GAS PHASE VIBRATIONAL SPECTROSCOPY OF WEAKLY VOLATIL SAFE TAGGANTS USING A SYNCHROTRON SOURCE

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The high performances of the AILES beamline of SOLEIL allow to study at medium resolution (0.5 cm^{-1}) the gas phase THz vibrational spectra of weakly volatil 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[a] [b]. 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, and so requires very high sensitive spectrometers. Moreover a specially designed heated multipass-cell have been developped for the gas phase study of very weak vapor pressures. Thanks to skills acquired during initial studies and recent experiments performed on AILES with solid PAHs[c], 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 safe taggants widely used for the detection of commercial explosives. These taggants are usually added to plastic explosives in order to facilitate 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. *This work is supported by the contract ANR-11-ASTR-035-01.*

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