

**COUPLED METHYL INTERNAL ROTATIONS IN HETEROCYCLIC
MOLECULES: THE MICROWAVE SPECTRA OF
2,4-DIMETHYLPYRROLE AND 2,3-DIMETHYLFURAN**

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The rotational spectra of the three isomers of methylpyrrole^{1,2,3} and 2,5-dimethylpyrrole⁴ as well as those of the two isomers of methylfuran^{5,6} and 2,5-dimethylfuran⁷ have been investigated. In both series, the effects of methyl internal rotations were observed. The barrier hindering the methyl torsion are mainly impacted by the positions of the methyl groups on the aromatic ring, which do not only reflect the steric but also electronic properties of the molecules.

In the present work, we studied two further cases with two methyl tops, 2,3-dimethylfuran and 2,4-dimethylpyrrole. The spectra were measured using a molecular jet Fourier transform microwave spectrometer operating from 2 to 26.5 GHz. The barriers to internal rotation were determined for both molecules. The hyperfine splittings due to the quadrupole coupling of the ¹⁴N nucleus in 2,4-dimethylpyrrole were fully resolved. The quadrupole coupling constants χ_{aa} , χ_{bb} , and χ_{cc} were determined with high accuracy and calculated well using Bailey's method.⁸ The obtained barriers were finally compared to those found for other molecules in the series to observe a trend for methyl internal rotational barriers in pyrrole and furan derivatives.

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