Synthesis and Characterization of N-Methyl-Substituted Germocanes. Crystal Structure of $MeN(CH_2CH_2O)_2GeBr_2$

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The reaction of $GeHal_4$ with $MeN(CH_2CH_2OSiMe_3)_2$ affords dihalogermocanes $MeN(CH_2CH_2O)_2GeHal_2$ (**1**, Hal = Br; **2**, Hal = Cl). Treatment of $Me_2Ge(NMe_2)_2$ with $MeN(CH_2CH_2OH)_2$ leads to dimethylgermocane $MeN(CH_2CH_2O)_2GeMe_2$ (**3**). The composition and structure of **1-3** were established by elemental analyses, ^1H, ^{13}C NMR spectroscopy, and mass spectrometry. The crystal structure of **1** is reported; structural data obtained from geometry DFT optimization on **1** are in good agreement with experimental results. Values of the electron density in the N→Ge bond critical point and the Laplacian of charge density for **1-3** indicate a closed-shell interaction between the Ge and N atoms.

Key words: Germocanes, Transannular Interaction, Crystal Structure, DFT Calculations