THE ν_5 BAND OF CH_3CD_3: HIGH RESOLUTION SPECTRUM AND GLOBAL THREE-BAND ANALYSIS

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The lowest frequency parallel fundamental band ν_5 of CH_3CD_3 near 900 cm^{-1} was measured at low temperature with a resolution of 0.0021 cm^{-1} using Fourier transform spectroscopy. The band is weak, and an absorption path of 60m was used. Large torsional splittings due to inter-vibrational coupling have been observed. Building on previous studies of the torsional levels in the ground vibrational state and and in the methyl rocking state ($\nu_{12} = 1$), a three-band analysis including this most recent data has been completed. The combined data set of more than 2,200 frequencies was fitted to within experimental accuracy using a 43-term model Hamiltonian. The results were found to bear a striking resemblance to those of an earlier, analogous study of CH_3SiH_3. In both cases, Fermi coupling between the ($\nu_5 = 1$) state and the ground state was found to be the dominant interaction responsible for the observed torsional splittings. Inclusion of this coupling results in a simplification of the ground-state Hamiltonian, so that only eight additional terms were required with the introduction of the ν_5 band.