MICROWAVE SPECTRA OF DINITROTOLUENE ISOMERS: A NEW STEP TOWARDS THE DETECTION OF EXPLOSIVE VAPORS

MHAMAD CHRAYTEH, *Laboratoire de Physico-Chimie de l'Atmosphère, Université du Littoral Côte d'Opale, Dunkerque, France*; PASCAL DRÉAN, MANUEL GOUBET, *UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, University of Lille, CNRS, F-59000 Lille, France*; ANTHONY ROUCOU, ARNAUD CUISSET, *Laboratoire de Physico-Chimie de l'Atmosphère, Université du Littoral Côte d'Opale, Dunkerque, France*.

The spectroscopic characterization of explosives taggants, like nitrotoluenes (NT) used for the TNT detection, is a research subject of growing interest. Recently, the spectroscopic studies of the three NT isomers in the microwave and millimeter-wave ranges were reported[1,2]. We present the gas-phase rotational spectroscopic study of weakly volatile dinitrotoluenes (DNT) isomers. The pure rotational spectrum of, 2,4-DNT and 2,6-DNT was recorded in microwave range (2-20 GHz) using a Fabry-Perot Fourier-transform microwave (FP-FTMW) technique coupled to a pulsed supersonic jet. The spectral analysis was supported by quantum chemical calculations carried out at the B98/cc-pvtz and MP2/cc-pvtz levels of theory. The spectra of DNT were complicated by the presence of two ^{14}N nucleus giving rise to congested hyperfine structures. The methyl group internal rotation barriers were calculated at the B98/cc-pvtz level of theory to be V_3=563 $\mathrm{cm}^{-1}$and V_3= 696 $\mathrm{cm}^{-1}$for 2,4- and 2,6-DNT, respectively. Although no splitting due to internal rotation was observed for 2,6-DNT, several splittings were observed for 2,4-DNT and their analysis in under progress. The semi-rigid and the nuclear quadrupole couplings descriptions obtained from the spectral analysis are presented. An anisotropic internal rotation of the coupled -$\mathrm{CH_3}$ and -$\mathrm{NO_2}$ torsional motions, as already mentioned for 2-NT[1], will be discussed for 2,4-DNT.

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