

Conformational analysis of 2-substituted 1-nitro-and 1-bromo-1-nitroethenes

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Abstract

Conformational analysis of 2-trichloromethyl(ethoxycarbonyl)-1-nitro-and 2-trichloromethyl-(ethoxycarbonyl)-1-bromo-1-nitroethenes was performed using the dipole moment method, IR spectroscopy, and DFT quantum-chemical calculations (B3LYP/6-31G*). The nitro and ester (or trichloromethyl) groups in the molecules of these compounds were found to occupy trans positions with respect to the double C=C bond, i.e., the nitroalkenes have E, and their bromine-containing analogs, Z configuration; the compounds having an ethoxycarbonyl group are characterized by s-cis orientation of the C=C and C=O bonds. © Nauka/Interperiodica 2007.

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