FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND FTMW-MILIMETER WAVE DOUBLE RESONANCE SPECTROSCOPY OF ClOO.

KOHSUKE SUMA,YOSHIHIRO SUMIYOSHI and YASUKI ENDO, *Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8902, Japan*.

Many a-type (9GHz-39GHz) and b-type transitions (80GHz) of ClOO for ^{35}Cl and ^{37}Cl isotopomers are observed using Fourier transform microwave (FTMW) and FTMW-mmw (millimeter wave) double resonance spectroscopy. The rotational, centrifugal, spin rotation coupling, and hyperfine coupling constants are determined by least squares fits of the observed spectra. Highly accurate *ab initio* calculations at MRCI/aug-cc-pV5Z are also performed, which reproduce the experimental results well. Other sigle reference methods are turned out to be inappropriate for ClOO, because it is indispensable to take account of static and dynamic electronic correlations simultaneously. The r_e structure is determined using the force field obtained by the *ab initio* calculations; r_e(OO) = 1.204Å, r_e(ClO) = 2.081Å, and θ_e(ClOO)= 115.0° . The nature of anomalous ClO bond become clear by the present experiments and *ab initio* calculations.