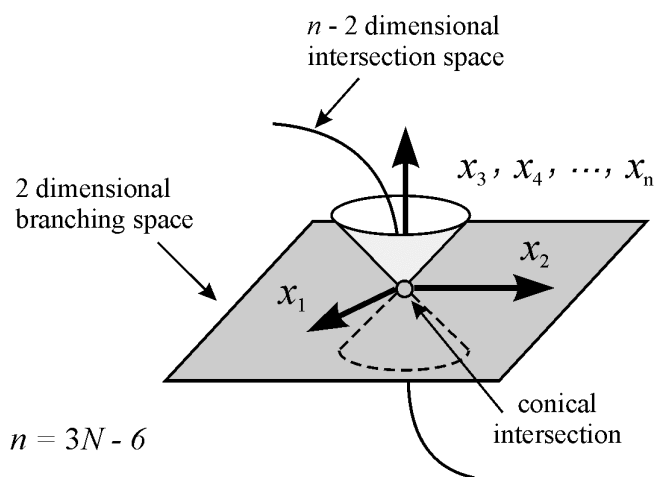


conical intersection

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

Note 1: In a polyatomic molecule two *potential energy surfaces* are allowed to cross along a $(3\tilde{N} - 8)$ -dimensional subspace of the $(3\tilde{N} - 6)$ -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 $(3\tilde{N} - 8)$ directions, the energies of the *ground* and *excited state* remain degenerate; movement in the branching plane lifts the degeneracy.

Note 2: From a mechanistic point of view, conical intersections often provide the channel mediating *radiationless deactivation* and *photochemical reaction*.



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