CHIRPED-PULSE FTMW SPECTRA OF FLUORINATED MOLECULES: 1,1,1-TRIFLUORO-2-BUTANONE AND 3,3,3-TRIFLUOROPROPIONIC ACID

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The pure rotational spectra of 1,1,1-trifluoro-2-butanone and of 3,3,3-trifluoropropionic acid have been investigated using the new chirped-pulse Fourier transform microwave (cp-FTMW) spectrometer at the University of Manitoba. Transitions due to the monosubstituted isotopologues with ^{13}C in natural abundance were assigned using spectra from both the broadband instrument and the conventional Fourier transform microwave (FTMW) spectrometer. The observed spectra are consistent with planar structures of the species in the ground vibrational states. Quantum chemistry calculations, at the MP2/6-311++G(d,p) level, have been carried out in order to obtain information about the structure, relative stability and difference in populations of the conformers under study.