Hartree-Fock limit, where the basis set is essentially complete, and use the term self-consistent-field (SCF) solution for one obtained with a finite, possibly small, basis set. We use the terms Hartree-Fock and SCF interchangeably, however, and specifically refer to the Hartree-Fock limit when necessary. The SCF procedure is as follows:

1. Specify a molecule (a set of nuclear coordinates $\{\mathbf{R}_A\}$, atomic numbers $\{Z_A\}$, and number of electrons N) and a basis set $\{\phi_\mu\}$.
2. Calculate all required molecular integrals, $S_{\mu\nu}$, $H_{\mu\nu}^{core}$, and $(\mu\nu|\lambda\sigma)$.
3. Diagonalize the overlap matrix $\mathbf{S}$ and obtain a transformation matrix $\mathbf{X}$ from either (3.167) or (3.169).
4. Obtain a guess at the density matrix $\mathbf{P}$.
5. Calculate the matrix $\mathbf{G}$ of equation (3.154) from the density matrix $\mathbf{P}$ and the two-electron integrals $(\mu\nu|\lambda\sigma)$.
6. Add $\mathbf{G}$ to the core-Hamiltonian to obtain the Fock matrix $\mathbf{F} = \mathbf{H}^{core} + \mathbf{G}$.
7. Calculate the transformed Fock matrix $\mathbf{F}' = \mathbf{X}^\dagger \mathbf{FX}$.
8. Diagonalize $\mathbf{F}'$ to obtain $\mathbf{C}'$ and $\boldsymbol{\epsilon}$.
9. Calculate $\mathbf{C} = \mathbf{XC}'$.
10. Form a new density matrix $\mathbf{P}$ from $\mathbf{C}$ using Eq. (3.145).
11. Determine whether the procedure has converged, i.e., determine whether the new density matrix of step (10) is the same as the previous density matrix within a specified criterion. If the procedure has not converged, return to step (5) with the new density matrix.
12. If the procedure has converged, then use the resultant solution, represented by $\mathbf{C}, \mathbf{P}, \mathbf{F}$, etc., to calculate expectation values and other quantities of interest.

We will describe the calculation of expectation values like the energy, dipole moment, etc., and other quantities of interest like population analyses shortly (Subsection 3.4.7) but let us first consider some of the practical questions involved in each of the twelve steps.

Within the Born-Oppenheimer approximation, what we have done in the above procedure is to determine an electronic wave function $|\Psi_0\rangle$ (and hence an electronic energy E_0) for a collection of N electrons in the field of a set of M point charges (the M nuclei with charges Z_A). By adding the classical nuclear-nuclear repulsion to the electronic energy we will have a total energy as a function of a set of nuclear coordinates $\{\mathbf{R}_A\}$. By repeating the calculation for different nuclear coordinates we can then explore the potential energy surface for nuclear motion. A common calculation is to find the set $\{\mathbf{R}_A\}$ which minimize this total energy; this is a calculation of the equilibrium geometry of a molecule. The procedure is valid for any collection of point charges. In particular, "supermolecule" calculations, which use a set of nuclear charges representative of more than one molecule, are common for exploring, for example, intermolecular forces.