NMR Spectroscopy of Tetra(propyn-1-yl)silane in the Solid State and in Solution

Bernd Wrackmeyer[a], Oleg L. Tok[a], and Amin Badshah[b]

[a] Universität Bayreuth, Anorganische Chemie II, D-95440 Bayreuth, Germany
[b] Department of Chemistry, Quaid-I-Azam University, Islamabad, Pakistan

Reprint requests to Prof. Dr. B. Wrackmeyer.
E-mail: b.wrack@uni-bayreuth.de

Z. Naturforsch. **58b,** 809 – 812 (2003); received May 5, 2003

The crystal structure of tetra(propyn-1-yl)silane, Si(C≡C-Me)$_4$ **1**, has revealed a completely asymmetric molecule (point group C_1). Since this finding concerns a single crystal, the bulk material of **1** was studied by solid-state ^{29}Si and ^{13}C MAS NMR. This confirmed the result of the X-ray analysis, and by comparison with previous NMR measurements of the tin analogue **1(Sn)** it is concluded that **1** and **1(Sn)** must have very similar solid-state structures which are in contrast to those known for other tetra(alkyn-1-yl)silicon and -tin compounds. The NMR data set of **1** in solution was completed by determination of the magnitude of coupling constants $^1J(^{13}C,^{13}C)$.

Key words: Alkynes, Silane, NMR, Solid State