# Software Spec – ElectronicConfiguration Class

Public Class ElectronicConfiguration

Encapsulates an electronic configuration (1s2 2s2 2p6 etc) and exposes methods to retrieve the occupancy of each orbital.

Implementation – store as a collection or list, keyed by the primary quantum number N concatenated with L quantum number, delimited. Ex: 2p6 🡪 key = “2p”, value = 6.0. OR have an enumeration of orbitals, ex: 1s = 0, 2s = 1, 2p = 2, 3s = 3, etc., and store occupation as corresponding array value. The former method may be superior from a parsing perspective. Can enumerate L value as s = 0, p = 1, d = 2, etc.

Should be able to parse input as full list of orbitals, and also referenced to noble gas configuration, ex: “[Kr] 4d10 5p2”

Should also handle input format string omitting occupation if = 1, ex: “1s” = “1s1”

Sub New(configuration as String)

* Parses the input string
* Throws an InvalidOperationException if the input string is not properly formatted.

Function Occupancy(n as Integer, l as Integer) as Double

* Returns the number of electrons in the orbital defined by quantum number n and angular momentum l.

Overloads Function Occupancy() as Double

* Returns the total number of electrons in the configuration. Can be fractional.
* Empty configuration has ElectronCount = 0.

Function ToString() as String

* Returns the configuration formatted as a space-delimited string. Ex: “1s2 2s2 2p5”
* Empty configuration returns an empty string.