GAS PHASE THZ SPECTROSCOPY OF ORGANOSULFIDE AND ORGANOPHOSPHOROUS COMPOUNDS USING A SYNCHROTRON SOURCE

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This study concerns the gas phase rovibrational spectroscopy of organosulfide and organophosphorous which are considered as non toxic model compounds in the analysis of chemical weapon materials, high pathogenic and mutagenic agents, and other environmentally interesting air-borne species. The coupling of the synchrotron radiation with multipass cells and the FTIR spectrometer allowed to obtain very conclusive results in term of sensitivity and resolution and improved the previous results obtained with classical sources.[a] For DMSO, using an optical path of 150 m the spectra have been recorded at the ultimate resolution of 0.001 cm^{-1} allowing to fully resolve the rotational structure of the lowest vibrational modes observed in the THz region. In the $290 - 420$ cm^{-1} region, the rovibrational spectrum of the perpendicular and parallel vibrational bands associated with, respectively, the asymmetric ν_{23} and symmetric ν_{11} bending modes of DMSO have been recorded with a resolution of 1.5×10^{-3} cm^{-1}. [b] The gas phase vibrational spectra of organophosphorous compounds were measured by FTIR spectroscopy using the vapor pressure of the compounds. Except for TBP, the room temperature vapor pressure was sufficient to detect all active vibrational modes from THz to NIR domain. Contrary to DMSO, the rotational patterns of alkyl phosphates and alkyl phosphonates could not be resolved; only a vibrational analysis may be performed. Nevertheless, the spectral fingerprints observed in the THz region allowed a clear discrimination between the molecules and between the different molecular conformations. [c]

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