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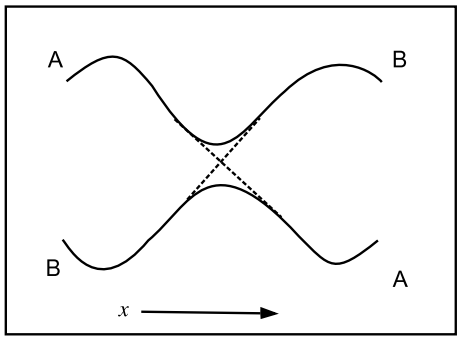
avoided crossing

of potential-energy surfaces

Frequently, two Born–Oppenheimer electronic states (A, B) change their energy order as molecular geometry (x) is changed continuously along a path. In the process their energies may become equal at some points (the surfaces are said to cross, dotted lines in the figure), or only come relatively close (the crossing of the surfaces is said to be avoided). If the electronic states are of the same symmetry, the surface crossing is always avoided in diatomics and usually avoided in polyatomics.



Synonymous with intended crossing.

Source:

PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

