singlet-triplet crossing

Point of intersection between the potential energy surfaces of states of different multiplicity.

Note:

The intersection belongs to a (3N-7)-dimensional subspace of the (3N-6)-dimensional nuclear coordinate space and therefore appears as a line on a two-dimensional energy surface (N is the number of nuclei). In this case the branching plane is one-dimensional and is defined by the gradient difference vector x_1 .

Source:

PAC, 2007, 79, 293 (Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)) on page 421