuration 1s22s22p63s1. The outer energy level is n = 3 and there is one valence electron. The attraction between this lone valence electron and the nucleus with 11 protons is shielded by the other 10 core electrons. The electron configuration for cesium is 1s22s22p63s23p64s23d104p65s24d105p66s1. While there are more protons in a cesium atom, there are also many more electrons shielding the outer electron from the nucleus. The outermost electron, 6s1, therefore, is held very loosely. Because of shielding, the nucleus has less control over this 6s1 electron than it does over a 3s1 electron. Effective Nuclear Charge The magnitude of the shielding effect is difficult to calculate precisely. As an approximation, we can estimate the effective nuclear charge on each electron. Effective nuclear charge diagramDiagram of the concept of effective nuclear charge based on electron shielding. The effective nuclear charge (often symbolized as Zeff or Z*) is the net positive charge experienced by an electron in a multi-electron atom. The term “effective” is used because the shielding effect of negatively charged electrons prevents higher orbital electrons from experiencing the full nuclear charge. The effective nuclear charge on an electron is given by the following equation: Zeff = Z – S where Z is the number of protons in the nucleus (atomic number), and S is the number of electrons between the nucleus and the electron in question (the number of nonvalence electrons). Example: Consider a neutral neon atom (Ne), a sodium cation (Na+), and a fluorine anion (F–). What is the effective nuclear charge for each? Solution: Start by figuring out the number of nonvalence electrons, which can be determined from the electron configuration. Ne has 10 electrons. The electron configuration is 1s22s2 2p6. The valence shell is shell 2 and contains 8 valence electrons. Thus the number of nonvalence electrons is 2 (10 total electrons – 8 valence). The atomic number for neon is 10, therefore: Zeff(Ne) = 10 – 2 = 8+ Flourine has 9 electrons but F– has gained an electron and thus has 10. The electron configuration is the same as for neon and the number of nonvalence electrons is 2. The atomic number for F– is 9, therefore: Zeff(F–) = 9 – 2 = 7+ Sodium has 11 electrons but the Na+ ion has lost an electron and thus has 10. Once again, the electron configuration is the same as in the previous examples and the number of nonvalence electrons is 2 (by losing one electron, the valence shell becomes the n=2 shell). The atomic number for Na+ is 11, therefore: Zeff(Na+) = 11 – 2 = 9+ In each of the above examples (Ne, F–, Na+) an atom has 10 electrons but the effective nuclear charge varies because each has a different atomic number. The sodium cation has the largest effective nuclear charge, which results in electrons being held the tightest, and therefore Na+ has the smallest atomic radius.

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