METHYL GROUP INTERNAL ROTATION IN THE PURE ROTATIONAL SPECTRUM OF 1,1-DIFLUOROACETONE

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We have used chirped pulse Fourier transform microwave spectroscopy to record the pure rotational spectrum of the title molecule. The spectrum was doubled owing to the internal rotation of the methyl group. The spectrum has been assigned and two approaches to the spectral analysis have been performed. In the first case, the A and E components were fit separately using a principal axis method with the SPFIT code of Pickett. In the second case, the A and E states were fit simultaneously using the ERHAM code. For a satisfactory analysis of the spectral data it has been found that the choice of Hamiltonian reduction, i.e. Watson A or S, is very important. The barrier to the internal rotation has been determined to be 261.1(8) cm^{-1} and it will be compared to that of acetone and other halogenated acetone species recently studied in our laboratory.