THE PURE ROTATIONAL SPECTRUM OF PERFLUOROOCTANONITRILE, $C_7F_{15}CN$, STUDIED USING CAVITY- AND CHIRPED-PULSED FOURIER TRANSFORM MICROWAVE SPECTROSCOPIES

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Fourier transform rotational spectroscopy has been used to collect the spectrum of perfluorooctanonitrile. The spectrum was weak and only one conformer was observed. The assigned spectrum currently consists of both a- and b-type transitions spanning J = 8 to 40. The rotational constants are small, A = 681.37155(18) MHz, B = 126.116097(48) MHz, and C = 124.284824(49) MHz. The spectroscopic constants together with quantum chemical calculations have been used to identify the structure of the observed conformer. Notably the helical nature of the perfluoro alkyl chain is fully in evidence. Further calculations confirm that the nitrogen quadrupole coupling tensor is such that nitrogen hyperfine splitting will not be observable at the high J transitions recorded in our experiments. Spectroscopic constants and a discussion of the molecular structure will be presented.