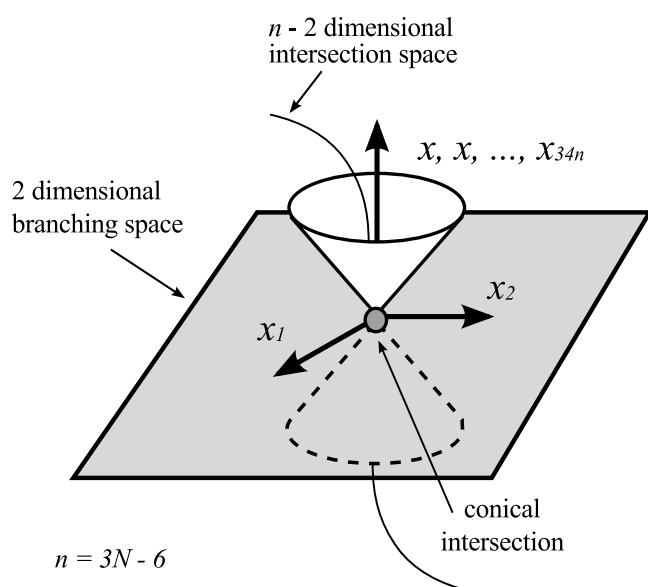


conical intersection

Point of crossing between two electronic states of the same spin multiplicity (most commonly singlets or triplets).

Notes:

1. In a polyatomic molecule two potential energy surfaces are allowed to cross along a $(3N - 8)$ -dimensional subspace of the $(3N - 6)$ -dimensional nuclear coordinate space (the intersection space) even if they have the same spatial/spin symmetry (N is the number of nuclei). Each point of the intersection space corresponds to a conical intersection. If the energy is plotted against two special internal geometrical coordinates, x_1 and x_2 , which define the so-called branching plane, the potential energy surface would have the form of a double cone in the region surrounding the degeneracy. In the remaining $(3N - 8)$ directions, the energies of the ground and excited state remain degenerate; movement in the branching plane lifts the degeneracy.
2. From a mechanistic point of view, conical intersections often provide the channel mediating radiationless deactivation and photochemical reaction.



Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 317