

TUNNELING SPLITTINGS FOR THE NOMINAL OO STRETCHING AND OTHER VIBRATIONS OF TROPOLONE ISOTOPOMERS OBSERVED IN THE LOW FREQUENCY INFRARED SPECTRUM

RICHARD L. REDINGTON and THERESA E. REDINGTON, *Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX 79409*; ROBERT L. SAMS, *Wiley Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352*.

Fourier transform infrared spectra including resolved spectral doublets for many transitions are reported for gaseous tropolone(OH), tropolone(OD), and (18-O,18-O)tropolone(OH) in the 800 to 150 cm^{-1} spectral range. The known zero-point tunneling splitting values $\Delta_0 = 0.974\text{cm}^{-1}$ for tropolone(OH) (Tanaka et al.) and 0.051cm^{-1} for tropolone(OD) (Keske et al.) allow vibrational state-specific tunneling splittings Δ_v to be estimated for fundamentals including the three with the strongest OO stretching displacements [cf. for tropolone(OH) $\nu_{13} = 435.22\text{cm}^{-1}$ with $\Delta_{13} = 1.71\text{cm}^{-1} = 1.76 \Delta_0$, and for tropolone(OD) $\nu_{13} = 429.631\text{cm}^{-1}$ with $\Delta_{13} = 0.311\text{cm}^{-1} = 6.10 \Delta_0$]. In addition to revealing isotope-dependent Δ_v splittings the FTIR study demonstrates effects due to dynamic couplings and potential function anharmonicity. Vibrational reassignments are fostered and the pattern of Δ_v tunneling splitting values is interpreted to underscore the intrinsic multidimensionality of the tautomerization process in this nonrigid 15 atom molecule.