NEW REACTION IN PYRIMIDINE SERIES

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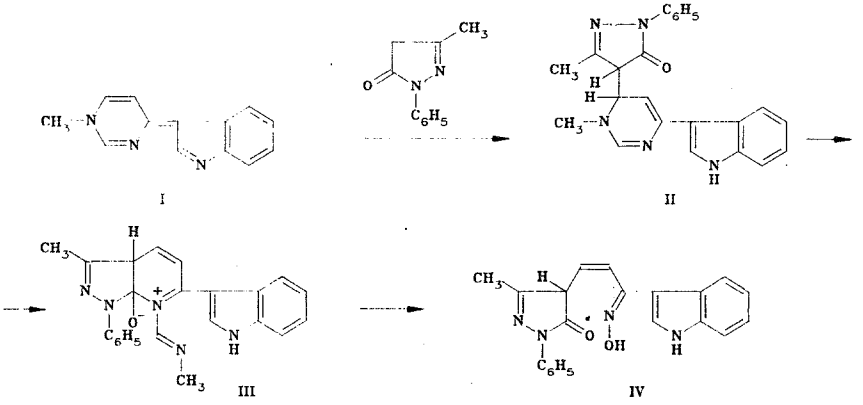
We discovered a new reaction in the pyrimidine series, namely the reaction of the anhydro-base 4-(3-indolyl)pyrimidine (I) with 1-phenyl-3-methylphrazolon-5-one:



The reaction proceeds by a double rearrangement scheme. First, as usual, the reagent adds to the $C_{(6)}$-atom of the pyrimidine ring. This is followed by ring opening in adduct II, and closure of a new ring with the participation of an electron-excess pyrimidine nitrogen atom and the carbonyl group of pyrazolone, into betaine III. Then, there is no aromatization of betaine III to pyranolopyridine, as in several similar cases [1, 2], but a repeated cyclization by a scheme of a sigmatropic rearrangement, leading to oxime IV. This reaction is completely new, not only for pyrimidine bases, but also for nitrogen-containing heterocycles, in general. A very remote analogy can be found in one single source only [3].

Compound IV was obtained by reaction between equimolar amounts of anhydro-base I and 1-phenyl-3-methylpyrazol-5-one in acetonitrile at room temperature for 3 h, yield 21%, mp 186-188°C (from acetone); IR spectrum: 1010 (NO); 1630 cm^{-1} (C=O). In the mass spectrum, a peak of M^+ with m/z 358 is recorded. The experimentally found isotopic correction (24.65%) corresponds well to the calculated one (25.05). The empirical formula was found from a high resolution mass spectrum (found 358.1143; calculated 358.1440). At the first stage of fragmentation, the OH particles are eliminated (found 341.1426, calculated for formula of ion $C_{21}H_{17}N_4O$ 341.1402). This phenomenon is typical of compounds containing an oxime group. In general, the character of the fragmentation strictly confirms the structure of the compound obtained.

LITERATURE CITED

1. T. V. Stupnikova, T. V. Nuzhnaya, and A. N. Vdovichenko, Khim. Geterotsikl. Soedin., No. 4, 555 (1983).
2. T. V. Stupnikova, T. V. Nuzhnaya, N. A. Klyuev, and A. Yu. Chervinskii, Khim. Geterotsikl. Soedin., No. 2, 212 (1982).
3. S. S. Radkova, S. Baranov, and R. O. Kochkanyan, Summaries of Lectures of the IIIrd Symposium on Chemistry and Technology of Heterocyclic Compounds in Combustible Fossils [in Russian], Donetsk (1978), p. 44.

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