

SUBSTITUTION STRUCTURES OF MULTIPLE SILICON-CONTAINING SPECIES BY CHIRPED PULSE FTMW SPECTROSCOPY

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The structures of CH₃SiHF-NCO, 1-X-silacyclopropane (X = cyano, isocyanato), 1,1,3,3-tetrafluoro-1,3-disilacyclopentane and its hydrogen analogue (1,3-disilacyclopentane), and 1-isocyanato-silacyclohexane have been studied by chirped pulse FTMW spectroscopy in the 6-18 GHz band. Multiple conformers for some of the species were also detected: *anti* and *gauche* for both silacyclopentyl species, and axial and equatorial for the silacyclohexane. Heavy atom substitution structures were determined, with all possible single ¹³C, ²⁹Si/³⁰Si and most ¹⁵N isotopologues assigned in natural abundance. Nitrogen hyperfine and distortion parameters for all species have been determined, and the barrier for methyl internal rotation for CH₃SiHF-NCO has been determined as 481(20) cm⁻¹, close to the B3LYP/6-311++g(d,p) barrier of 450 cm⁻¹. A summary of the microwave and structural results for the aforementioned molecules will be presented. In addition, emphasis will be placed on the use of previously discussed^{ab} automated fitting techniques as a means of efficient and fast assignment of isotopologues in spectra with increasingly large line densities.

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