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instability of Hartree–Fock solution

Existence of additional solutions to the equations of the Hartree–Fock method occurring usually in the case when potential energy surfaces of different electronic states are drawn close together. Within the spin-restricted Hartree–Fock method (RHF), singlet and triplet instabilities are distinguished. The former involves the existence of another solution with lower energy and the electron distribution of lower symmetry. It may be regarded as an indication that the initially assumed molecular shape needs correction. The triplet instability involves rejection of the condition of double occupancy of molecular orbitals and thus transition to the spin-unrestricted Hartree–Fock method (UHF). The triplet instability is a necessary, but insufficient, condition for the conclusion as to the biradical character of the ground state of a given system.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1946

