

## RITZ ASSIGNMENT AND AWAT ANALYSIS OF THE RING-PUCKERING HOT BANDS OF OXETANE

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The oxetane molecule consists of 10 atoms, corresponding to 24 vibrational degrees of freedom. These include one large-amplitude vibration, i.e., the ring puckering, with its fundamental at approximately  $53\text{ cm}^{-1}$ . The first rotationally resolved spectrum of these transitions has been reported recently. We have investigated the oxetane spectrum between  $52$  and  $162\text{ cm}^{-1}$ . Six different  $\Delta v_{\text{rp}} = 1$  rotation-puckering transitions are observed in this region. Preliminary analyses of the lowest three bands have already been presented<sup>abc</sup>. In the present contribution we complete our assignment work in the investigated spectral region. We shall present the results of fitting our FIR assignments and previously published MW and MMW data with the AWAT1 program (Watson Hamiltonian for an asymmetric rotor, A-reduction, programmed by K. M. T. Yamada), and with an equivalent program now incorporated into the Ritz program, for levels up to  $v_{\text{rp}} = 5$ . Watsonian frequency predictions have been used as a feed-back for the assignments in the most dense and entangled spectral regions. An analysis of the dependence of the rotational constants and of the quartic centrifugal distortion constants of the Watsonian on the puckering state will also be attempted.

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<sup>a</sup>M. Winnewisser, M. Kunzmann and M. Lock, 53rd Ohio State University International Symposium on Molecular Spectroscopy, Columbus, June 15–19, 1998, TD04

<sup>b</sup>G. Moruzzi, M. Kunzmann, B. P. Winnewisser and M. Winnewisser, 15th International Conference on High Resolution Molecular Spectroscopy, Prague, Czech Republic, August 30 – September 3, 1998, H7

<sup>c</sup>G. Moruzzi, M. Kunzmann, B. P. Winnewisser and M. Winnewisser, 16th International Colloquium on High Resolution Molecular Spectroscopy, Dijon, France, September 6–10, 1999, F20