

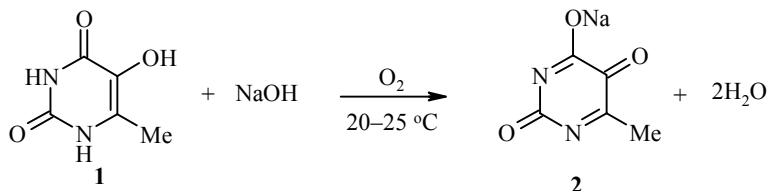
CHANGES IN THE PYRIMIDINE RING ON INTERACTION OF 5-HYDROXY-6-METHYLURACIL WITH SODIUM HYDROXIDE

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Keywords: 5-hydroxy-6-methyluracil, sodium salt of 4-hydroxy-6-methylpyrimidine-2,5-dione, oxidation.

Pyrimidine derivatives are known to be physiologically active compounds [1]. In particular, 5-hydroxy-6-methyluracil (**1**) has a wide range of pharmacological properties [2]. However its chemical and physico-chemical properties have not been adequately studied.

We have shown (IR, UV, and ^{13}C NMR spectroscopic data) for the first time that treatment of compound **1** with sodium hydroxide in a 1:1 molar ratio in water solution causes oxidation of the 5-hydroxy derivative of uracil by aerial oxygen to give product **2** with *p*-quinonoid conjugation in the pyrimidine ring.



It had been reported previously [3] that oxidation of 6-amino-5-hydroxyuracil gave 5,6-dihydroxy-, 5-hydroxy-6-oxo-, or 5,6-dioxo derivatives, depending on the reaction conditions, but that there was no change in the carbonyl groups at C₍₂₎ and C₍₄₎. In our opinion, the formation of compound **2** is explained by both the unexpected oxidation at C₍₆₎ and by the stabilization of the product as the sodium salt of the lactim form with *p*-quinonoid conjugation.

Reaction of 5-Hydroxy-6-methyluracil with Sodium Hydroxide. Compound **1** (0.346 g, 0.005 mol) was added to NaOH solution (487 ml, 0.005 M). The reaction mixture was stirred at 20–25°C for 50 h. After removal of the solvent on a rotary evaporator, compound **2** (0.240 g, 60.1%) was obtained as moderate hygroscopic red-brown crystals.

Sodium Salt of 4-Hydroxy-6-methylpyrimidine-2,5-dione (2). Mp 115–116°C. IR spectrum, ν , cm⁻¹: 3344, 1724 (C₍₂₎=O), 1664 (C₍₄₎=O), 1628 (C=N), 1600 (C=N), 1552, 1463, 1408, 1336, 1208, 1176, 1096, 1024, 928, 776. ^{13}C NMR spectrum (D₂O): 165.12 (C₍₂₎), 177.19 (C₍₄₎), 183.82 (C₍₅₎), 158.61 (C₍₆₎), 25.65 (Me). Found, %: C 26.8; H 3.3; N 13.3; Na 11.8. C₅H₃N₂O₃Na·H₂O. Calculated, %: C 27.7; H 4.1; N 12.9; Na 10.6.

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