SPONTANEOUS CONVERSION OF A 2H-PYRAN TO A FURAN DERIVATIVE

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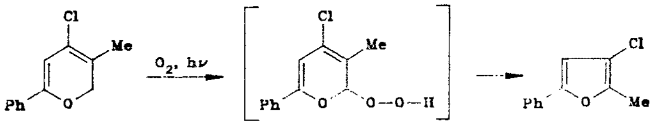
We found that 3-methyl-6-phenyl-4-chloro-2H-pyran (I), obtained from benzoyl chloride and isopropenylacetylene, is spontaneously converted to 2-methyl-5-phenyl-3-chlorofuran (III) at room temperature with the yield of 55-60%.



I II III

The reaction is an autoxidation initiated by light [1]; it proceeds via the intermediate formation and decomposition of the hydroperoxide having the hypothetical structure (II) [2]. The process is completed after 20 h in light with the admission of air [31 mg of (I) in 2 ml of CCl_4]; it is accelerated by the passage of oxygen (1 h, 30 min), and is significantly retarded in an inert atmosphere (argon, 45 h). When the reaction mixture is irradiated with a low-pressure mercury lamp, the duration of the reaction comprises 1 h [2.5 mg of (I) in 300 ml of CCl_4]; the duration is 3 h without the irradiation.

2-Methyl-5-phenyl-3-chlorofuran (III). This compound has n_D^{20} 1.5891 and the R_f 0.59 (Silufol, hexane, detection by UV light). The IR spectrum (thin layer) is as follows: 3135 (C—H of the furan ring), 3090, 3070, 3040 (C—H of the benzene ring), 1598, 1554, and 1485 cm^{-1} (C—C of the aromatic rings). The PMR spectrum ($CDCl_3$) is as follows: 2.36 (3H, singlet, $2\text{-}CH_3$), 6.57 (1H, singlet, 4-H), and 7.22-7.65 ppm (5H, multiplet, the phenyl group). The ^{13}C NMR spectrum ($CDCl_3$) is as follows: 11.2 (quartet, $2\text{-}CH_3$), 106.7 (doublet, $C_{(4)}$), 112.8 (singlet, $C_{(3)}$), 147.1 and 151.3 (singlet, $C_{(2)}$, $C_{(4)}$), 123.4 (doublet, $C_{(2')}$, $C_{(6')}$), 127.5 (doublet, $C_{(4')}$), 128.7 (doublet, $C_{(3')}$, $C_{(5')}$), and 130.2 (singlet, $C_{(1')}$). The mass spectrum has M^+ 192.194.

LITERATURE CITED

1. K. Ingold, The Theoretical Basis of Organic Chemistry [Russian translation], Mir, Moscow (1973), p. 489.
2. E. G. E. Hawkins, Organic Peroxides, Van Nostrand (1962).

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