LARGE AMPLITUDE TORSIONS IN NITROTOLUENE ISOMERS STUDIED BY ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMISTRY CALCULATIONS

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The monitoring of gas phase mononitrotoluenes is crucial for defence, civil security and environmental interests since they are used as taggant for TNT detection. Rotational spectra of the three isomers of nitrotoluene have been recorded at low and room temperatures using a supersonic jet Fourier Transform microwave (MW) spectrometer and a millimeter-wave frequency multiplier chain, respectively. Supported by quantum chemistry calculations, the spectral analysis of pure rotation lines in the vibrational ground state has allowed to characterise the rotational energy, the hyperfine structure due to the ^{14}N nucleus and the internal rotation splittings arising from the methyl group. An anisotropic internal rotation of coupled -CH_3 and -NO_2 torsional motions was identified for the ortho isomer by quantum chemistry calculations and discussed from the results of its MW analysis. The study of the internal rotation splittings in the spectra of three NT isomers allowed to characterise the internal rotation potentials of the methyl group and to compare them with other mono-substituted toluene derivatives in order to study the isomeric influence on the internal rotation barrier. [b, c]

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[b] Roucou *et al., CHEMPHYSCHEM,* **21(22), 2523-2538, (2020).**

[c] Roucou *et al., CHEMPHYSCHEM,* **19, 1056-1067, (2018).**