HIGH RESOLUTION MID-INFRARED SPECTRUM OF A RING MODE OF JET COOLED TRIMETHYLENE OXIDE

BRYAN J. WINN and MARK D. MARSHALL, *Department of Chemistry-2243, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000*.

The interesting low-frequency ring-pucker vibration in the far infrared region of trimethylene oxide (oxetane) has been the subject of previous, extensive investigations. Ueda and Shimanouchi [a] found that by studying difference bands in the near-IR originating from C-H stretching and ring-puckering modes, values for the puckering energy levels could be obtained that agree well with the far-IR data. Recently, we have obtained a high resolution, diode laser, mid-IR spectrum of trimethylene oxide seeded in a pulsed-jet expansion with argon, (The rotational and vibrational temperatures are approximately 5 K and 50 K, respectively.) in the expectation that the effect of the ring mode on the puckering vibration could be determined. Preliminary analysis of the spectrum yields the following, previously undetermined upper-state rotational constants for this mode, A' = 0.4009 cm^{-1}, B' = 0.3909 cm^{-1}, and C' = 0.2204 cm^{-1}. The band origin ν_0 is determined to be 908.427 cm^{-1}, which represents greater accuracy and precision than the previously available value of 908.7 cm^{-1}. [b]

[a] T. Ueda and T. Shimanouchi, J. Chem. Phys. 47, 5018 (1967).

[b] R. A. Kydd, H. Wieser, and W. Kiefer, Spectrochim. Acta 39A, 173 (1983).