

RHF, ROHF, UHF Methods

The table below summarizes some properties of RHF, ROHF and UHF methods.

Method	RHF	ROHF	UHF
Initials of	Restricted Hartree-Fock	Restricted Open shell Hartree-Fock	Unrestricted Hartree-Fock
For system with multiplicity	1	All multiplicities	All multiplicities
Do α and β electronic orbitals have the same spatial part?	Yes	Yes	For multiplicity 1, yes. For other multiplicities, no
Relative energy for multiplicity 1	Identical energy	Identical energy	Identical energy
Relative energy for multiplicity different than 1	Not relevant	Higher than E(UHF)	Lower than E(ROHF)
Advantages for multiplicity different than 1	Not relevant	<ul style="list-style-type: none">Orbital analysis is simpler than UHF.The total calculated spin of the system is accurate.	The calculated energy is lower than E(ROHF)
Disadvantages for multiplicity different than 1	Not relevant	The calculated energy is higher than E(UHF)	The total calculated spin of the system is not accurate