

## Formation enthalpies and energies of dissociation bonds C-NO<sub>2</sub> in the series of nitrobenzene derivatives

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### Abstract

With the use of different bases of hybrid method of density potential B3LYP there have been calculated formation enthalpies and dissociation energies of the bond C-NO<sub>2</sub> (D(C-N)) of nitrobenzene, isomeric dinitrobenzenes, nitrotoluenes, nitroanilines and nitrophenols. Basic characteristics of the influence of molecular structure on the change of formation enthalpy have been analyzed. For *o*-nitrophenol and *o*-nitroaniline there has been noted the influence of intramolecular hydrogen bond. The computed values of D(C-N) have been used for discussing the influence of the molecular structure on the changes of activation energy of the radical gas-phase dissociation in the series of the listed substances.