

complete active space self-consistent field (CASSCF)

Computational scheme employed in multiconfigurational SCF theory especially suitable for studies of reactivity of excited states. The wavefunction is defined by selecting the set of active orbitals involved in the excitation or chemical reaction under investigation and is constructed as a linear expansion in the set of configuration functions that can be generated by occupying the active orbitals in all ways consistent with an overall spin and space symmetry (full configuration interaction, CI).

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 315