THE PURE ROTATIONAL SPECTRA OF THE TWO LOWEST ENERGY CONFORMERS OF n-BUTYL ETHYL ETHER

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An experimental study has been performed shedding light on the conformational energies of n-butyl ethyl ether. Rotational spectroscopy between 7.8 GHz and 16.2 GHz has identified two conformers of n-butyl ethyl ether, $C_4H_9OC_2H_5$. In these experiments spectra were observed as the target compound participated in an argon expansion from high to low pressure causing molecular rotational temperatures to be below 4 K. For one conformer, 95 pure rotational transitions have been recorded, for the second conformer, 20 pure rotational transitions were recorded. Rotational constants and centrifugal distortion constants are presented for both butyl ethyl conformers. The structures of both conformers have been identified by exploring the multi-dimensional, molecular potential energy surface using ab initio calculations. From the numerous low energy conformers identified using ab initio methods, the three lowest conformers were pursued at increasingly higher levels of theory, i.e. complete basis set extrapolations and also coupled cluster methods. The two conformers observed experimentally are only revealed to be the two lowest energy conformers when high levels of quantum chemical methodologies are employed.