A PURE ROTATIONAL STUDY OF TWO NEARLY-EQUIVALENT STRUCTURES OF HEXAFLUOROACETONE IMINE

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The rotational spectrum of hexafluoroacetone imine, $(CF_3)_2C{=}NH$, has been observed on a chirped pulse Fourier transform microwave spectrometer. Each of the singly substituted ^{13}C isotopologues and the ^{15}N isotopologue have been observed in natural abundance on a Balle-Flygare cavity type spectrometer. The r_0 and r_S structures have been determined for the heavy atom backbone. Both *a*-type and *b*-type transitions exhibit doubling with a spacing of about 15 kHz to 40 kHz. A change in an ∠NCCF dihedral angle appears to be the source of the doubling, and each set of transitions can be fit to two unique conformers of hexafluoroacetone imine. This structural difference produces two sets of rotational constants that have differences in experimental values on the order of kHz.