ROTATIONAL SPECTRA OF TWO CONFORMATIONS OF NICOTINE

R. J. LAVRICH,R. D. SUENRAM,D. F. PLUSQUELLIC and S. DAVIS, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg,MD 20899*.

Nicotine consists of two ring systems joined through a C-C bond: N-methylpyrrolidine and pyridine. Conformational flexibility occurs along three coordinates: (1) ring puckering of the pyrrolidine ring, (2) inversion of the N-methyl group between axial and equatorial positions and (3) relative orientation of the two ring systems by rotation about the C-C bond joining them.

Two conformations of nicotine have been assigned using the Fouier-transform microwave spectrometers at NIST. Due to the presence of two ^{14}N nuclei, the resulting rotational transitions appear as broad clusters of partially resolved lines typically spanning 50 kHz to 100 kHz. Approximate line centers were estimated near the center of the resulting hyperfine clusters and fit using the graphical interface fitting program JB95. For conformer I, the fit of 104 a- and c-type transitions yield the following rotational constants; A = 2059.558(3) MHz, B = 579.8571(9) MHz, and C = 549.3357(9) MHz. For conformer II, 70 a- and c-type transitions were measured yielding; A = 2045.661(5) MHz, B = 583.242(1) MHz, and C = 552.844(1) MHz.