RE-INVESTIGATION OF THE ν_3-ν_6 CORIOLIS INTERACTION IN TRIFLUOROIODOMETHANE

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We re-investigate the ν_3-ν_6 Coriolis interaction in CF_3I as part of the testing and evaluation of a newly constructed chirped-pulse Fourier-transform microwave (CP-FTMW) spectrometer in the 2–8 GHZ region. We observe vibrational satellites and ^{13}C peaks in natural abundance. We report low-*J* vibrational satellites for the ν_6 level for the first time. The observed frequencies deviate significantly from the prediction of of the fit model reported by Walters and Whiffen[a] and more recently by Willeart *et al.*,[b] which motivates us to re-evaluate the fit model using the combined dataset of microwave and millimeter-wave transition frequencies. The results of our fit to the combined dataset will be presented. The analysis allows us to make an improved determination of ν_6 frequency, which has never been observed directly by IR spectroscopy.

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[a]Walters, S.W. and D.H. Whiffen, Rotational spectrum of trifluoroidomethane. Journal of the Chemical Society, Faraday Transactions 2: Molecular and Chemical Physics, 1983. 79(6): p. 941-949.

[b]Willaert, F., et al., High resolution investigation of the v3 band of trifluoromethyliodide (CF3I). Journal of Molecular Spectroscopy, 2015. 315: p. 16-23.