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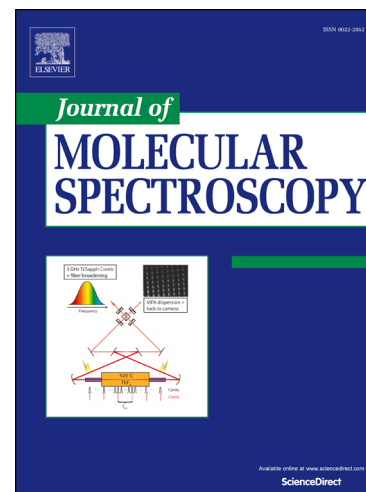
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The Microwave Spectrum of Phenylpropionic Acid

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Abstract

The microwave spectrum for phenylpropionic acid was measured in the 4.8-10 GHz frequency range using a Flygare-Balle type pulsed-beam Fourier transform microwave spectrometer. 34 a-type and 11 b-type rotational transitions were measured and assigned for the most abundant isotopologue. Based on the measured transitions, the rotational constants were determined to be $A = 3859.823(33)$ MHz, $B = 443.54379(10)$ MHz, and $C = 398.09128(13)$ MHz. The centrifugal distortion constants were determined to be $D_J = 0.00286(66)$ kHz and $D_{JK} = 0.1030(82)$ kHz. DFT(B3LYP) and MP2 calculations were performed with aug-cc-pVTZ basis and the calculated rotational constants compare well with experimentally determined values.

Keywords: Microwave Spectroscopy; Rotational Constants; Molecular Structure
Calculations

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