STATE-SPECIFIC DOUBLETS IN THE FTIR SPECTRUM OF GASEOUS TROPOLONE

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The FTIR absorption spectrum of tropolone vapor at 25°C and 32 m path length has been recorded from 960 to about 700 cm^{-1} at a resolution of 0.0025 cm^{-1}. Twenty-nine cold band and hot band spectral tunneling doublets are assigned. They are marked by sharp type A or type C Q branch spikes. Twenty-six vibration-contortion state-specific tunneling splittings are estimated for tropolone vapor in the ground electronic state. About half of these states show quenching of tunneling due to increased effective barriers and/or path lengths. The COH torsion and contortion fundamentals show resolved Q subband structure indicating vibration-contortion-rotation state-specific behavior. The analysis is guided by predictions of the independent {tunneling skeleton}{tunneling H atom} tautomerization model previously applied to the vibrational spectrum and tautomerization mechanism of tropolone. Several parallels are seen between the vibrational interactions arising in our studies of the tautomerization of tropolone and those appearing in recent articles discussing possible behaviors in the active sites of enzymatic H transfer reactions.