

Answer on the question #54596 – Chemistry – General chemistry

Question:

What is meant by effective nuclear charge? What are the factors that determine the effective nuclear charge? How is it calculated?

Answer:

It 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 by the repelling effect of inner-layer electrons. The effective nuclear charge experienced by the outer shell electron is also called the core charge. It is possible to determine the strength of the nuclear charge by the oxidation number of the atom.

Calculation:

In an atom with one electron, that electron experiences the full charge of the positive nucleus. In this case, the effective nuclear charge can be calculated from Coulomb's law.

However, in an atom with many electrons the outer electrons are simultaneously attracted to the positive nucleus and repelled by the negatively charged electrons. The effective nuclear charge on such an electron is given by the following equation:

$$Z_{\text{eff}} = Z - S$$

where

Z is the number of protons in the nucleus (atomic number), and

S is the average number of electrons between the nucleus and the electron in question (the number of nonvalence electrons).

S can be found by the systematic application of various rule sets, the simplest of which is known as "Slater's rules" (named after John C. Slater). Douglas Hartree defined the effective Z of a Hartree–Fock orbital to be:

$$Z_{\text{eff}} = \frac{\langle r \rangle_{\text{H}}}{\langle r \rangle_{\text{Z}}}$$

where

$\langle r \rangle_{\text{H}}$ is the mean radius of the orbital for hydrogen, and

$\langle r \rangle_{\text{Z}}$ is the mean radius of the orbital for an electron configuration with nuclear charge Z.