

## SYNTHESIS AND STRUCTURE OF N-FORMYLCYTISINE

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In order to obtain new 1,4-dihydropyridine derivatives containing the alkaloid cytosine substituent in the 4-position of the dihydropyridine ring, we used the known method [1]. Formylation of cytosine with formic acid was synthesized N-formylcytosine (**1**).

It was established that the bond lengths and valence angles in the cytosine backbone of structure **1** are standard and close to the corresponding values in N-methylcytosine [2], N-cyanomethylcytosine [3]. The exception is made by the valence angles at the N12 atom. Thus, in the molecules of N-methylcytosine and N-cyanomethylcytosine, the coordination of the N12 atom is pyramidal (the sum of the valence angles is 335.7° and 334.0°), whereas in molecule **1** the coordination is plano-trigonal (the sum of the valence angles is 359°). The difference in the coordination of the N12 nitrogen atom is due to the presence of a mesomeric effect between the unshared electron pair of the nitrogen atom and the double bond C14=O2.

The dihydropyridine ring is flat with an accuracy of  $\pm 0.009$  Å, the carbonyl O1 atom almost lies in the plane of the remaining atoms, the deviation is 0.05 Å. The tetrahydropyridine ring N1C6C7C8C9C10 assumes the conformation of the distorted sofa ( $\Delta C_2^{7,13} = 1.03^\circ$ ) with the exit of the bridging C8 atom from the middle plane of the remaining atoms of the cycle at 0.71 Å. The piperidine ring is in the conformation of an almost ideal chair ( $\Delta C_2^{7,13} = 1.03^\circ$ ). The carbonyl group lies in the plane of C11N12C13 atoms (torsion angle C13N12C14O2 = 0.96°).

### References:

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