FAR INFRARED LMR SPECTROSCOPIC MEASUREMENTS OF THE QUASI-LINEAR MOLECULE DCCN

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FIR laser magnetic resonance spectra of the quasilinear free radical DCCN, produced by fluorine atom abstraction of deuterium from deuterated acetonitrile (CD_3CN), has been measured at laser wavelengths between 46 and 136 μm. The spectra have been analyzed using a triplet asymmetric rotor Hamiltonian. Included in the fitting data set are the millimeter wave data [a] for the ν_5 = 0 and 1 levels. This analysis has allowed the determination of some Zeeman constants and the refinement of the molecular constants of DCCN.

[a] M. C. McCarthy, C. A. Gottlieb. A. L. Cooksy, and P. Thaddeus, J. Chem. Phys. 103, 7779, (1995).