FURTHER STUDIES OF THE PERCHLORIC ACID ROTATIONAL SPECTRUM

J. J. Oh*, B. J. Drouin†, and E. A. Cohen†
*Department of Chemistry, SookMyung Womens University, Seoul, Korea
†Jet Propulsion Laboratory, California Institute of Technology
Pasadena, California 91109-8099, U. S. A.

$HClO_4$ is a nearly spherical rotor with a moderately low 3–fold barrier to internal rotation, ($s \approx 5.15$). The a molecular axis is nearly coincident with the internal rotation axis of the OH and ClO_3 groups. Only A torsional states are allowed. The rotational energies are dominated by the K dependent solutions of the Mathieu equation and have little resemblance to those of a normal asymmetric rotor. For the $HClO_4$ ground torsional state, more than 700 features between 52 and 645 GHz with $J \leq 61$ and $K \leq 47$ of the two major isotopic species have been assigned and fitted. Because of the unusual distribution of energy levels, these include many perturbation enhanced transitions involving large changes in the K quantum number. Low lying excited torsional state spectra also have been assigned. Details of the fitting will be shown. The derived molecular parameters, which include rotational, centrifugal distortion, quadrupole coupling, and torsion–rotation interaction constants as well as the barrier to internal rotation, will be presented. Structural implications will be discussed.