Synthesis and Crystal Structure of the Germatrane E-$N(CH)_2CH_2O_3GeC(Br)=C(Br)Ph$

Anastasia A. Selina[a], Sergey S. Karlov[a], Klaus Harms[b], Daniil A. Tyurin[a], Yuri F. Oprunenko[a], Jörg Lorberth[b], and Galina S. Zaitseva[a]

[a] Chemistry Department, Moscow State University, Leninskie Gory, 119899 Moscow, Russia
[b] Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35032 Marburg / Lahn, Germany

Reprint requests to Prof. Dr. J. Lorberth or Dr. S. S. Karlov.
E-mail: lorberth@staff.uni-marburg.de or sergej@org.chem.msu.su

Z. Naturforsch. **58b,** 613 – 619 (2003); received January 9, 2003

The reaction of (phenylacetylenyl)triethoxygermane, $(EtO)_3GeC{\equiv}CPh$ (**3**), with bromine in $CHCl_3/CCl_4$ solution leads to a mixture of Z- and E- $(EtO)_3GeC(Br)=C(Br)Ph$ (**4**) in the ratio Z/E = 3/1. Treatment of this product with $N(CH_2CH_2OH)_3$ affords a mixture of Z- and E-$N(CH_2CH_2O)_3GeC(Br)=C(Br)Ph$ (**2**) in high yield. Compound E-**2** was isolated in 16% yield. The molecular composition and the structure of all new compounds have been established by elemental analyses, ^1H and ^{13}C NMR spectroscopy. The crystal structure of E-**2** is reported. The possible reasons for the different Z/E ratios in the products of the bromination of **3** and $N(CH_2CH_2O)_3GeC{\equiv}CPh$ (**1**) are discussed using DFT calculations.

Key words: Germatrane, Bromination, Alkynes, DFT Calculations