VIBRONIC ANALYSIS OF THE $\widetilde{A}^2E''$ STATE OF NO_3 RADICAL

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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 $\widetilde{A}^2E''$ 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 (ν_3 and ν_4 respectively). We have taken a moderate resolution CRDS spectrum of the $\widetilde{A}^2E''$-$\widetilde{X}^2A_2'$ transition of the NO_3 radical under jet-cooled conditions. We resolve ~ 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 ν_3 and ν_4 and possible bilinear coupling between the totally symmetric stretch, ν_1, and ν_4. We conclude that the JT coupling in ν_4 is quite weak. Satisfactory spectral fits can be obtained assuming weak JT coupling for ν_3 also, though there is some evidence of strong JT coupling for ν_3 and the strengths and weaknesses of each case are discussed.

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[b]Codd, T. et al. 67^{th} Int. Symp. Molec. Spec. (2012)