APPROACHING THE FREE ROTOR LIMIT: EXTREMELY LOW METHYL TORSIONAL BARRIER OBSERVED IN THE MICROWAVE SPECTRUM OF 2,4-DIMETHYLFLUOROBENZENE

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Dimethylfluorobenzene isomers (DMFB) are aromatic heterocyclic volatile organic compounds (VOCs). These VOCs are methylated toluene derivatives, one of the most prevalent aromatic hydrocarbons in the troposphere and considered as atmospheric pollutants. The spectrum of 2,4-dimethylfluorobenzene (24DMFB) has been recorded between 2.0 and 26.5 GHz using the LISA molecular jet Fourier transform microwave spectrometer with an estimated measurement accuracy of 4 kHz. Due to the internal rotation of two inequivalent methyl groups, all rotational transitions split into quintets. The spectral analysis was challenging due to the fact that one of the two methyl groups in 24DMFB have a torsional barrier of about 1 cm^{-1}, leading to large splittings between the torsional species. Using the *SFLAMS*[a] program, the assignments were checked by fitting separately each of the five torsional species. A global fit of 813 torsional lines was performed using the programs *XIAM*[b], *ntop*[c] and *BELGI-Cs-2Tops*[d] giving standard deviations of 578.4 kHz, 13.3 and 4.7 kHz, respectively. The torsional barriers of the methyl groups in the *ortho* and *para* positions were determined to be 226.2087(16) and 1.4387(58) cm^{-1}, respectively.[e]

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