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Quantum-chemical study of force fields of 4-nitro-5-metilbenzofuroksan and 4-nitro-7-metilbenzofuroksan

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Abstract

In the framework of density functional theory there have been examined the electronic structure of 4-nitro-5-methyl-benzofuroksan and 4-nitro-7-metilbenzofuroksan, computed the matrix of force constants in Cartesian coordinates and X_δ^0. The features of the force fields of the molecules examined have been revealed.