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LETTERS TO THE EDITOR

Synthesis of 3-Phenoxyphenylmethoxypropionitrile

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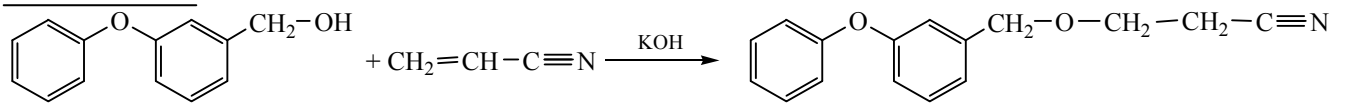
Nitriles of the series of diphenyl oxide functional derivatives, whose molecules contain in the side chain different functionalities along with nitrile group, are of great interest. These compounds exhibit the biological activity of various types and also they can be used as starting materials for the synthesis of some derivatives possessing medical-biological properties.

New effective synthetic approach to 3-phenoxyphenylmethoxypropionitrile, starting from 3-phenoxybenzyl alcohol and acrylonitrile, was developed. This compound is a 3-phenoxyphenyl-containing product new by structure and can be of interest as semiproduct in the synthesis of biologically active compounds.

There is a special interest in the synthesis of molecules, which besides diphenyloxide fragment and nitrile group contain in the side chain functional groups, since combination of different pharmacophores in the structure must lead to expansion of biological activity range of the target compounds [1–4].

The 3-phenoxyphenylmethoxypropionitrile was obtained by the reaction of 3-phenoxybenzyl alcohol with acrylonitrile in anhydrous benzene in the presence of 40% solution of potassium hydroxide along the following scheme:



The synthesis was performed at reagents molar ratio 3-phenoxybenzyl alcohol:acrylonitrile 1:1.2–1.5 at the boiling point of benzene, 80–82°C.

The obtained nitrile was isolated by the vacuum distillation [bp 182–185°C (3 mm Hg)] as colorless liquid in 85% yield.

The structure and the composition of nitrile obtained was confirmed with IR and ^{1}H NMR spectroscopy.

3-Phenoxyphenylmethoxypropionitrile. A mixture of 10 g (0.05 mol) of 3-phenoxybenzyl alcohol, 4.2 g (0.075 mol) of acrylonitrile, 20 ml of anhydrous benzene, and 1.5 ml of 40% potassium hydroxide solution was stirred for 5 h at 80–82°C. Then the reaction mixture was filtered; the benzene layer was separated, washed with distilled water to neutral pH, concentrated, and distilled. Yield 10.7 g (0.042 mol, 85%), bp 182–185°C (3 mm Hg). IR spectrum, ν, cm^{-1}: 2218 (C≡N); 980 (C–O–C). ^{1}H NMR spectrum, δ, ppm: 6.659–7.102 m (9H, $C_6H_5OC_6H_4$); 4.245 s (2H, Ar–CH_2–); 3.320–3.362 t (2H, O–CH_2–); 2.232–2.275 t (2H, –CH_2–CN).

IR spectrum was recorded on a SPEKORD M-82 and PERKIN-ELMER instruments (film). ^{1}H NMR spectrum was registered on a Varian Mercury 300BB instrument relative to internal HMDS in carbon tetrachloride.

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