The Restricted Hartree Fock (RHF) Algorithm is a way of approaching the lowest energy of an electronic system. The restriction comes from the property that only even numbers of electrons (Nelec) can be treated. The RHF equations solve the eigenvalue problem of

$$FC = C\epsilon \, . \tag{1}$$

In (1) F is the Fock matrix, C is the matrix of eigenvectors and ϵ is the diagonal matrix of eigenvalues. The Fock matrix is given by

$$F_{\mu\nu} = H_{\mu\nu} + P_{\lambda\sigma} * [2(\mu\nu|\sigma\lambda) - (\mu\lambda|\sigma\nu)] \, . \tag{2}$$

H is the one-electron matrix, P the density matrix and $(\mu\nu|\sigma\lambda)$ is the two-electron matrix given in chemists notation. In (2) and below we use the Einstein convention that is summing over every index which occurs more then once. The one-electron-matrix and the two-electron-matrix are constant inputs for the RHF algorithm. Therefore we can treat them as given. The density matrix is given by

$$P_{\mu\nu} = \sum_{a}^{Nocc} C_{\mu a} C^{*}_{\nu a} \, . \tag{3}$$

$Nocc$ stands for the number of occupations and is given as $\frac{Nelec}{2}$. We obtain C from decomposing F into its eigendecomposition.

$$C = \text{matrix of eigenvectors}(F) \tag{4}$$

The eigenvectors are sorted in ascending order based on the values of the eigenvalues. The density is built from the $Nocc$ eigenvectors corresponding to the lowest eigenvalues. The resulting electronic energy (E) is given by

$$E = P_{\nu\mu}(H_{\mu\nu} + F_{\mu\nu}) \, . \tag{5}$$

To obtain the total energy, the nuclear energy is added to the electronic energy. The RHF-algorithm is solved by iteratively computing (3), (2) and (4) while checking for convergence with (5).