

Internal rotation potential and pure rotational spectroscopy of 3-nitrotoluene

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Nitrotoluene compounds are semi-volatile organic molecules of environmental and military interest. They are widely used in dyestuff, pesticides, rubber and pharmaceutical manufacturing [1]. Persistent in natural conditions, they are difficult to oxidize due to the strong electron-withdrawing effect of the nitro group [2]. Moreover, they are derivative products and taggants of the very well-known explosive TNT.

In a previous study, gas phase Far-IR vibrational cross-sections have been measured using FT-FarIR spectroscopy based on the AILES beamline of the SOLEIL synchrotron facility [3]. Even at the maximum resolution of the interferometer, it was not possible to resolve rotationally the Far-IR spectra at room temperature. In this study, we present the first high resolution analysis of 3-nitrotoluene (3-NT).

Pure rotational measurements were performed in jet-cooled conditions and at room temperature using the Fourier Transform MicroWave (FTMW) spectrometer [4] located at the PhLAM (2-20 GHz range) and the submm/THz frequency multiplication chain [5] located at the LPCA (70-220 GHz range), respectively.

The FTMW data have been analysed using the BELGI-Cs program [6] taking into account both the internal rotation motion and the hyperfine structure of 3-NT. The FTMW measurements allowed a first determination of the rotational constants, of the quartic centrifugal distortion constants, of the hyperfine structure constants due to the nuclear quadrupole coupling of nitrogen and of the internal rotation parameters characterized by a very low barrier height (calculated at about 6 cm^{-1}).

In the submillimeter domain, a weak and very congested spectrum with many blended lines was observed because of the high number of low-frequency vibrational and torsional excited states. The analysis has been achieved by combining Kisiel's (ASCP and SVIEW) and Pickett's (SPFIT SPCAT) programs in support to the use of the BELGI-Cs program. The analysis permitted a determination of high order internal rotation parameters, and therefore a determination of the internal rotation potential.

References

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