ROTATIONAL SPECTRA OF 4,4,4-TRIFLUOROBUTYRIC ACID AND THE 4,4,4-TRIFLUOROBUTYRIC ACID-FORMIC ACID COMPLEX

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The pure rotational spectra of 4,4,4-trifluorobutyric acid, $CF_3CH_2CH_2COOH$, and its complex with formic acid, were studied by a pulsed nozzle, chirped-pulse Fourier transform microwave spectrometer in the frequency range of 8-12 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 and the structure of the 4,4,4-trifluorobutyric acid-formic acid complex using B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVTZ calculations. The experimental spectroscopic constants are compared to those obtained from $ab\ initio$ calculations.