

## LITERATURE CITED

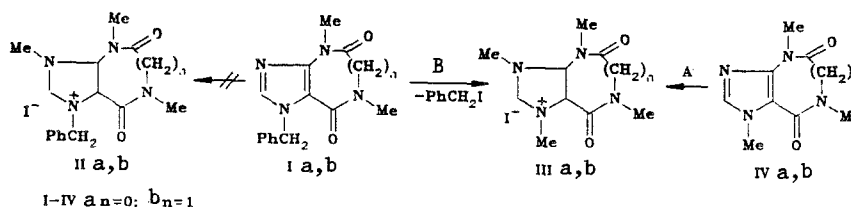
1. Yu. M. Volovenko, S. V. Litvinenko, and F. S. Babichev, Dokl. Akad. Nauk Ukrainian SSR, Ser. B, No. 4, 37 (1988).

## NEW SYNTHESIS OF CAFFEINE METHIODIDE AND ITS HOMOLOG

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It has been found that on heating 7-benzyltheophyllin (Ia) with an excess of methyl iodide in DMF, instead of the expected salt (IIa), there is obtained caffeine methiodide (IIIa).



The homolog of Ia (Ib) is converted under similar conditions into 1,4,7-trimethylimidazo[4,5-e][1,4]diazepin-(6H)-5,8-dione methiodide (IIIb). In each case, benzyl iodide was detected in the reaction mixture.

The structures of (IIIa) and (IIIb) were confirmed by direct synthesis from caffeine (IVa) and its homolog (IVb).

**Caffeine Methiodide (IIIa).** A. A mixture of 1.8 g (0.01 mole) of caffeine, 25 ml of DMF, and 2.5 ml of methyl iodide was boiled for 6 h. The solid which separated was filtered off, washed with ether, and the filtrate diluted with ether to give a further small amount of product. Overall yield 2.5 g (79%), mp 360°C (subl.).

B. A mixture of 2.7 g (0.01 mole) of 7-benzyltheophyllin, 20 ml of DMF, and 2.5 ml of methyl iodide was boiled for 6 h. The solvent was removed under reduced pressure, and the crystalline solid filtered off to give 2.7 g (83%) of product, mp 360°C (subl.).

A mixed melting point with the material obtained by method A gave no depression.

**1,4,7-Trimethyl-5,6,7,8-tetrahydro-4-imidazo[4,5-e][1,4]diazepine-5,8-dione (IIIb) Methiodide.** A. Compound (IIIb) was obtained as described in [1].

B. A mixture of 2.8 g (0.01 mole) of (Ib), 20 ml of DMF, and 3 ml of methyl iodide was boiled for 4 h. The solvent was removed under reduced pressure, and the dry residue treated with a mixture of acetone and ether (1:1) and kept overnight. The solid was filtered off, and washed with ether to give 3.2 g (92%) of product, mp 200-202°C.

## LITERATURE CITED

1. É. I. Ivanov, Dissertation for Candidate Chem. Soc., Odessa (1980).

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