For example, the following Geometry, Lattice and Crystal Spec sections define a body centered lattice of H atoms where the length of the c lattice vector is the first Walsh Variable.

```
Geometry Crystallographic
5
1 H 0 0 0
2 H 0.5 0.5 0.5
3 H 1 0 0
4 H 0 1 0
5 H 0 0 1

Lattice
3
5 5 5
1 3
1 4
1 5

Crystal Spec
; a   b   c
  1   1   1000
; alpha   beta   gamma
   90       90       90
```

5.1.4 Electrons (potentially required)

The line following this keyword should have the number of valence electrons in the molecule (or unit cell for an extended system).

5.1.5 Charge (potentially required)

The line following this keyword should have the charge on the molecule (or unit cell for an extended system).

Either the Charge or Electrons keywords must appear in the input file.

5.1.6 Alternate Occups

This keyword is for looking at the effects of changing the number of electrons in the unit cell upon the position of the Fermi level, the average energy, and orbital occupations. This is a far more efficient way of probing these changes than rerunning the calculation with alternate electron numbers.

On the line following the keyword, the number of alternate occupations (num_occups) should be given. The next line contains the step that is to be taken between occupations.

For example, the following input fragment would result in the program doing a calculation with 5 electrons, then printing out the Fermi level, average energy, net charges, and orbital occupations for 4.8,4.6,4.4,4.2, and 4.0 electrons per unit cell.

```
Electrons
```

```
5

Alternate Occup
; num_occups
5
; the step
-.2
```

5.1.7 Parameters (optional)

NOTE: If this keyword appears in the file it *must* follow the Geometry keyword in the input file.

There should be a line following this keyword for each type of custom atom which is being defined. Recall that a custom atom is defined by replacing the first occurance of that atom's label in the Geometry specification with an asterix: *. If there are multiple custom atom types, then define them in this section in the order in which they occurred in the Geometry section.

The format of a parameter specification is:

Symbol Atomic_Number Num_Valence_Electrons n_s ζ_s IP_s n_p ζ_p IP_p n_d $\zeta 1_d$ IP_d *c1* $\zeta 2_d$ *c2*

In this specification, the ζ values are the radial exponents of the Slater type orbitals and the H_{ii} values are the valence state ionization potentials (diagonal elements of the hamiltonian) for each AO. Here's an example of a section of input file where 3 different custom atoms are defined:

```
Geometry
8
1 *      .000000000      .000000000      .000000000
2 O    1.952000000    1.952000000      .000000000
3 *    1.952000000      .000000000    -.3
4 O    1.952000000      .000000000    1.4862
5 *    0.000000000    1.952000022    1.9422
6 O    3.904000044      .000000000      .000000000
7 O      .000000000    3.904000044      .000000000
8 O      .000000000    0.0            4.152

Parameters
O   8 6 2 2.275 -32.3 2 2.275 -14.8
Ti 22 4 4 1.075 -8.970 4 1.075 -5.400 3 4.55 -10.81 .4206 1.400 .7839
Pb 82 4 6 2.50  -16.70 6 2.06 -8.000
```

In this example, atom 1 is an O, atom 3 is a Ti, and atom 5 is a Pb. Atoms 2,4,6,7, and 8 will use the same parameters as atom 1. **Clarification:** The parameters specified here for O are the default parameters. I only put them in this example to demonstrate a point.

5.1.8 Molecular (mandatory for molecular calculations)

Indicates that a molecular calculation (not an extended one) is being performed. Otherwise it is assumed that the calculation is on an extended system.