

Conformational analysis of 2-aminophenyl-, 2-aminobenzyl-, and 2-nitrobenzyl(diphenyl)phosphine oxides

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Abstract

The polarity and conformations of 2-aminophenyl-, 2-aminobenzyl-, and 2-nitrobenzyl(diphenyl)-phosphine oxides were studied by the dipole moment method, IR spectroscopy, and quantum chemical calculations. 2-Aminophenyl- and 2-aminobenzyl(diphenyl)phosphine oxides were found to exist preferentially as conformers with intramolecular hydrogen bond. 2-Nitrobenzyl(diphenyl)phosphine oxide is likely to be represented by equilibrium mixture of three conformers in which the phosphoryl and nitro groups are oriented syn or anti with respect to the PCsp³ Csp² fragment. © 2014 Pleiades Publishing, Ltd.

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