borrowed from
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Slater's Simple Rules

For an atom with nuclear charge $+Ze$, the total energy is

$$E = -13.606\,eV \sum_{\substack{i \\ \text{all electrons}}} \frac{(Z-S_i)^2}{n_i^2}$$

S_i = shielding constant for electron i in orbital n_i, ℓ_i

n_i = principle quantum number of electron i in orbital n_i, ℓ_i

S_i computed from Slater's rules attached

Example $Li\ (1s)^2(2s)^1$

slater's rules give $S_{1s} = 0.30$ and $S_{2s} = 2(0.85) = 1.70$

$$E_{Li} = -13.606\,eV\left[2\left(\frac{3-0.30}{1}\right)^2 + 1\left(\frac{3-1.70}{2}\right)^2\right] = -204.1\,eV$$

Exp value = $-203.5\,eV$ pretty good

Li^- $(1s)^2(2s)^2$

$S_{1s} = 0.30$ $S_{2s} = 2(0.85) + 1(0.35) = 2.05$

$$E_{Li^-} = -13.606\,eV\left[2\left(\frac{3-0.30}{1}\right)^2 + 2\left(\frac{3-2.05}{2}\right)^2\right]$$
$$= -204.5\,eV$$

Gives Electron Affinity of $Li = 0.4\,eV = -204.1 + 204.5\,eV$

Exp Value $= 0.62\,eV$ not bad

Li^+ $(1s)^2$ $S_{1s} = 0.30$ $E_{Li^+} = -13.606\,eV\left[2\left(\frac{3-0.30}{1}\right)^2\right]$

$= -198.4$

Ionization Potential $Li = -198.4\,eV + 204.1\,eV = 5.7\,eV$

$IP(Li) = 5.4\,eV$

SLATER-TYPE ORBITALS

Slater-type orbitals are of the form

$$R_{n\ell} = [(2\zeta)^{2n+1}/(2n)!]^{\frac{1}{2}} r^{n-1} \exp(-\zeta r)$$

where the orbital exponent ζ is $(Z-s_{n\ell})/n$ where the screening constant $s_{n\ell}$ may be obtained by several ways:

a) Use of Slater rules
b) Variational calculations such as that by Clementi and Raimondi give the best ζ's for ground state configuration.
c) Rules for dependence of the screening constants upon all of the electrons may also be obtained from calculations such as b). These are the Clementi and Raimondi rules, which could be considered as a refinement of the simple Slater rules.

Slater rules:

Slater's rules for finding approximate orbital exponents of *K*-, *L*-, and *M*-shell Slater AO's are as follows. The orbital exponent ζ is taken as $(Z - s_{nl})/n$, where n is the principal quantum number and Z is the atomic number. The screening constant s_{nl} is calculated as follows: The AO's are divided into the following groups:

$(1s)$ $(2s, 2p)$ $(3s, 3p)$ $(3d)$

To find s_{nl}, the following contributions are summed: (a) Zero from electrons in groups outside the one being considered. (b) 0.35 from each other electron in the group considered, except that 0.30 is used in the 1*s* group. (c) For an *s* or *p* orbital, 0.85 from each electron with n one less than the orbital considered and 1.00 from each electron still further in. For a *d* orbital, 1.00 for each electron inside the group.

Clementi and Raimondi rules;

$$\begin{aligned}
s_{1s} &= 0.3[N(1s) - 1] + 0.0072[N(2s) + N(2p)] \\
&\quad + 0.0158[N(3s) + N(3p) + N(4s) + N(3d) + N(4p)] \\
s_{2s} &= 1.7208 + 0.3601[N(2s) + N(2p) - 1] \\
&\quad + 0.2062[N(3s) + N(3p) + N(4s) + N(3d) + N(4p)] \\
s_{2p} &= 2.5787 + 0.3326[N(2p) - 1] - 0.0773N(3s) \\
&\quad - 0.0161[N(3p) + N(4s)] - 0.0048N(3d) + 0.0085N(4p) \\
s_{3s} &= 8.4927 + 0.2501[N(3s) + N(3p) - 1] + 0.0778N(4s) \\
&\quad + 0.3382N(3d) + 0.1978N(4p). \\
s_{3p} &= 9.3345 + 0.3803[N(3p) - 1] + 0.0526N(4s) \\
&\quad + 0.3289N(3d) + 0.1558N(4p) \\
s_{4s} &= 15.505 + 0.0971[N(4s) - 1] + 0.8433N(3d) \\
&\quad + 0.0687N(4p) \\
s_{3d} &= 13.5891 + 0.2692[N(3d) - 1] + 0.1063N(4p) \\
s_{4p} &= 24.7782 + 0.2905[N(4p) - 1]
\end{aligned}$$

Equation (1)

where $N(n'l')$ is the number of electrons occupying the $(n'l')$ subshell