MICROWAVE SPECTROSCOPY OF 1,1-DIFLUOROCYANOMETHYL RADICAL, $\dot{C}F_2CN$

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The pure rotational spectrum of 1,1-difluorocyanomethyl radical, $\dot{C}F_2CN$, 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 $\dot{C}F_2CN$ were fit by Pickett's SPFIT suite of programs. The experimentally determined rotational constants are: A_0 = 11010.58(1) MHz, B_0 = 4081.6917(1) MHz, and C_0 = 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 amuÅ^2, indicates that $\dot{C}F_2CN$ has a non-planar geometry. This is not the case in its isoelectronic analog, 1,1-difluoropropargyl, $\dot{C}F_2CCH$ [a].

[a] L. Kang, S. E. Novick; *J. Chem. Phys.* **125**, 054309, (2006)