Hartree-Fock Wavefunctions

There are three types of Hartree-Fock Wavefunctions:

Restricted Hartree-Fock (RHF or HF)

Used for closed shell atoms or molecules such as He, H_2O, NH_3, CH_3COOH, etc. Most molecules fall in this group. They have an even number of electrons, a singlet spin state, and zero orbital angular momentum. Each spatial Hartree-Fock orbital is occupied by two electrons, an α and a β.

Restricted open shell Hartree-Fock (ROHF)

Used for open shell atoms and molecules such as O, H_2O^+, OH, O_2, etc.
These systems may have an even or odd number of electrons and are characterized by a non-zero spin or orbital angular momentum. Spatial orbitals may be singly or doubly occupied.

Unrestrcited Hartree-Fock (UHF)

These are used for the same class of molecules as the ROHF. The difference is that the spatial orbitals for the α and β electrons are different. There are no doubly occupied spatial orbitals.