

## THE ANALYSIS OF THE GROUND STATE OF ASYMMETRICALLY DEUTERATED METHOXY RADICALS: AN ALTERNATIVE APPROACH

DMITRY G. MELNIK and ROBERT F. CURL, *Department of Chemistry and Rice Quantum Institute, Rice University, Houston, TX 77005*; JINJUN LIU, JOHN T. YI and TERRY A. MILLER, *The Ohio State University, Dept. of Chemistry, Laser Spectroscopy Facility, 120 W. 18th Avenue, Columbus, Ohio 43210*.

The global analysis of the spectra of asymmetrically deuterated methoxy radicals obtained in high resolution spectroscopy of  $3_0^2$  and  $(6')_0^1$  bands of  $\tilde{A}^2 A' \leftarrow \tilde{X}^2 E$  electronic transition<sup>a</sup>, as well as the previously reported microwave<sup>b</sup> data has been performed to obtain the molecular constants of the ground state of these species. For this purpose, a molecular Hamiltonian in which the coordinate system has one axis aligned with the C-O bond of the molecule, was used to analyze the combination differences derived from LIF data together with raw microwave spectrum. The quality of the fit is consistent with the experimental accuracy of both microwave and LIF measurements. The results of the analysis and the correlation of different models are discussed.

---

<sup>a</sup>see abstracts for previous talks in this section

<sup>b</sup>D.Melnik, V.Stakhursky, V.A.Lofovsky, T. A. Miller, B. C. Moore and F. C. De Lucia, *WJ09, 59<sup>th</sup> International Symposium on Molecular Spectroscopy*, June 2004