METHYL INTERNAL ROTATION AND $^{14}$N QUADRUPOLE COUPLING IN 2-METHYLPYRROLE AND 2,5-DIMETHYL PYRROLE: A COMPARATIVE STUDY

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The torsional barriers of methyl groups attached to aromatic compounds are hard to predict. In addition, studying the $^{14}$N quadrupole hyperfine structure gives us information on the electric field gradient at the site of the $^{14}$N nucleus and consequently on the nature of its chemical bonds. All these reasons motivated us to investigate two methyl derivatives of pyrrole, 2-methylpyrrole (2MP) and 2,5-dimethylpyrrole (25DMP), using a combination of quantum chemical calculations and Molecular Jet Fourier-Transform MicroWave (MJ-FTMW) spectroscopy.

The microwave spectra of 2MP and 25DMP were recorded using two MJ-FTMW spectrometers operating in the frequency ranges from 2.0 to 26.5 GHz$^1$ and 26.5 to 40.0 GHz$^2$. The splittings arising from the internal rotation of the methyl groups as well as the $^{14}$N quadrupole hyperfine structure were successfully assigned. All spectra of 2MP and 25DMP are presently analyzed using the programs XIAM$^3$ and BELGI-$C_s$-hyperfine for 1 top$^4$ and 2 tops, respectively. From the splittings due to the internal rotation of the methyl groups, the barrier heights of the methyl group in 2MP and 25DMP can be obtained. The $^{14}$N quadrupole coupling constants are accurately determined.

In both cases, 2MP and 25DMP, the methyl groups are adjoining the nitrogen atom, therefore a comparison of the respective $V_3$ values can be made. Due to the $C_s$ symmetry of ring systems, the $c$ axes are principal axes of both the inertia and the quadrupole coupling tensor, and the values of $\chi_{cc}$ could be directly compared with other aromatic five-membered rings. Different signs of the $\chi_{cc}$ constant can be explained by the different chemical bond situations.

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