

PRELIMINARY MODELING OF CH₃D FROM 4000 TO 4550 cm⁻¹

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New line positions, intensities and quantum assignments were obtained for ¹²CH₃D between 4000 and 4550 cm⁻¹ using high resolution spectra recorded with two Fourier transform spectrometers and enriched gas samples (98%-Deuterium) at room and cold (80 K) temperatures. The effective Hamiltonian and the effective Dipole moment expansions were expressed in terms of irreducible tensor operators adapted to symmetric top molecules. Over 4000 positions and 1300 line intensities in this region were reproduced with RMS values of 0.007 cm⁻¹ and 14%, respectively. With these new results included, the simultaneous modeling of the four lowest polyads of ¹²CH₃D from 0 to 4550 cm⁻¹ [Ground State, Triad (1000–1600 cm⁻¹), Nonad (2000 to 3300 cm⁻¹), and Enneadecad (3400 to 4600 cm⁻¹)] permitted over 19000 observed positions to be fitted within 0.003 cm⁻¹.^a

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