CONFORMATIONS AND BARRIERS TO METHYL GROUP INTERNAL ROTATION IN TWO ASYMMETRIC ETHERS: PROPYL METHYL ETHER AND BUTYL METHYL ETHER

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The conformational preferences of the O-C-C-C unit are important in many biological systems[a] with the unit generally preferring a gauche configuration compared to an anti configuration. Butyl methyl ether and propyl methyl ether provide very simple systems for this phenomenom to manifest. Pure rotational spectra of the title molecules have been recorded using chirped pulse Fourier transform microwave spectroscopy (CP-FTMW). In the case of butyl methyl ether, only one conformer has been observed. This conformer has torsional angles of COCC = 180°, OCCC = 62° and CCCC = 180° (anti-gauche-anti) and rotational constants of A = 10259.4591(33) MHz, B = 1445.6470(13) MHz, and C = 1356.2944(14) MHz. The rotational spectrum was doubled and has been analyzed to produce an effective barrier to methyl group internal rotation of 780(35) cm^{-1}. A prior rotational spectroscopic study on propyl methyl ether had focused only on the high energy anti-anti conformer.[b] We have analyzed spectra from the lowest energy anti-gauche conformer and the spectroscopic constants will be presented. A summary of the differences in conformational energies and methyl group internal rotation barriers for the class of aliphatic asymmetric ethers will be presented.

[a] K. N. Houk, J. E. Eksterowicz, Y.-D. Wu, C. D. Fuglesang, D. B. Mitchell. *J. Am. Chem. Soc.* **115** (4170), 1993.
[b] Hiroshi Kato, Jun Nakagawa, Michiro Hayashi. *J. Mol. Spectrosc.* **80** (272), 1980.