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

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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 $150\mathrm{cm}^{-1}$ spectral range. The known zero-point tunneling splitting values Δ_0 = $0.974\mathrm{cm}^{-1}$ for tropolone(OH) (Tanaka et al.) and $0.051\mathrm{cm}^{-1}$ 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) ν_{13} = $435.22\mathrm{cm}^{-1}$ with Δ_{13} = $1.71\mathrm{cm}^{-1}$ = 1.76 Δ_0, and for tropolone(OD) ν_{13} = $429.631\mathrm{cm}^{-1}$ with Δ_{13} = $0.311\mathrm{cm}^{-1}$ = 6.10 Δ_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.