

Letters to the Editor

Reaction of divinyl selenide with thiourea

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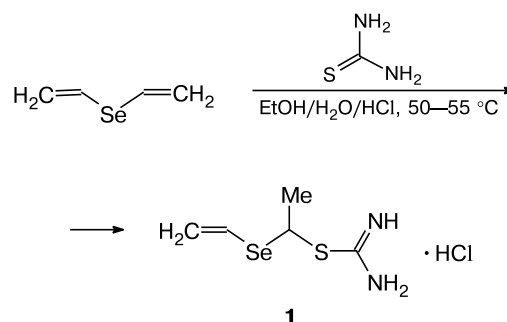
It is known^{1,2} that the reaction of divinyl sulfide with thiourea and its derivatives proceeds in aqueous ethanol in the presence of strong acids (for example, HCl) at 40–55 °C and leads to the cyclization products, viz., 4-amino-2,6-dimethyl-2*H*,6*H*-1,3,5-dithiazinium salts. Formation of these heterocyclic compounds occurs through the addition of the sulfur and nitrogen atoms of thiourea at the double bonds of divinyl sulfide. There is no information on the reaction of divinyl selenide with thiourea in the literature.

We have studied the reaction of divinyl selenide with thiourea under conditions similar to those of the reaction of divinyl sulfide with thiourea. It was found that the reaction leads to the earlier unknown *S*-(1-vinylseleno)ethylisothiurea hydrochloride (**1**) in 89% yield rather than to the cyclization product (Scheme 1).

The reaction was carried out by heating (50–55 °C, 10 h) of equimolar amounts of the reagents in ethanol–0.1 *M* HCl mixture (v/v, 5 : 1). An increase in the reaction time and in the temperature (to 75 °C) did not cause the cyclization of product **1**.

Hydrochloride **1** is a crystalline compound of light yellow color. Its structure was confirmed by ¹H, ¹³C, and ⁷⁷Se NMR spectroscopy and elemental analysis data.

Scheme 1



We suggest that the unexpected result of the reaction in case of divinyl selenide (as compared with divinyl sulfide) is caused by the lower activity of vinylseleno group toward addition of the amino group in the presence of acid as compared to the vinylthio group. The reaction proceeds as the addition of the thiol function at the double bond and stops at this stage, giving no cyclization product, since the vinylseleno group is not active enough for the addition of the amino group in the presence of HCl. It can be suggested that compound similar to prod-

uct **1**, yet containing sulfur atom instead of selenium one, is the intermediate in the cyclization reaction of divinyl sulfide with thiourea.^{1,2}

NMR spectra were recorded on a Bruker DPX-400 spectrometer (400.1 (¹H), 100.6 (¹³C), and 76.3 (⁷⁷Se) MHz) in CDCl₃.

S-[(1-Vinylseleno)ethyl]isothiuronium chloride (1), m.p. 78–82 °C. Found (%): C, 24.68; H, 4.63; Cl, 14.36; N, 11.36; S, 12.73; Se, 32.03. C₅H₁₁ClN₂SSe. Calculated (%): C, 24.45; H, 4.51; Cl, 14.45; N, 11.40; S, 13.03; Se, 32.16. ¹H NMR, δ: 1.72 (d, 3 H, CHCH₃, *J* = 6.8 Hz); 5.58 (q, 1 H, CHCH₃, *J* = 6.8 Hz); 5.63 (d, 1 H, CH=, *J* = 17.4 Hz); 5.85 (d, 1 H, CH=, *J* = 9.7 Hz); 6.87 (dd, 1 H, SeCH=, *J* = 9.7 Hz, *J* = 17.4 Hz); 9.34 (br.s, 2 H, NH₂); 9.60 (br.s, 2 H, =NH • HCl). ¹³C NMR, δ: 23.2 (CH₃); 36.1 (CH); 121.7 (CH₂=); 124.7 (SeCH=); 169.3 (C=NH). ⁷⁷Se NMR, δ: 417.2.

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