

**POLARITY AND STRUCTURE OF
POLYFUNCTIONAL NITROETHENES**

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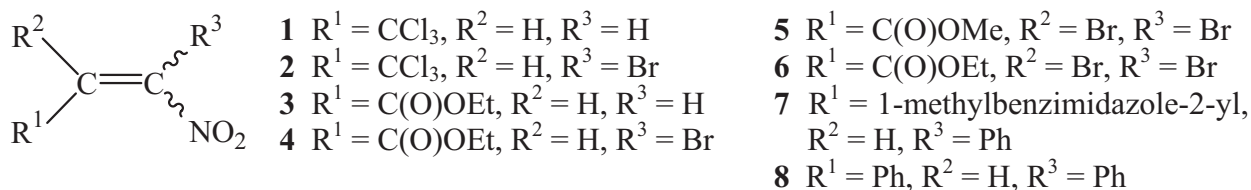
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Polyfunctional nitroethenes are convenient compounds for a study of general theoretical problems of organic chemistry as well as for synthesis of biologically active substances.

We have determined polarities of nitroethenes **1-8** in benzene solution, and have studied spatial structures of **1-8** by the methods of dipole moments, NMR and IR spectroscopy, X-ray analysis and quantum chemical calculations (DFT B3LYP/6-31G*).



It was established that the nitro and ester (or trichloromethyl) groups are *trans*-arranged in the molecules of **1-4**, i.e. nitroalkenes have *E*-configuration, their bromo-containing analogues have *Z*-configuration, and *s-cis*-orientation of the C=C and C=O double bonds is preferred for nitroacrylates **3**, **4**. The polarities of **1**, **2** in CH₂Cl₂ and C₆H₆ solutions were calculated using B3LYP/6-31G* method within the limits of SCIPCM model. Detailed interpretation of the experimental Fourier-transform IR spectra of **1-4** was carried out on the basis of the computation of their vibration spectra. Alkyl 2,3-dibromo-3-nitroacrylates **5**, **6** have untrivial *Z*-configuration in solution. It was found that 2-(1-methylbenzimidazole-2-yl)-1-nitro-1-phenylethene **7** has *Z*-configuration in crystal, and the energetically advantageous *E*-isomer of **7** (theoretical data) exists in solution; 1,2-diphenyl-1-nitroethene **8** has *E*-form. For all compounds, the computational results are in a good agreement with the experimental data obtained.

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