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Molecular structure of nitrobenzene and a series of its monofunctional derivatives in gaseous state

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Abstract

With the use of hybrid method of density functional B3LYP with different bases geometrical parameters of nitrobenzene, isomeric dinitrobenzenes, nitrotoluenes, nitroanilines, nitrophenols have been defined. Influence of chemical structure on the change of geometric parameters of the reaction center of molecules (C-NO_2) in the series of the studied substances has been investigated. It has been established that donor substituents: CH_3, NH_2, OH cause diminution of bond length C-NO_2 in *para*-isomers, as well as in *orto*-nitroaniline and *orto*-nitrophenol. The given results could be explained with the action of the direct polar coupling of donor substituents with the acceptor by NO_2-group. In *orto*-nitrophenol and *orto*-nitroaniline an important additional factor is the formation of intramolecular hydrogen bonds. In dinitrobenzenes the value r(C-NO_2) slightly increases. On the basis of the above mentioned factors one can explain the change of other geometric parameters of the reaction center.