

Hartree-Fock Wavefunctions

<u>Wavefunction</u>	<u>Applicability</u>	<u>Characteristics</u>
RHF	Closed shell molecules around equilibrium	Cannot break bond
ROHF	Open shell molecules around equilibrium	Cannot break bond Eigenfunction of S^2 & S_z
UHF	Open & closed shell molecules At equilibrium and often far from it	Not an eigenfunction of S^2 , but is an eigenfunction of S_z