

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 CH₃CH₂-CH₂CH₂OH bond, *trans* (*t*) and two *gauche*'s (*g*, *g'*) to the CH₃CH₂CH₂-CH₂OH 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(CH₃)₂C-CH₂OH bond and one isomer lacking *a*-type spectra to *trans* to the CH₂-OH bond.