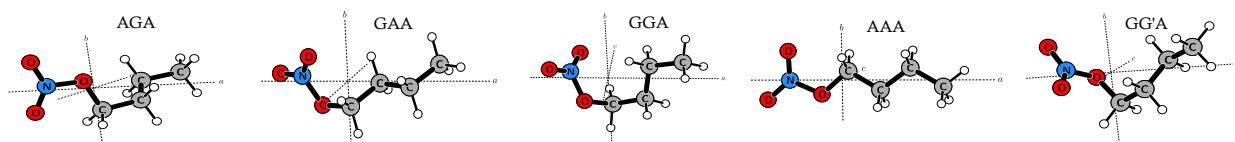


CONFORMATIONAL ISOMERISM OF N-BUTYL NITRATE STUDIED BY MICROWAVE SPECTROSCOPY

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The rotational spectrum of n-butyl nitrate was measured with a chirped pulse Fourier transform microwave spectrometer over the range of 7-13 GHz. This allowed for the identification and assignment of five conformers, AGA, GAA, GGA, AAA, and GG'A with intensity ratios of approximately 1 : 0.2 : 0.2 : 0.1 : 0.1. These conformers were subsequently investigated by Balle-Flygare Fourier transform microwave spectroscopy in order to resolve the nuclear electric quadrupole coupling splitting and for further transitions to be collected, allowing improved fitting. Isotopic substitutions at natural abundance were also observed for the AGA conformer. Quantum chemical calculations reveal that the AGA conformer is the lowest in energy. A variety of computational methods were used to explore the energy ordering and barriers between inter-conversion of the lowest lying energy conformers. This work extends a series of other alkyl nitrate works studied by microwave and mm-wave spectroscopy.^{a b c}



^aMethyl Nitrate; W.B. Dixon, E.B. Wilson, *J. Chem. Phys.*, **35**, 191 (1961)

^bEthyl Nitrate; D.G. Scroggrin, J.M. River, E.B. Wilson, *J. Chem. Phys.*, **60**, 1376 (1974); J. Thomas, I. Medvedev, D. Dolson, ISMS 2014

^cn-Propyl Nitrate; W. Orellana, S.L. Stephens, S.E. Novick, S.A. Cooke, C. Brauer, T.A. Blake, ISMS 2019