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

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The structures of $CH_3SiHF$-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 silacyclopropyl species, and axial and equatorial for the silacyclohexane. Heavy atom substitution structures were determined, with all possible single $^{13}$C, $^{29}$Si/$^{30}$Si and most $^{15}$N isotopologues assigned in natural abundance. Nitrogen hyperfine and distortion parameters for all species have been determined, and the barrier for methyl internal rotation for $CH_3SiHF$-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.

[a] A. L. Steber, J. L. Neill, M. T. Muckle, B. H. Pate, D. F. Plusquellic, V. Lattanzi, S. Spezzano, M. C. McCarthy. 65th OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 2010, TC10.

[b] E. B. Kent, M. N. McCabe, M. A. Phillips, B. P. Gordon, S. T. Shipman. 66th OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 2011, RH01.