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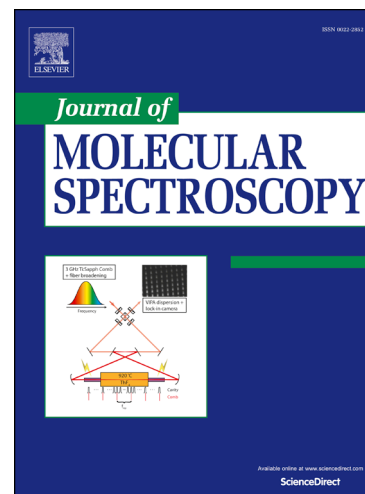
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Rotational Spectra of 4,4,4-Trifluorobutyric Acid and the 4,4,4-Trifluorobutyric Acid-Formic Acid Complex

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ABSTRACT: The pure rotational spectra of 4,4,4-trifluorobutyric acid, $\text{CF}_3\text{CH}_2\text{CH}_2\text{COOH}$, and its complex with formic acid were studied by a pulsed nozzle, chirped-pulse Fourier transform microwave spectrometer in the frequency range of 7-13 GHz. The rotational constants and centrifugal distortion constants were determined for the first time. Quantum chemical calculations were carried out exploring possible conformations of 4,4,4-trifluorobutyric acid and the structure of the 4,4,4-trifluorobutyric acid-formic acid complex using B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVTZ calculations. Only one conformer was observed for 4,4,4-trifluorobutyric acid and its complex with formic acid, in agreement with the calculations.

KEY WORDS: microwave spectroscopy, chirped pulse, *ab initio* calculations, structure, 4,4,4-trifluorobutyric acid, 4,4,4-trifluorobutyric acid-formic acid

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