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

Vereshchagina Y., Alimova A., Chachkov D., Ishmaeva E., Artyushin O., Sharova E., Klimovitskii A., Khanafieva R.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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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