Molecular structure and electric properties of *N*-methyl-*N*-nitroaniline and its derivatives.

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Streszczenie

A comparative study of the molecular structure of*N*-methyl-*N*-nitroaniline and its derivatives is carried out employing the Kerr effect and dipole moments methods in combination with the crystallographic analysis. The obtained experimental structural data agree with the quantum-chemical calculations by the B3LYP/6-31G* and MP2/3-21G* methods. The measurement and calculation results are used to draw conclusions about the mutual interaction and role of various substituents to the *N*-methyl-*N*-nitroaniline molecule.

Słowa kluczowe

Molecular structure, Dipole moment, Kerr constant, N-methyl-N-nitroaniline and its derivatives, N, N-dimethylnitramine

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