

complete active space self-consistent field second-order perturbation theory (CASPT2)

Theoretical scheme suitable for computations of accurate excitation energies and reaction barriers. In the first step, electron correlation is taken into account only to a certain extent by using a *CASSCF* formalism (the so called non-dynamic correlation), whereas the remaining electron correlation (the so called dynamic correlation) is included through the use of second-order perturbation theory.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 316