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3-Aryl(hetaryl)-3-hydroxy-2-phosphorus-substituted acrylonitriles. Synthesis and experimental and theoretical conformational analysis

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Abstract

Under conditions of the phase transfer catalysis, acylation of (thio)phosphorylacetonitriles by (het)aroyl chlorides affords the Z-enol forms of C-acylation products in high yields. Their configurations were studied by IR spectroscopy, dipole moment measurements, and ab initio quantum-chemical calculations [B3LYP/6-31G(d)]. The C=C double bond and the phosphoryl or thiophosphoryl group have an s-cis arrangement. The possibility of strong intramolecular hydrogen bonding in these conformers is the governing factor responsible for the three-dimensional structures of the compounds under investigation. Derivatives of nicotinic acid existing in the individual form as zwitterions are the only exceptions.

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Keywords

(thio)phosphorylacetonitriles, 3-alkyl-2-(thio)phosphoryl-substituted acrylonitriles, 3-aryl(hetaryl)-3-hydroxy-2-phosphorus-substituted acrylonitriles, Dipole moments, Enols, IR spectroscopy, Phase transfer catalysis, Z and E isomers