LOW BARRIERS TO INTERNAL ROTATION IN THE MICROWAVE SPECTRUM OF 2,5-DIMETHYLFLUOROBENZENE

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We investigated the rotational spectrum of 2,5-dimethylfluorobenzene which contains two coupled large amplitude motions of the methyl groups. The methyl internal rotations can be used to examine the molecular structure[1] as steric and electronic environments around the methyl group affect its torsional barrier. Electronic properties play a particularly important role in aromatic molecules with the presence of a π-conjugated double bond system. 2,5-dimethylfluorobenzene was studied in the frequency range from 2 GHz to 26.5 GHz using a pulsed molecular jet Fourier transform microwave spectrometer. The experimental results are combined with quantum-chemical calculations. The internal rotations of two inequivalent methyl groups with low torsional barriers (around 16 cm^{-1} and 226 cm^{-1}, respectively) lead to the splitting of all rotational transitions into quintets, resulting in separations of hundreds of MHz in the microwave spectrum. Spectral analysis and modeling of the observed splittings were performed using the programs *XIAM*[2] and *BELGI-C_s-2Tops*,[3] whereby the latter achieved measurement accuracy. The experimental results were compared with those of quantum chemistry calculations.

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