

branching plane

At a conical intersection point, the plane spanned by the gradient difference vector (\mathbf{x}_1) and the gradient of the interstate coupling vector (\mathbf{x}_2):

$$\mathbf{x}_1 = \frac{\partial(E_2 - E_1)}{\partial Q} \mathbf{q}$$

$$\mathbf{x}_2 = \langle \mathbf{C}_1^t \left(\frac{\partial H}{\partial Q} \right) \mathbf{C}_2 \rangle \mathbf{q}$$

where \mathbf{C}_1 and \mathbf{C}_2 are the configuration interaction eigenvectors (i.e., the excited and ground-state adiabatic wavefunctions) in a conical intersection problem, H is the conical intersection Hamiltonian, \mathbf{Q} represents the nuclear configuration vector of the system, and thus \mathbf{q} is a unit vector in the direction of vector \mathbf{q} . E_1 and E_2 are the energies of the lower and upper states, respectively.

Note:

The branching plane is also referred to as the ***g-h*** plane. Inspection of \mathbf{x}_1 and \mathbf{x}_2 provides information on the geometrical deformation imposed on an excited state molecular entity immediately after decay at a conical intersection. Consequently, these vectors provide information on the ground-state species that will be formed after the decay.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 309