

A COMPARISON OF THE MOLECULAR STRUCTURES OF $C_4H_9OCH_3$, $C_4H_9SCH_3$, $C_5H_{11}OCH_3$, AND $C_5H_{11}SCH_3$ USING MICROWAVE SPECTROSCOPY

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Pure rotational spectra of the title molecules have been recorded using chirped pulse Fourier transform microwave spectroscopy. Under our experimental conditions only one conformer has been observed for each of the four compounds. These conformers have torsional angles of $CXCC = 180^\circ$, $XCCC = 60^\circ$, $CCCC = 180^\circ$, and, for the $C_5H_{11}-X-CH_3$ species, $CCCC_{Methyl} = 180^\circ$. These angles correspond to anti-gauche-anti conformations for the butyl methyl ether/thioether species, and anti-gauche-anti-anti conformations for the pentyl methyl ether/thioether species. Splittings due to the internal rotation of the $X-CH_3$ group are observed in both butyl species but are not observed in the pentyl species. The barrier to the $X-CH_3$ internal rotation has been investigated through spectral analyses and quantum chemical calculations. The differences in the internal rotation barrier between the ethers and thioethers will be discussed and will further be compared to the barriers obtained for similar molecules.