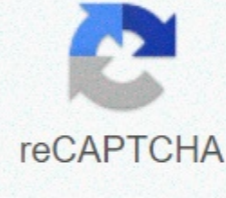




I'm not robot



Continue

## What is zeff in chemistry

Training objectives To understand the basics of electron protection and penetration For an atom or ion with only one electron, we can calculate potential energy by examining only electrostatic pull between a positively charged core and a negatively charged electron. However, when more than one electron is present, the total energy of the atom or ion depends not only on the attractive interactions of the electron-core, but also on the repulsive interactions of electrons-electrons. When there are two electrons, the repulsive interactions depend on the positions of both electrons at a given moment, but because we can not specify the exact positions of the electrons, it is impossible to accurately calculate the repulsive interactions. Consequently, we must use approximate methods to combat the impact of electronic repulsions on orbital energies. These effects are the basis for periodic trends in elementary properties that we will explore in this section. If the electron is far from the nucleus (i.e., if the distance  $r$  between the nucleus and the electron is large), then at any time many other electrons will be between this electron and the nucleus (Fig. 1). Thus, electrons will cancel part of the positive core charge and thereby reduce the attractive interaction between it and the electron further. As a result, the electron further experiences an effective nuclear charge ( $Z_{\text{eff}}$ ) that is less than the actual nuclear charge ( $Z$ ). This effect is called electronic protection. Figure 1: This image shows how internal electrons can protect other electrons from nuclear charge. (CC BY-SA 3.0; by NickNax). As the distance between the electron and the core approaches infinity,  $Z_{\text{eff}}$  is approaching a value of 1, as all other ( $Z - 1$ ) electrons in a neutral atom are, on average, between it and the core. If, on the other hand, the electron is very close to the nucleus, then at any moment most other electrons are farther from the nucleus and do not protect the nuclear charge. When ( $r = 0$ ), the positive charge experienced by the electron is approximately a full nuclear charge, or ( $Z_{\text{eff}} = Z$ ). At intermediate values  $r$  the effective nuclear charge is somewhere between 1 and  $Z$ : ( $1 \leq Z_{\text{eff}} \leq Z$ ) that ( $Z_{\text{eff}} = Z$ ) only for hydrogen and only for helium ( $Z_{\text{eff}}$ ) and ( $Z$ ) can be compared by magnitude (Figure 2). Protective protection refers to the main electrons repulsed by the output electrons, which reduces the effective core charge on the output electrons. Consequently, the nucleus has less traction on the output electrons because it is protected from them.  $Z_{\text{eff}}$  can be calculated by reducing the amount of protection against the total nuclear charge effective nuclear charge of the atom is given by an equation:  $Z_{\text{eff}} = Z - S$  where  $S$  is the atomic number (number of protons in the nucleus) and  $S$  is a protective constant. The value ( $Z_{\text{eff}}$ ) will provide information about how much charge the electron actually feels. Equation 1 can be seen 4) effective nuclear charge of the atom increases as the number of protons in the atom increases (Fig. 2). So as we go from left to right on the periodic table, the atom's effective nuclear charge increases in strength and keeps other electrons closer and denser to the nucleus. As we will discuss later in the section, this phenomenon may explain the decline in atomic radii we see as we go through the periodic table as electrons are held closer to the core due to increased proton count and increased effective nuclear charge. Figure 2: The link between the effective  $Z_{\text{eff}}$  nuclear charge and the atomic number  $Z$  for the output electrons of the elements of the first three rows of the periodic table. With the exception of hydrogen, ( $Z_{\text{eff}}$ ) is always smaller than ( $Z$ ), and ( $Z_{\text{eff}}$ ) increases from left to right when you go over the string, ( $S = \sum_{i=1}^{n-1} S_i$ ) where ( $S_i$ ) is the protection of  $i$ th electron. Electrons that are protected from full core charge experience effective nuclear charge ( $Z_{\text{eff}}$ ) core that is to some extent less than the full nuclear charge that the electron would have felt in a hydrogen atom or hydrogen ion. From the equations 1 and 2, ( $Z_{\text{eff}}$ ) for a particular electron can be approximately, these are the protection constants for this electron of all other electrons in the form. A simple approximation is that all other electrons shield equally and completely ( $S_i = 1$ ) This rough approximation is demonstrated in the example 1. Example 1: Fluoride, neon, and sodium What is the effective attraction ( $Z_{\text{eff}}$ ), which experience valence electrons in three isoelectronic species: fluoride anion, neutral neon atom and sodium atom? Solution Each species has 10 electrons, and the number of electrons of non-valence is 2 (10 common electrons - 8 valence), but the effective nuclear charge varies because each has a different atomic number ( $Z$ ). This is the 1 and 2 formula program. We use the simple assumption that all electrons shield the same and completely valent electrons (Equation 1). The charge ( $Z$ ) core of the fluoride atom is 9, but valence electrons are visibly drifted by the main electrons (four electrons from orbital 1 and 2s) and partly 7 electrons in 2p Scheme of fluoride atom showing the extent of effective nuclear charge. (CC BY-SA-3.0; from NikNaks).  $Z_{\text{eff}}(\text{F}^-) = 9 - 2 = 7$   $Z_{\text{eff}}(\text{Ne}) = 10 - 10 = 0$   $Z_{\text{eff}}(\text{Na}^+) = 11 - 2 = 9$  So sodium twisting has the highest effective nuclear charge. This also indicates that ( $\text{Na}^+$ ) has the smallest radius of these species, and that's right. Exercise 1: Types of sodium What is an effective attraction ( $Z_{\text{eff}}$ ) experiencing electrons of valence in sodium anion, neutral sodium atom and sodium atom? Use a simple approximation for protective constants. Compare your result for the sodium atom with the more accurate value in the table 1 and suggested origin for the difference. Reply  $Z_{\text{eff}}(\text{Na}^-) = 11 - 2 = 9$   $Z_{\text{eff}}(\text{Na}) = 11 - 2 = 8$   $Z_{\text{eff}}(\text{Na}^+) = 11 - 2 = 9$  in table 1 for ( $\text{Na}$ ) — 10.63 and 8 ratings, which were rated higher. This means that a simple approximation (Equation 1) overestimates the protective constant ( $S$ ), but the actual ( $Z_{\text{eff}}$ ), which has an electron on a given orbital basis, depends not only on the spatial distribution of the electron in this orbital, but also on the distribution of all other electrons present. This causes large differences in ( $Z_{\text{eff}}$ ) for different items, as shown in 2 for elements of the first three rows of the periodic table. Penetration describes the proximity to which the electron can approach the nucleus. In multi-electron systems, electron penetration is determined by the relative density of electron electrons (probability density) near the nucleus of the atom (Fig. 3). Electrons in different orbitals have different density of electrons around the nucleus. In other words, penetration depends on the shell ( $n$ ) and the shell ( $l$ ). For example, electron 1s (Fig. 3; purple curve) has a higher density of electrons near the nucleus than the 2p electron (Fig. 3; red curve) and has greater penetration. This is due to protective constants as 1s electrons are closer to the nucleus than the 2p electron, hence 1s electron 2p screens are almost ideal ( $S=1$ ). However, the 2s electron has a lower protective constant ( $S \approx 1$ ) because it can penetrate close to the nucleus in a small area of electron density within the first spherical node (Fig. 3; green curve). Orbital penetration. Comparison of radial probability distribution Orbiters 2s and 2p for different states of the hydrogen atom show that orbital orbit 2s penetrates into orbital 1s more than orbital 2p. So when the electron is in a small inner fraction of orbital particle 2s, it feels a relatively large value ( $Z_{\text{eff}}$ ), causing orbital orbital energy 2s to be lower than orbital energy 2p. For the same shell value ( $n$ ) the penetrating value of the electron follows this trend in the sub-shells (Figure 3):  $S \approx p \approx d \approx f$ . Penetration describes the proximity of electrons in orbit to the nucleus. Electrons that have more penetration can approach the nucleus and effectively block the charge from electrons that have less proximity. Table 1: Effective nuclear charges for selected Atom Sublevel  $Z_{\text{eff}}$  H 1s 1 He 1s 2 1.69 Li 1s, 2s 3 2.69, 1.28 Be 1s, 2s 4 3.68, 1.91 B 1s, 2s, 2p 5 4.68, 2.58, 2.42 F 1s, 2s, 2p 9 8.65, 5.13, 5.10 Na 1s, 2s, 2p, 3s 11 10.63, 6.57, 6.80, 2.51 Dani E. Clementi and D. L. Raymond: Journal of Chemical Physics 38, 2686 (1963). Due to the influence of protective and various radial distributions of orbitals with the same value  $n$ , but different values  $l$ , different subshells do not divide in the multi-electronic atom. For a given  $n$  value, orbital  $ns$  are always lower in energy than orbital  $np$ , which are lower in energy than in orbital orbitals, and so on. As a result, some subshells with higher core quantum numbers are actually lower in energy than subshells with a lower value of  $n$ ; for example, orbital 4s is lower in energy than orbital 3d for most atoms. Better protection assessment: Slater Rules Concepts of electron protection, orbital penetration and effective nuclear charge were introduced above, but we did it qualitatively (e.g. Equations 1 and 2). A more accurate model for assessing electronic protection and the appropriate effective nuclear charge tested is the Slater Rules. However, the application of these rules is outside the scope of this text. The calculation of orbital energies in atoms or ions with more than one electron (multielectronic atoms or ions) is complicated by repulsive interactions between electrons. The concept of electron protection, in which electrons interfere, act to reduce the positive nuclear charge experienced by the electron, allows hydrogen orbiters to be used and an effective nuclear charge ( $Z_{\text{eff}}$ ) to describe electron distributions in more complex atoms or ions. The extent to which orbital with different  $l$  values and the same value  $n$  overlapping or penetration of filled inner shells leads to slightly different energies for different sub-points in the same main shell in most atoms. Atoms.