5-BENZYLURACIL AND ITS DERIVATIVES

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5-(Hydroxybenzyl)uracils are obtained by condensation of 5-hydroxymethyluracil (I) with phenols in the presence of CF_3COOH [1]. However, the activity of CF_3COOH is insufficient for aromatic compounds that do not contain electron-donor substituents. Thus, according to PMR data, the reaction between equivalent amounts of I and C_6H_6 in CF_3COOH is complete only after 3 days. However, benzene derivatives containing electron-acceptor substituents are practically unreactive. Anhydrous HP, in which even benzotrifluoride reacts, is a considerably more efficient agent.

A two-to threefold excess of the aromatic compound was added to a 3-5% solution of I in HF at 0°C. After 2 h, the HF was evaporated at room temperature, and the residue was crystallized from aqueous acetic acid. This method was used to obtain the following compounds. 5-Benzyluracil, with mp 278° (decomp.) was obtained in 52% yield from benzene. 5-(4'-Methylbenzyl)uracil, with mp 265-268°, was obtained in 59% yield from toluene. UV spectrum (in methanol): λ_{max} 265 nm, log ε 4.02. PMR spectrum, δ, ppm: 1.87 s,* 3.29, 6.71, 7.42 (3:2:4:1). Found: C 66.4; H 5.5; N 13.0%. $C_{12}H_{12}N_2O_2$. Calculated: C 66.1; H 5.6; N 13.0%. 5-(3'-Trifluoromethylbenzyl)uracil, with mp 222°, was obtained from benzotrifluoride. ^{19}F NMR spectrum: 6.9 s ppm. IR spectrum (KBr): 716, 799 cm^{-1} (metasubstitution). Found: N 10.6%. $C_{12}H_9F_3N_2O_2$. Calculated: N 10.8%. 5-(2',3',5',6'-Tetrafluoro-4'-ethoxybenzyl)uracil, with mp 280-282°, was obtained in 62% yield from 2,3,5,6-tetrafluorophenetole. UV spectrum: λ_{max} 264 nm, log ε 3.78. PMR spectrum, δ, ppm: 1.00 t, 3.40 s, 3.96 q, 7.04 s (3:2:2:1). ^{19}F NMR spectrum: 70.0 m and 83.1 ppm (1:1). Found: C 49.2; H 3.2; F 23.6; N 8.5%. $C_{13}H_{10}F_4N_2O_3$. Calculated: C 48.8; H 3.1; F 23.9; N 8.7%.

LITERATURE CITED

1. R. Brossmer, Angew. Chem., Int. Ed. in English, 6, 702 (1967).

*Here and subsequently, in CF_3COOH with tetramethylsilane as the external standard (the ^{19}F chemical shifts are relative to the solvent). Abbreviations: s is singlet, d is doublet, t is triplet, q is quartet, and m is multiplet.

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