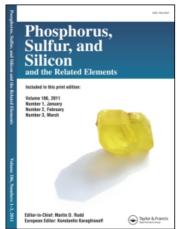
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Conformational Analysis of Halogenonitroethenes and Halogenonitroethenephosphonates in Solution

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CONFORMATIONAL ANALYSIS OF HALOGENONITROETHENES AND HALOGENONITROETHENEPHOSPHONATES IN SOLUTION

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Spatial structure of 2-cyclohexylamino(1)- and 2-piperidino(2)-1-bromo-1-nitro-2-phenylethenes was studied by PMR, IR spectroscopy, and method of dipole moments (DM). Both molecules had E-configuration (Ph and NO₂ are trans-arranged). High polarity of compounds 1, 2 (about 7 D) and IR spectral data indicate significant contribution of bipolar forms into these structures. Structure of β -nitrosubstituted vinylphosphonates 3–5 was studied by NMR 1 H, 31 P, UV, and IR spectroscopy, and DM. We determined that these compounds existed in

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a state of totality of s-trans-conformations. Forms with gauche-trans-orientation of C—Cl and C—O bonds prevailed in conformational transitions determined by internal rotation around $P\text{-}Csp^2$ and $Csp^3\text{-}Csp^3$ bonds.