Molecular and crystal structures of *N*-methyl-*N*-nitro- 2-chloroaniline.

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Streszczenie

The crystal structure of *N*-methyl-*N*-nitro-2-chloroaniline is determined by X-ray diffraction [a = 9.218(2) Å, b = 12.593(3) Å , c = 14.510(2) Å, space group *Pbca*, and Z = 8]. The structure is solved by the direct method and refined in the anisotropic approximation to R = 0.0377. All hydrogen atoms are localized. The structural parameters obtained agree with the data of the *ab initio* quantum-chemical B3LYP/6-31G** calculations. The data obtained are compared with those for *N*-methyl-*N*-nitro-4-chloroaniline. Conclusions on the interaction of the functional groups in the molecule are drawn.

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