A STUDY OF THE CONFORMATIONAL ISOMERISM OF N-PROPYL NITRATE BY MICROWAVE SPECTROSCOPY

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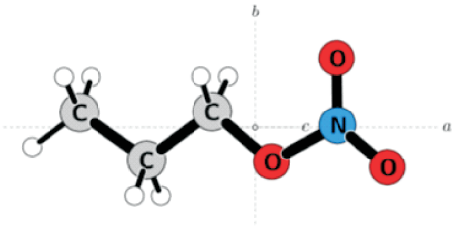
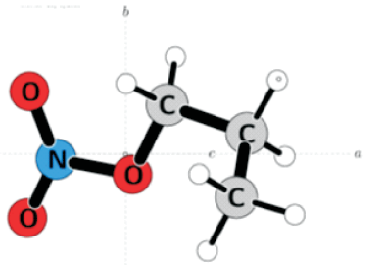
The rotational spectrum of n-propyl nitrate was measured in the frequency range between 6-18 GHz using a Balle-Flygare Fourier transform microwave jet/cavity spectrometer. Parent, ^{13}C and ^{15}N isotopologue transitions for the lower-energy anti-gauche (AG) conformer were found using this instrument. The search for spectra from other conformers was performed using a broadband chirped-pulse jet spectrometer. Transitions from the anti-anti (AA) conformer were observed in this manner. Parent, ^{13}C and ^{15}N isotopologue transitions for the AA conformer were rescanned using the cavity instrument to improve resolution and the signal-to-noise ratio. Rotational, centrifugal distortion, and nuclear electric quadrupole coupling constants for all conformers/isotopologues were fit using Pickett's SPFIT program. The structure of n-propyl nitrate will be discussed in light of these results.



Anti-Anti



Anti-Gauche