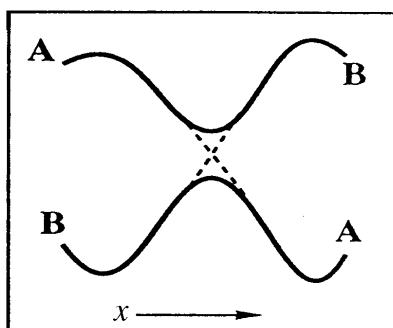


avoided crossing (of potential-energy surfaces)

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*.
1996, 68, 2229