

The Molecular Structures and Conformational Preferences of Bis(dimethylstibyl)-Sulfane and -Tellurane, $E(\text{SbMe}_2)_2$, $E = \text{S}$ or Te , $\text{Me} = \text{CH}_3$, by Density Functional Theory Calculations and Gas Electron Diffraction

Arne Haaland^{*a}, Dmitry J. Shorokhov^a, Hans Vidar Volden^a,
Hans Joachim Breunig^{*b}, Michael Denker^b, Roland Rösler^b

^a Department of Chemistry, University of Oslo, Box 1033 Blindern, N-0315 Oslo, Norway

^b Universität Bremen, Fachbereich 2 (Chemie), Postfach 330440, D-28334 Bremen, Germany

Z. Naturforsch. **53b**, 381–385 (1998); received November 7, 1997

Distibylsulfane, Distibyltellurane, Density Functional Theory Calculations,
Gas Electron Diffraction

Density functional theory calculations on $E(\text{SbMe}_2)_2$, $E = \text{S}$ or Te , $\text{Me} = \text{CH}_3$, indicate that the equilibrium structures are *syn-syn* or near *syn-syn* conformers with overall C_{2v} or C_2 symmetry. The calculations further indicate the existence of *syn-anti* conformers about 4 kJ mol⁻¹ ($E = \text{S}$) or 1 kJ mol⁻¹ ($E = \text{Te}$) above the equilibrium structure. Gas electron diffraction data show that both conformers are present in gaseous $\text{S}(\text{SbMe}_2)_2$, while the presence of the *syn-anti* conformer in gaseous $\text{Te}(\text{SbMe}_2)_2$ is uncertain. The Sb–S and Sb–Te bond distances are 241.4(4) and 278.1(3) pm, respectively, the valence angles of the *syn-syn* conformers are $\angle\text{SbSSb} = 98.7(5)^\circ$ and $\angle\text{SbTeSb} = 91(2)^\circ$.

* Reprint requests to Prof. A. Haaland.