VIBRATIONAL OVERTONES OF SOME DEUTERATED PROPANES

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The CH stretching overtone spectra of two deuterated propanes, CD_3CHDCD_3 and $CD_3CH_2CD_3$, have been measured between 2800 and 16000 cm⁻¹. They evidence Fermi resonances in all the spectra wavenumbers. A reconstruction of all the overtone spectra of the two molecules with the same anharmonic potential indicates that Fermi resonances occurs principally with combination states involving angle deformations inside the methylene chromophore. The Fermi resonances with combination states involving CC stretching are modelled but seem to be weaker. Couplings with the methyl modes occurs only incidently and have only effects on some band intensities.