Gas-phase vibrational spectroscopy of explosive derivatives and safe taggants

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The high performances of the AILES beamline of SOLEIL [1] allow studying the gas-phase vibrational spectra of weakly volatile compounds. Between 2008 and 2010 we recorded and analyzed the THz/Far-IR spectra of phosphorous-based nerve agents thanks to sufficient vapour pressures from liquid samples at room temperature [2,3]. Recently, we extended these experiments towards the vibrational spectroscopy of vapour pressures from solid samples. This project is quite challenging since we target lower volatile compounds, so this requires very high sensitive spectrometers. Moreover a specially designed heated multipass-cell has been developed for the gas-phase study of very weak vapor pressures. From the skills acquired during initial studies and recent experiments performed on AILES with solid PAHs [4], we have recorded and assigned the gas-phase vibrational fingerprints from the THz to the NIR spectral domain (10-4000 cm-1) of a set of targeted nitro-derivatives. The study was focused onto the para-, ortho-mononitrotoluene (p-NT, o-NT), the 1,4 dinitrobenzene (1,4 DNB), the 2,3-dimethyl-2,3-dinitrobutane (DMNB), and 2,4 and 2,6-dinitrotoluene (2,4-2,6 DNT), which are TNT derivatives widely used for the detection of commercial explosives or taggants usually added to the identification of plastic explosives from their vapour detection. Therefore, there is a continuous interest for their detection and identification in realistic conditions via optical methods. A first step consists in the recording of their gas-phase vibrational spectra. These expected spectra focused onto molecules involved into defence and security domains are not yet available to date and will be very useful for the scientific community.
A first database of explosive derivatives and taggants is under construction. The results obtained in gas-phase are compared with more studied vibrational spectra of taggants diluted in pellets and with harmonic and anharmonic DFT calculations. *This work is supported by the contract ANR-11-ASTR-035-01 in collaboration with the EADS company.*

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