

## spin contamination

In unrestricted Hartree–Fock method, the wavefunctions obtained are eigenfunctions of the Hamiltonian and the spin projection  $S_z$  operators, but not eigenfunctions of the  $S^2$  operator. As a result, the wavefunctions of the doublet systems are spin-contaminated to some extent by admixtures of quartet, sextet, and higher spin states. The eigenvalues of the  $S^2$  operator are given as a measure of the spin contamination.

**Source:**

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1962