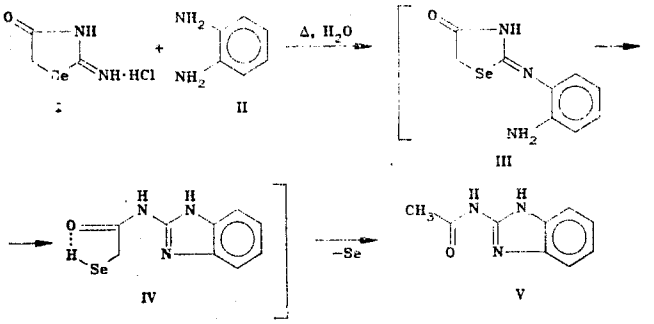
CYCLOCONVERSION OF 2-IMINOSELENAZOLID-4-ONE WITH o-PHENYLENEDIAMINE TO 2-ACETAMIDOBENZIMIDAZOLE

V. F. Lipnitskii and O. P. Shvaika

UDC 547.789.8'785.5'553.1.04

We have established that 2-acetamidobenzimidazole is formed in a yield that is close to quantitative when 2-iminoselenazolid-4-one hydrochloride is refluxed in water for 3 h with an equivalent amount of o-phenylenediamine. Selenium, which is eliminated by hot filtration during recrystallization, is liberated during the reaction. The cycloconversion can be interpreted by the scheme



Intermediates III and IV could not be isolated. The deselenization that occurs during the cycloconversion leads to the unexpected conversion of the methyleneselenol grouping to a methyl group (V). One of the conditions for this conversion is apparently the presence of an electron-acceptor function in the β position relative to the selenol group, since, when this is not the case, substituted alkane-selenols retain selenium when they are heated to 160°C and undergo cyclization with the participation of the selenol group or form diselenides [1].

2-Acetamidobenzimidazole (V). This compound had mp 312-315°C (subl., from ethanol). IR spectrum (in mineral oil): ν_{NH} 3270-3320, $\nu_{amide\ I}$ 1690, and $\nu_{C=N}$ 1640 cm^{-1}. PMR spectrum with tetramethylsilane as the internal standard (in CF_3COOH): 2.50 (s, CH_3) and 7.46-7.83 ppm (m,4H, aromatic); (in DMSO): 11.60-11.83 ppm (d, NH). Compound V was readily soluble in acetic acid, moderately soluble in methanol, ethanol, and dioxane, only slightly soluble in benzene, and insoluble in water. The composition of V was confirmed by the results of elementary analysis for C, H, and N, and the structure was proved by alternative synthesis by acylation of 2-aminobenzimidazole by heating in acetic anhydride.

LITERATURE CITED

1. W. H. H. Gunther, in: Organic Selenium Compounds: Their Chemistry and Biology, Wiley, New York–London (1973), p. 44.

Institute of Physical Organic Chemistry and Coal Chemistry, Academy of Sciences of the Ukrainian SSR, Donetsk 340114. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 8, pp. 1135-1136, August, 1985. Original article submitted January 30, 1985.

 0009-3122/85/2108-0954$09.50