THE MICROWAVE SPECTRUM OF THE DIFLUOROCYANOMETHYL RADICAL, $\dot{C}F_2CN$

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The pure rotational spectrum of the open shell difluorocyanomethyl radical, $\dot{C}F_2CN$, has been measured using two Balle-Flygare-type cavity Fourier-Transform-Microwave (FTMW) spectrometers both equipped with pulsed discharged nozzles. A total of 156 transitions (from N = 1 – 0 to 6 – 5, and K_a = 0, 1, 2, 3) in the electronic ground state were observed between 6.5 GHz and 38.4 GHz with a typical linewidth of approximately 5 kHz full-width-half-maximum. A Hamiltonian that included semi-rigid rotor, spin-rotation, and nuclear hyperfine parameters was fit to the observed data set and these parameters have been interpreted and compared to similar radicals. Excellent agreement between experimental and uB3LYP/aug-cc-pVQZ calculated rotational constants, the experimental inertial defect, -0.6858(2) uÅ^2, and the failure of a coupling scheme in which the fluorine nuclei are treated as identical and related by a C_{2v} symmetry axis combine to indicate a nonplanar structure for the $\dot{C}F_2CN$ radical.