CO2 LASER PHOTOACOUSTIC SPECTROSCOPY OF SOME HAZARDOUS MOLECULES

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Laser photoacoustic spectra of RDX, TNT, heroin, morphine and narcotine in the powder form and of methanol, ethanol and trichloroethylene in the varpor phase have been recorded in the 9.6 and 10.6 μ m regions using a rotational line tunable CO₂ Iser. The persistent vibrational bands in RDX are observed at 1045, 941 cm⁻¹ and those in TNT are at 978, 946 cm⁻¹. The characterstic bands in heroin are at 976, 944 cm⁻¹, in morphine at 973, 949 cm⁻¹ and in the narcotine at 1043, 936 and 929 cm⁻¹. Assignments of the vibrational bands in terms of normal modes have been made with the help of ab initio calculations of molecular geometries and the intramolecular force constants. In the case of vapor phase spectra, the rotational contours with two prominent peaks in methanol and ethanol are observed in the 9.6 μ m region whereas trichloroethylene exhibits three peaks in its rotational contour in the 10.6 μ m region.