3-PHENYL-5-(γ -HYDROXYPROPYL)ISOXAZOLE

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We discovered a new reaction in the series of 5-(γ -hydroxypropyl)isoxazole derivatives (I), and specifically the reaction of (I) with bromine, which in the presence of pyridine leads to the first member of spiro[isoxazoline-5,2'-tetrahydrofuran] (II) in 95% yield. This transformation can be regarded as being

$$C_{6}H_{5} \xrightarrow{\parallel} C_{6}H_{5} \xrightarrow{\parallel} C_{6}H_{5} \xrightarrow{\parallel} O \longrightarrow{\parallel} O \xrightarrow{\parallel} O \xrightarrow{\parallel} O \xrightarrow{\parallel} O \longrightarrow{\parallel} O \xrightarrow{\parallel} O \xrightarrow{\parallel} O \longrightarrow{\parallel} O \xrightarrow{\parallel} O \longrightarrow{\parallel} O \longrightarrow{\parallel} O \xrightarrow{\parallel} O \longrightarrow{\parallel} O$$

important proof for the intermediate formation of the σ -complex when an isoxazole is reacted with bromine.

$$\begin{array}{c|c} C_6H_5 & & Br & H \\ \hline & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

According to [1], an intermediate product of this type is formed in the bromination of a 5-phenacyl-3-phenyl-isoxazole oxime. Heterocycle (I) was obtained in 75% yield by the reaction of benzonitrile N-oxide with 1-propyn-5-ol as described in [2]. Compound (I), mp 53-55°C (1:1 hexane—benzene). Found: C 71.25; H 6.54; N 6.91%. $C_{12}H_{13}NO_2$. Calculated: C 70.93; H 6.40; N 6.89%. NMR spectrum (δ , ppm, in CDCl₃): 6.28 s (CH), 2.04 s (OH), 3.66 t (CH₂O), 2.84 t (CH₂—C=), 1.94 m (CCH₂C). Compound (II), mp 47-48°C (from hexane). Found: C 51.39; H 4.35; N 5.17; Br 28.56%. $C_{12}H_{12}BrNO_2$. Calculated: C 51.06; H 4.26; N 4.96; Br 28.37%. NMR spectrum (δ , ppm, in CCl₄): 4.94 s (CH—Br), 4.60 t (weak splitting, CH₂O), ~2.17 m (2 CH₂).

LITERATURE CITED

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