ATOMIC MODELS

Effective Nuclear Charge (Z) and Slater's Rules*

In many-electron systems, the electrons in the interior act as a shield, reducing the effect of the nucleus on the outer electrons. In multi-electron atoms, the electron in an orbital is pulled by the nucleus while it is pushed by other electrons in the atom. The amount of the nuclear charge that sees each electron is called an effective nuclear charge (often symbolized as Z_{eff} *or* Z^**) and the amount of the lowering charge of the nucleus is called the shielding or screening constant (P).*

The effective nuclear charge on an electron is given by the following equation:

$Z^* = Z - P$ *(Z= atomic number)*

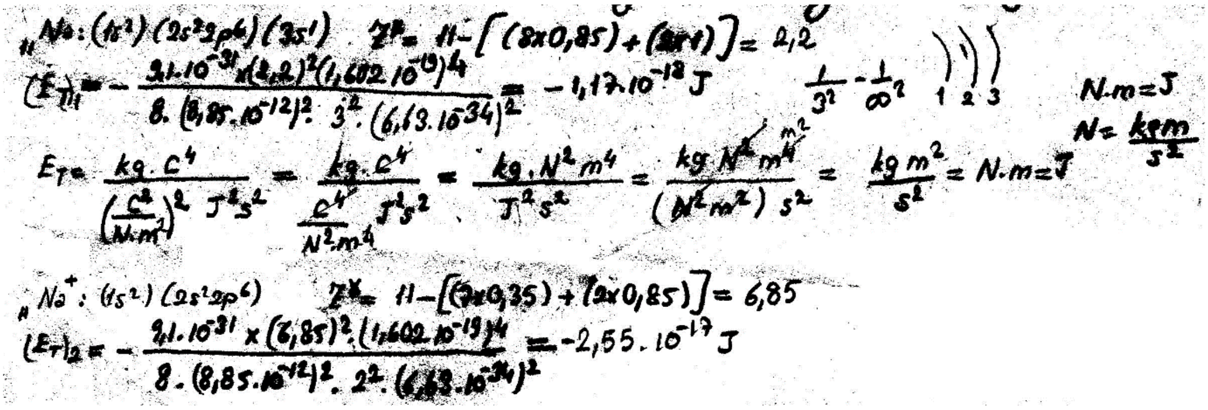
The rules for finding the effective nuclear charge was provided by J.C. Slater in 1930:

1. *Write the electron configuration for the atom using the following design (Aufbau);*
   $[_nX] = (1s)\ (2s\ 2p)\ (3s\ 3p)\ (3d)\ (4s\ 4p)\ (4d)\ (4f)\ldots$
2. *Any electrons to the right of the electron of interest contributes no shielding. Shielding effect is 0.*
3. *All other electrons in the same* (ns np) *group as the electron of interest shield to an extent of 0.35 nuclear charge units. The contribution of the neighboring 1s electron to the shield for the 1s electron is 0.30.*
4. *If the electron of interest is a* s *or* p *electron: All electrons with one less value of the principal quantum number shield to an extent of 0.85 units of nuclear charge. All electrons with two less values of the principal quantum number shield to an extent of 1.00 units.*
5. *If the electron of interest is an* d *or* f *electron: All electrons to the left shield to an extent of 1.00 units of nuclear charge. The contribution of electrons in this group is 0.35.*

In the Bohr energy equation for multi-electron systems, Z is taken instead of Z . Because there is shielding.*

$$E_T = -\frac{m \,.\, Z^{*2} \,.\, e^4}{8\varepsilon_o^2 \,.\, n^2 \,.\, h^2}$$

Calculate the first two ionization energies of Na using the Slater's rule.



