Jahn-Teller effect and group theory

Martin Breza

Department of Physical Chemistry, Slovak Technical University, SK-81237 Bratislava, Slovakia.

A group-theoretical treatment is used to solve the problem of searching the stable structures obtained by the symmetry descent of high-symmetric non-linear parent systems in a degenerate electronic state due to Jahn-Teller effect. The methods of epikernel principle of Ceulemans (based on Jahn-Teller active coordinates obtained by the first-order perturbation theory) and step-by-step descent in symmetry of Breza (based on consecutive splitting the degenerate electronic states due to a symmetry descent) are explained. Both methods are illustrated by several examples and their results are compared with the structures obtained by high-level quantum-chemical calculations.

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