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Study of the structure of 1-nitro-3,3,3-trifluoro- and 1-nitro-3,3,3-tribromopropenes by the methods of dipole moments and quantum chemistry

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Abstract

© 2014 Pleiades Publishing, Ltd. Method of dipole moments and quantum-chemical calculations allowed establishing that 1-nitro-3,3,3-trifluoro- and 1-nitro-3,3,3-tribromopropenes have the E-configuration (the nitro group and the trihalomethyl substituent are in the trans-position); the obtained characteristics were compared with the corresponding data for the trichloromethyl-containing analog.

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