$_{11}Na: (1s^2)(2s^2 2p^6)(3s^1) \quad Z^* = 11-[(8\times 0{,}85)+(2\times 1)] = 2{,}2$

$(E_T)_1 = -\dfrac{9{,}1.10^{-31}\times(2{,}2)^2(1{,}602.10^{-19})^4}{8.(8{,}85.10^{-12})^2.\,3^2.(6{,}63.10^{-34})^2} = -1{,}17.10^{-18}\,J$

$\dfrac{1}{3^2}-\dfrac{1}{\infty^2}$

$N.m = J$

$N = \dfrac{kg\,m}{s^2}$

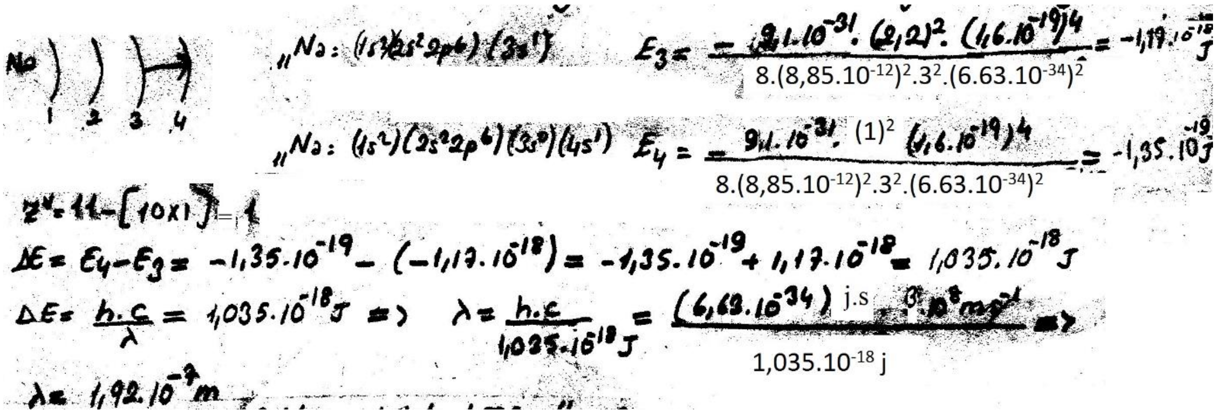
$E_T = \dfrac{kg.C^4}{\left(\frac{C^2}{N.m^2}\right)^2 J^2 s^2} = \dfrac{kg.\cancel{C^4}}{\frac{\cancel{C^4}}{N^2.m^4} J^2 s^2} = \dfrac{kg.N^2 m^4}{J^2 s^2} = \dfrac{kg\,\cancel{N^2}\,\overset{m^2}{\cancel{m^4}}}{(\cancel{N^2}\cancel{m^2})\,s^2} = \dfrac{kg\,m^2}{s^2} = N.m = J$

$_{11}Na^+: (1s^2)(2s^2 2p^6) \quad Z^* = 11-[(7\times 0{,}35)+(2\times 0{,}85)] = 6{,}85$

$(E_T)_2 = -\dfrac{9{,}1.10^{-31}\times(6{,}85)^2.(1{,}602.10^{-19})^4}{8.(8{,}85.10^{-12})^2.\,2^2.(6{,}63.10^{-34})^2} = -2{,}55.10^{-17}\,J$

Calculate the wavelength of the largest wavelength that the vaporized Na atom can absorb.

The largest wavelength ray means the ray with the smallest energy. The smallest energy means the electron passes only one upper orbital. When the electron passes the highest energy orbital, ionization occurs.



