FOURIER TRANSFORM MICROWAVE SPECTRA OF n-BUTANOL AND ISOBUTANOL

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We have investigated two butanols, normal (1-butanol) and iso (2-methyl-1-propanol), by Fourier transform microwave spectroscopy, focusing attention mainly to internal motion and rotational isomerism. We anticipate that n-butanol exists in fourteen rotational isomers with the combination of the following conformations: $trans$ (T) and $gauche$ (G) with respect to the CH_3CH_2-CH_2CH_2OH bond, $trans$ (t) and two $gauche$'s (g, g') to the $CH_3CH_2CH_2$-CH_2OH bond, and two or three potential minima in the internal rotation of OH, and that isobutanol in five. We scanned the frequency region from 7 to 25 GHz using a heated nozzle, and detected six and three isomers for n-butanol and isobutanol, respectively: three with Ar as a buffer gas and three with Ne instead of Ar for n-butanol, whereas Ar was employed for isobutanol. The observed spectral lines were assigned by comparing the experimental moments of inertia and the observed spectral intensities with those calculated by $ab\ initio$ MO at the MP2/6-311++G(d,p) level. We thus concluded that five conformers detected for n-butanol are T-form and one G-form and that three observed isomers of isobutanol are $gauche$ with respect to the $H(CH_3)_2C$-CH_2OH bond and one isomer lacking a-type spectra to $trans$ to the CH_2-OH bond.