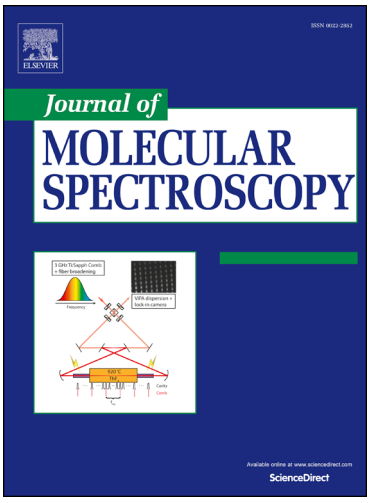

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PII: S0022-2852(17)30237-0
DOI: https://doi.org/10.1016/j.jms.2017.09.008
Reference: YJMSP 10957

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 15 May 2017
Revised Date: 21 September 2017
Accepted Date: 21 September 2017

Please cite this article as: L. Ferres, W. Stahl, I. Kleiner, H. Vinh Lam Nguyen, The Effect of Internal Rotation in *p*-Methyl Anisole Studied by Microwave Spectroscopy, *Journal of Molecular Spectroscopy* (2017), doi: https://doi.org/10.1016/j.jms.2017.09.008

The Effect of Internal Rotation in *p*-Methyl Anisole Studied by Microwave Spectroscopy

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Keywords: structure determination, phenyl ring, rotational spectroscopy, microwave spectroscopy, large amplitude motion, internal rotation

Abstract

The Fourier transform microwave spectrum of *p*-methyl anisole, $CH_3C_6H_4OCH_3$, was measured in the frequency range from 2 to 26.5 GHz under molecular jet conditions. The conformer analysis yielded only one stable conformer, in which all heavy atoms are co-planar, and which was identified after analyzing the spectrum by comparison with the results from quantum chemical calculations. The barrier of the V_3 potential of the ring methyl rotor was found to be 49.374548(1) cm^{-1}, and was compared with that found in other para-substituted toluenes as well as in *o*-methyl anisole. A comparison between two theoretical approaches treating internal rotations, the rho axis method (program *BELGI-*C_s) and combined axis method (program *XIAM*), is also performed.