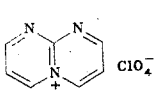
PYRIMIDO[1,2-a]PYRIMIDINIUM PERCHLORATE

V. A. Chuiguk, N. N. Vlasova,
and N. E. Kruglyak

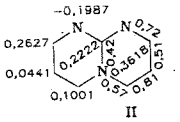
UDC 547.859

The pyrimido[1,2-a]pyrimidinium ion was previously known in the form of perchlorates of 2,8-diaryl derivatives, which were obtained by condensation of 2-amino-4-arylpyrimidines with aryl β-chlorovinyl ketones or benzoylacetaldehyde dimethylacetal with the participation of perchloric acid; unsubstituted salts, monosubstituted salts, and salts with two alkyl substituents or alkyl and aryl substituents in different rings could not be obtained by this method [1].

We also were unsuccessful in our attempts to condense 2-amino-, 2-amino-4-phenyl-, 2-amino-4-methyl, and 2-amino-4,6-dimethylpyrimidines with acetylacetone, a β-chlorovinyl aldehyde (2-methyl-3-chloro-2-butenal), and a malonaldehyde acetal (1,1,3,3-tetraethoxypropane) with the exception of a single case, viz., condensation of 2-aminopyrimidine with tetraethoxypropane. The reaction takes place in methanol or acetic acid solution in the presence of perchloric acid with heating on a water bath for a few minutes and subsequent standing at room temperature for a few hours; unsubstituted pyrimido[1,2-a]pyrimidinium perchlorate, with mp 262°C [dec., from acetic acid—formic acid (1:1)], is formed in 25-30% yield:



I



II

The structure of salt I is confirmed by its PMR spectrum [CF_3COOH, hexamethyldisiloxane (HMDS)]: 7.70 (m, 2H, 3- and 7-H), 8.92 [dd, 2H, 4- and 6-H, $J_{4,3(6,7)} = 7$, $J_{4,2(6,8)} = 1.5$ Hz], and 9.20 ppm [dd, 2H, 2- and 8-H, $J_{2,3(8,7)} = 4$, $J_{4,2(6,8)} = 1.5$ Hz]. The molecular diagram of cation II obtained by the SCF CNDO (self-consistent-field complete neglect of differential overlap) method from the PPP-1 program is in agreement with the PMR spectrum, in particular in conformity with the calculation, $\delta_{2(8)}\text{-H} > \delta_{4(6)}\text{-H}$, and $J_{4,3(6,7)} > J_{2,3(8,7)}$, since the order of the 2—3 (8—7) bond is lower than the order of the 3—4 (6—7) bond.

The results of elementary analysis of salt I were in agreement with the calculated values.

LITERATURE CITED

1. A. N. Nesmeyanov and M. I. Rybinskaya, Dokl. Akad. Nauk SSSR, 125, 97 (1959).

T. G. Shevchenko Kiev State University, Kiev 252017. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 5, pp. 704-705, May, 1984. Original article submitted October 10, 1983.

0009-3122/84/2005-0573$08.50