

## Quantum-chemical approach to the choice of heterogenous catalyst for the synthesis of *N*-methylaniline

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**Keywords:** *structure-property-catalytic activity, vibration frequency, amplitude of vibration, resonance, catalyst composition.*

### Abstract

The fact of correlation of boundary shot-wave radiation frequency has been established in vibration spectra used in production of heterogeneous catalysts with vibration spectra of the transformable groups and bonds in reagents and products of chemical transformations. The hypothesis has been suggested for explaining the effect of heterogeneous catalysts in controlled chemical synthesis. Examples of selecting the composition of catalysts for the synthesis of *N*-methylaniline basing on the mechanism of chemical transformations and the results of quantum-chemical calculations have been given.