JAHN-TELLER ANALYSIS OF THE VIBRONIC STRUCTURE OF THE $\widetilde{X}^2\mathrm{E}_1''$ STATE IN THE CYCLOPENTADIENYL RADICAL

BRIAN E. APPLEGATE, ANDREW J. BEZANT, AND TERRY A. MILLER, *The Ohio State University, Dept. of Chemistry, Laser Spectroscopy Facility, 120 W. 18th Avenue, Columbus, Ohio 43210*; TIMOTHY A.BARCKHOLTZ, *JILA, National Institute of Standards and Technology and The Department of Chemistry and Biochemistry, University of Colorado Boulder, Colorado 80309*.

While room temperature wavelength resolved emission spectra of the $\widetilde{A}^2\mathrm{A}_2''$-$\widetilde{X}^2\mathrm{E}_1''$ transition have existed for nearly 20 years[a], the vibrational assignment of these spectra has remained elusive. The major difficulty with the vibrational analysis is attributable to complications arising from the dynamic Jahn-Teller effect in the $\widetilde{X}$ state. Newly obtained jet-cooled laser excited wavelength resolved fluorescence emmision spectra, in conjunction with recent [b]calculations aimed at predicting the relevant Jahn-Teller constants have now made the complete analysis of the available spectral data possible. The transitions involving the Jahn-Teller active vibrations have been analyzed in terms of the three lowest energy harmonic vibrations of the appropriate symmetry (e_2'), assuming only linear Jahn-Teller interactions. Additional features of the spectrum may be described in terms of the fundamentals, overtones, and combination bands of the non-Jahn-Teller active vibrations as well as combinations involving the Jahn-Teller active modes.

[a]Nelson H. H.; Pasternack L.; McDonald J. R., *Chem. Phys*, **1983**, *74*, 227.
[b]Applegate B. E.; Barckholtz T. A.;Miller T. A., *to be published*