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Dipole moments and structure of ortho-diphenyl(diethyl)phosphinoyl- substituted benzyl alcohols, phenols, and their derivatives

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Abstract

The method of dipole moments and DFT B3LYP/6-31G*quantum-chemical calculations were used to study the structures of ortho-substituted aryl-and arylmethyldiphenyl(diethyl)phosphine oxides. It was established that methyl ethers of phosphorus-containing benzyl alcohols and phenols exist as equilibrium mixtures of several conformers with prevalence of forms with the weakest steric interactions. Preferred conformers of o-[(diethylphosphinoyl)methyl]benzyl alcohol and i-[(diphenylphosphinoyl)methyl]phenol contain an intramolecular hydrogen bond between the hydroxyl hydrogen atom and phosphinoyl oxygen atom. © 2008 MAIK Nauka.

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