

Jahn–Teller effect

Molecular distortions due to an electronically degenerate ground state. For non-linear molecular entities in a geometry described by a point symmetry group possessing degenerate irreducible representations there always exists at least one non-totally symmetric vibration that makes electronically degenerate states unstable at this geometry. The nuclei are displaced to new equilibrium positions of lower symmetry causing a splitting of the originally degenerate states (first-order Jahn–Teller effect).

Note:

Effect due to the odd terms in the vibronic perturbation expansion. In the case of molecules with a non-degenerate ground electronic state but with a low-lying degenerate excited state, distortions of proper symmetry arise that result in mixing of the ground and excited states, thereby lowering the ground-state energy (pseudo Jahn–Teller effect). The pseudo Jahn–Teller effect manifests itself in fluxional behaviour (see fluxional molecules) and stereochemical non-rigidity of molecules and ions. The Jahn–Teller effect generates a surface crossing (e.g., a conical intersection) whereas a pseudo Jahn–Teller effect generates an avoided crossing.

See also: Renner–Teller effect

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 360