

ROTATIONAL ANALYSIS OF THE NEAR INFRARED SINGLET-TRIPLET ELECTRONIC SPECTRUM OF OZONE

A. J. BOUVIER, D. INARD, S. CHURASSY and R. BACIS, *Laboratoire de Spectrométrie Ionique et Moléculaire (associé au CNRS U.M.R. 5579), Université Claude Bernard Lyon I, 43, Bd. du 11 Novembre 1918, 69622 Villeurbanne Cedex, France*; J. BRION and J. MALICET, *Laboratoire de Chimie-Physique, Faculté des Sciences de Reims, G.S.M.A., C.N.R.S., U.R.A.D., 1434, B.P. 347-51062, Reims, France*; and R. H. JUDGE, *Department of Chemistry, University of Wisconsin-Parkside, Kenosha, WI, U.S.A. 53141-2000*.

High Resolution Fourier Transform Infrared Spectrometry was used to study the rotational fine structure of the lowest energy singlet-triplet electronic spectrum of ozone, $^{16}\text{O}_3$ and $^{18}\text{O}_3$ near 9300 cm^{-1} . With a near pure case (b) coupling model, approximately 100 lines were assigned in the spectrum of $^{16}\text{O}_3$. A combined least-squares/band contour analysis yielded an overall standard deviation of 0.045 cm^{-1} . The fit to the $^{18}\text{O}_3$ spectrum used approximately 30 lines and gave a slightly higher overall standard deviation. The rotational analysis has established that the upper state is 3A_2 in agreement with recent theoretical calculations. Numerous perturbations are observed in the spectrum of both isotopomers and limited our least-squares fit to the three rotational constants, the symmetric top distortion constants, the three spin-rotation constants and the alpha spin-spin constant. The talk will feature an overview of the rotational analysis along with a brief discussion of the perturbations seen in the spectrum.