Synthesis and Characterization of Cl_2HSi-O-NMe_2

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O-(Dichlorosilyl)-*N*,*N*-dimethylhydroxylamine, $Cl_2HSiONMe_2$, was synthesised by the reaction of *O*-lithio-*N*,*N*-dimethylhydroxylamine with an excess of trichlorosilane. The compound was characterised by multinuclear NMR spectroscopy (^1H, ^{13}C, ^{15}N, ^{29}Si), gas-phase IR spectroscopy and mass spectrometry. The structure of $Cl_2HSiONMe_2$ was determined by gas-phase electron diffraction. It exists as two conformers in the vapour, named *anti* and *gauche* after the position of the SiH hydrogen atom relative to the SiON skeleton. The *anti*:*gauche* ratio in the vapour was determined to be 40:60. The *anti* conformer shows only a weak attractive interaction between the geminal donor and acceptor centres N and Si [angle Si-O-N 111.1(20)°], whereas these interactions are stronger in the *gauche* conformer [angle Si-O-N 98.8(12)°]. Further structure-determining forces from weak hydrogen bridges of the Si-Cl···H-C type and van der Waals repulsive forces are also discussed. The experimental results are in reasonable agreement with *ab initio* calculations at the MP2/6-311++G** level of theory.

Key words: Silicon, Hydroxylamine, Donor Bonds, Electron Diffraction