THE ROTATIONAL SPECTRUM AND MOLECULAR PROPERTIES OF CHLORYL CHLORIDE, $ClClO_2$

HOLGER S. P. MÜLLER, AND EDWARD A. COHEN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109*.

$ClClO_2$ is slightly higher in energy than its structural isomer ClOOCl,[a] which has been implicated in polar ozone depletion processes. $ClClO_2$ may be formed from other Cl_xO_y compounds on or in stratospheric ices.[b c] Therefore, its millimeter and submillimeter spectrum has been studied in a flowing system as a product of the $FClO_2$ + HCl reaction. The pyramidal $ClClO_2$ is an asymmetric prolate top, κ = -0.7598 for $^{35}Cl^{35}ClO_2$. It has C_s symmetry with a strong dipole component along the c-axis and a smaller one along the a-axis. The highest quantum numbers accessed are larger than 50 and 30 for J and K_a, respectively, permitting rotational and centrifugal distortion constants to be determined precisely. Splittings due to both Cl nuclei have been resolved, and a quadrupole analysis will be presented. The molecular structure has been derived from isotopomers involving ^{35}Cl and ^{37}Cl. The results will be compared with those from an earlier matrix-isolation study,[d] from $ab\ initio$ calculations,[a] and from data of related molecules.

[a] T. J. Lee, C. McMichael Rohlfing, and J. E. Rice, J. Chem. Phys., **97**, 6593, (1992)
[b] C. J. Pursell, J. Conyers, and C. Denison, J. Phys. Chem., **100**, 15450, (1996)
[c] J. D. Graham, J. T. Roberts, L. D. Anderson, and V. H. Grassian, J. Phys. Chem. **100**, 19551, (1996)
[d] H. S. P. Müller and H. Willner, Inorg. Chem. **31**, 2527, (1992)