STRUCTURAL STUDIES OF CH_3SiF_2-X (X = NCO, Cl) BY MICROWAVE SPECTROSCOPY

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The structures of CH_3SiF_2-NCO and CH_3SiF_2-Cl have been studied by molecular rotational spectroscopy in the 6.5-18 GHz band. The rotational spectrum was measured by cavity Fourier transform microwave (FTMW) and chirped-pulse FTMW spectroscopy. The experiment targeted the study of CH_3SiF_2-NCO, but CH_3SiF_2-Cl was also observed as an impurity. Due to the dynamic range achieved on these spectra, all isotopologs with natural abundance $\geq$0.2% were assigned, which includes two doubly-substituted isotopologs for the chloride (^{29}Si/^{37}Cl and ^{30}Si/^{37}Cl). Strategies for obtaining the molecular structure for these two molecules using either a Kraitchman analysis (to obtain a partial substitution structure) or r_0 analysis (with additional constraints on the structure supplied by the theoretical structure) will be discussed. Derived structural parameters for the CH_3-SiF_2-X base structure are the same for the two compounds. The hyperfine and internal rotation effects in the spectra have been analyzed for all isotopologs and the Hamiltonian parameters are in very good agreement with ab initio results. The barriers to methyl group internal rotation for the two compounds 446(50) cm^{-1} and 463(3) cm^{-1} and are independent of the isotopic structure of the heavy atom frame.