SPECTROSCOPY OF CHLOROSYL FLUORIDE, FClO

HOLGER S. P. MÜLLER, *I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln, Germany*; and EDWARD A. COHEN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099*.

FClO has been proposed as an intermediate in reactions involving ClF, Cl_2O, and ClF_3O, and it has been suggested as a molecule of atmospheric interest. It has been prepared *in situ* by the hydrolysis of ClF_3. The pure rotational spectrum of FClO has been studied by conventional millimeter wave techniques and by microwave Fourier transform spectroscopy. Selected transitions were searched for using predictions based on an analysis of the ν_1 band.[a] Low field Stark measurements have been performed in the millimeter region. FClO is an asymmetric prolate top, κ = –0.8950 for $F^{35}ClO$, with a rather small dipole component of 0.093 (4) D along the a-axis and a larger one of 1.93 (5) D along the b-axis. Transitions with $0 \leq J \leq 54$ and $0 \leq K_a \leq 18$ were observed. Cl hyperfine splitting was generally observable throughout the spectrum with ^{19}F spin-rotation splitting observable as well in the microwave region. Structural parameters, harmonic force constants, and nuclear magnetic shielding parameters were derived and will be compared with data of related molecules, such as ClF_3, ClF, $FClO_2$, and $FClO_3$. High resolution infrared spectra were taken in the regions of the FCl stretching mode and bending mode around 600 and 310 cm^{-1}, respectively. A preliminary analysis indicates that the FCl stretch, near 596.86 cm^{-1} for $F^{35}ClO$, is in resonance with the dark overtone of δ near 617 cm^{-1}. A brief progress report will be given.

[a]H. S. P. Müller, paper MF04, presented at The 53rd Ohio State University International Symposium on Molecular Spectroscopy, Columbus, OH, June 1998