## TRIETHOXY (3-ISOTHIOCY ANATOPROPYL) SILANE

## M. G. Voronkov, O. S. Stankevich, and É. I. Dubinskaya

The reaction of triethoxy(3-aminopropyl)silane with carbon disulfide and ortho-chloroethyl formate in absolute ethanol gave triethoxy(3-isothiocyanatopropyl)silane for the first time. The presence of SCN and  $(C_2H_5O)_3Si$  groups in this compound enabled us to use it for the preparation of adsorbents and polymer coatings with biocidal activity.

Keywords: triethoxy(3-isothiocyanatopropyl)silane, triethoxy(3-aminopropyl)silane, carbon disulfide, orthochloroethyl formate.

Organic and organosilicon isothiocyanates are used in medicine as antibacterial and antifungal agents [1, 2]. We are the first to report a high-yield synthesis of triethoxy(3-isothiocyanatopropyl)silane (1) by the reaction of

triethoxy(3-aminopropyl)silane with carbon disulfide and *ortho*-chloroethyl formate in absolute ethanol.

 $(C_{2}H_{5}O)_{9}Si(CH_{2})_{3}NH_{2} + CS_{2} + C_{2}H_{5}ONa \xrightarrow{-C_{2}H_{5}OH}$   $\rightarrow (C_{2}H_{5}O)_{8}Si(CH_{2})_{3}NHCSSNa \xrightarrow{+CiCOOC_{2}H_{5}} (C_{2}H_{5}OH)_{3}Si(CH_{2})_{3}N = C = S$  (1)

The use of sodium ethylate in this reaction significantly raises the yield of 1 in comparison with the reactions, in which trimethylamine [3, 4] or N,N'-dicyclohexylcarbodiimide [5] are used for this purpose. Furthermore, the use of sodium ethylate also permitted more facile separation of the final reaction product in light of the formation of NaCl instead of  $(CH_3)_3N \cdot HCl$ , which is difficult to separate.

The presence of the  $(C_2H_5O)_3Si$  group in 1 permits us to use this compound for the preparation of adsorbents and biological coatings with biocidal activity.

## **EXPERIMENTAL**

The PMR spectra were taken on a JEOL FX-90Q (60 MHz) spectrometer using HMDS as the standard and  $CDCl_3$  as the solvent.

A mixture of 55.3 g (0.25 mole)  $(C_2H_5O)_3$ Si(CH<sub>2</sub>)<sub>3</sub>NH<sub>2</sub> and 20 g (0.26 mole) CS<sub>2</sub> was added dropwise to 5.75 g (0.25 mole) sodium in 250 ml absolute ethanol and heated at reflux for 5 h. The reaction mixture was cooled and 32.5 g (0.3 mole) ClCOOC<sub>2</sub>H<sub>5</sub> was added. The precipitate was filtered off and vacuum distillation gave 49.4 g (75%) 1, bp 108-109°C (1 mm Hg),  $d_4^{20}$  1.0278,  $n_D^{20}$  1.4595. Found, %: C 46.02; H 8.22; N 5.47; S 11.85; Si 10.33. C<sub>10</sub>H<sub>21</sub>NO<sub>3</sub>SSi. Calculated, %: C 45.62; H 7.98; N 5.32; S 12.16; Si 10.64. MR<sub>D</sub> found, %: 70.02; calculated, %: 71.15. PMR spectrum in CDCl<sub>3</sub> ( $\delta$ , ppm):

0.68 t (2H, CH<sub>2</sub>Si), 1.22 t (3H, CH<sub>3</sub>CO), 1.83 q (2H, CCH<sub>2</sub>C), 3.51 t (2H, CH<sub>2</sub>N), 3.83 q (2H, CH<sub>2</sub>O).

Irkutsk Institute of Organic Chemistry, Siberian Branch, Russian Academy of Sciences, 664033 Irkutsk. Translated from Izvestiya Akademii Nauk, Seriya Khimicheskaya, No. 11, pp. 2681-2682, November, 1992. Original article submitted March 3, 1992.

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