VIBRONIC ANALYSIS OF THE $\tilde{A}^2E''$ STATE OF NO$_3$ RADICAL

TERRANCE J. CODD, MOURAD ROUDJANE, MING-WEI CHEN$^a$, and TERRY A. MILLER, Laser Spectroscopy Facility, The Ohio State University, Columbus, Ohio 43210.

The nitrate radical is a key reactant in atmospheric chemistry leading to the formation of acid rain and is the primary oxidant in the night sky. The $\tilde{A}^2E''$ state of NO$_3$ is doubly degenerate and is therefore subject to Jahn-Teller (JT) coupling through the degenerate in-plane stretch and bend modes ($\nu_3$ and $\nu_4$ respectively). We have taken a moderate resolution CRDS spectrum of the $\tilde{A}^2E'' - \tilde{X}^2A'$ transition of the NO$_3$ radical under jet-cooled conditions. We resolve $\sim 20$ vibronic transitions and are able to assign many using an independent anharmonic oscillator model as was presented previously.$^b$ In order to gain a deeper understanding of the nature of the JT effect in this electronic state we have performed a vibronic analysis including linear and quadratic JT coupling terms for $\nu_3$ and $\nu_4$ and possible bilinear coupling between the totally symmetric stretch, $\nu_1$, and $\nu_4$. We conclude that the JT coupling in $\nu_4$ is quite weak. Satisfactory spectral fits can be obtained assuming weak JT coupling for $\nu_3$ also, though there is some evidence of strong JT coupling for $\nu_3$ and the strengths and weaknesses of each case are discussed.

$^a$Present address: University of Illinois at Urbana-Champaign, Urbana, IL 61801