

Accepted Manuscript

Conformational Preferences and Internal Rotation of Methyl Butyrate by Microwave Spectroscopy

Alicia O. Hernandez-Castillo, Chamara Abeysekara, Brian M. Hays, Isabelle Kleiner, Ha Vinh Lam Nguyen, Timothy S. Zwier

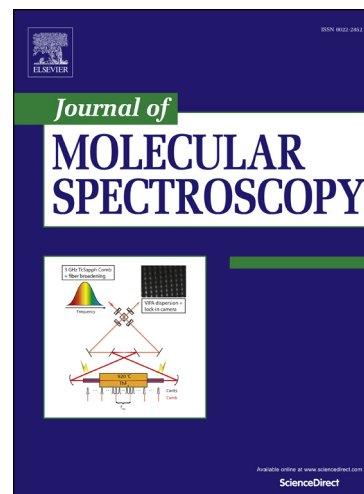
PII: S0022-2852(17)30050-4
DOI: <http://dx.doi.org/10.1016/j.jms.2017.03.016>
Reference: YJMSP 10873

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 29 January 2017
Revised Date: 3 March 2017
Accepted Date: 15 March 2017

Please cite this article as: A.O. Hernandez-Castillo, C. Abeysekara, B.M. Hays, I. Kleiner, H.V.L. Nguyen, T.S. Zwier, Conformational Preferences and Internal Rotation of Methyl Butyrate by Microwave Spectroscopy, *Journal of Molecular Spectroscopy* (2017), doi: <http://dx.doi.org/10.1016/j.jms.2017.03.016>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Conformational Preferences and Internal Rotation of Methyl Butyrate by Microwave Spectroscopy

Alicia O. Hernandez-Castillo¹, Chamara Abeysekara¹, Brian M. Hays¹,
Isabelle Kleiner², Ha Vinh Lam Nguyen^{2*}, and Timothy S. Zwier^{1*}.

¹Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907, USA

²Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS UMR 7583, Université Paris-Est Créteil, Université Paris Diderot, 61 avenue du Général de Gaulle, F-94010 Créteil cedex, France

Abstract

The broadband rotational spectrum of methyl butyrate from 8-18 GHz, recorded using a chirp-pulsed Fourier transform microwave (FTMW) spectrometer, was combined with high resolution FTMW measurements over the 2-26.5 GHz region to provide a comprehensive account of its microwave spectrum under jet-cooled conditions. Two low-energy conformers, one with a fully extended, heavy-atom planar *anti/anti* structure (**a,a**), and the other with a *gauche* propyl chain (**g±,a**), were assigned in the spectrum. Torsional A/E splittings due to the internal rotation of the methoxy methyl group were resolved for both lower energy conformers, and were fitted using the program *XIAM* and *BELGI*, providing an estimate of the barrier to methyl internal rotation of $V_3 \approx 420 \text{ cm}^{-1}$. The conformational landscape of methyl butyrate occurs on a two-dimensional potential energy surface, which was mapped out by quantum chemical calculations at the B2PLYP-D3BJ/aug-cc-pVTZ level of theory. The low torsional barrier about the C–C(=O)O bond leads to collisional removal of population originally in the (**a,g±**) and (**g±,g±**) minima into the (**a,a**) and (**g±,a**) minima, respectively, during the cooling in the expansion. Analysis of experimental intensities in the spectrum provide percent populations downstream in the expansion of $41 \pm 4 \%$ (**a,a**), and $59 \pm 6 \%$ (**g±,a**).

*To whom correspondence should be addressed. E-mail: lam.nguyen@lisa.u-pec.fr, zwier@purdue.edu

Key Words: methyl butyrate, rotational spectroscopy, large amplitude motions, conformational analysis

to be submitted to the Journal of Molecular Spectroscopy
18 pages, 3 Tables, 5 Figures

Download English Version:

<https://daneshyari.com/en/article/5413972>

Download Persian Version:

<https://daneshyari.com/article/5413972>

[Daneshyari.com](https://daneshyari.com)