Russian Journal of General Chemistry 2007 vol.77 N5, pages 894-898

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

Ishmaeva E., Gazizova A., Vereshchagina Y., Chachkov D., Anisimova N., Makarenko S., Smirnov A., Berestovitskaya V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Conformational analysis of 2-trichloromethyl(ethoxycarbonyl)-1-nitro-and 2-trichloromethy--(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.

http://dx.doi.org/10.1134/S1070363207050131