Cleavage of an Iron-Silicon Bond by Hexamethylphosphoric Triamide: Synthesis and Characterization of $[SiCl_3(HMPA)_3]^+[Fe(CO)_4SiCl_3]^-$

Van An Du[a], Stefan O. Baumann[a], Gregor N. Stipicic[b], and Ulrich Schubert[a]

[a] Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9, 1060 Vienna, Austria
[b] Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9, 1060 Vienna, Austria

Reprint requests to Prof. U. Schubert. Fax: +43-(0)1-58801-16599.
E-mail: uschuber@mail.zserv.tuwien.ac.at

Z. Naturforsch. **2009**, *64b,* 1553 – 1557; received August 10, 2009

Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

Addition of excess hexamethylphosphoric triamide (HMPA) to *cis*-$Fe(CO)_4(SiCl_3)_2$ led to the exclusive formation of the new complex $[SiCl_3(HMPA)_3]^+$ $[Fe(CO)_4SiCl_3]^-$ by cleavage of an iron-silicon bond. A reaction mechanism is presented, based on density functional theory calculations.

Key words: Iron-Silicon Bond Cleavage, Anionic Metal Silyl Complex, Hexacoordinate Silicon, DFT Calculations