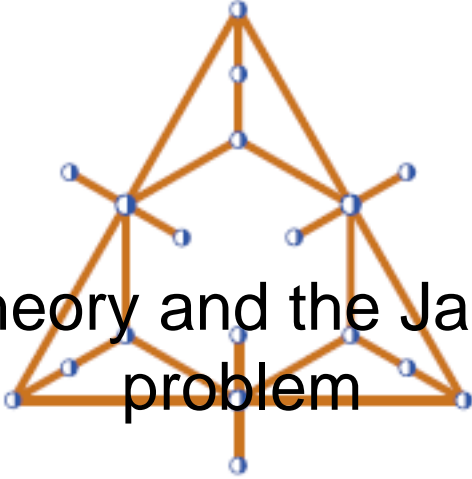


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Graph theory and the Jahn-Teller problem

Content :

In 1937 Jahn and Teller stated their remarkable theorem that all non-linear nuclear configurations are unstable for an orbitally degenerate electronic state. The instability will trigger a distortion to a lower symmetry that removes the cause of the degeneracy. In other words symmetry and degeneracy do not seem to go together and nature will always find ways to avoid such situations.

In the current contribution we will reformulate the Jahn-Teller theorem in graph-theoretical terms and show that an analogous connection exists between the degeneracy of eigenvalues in the graph spectrum and distortion patterns of the edges. This analogy has interesting consequences for both the molecular Jahn-Teller theorem and for spectral graph theory.

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