$_{11}Na: (1s^2)(2s^2 2p^6)(3s^1) \quad E_3 = -\dfrac{9{,}1.10^{-31}.(2{,}2)^2.(1{,}6.10^{-19})^4}{8.(8{,}85.10^{-12})^2.3^2.(6.63.10^{-34})^2} = -1{,}19.10^{-18}\,J$

$_{11}Na: (1s^2)(2s^2 2p^6)(3s^0)(4s^1) \quad E_4 = -\dfrac{9{,}1.10^{-31}.(1)^2\,(1{,}6.10^{-19})^4}{8.(8{,}85.10^{-12})^2.3^2.(6.63.10^{-34})^2} = -1{,}35.10^{-19}\,J$

$Z^* = 11-[10\times 1] = 1$

$\Delta E = E_4 - E_3 = -1{,}35.10^{-19} - (-1{,}17.10^{-18}) = -1{,}35.10^{-19} + 1{,}17.10^{-18} = 1{,}035.10^{-18}\,J$

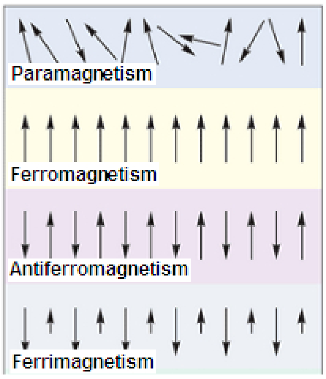
$\Delta E = \dfrac{h.c}{\lambda} = 1{,}035.10^{-18}\,J \Rightarrow \lambda = \dfrac{h.c}{1{,}035.10^{-18}\,J} = \dfrac{(6{,}63.10^{-34})\ j.s\ .\ 3.10^8\,m s^{-1}}{1{,}035.10^{-18}\,j} \Rightarrow$

$\lambda = 1{,}92.10^{-7}\,m$

Magnetic Properties

Substances may be classified by their response to externally applied magnetic fields as

1. ***Paramagnetic substances***
2. ***Diamagnetic substances***
3. ***Ferromagnetic substances***
4. ***Antiferromagnetic substances***
5. ***Ferrimagnetic substances***



Paramagnetic substances: Substances with an unpaired electron that are lightly pulled by large magnets. Whether a substance is paramagnetic or not can be understood examining radicals using esr (electron spin resonance) method. Many diseases such as cancer are because of radicals. If the food coming out of the microwave oven immediately is eaten, the radicals are eaten. The magnet is made from the paramagnetic materials at the nano extent and the molecular level.

Diamagnetic substances: Substances withouth an unpaired electron that are pushed by large magnets. Whether a substance is diamagnetic or not is determined by magnetical susceptibility measurements. Magnetical susceptibility measurements were done with Gouy scale or Evans method. The magnetic susceptibility of solids is determined by the Gouy method and the liquids by the Evans method. The measurement of magnetic susceptibility is made for paramagnetic substances. The result is how many unpaired electrons are found in a substance or coordination compound. If the magnetic susceptibility is less than zero, the substance is diamagnetic. Paramagnetic, superparamagnetic, and ferromagnetic substances have positive susceptibilities.

Ferromagnetic substances: Substances that are pulled thousands of times more than paramagnetic substances by magnetic field. This property is a solid state property. If a ferromagnetic substance is dissolved in acids, this property is lost. Ferromagnetic substances are rare in nature. They are natural magnets. Examples of antiferromagnetic substances: Ca_3O_4, Mn_3O_4. *In order to be a ferromagnetic substance, there must be ions containing unpaired electrons in the crystal lattice. These electrons must be aligned to strengthen each other.*

Antiferromagnetic substances: Substances that the magnetic moments are aligned in opposite directions and are equal in magnitude. In the presence of the strong magnetic field, antiferromagnetic substances are weakly magnetised in the direction the field. Examples of antiferromagnetic substances: MnO, FeO, CoO, NiO, Cr.

Ferrimagnetic substances: Substances that there are unequal number of parallel and antiparallel magnetic moments which leads to remain a net magnetization. Examples of ferrimagnetic substances: Typically ceramic materials with spinel structure $FeO.Fe_2O_3$, $NiO. Fe_2O_3$, $CuO. Fe_2O_3$. *The ferromagnetic, antiferromagnetic and ferrimagnetic substances change into paramagnetic at a particular temperature. This is due to alignment of spins in one direction.*