Trifluoromethylated Compounds with Si\(\text{NN}\) and Si\(\text{ON}\) Backbone, and the Crystal Structures of Trimethyl- and Trichloro(trifluoromethyl)silane

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Dedicated to Professor Otto J. Scherer on the occasion of his 75\textsuperscript{th} birthday

The reaction of (F\(_3\)C)Cl\(_2\)SiCl\(_3\) with the lithiated hydrazine LiN(Me)NMe\(_2\) gives the compound (F\(_3\)C)Cl\(_2\)SiN(Me)NMe\(_2\) (1) and in traces Cl\(_3\)SiN(Me)NMe\(_2\) (2). The reactions with LiN(SiMe\(_3\))NMe\(_2\) and LiONMe\(_2\) give (F\(_3\)C)Cl\(_2\)SiN(SiMe\(_3\))NMe\(_2\) (4) and (F\(_3\)C)Cl\(_2\)SiONMe\(_2\) (5), respectively. The compounds were characterised by multinuclear solution NMR, gas-phase IR spectroscopy and mass spectrometry. Information about conformational preferences of 1 and 4 can be extracted by comparing experimental IR spectra with those calculated by quantum chemical methods (B3LYP/6-311G**). The former show the gas phase of the β-donor-acceptor silanes 1 and 4 to be dominated by the anti conformations, while the calculations show a preference for the gauche conformers. The crystal structure of Cl\(_3\)SiN(Me)NMe\(_2\) (2) has been determined. The solid-state structures of the Ruppert reagent F\(_3\)C–SiMe\(_3\) (1) and its chlorine analogue F\(_3\)C–SiCl\(_3\) (2) have also been determined by X-ray diffraction of single crystals grown by in situ techniques.

Key words: Silicon, Trifluoromethylsilanes, Hydroxylamine, Hydrazine, Crystal Structure, Quantum Chemical Calculations