MICROWAVE SPECTROSCOPY OF 1,1-DIFLUOROCYANOMETHYL RADICAL, CF₂CN

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The pure rotational spectrum of 1,1-difluorocyanomethyl radical, CF₂CN, was measured between 7.0 and 26.5 GHz using a Fabry-Pérot cavity Fourier transform microwave (FP-FTMW) spectrometer. The a-type (K_a = 0, 1, 2) paramagnetic transitions were observed and assigned. The spectroscopic constants of CF₂CN were fit by Pickett’s SPFIT suite of programs. The experimentally determined rotational constants are: A₀ = 11010.58(1) MHz, B₀ = 4081.6917(1) MHz, and C₀ = 2989.9589(1) MHz. These constants are in a good agreement with the predicted values from density functional theory (DFT) calculation, UB3LYP/aug-cc-pVQZ. The inertial defect, Δ = -0.69 amuÅ², indicates that CF₂CN has a non-planar geometry. This is not the case in its isoelectronic analog, 1,1-difluoropropargyl, CF₂CCH.