

### **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*. N.B. This supersedes an earlier definition.

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