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 *o*-[(diphenylphosphinoyl)methyl]phenol contain an intramolecular hydrogen bond between the hydroxyl hydrogen atom and phosphinoyl oxygen atom.

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