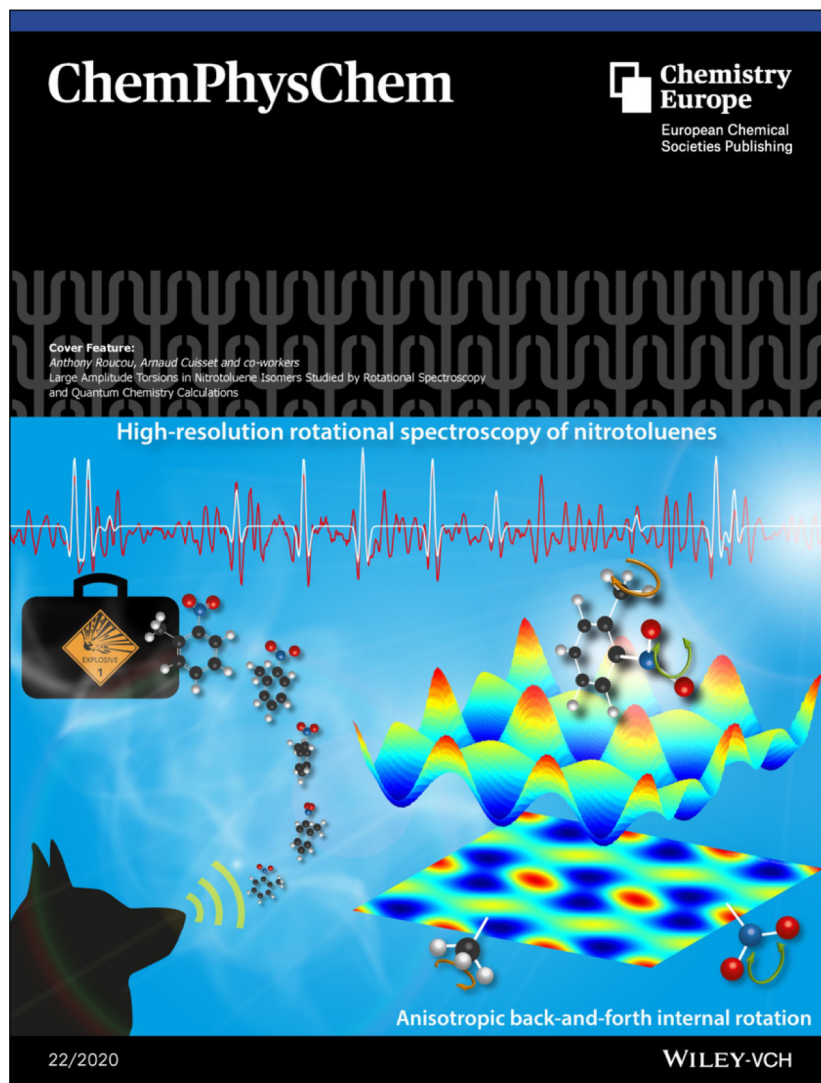


P5285: LARGE AMPLITUDE TORSIONS IN NITROTOLUENE ISOMERS STUDIED BY ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMISTRY CALCULATIONS



None of the actual methods allow an unambiguous detection of explosive and their taggants in the gas phase!

We present the 1st gas phase high resolution measurements of NT isomers using jet-cooled FTMW and room temperature mm-wave rotational spectroscopies supplemented with quantum chemistry calculations.

Assignments were complicated due to several effects:

- hyperfine splitting resolved in MW
- CH₃ internal rotation splitting resolved in MW and MMW (for 3-NT & 4-NT) and in MW (for 2-NT)
- NO₂ torsional splitting resolved in MW 2-NT

Several codes were required according to the barrier (BELGI, RAM36, XIAM,...)

Quantum chemistry calculations revealed a unexpected anisotropic behaviour with a back-and-forth movement of the methyl/nitro double torsion.

A specific hamiltonian has to be used for a reliable assignment of the 2-NT MW spectrum