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Laboratory (C_2H_6) and terrestrial (NO^+) IR spectroscopy

J.-M. Flaud

LISA, University Paris 12&7 and CNRS, 61 Av. General de Gaulle, 94010, Créteil,

France.(flaud@lisa.univ-paris12.fr / Fax: 33 145171564 / Phone: 33145171550)

Optical measurements of atmospheric minor constituents are carried out using spectrometers working in the UV-visible, infrared and microwave spectral ranges. In all cases the quality of the analysis and of the interpretation of the atmospheric spectra requires the best possible knowledge of the molecular parameters of the species of interest. To illustrate this point we will concentrate on recent laboratory studies of ethane demonstrating that at 12 μm the data available in the current databases are of rather poor quality. On the other hand there are a few cases where the spectroscopic properties of a molecule can be improved by using atmospheric spectra. As an example, recent NO^+ results derived from the MIPAS experiment will be presented.

The ν_9 fundamental band of ethane falls in the 12 μm region. It is the strongest band of ethane in a terrestrial window in the thermal infrared and is commonly used to determine ethane's abundance in the atmospheres of the Jovian planets and comets. Precise and accurate absolute intensities of this band are crucial for a correct interpretation of recent Cassini observations of ethane spectra in the atmospheres of Saturn and Titan. Using a spectrum of the ν_9 band of ethane recorded at 278 K at the Pacific Northwest National Laboratory, we demonstrate that the line parameters available in the HITRAN and GEISA databases do not reproduce the experimental data to within their accuracy. In fact, the integrated band intensity calculated at 296 K using both linelists are, respectively, a factor 1.57 larger and 1.44 smaller than the observed value. Using results from a recent global analysis of data involving the three lowest vibrational states of ethane and measurements of pressure broadening parameters, we have generated a new set of line parameters which provides a much more accurate description of the experimental spectrum of C_2H_6 in this region.

MIPAS (Michelson Interferometer for Passive Atmosphere Sounding) is a high spectral resolution interferometer (0.035 cm^{-1} unapodized) covering a very wide spectral range (from 4.16 to 16.4 μm) with high sensitivity which was successfully launched on the 1^{st} of March 2002 on the European Envisat satellite. MIPAS has measured spectra of the Earth's upper atmosphere in the 4.3 m region with the highest spectral resolution ever reached in this altitude region. This high spectral resolution lead to the determination of the frequency position of ro-vibrational NO^+ transitions with an unprecedented accuracy. It has been found that the spectral line positions of the NO^+ (1-0) ro-vibrational band are shifted by about 0.15 cm^{-1} with respect to those listed in the HITRAN 2004 compilation. Also, spectral line positions of the NO^+ (2-1) ro-vibrational band are shifted by approximately (0.05- 0.1) cm^{-1} with respect to those listed in the HITRAN 2004 compilation. A new set of Hamiltonian constants for NO^+ has been derived from MIPAS data producing a much improved prediction of the line positions of this species.