

Technical report on

**Spectral line parameters for
C₂H₆ and NO⁺**

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1. Purpose of the document

The purpose of this document is to describe the modifications made to the MIPAS database as far as the C₂H₆ and NO⁺ line parameters are concerned. The modifications described in the present document were applied to the version PF_3.2 of the database to generate the new version PF_3.3 available at the following web page:

http://www2.fci.unibo.it/~ridolfi/mipas_special_modes/db/

2. C₂H₆

The ethane molecule C₂H₆ is spectroscopically difficult to handle since it exhibits a large amplitude motion difficult to model. The only data available in the HITRAN [Rothman et al., 2003] and/or GEISA [Jacquinet-Husson et al., 2005] databases and useful for MIPAS concerns the 12.2 μm region. These parameters are quite dated, of rather poor quality and are not consistent: They are respectively, a factor 1.57 larger and 1.44 smaller than the observed value [Sharpe et al., 2004] respectively. A recent [Vander Auwera et al., 2007] study using results from a global analysis of data involving the four lowest vibrational states of ethane and measurements of pressure broadening parameters was performed. A new set of line parameters was generated which proved to be of much better quality providing a much more accurate description of the experimental spectrum of C₂H₆ in the 12 μm region. All the details concerning the new calculations and comparisons with the experiments are given in the corresponding paper.

The line list was generated in the MIPAS format including indexes for the quality of the various spectral parameters and included in the MIPAS database while all the previous parameters were removed.

3. NO⁺

During a recent study [Lopez-Puertas et al., 2006] it was shown that the line positions for the NO⁺ species given in the HITRAN database were not correct. Using all the literature available data as well as the MIPAS spectra a new line list was generated allowing one to provide precise line positions for the cold band (2-1 in the MIPAS notation) as well as the first hot band (3-2 in the MIPAS notation).

The line list for the MIPAS database was built as described below:

- 1- For the 2-1 and 3-2 bands new line positions were generated up to J=40 and the corresponding quality indexes were defined.

In order to be complete it was decided also to do the following:

- 2- For the 2-1 and 3-2 bands the old line positions were kept for J above J=40 since there is no way (except a new experiment) to decide if the new data are better or worse than the previous ones (extrapolation problem)
- 3- For the other hot bands the HITRAN data were kept

It should be underlined that the quality of the data described in bullets 2 and 3 could not be assessed properly.

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ANNEX 1

NO⁺ fundamental and first hot ro-vibrational line frequencies from MIPAS/Envisat atmospheric spectra,

Lopez-Puertas M., B. Funke, S. Gil-Lopez, J. Peralta-Calvillo and J.-M. Flaud, , J. Mol. Spectrosc., 237, 218-224 (2006)

Pdf file of the above paper from the web:

http://www2.fci.unibo.it/~ridolfi/mipas_special_modes/db/puertas_et_all_no+_2006.pdf

ANNEX 2

Toward an accurate database for the 12 μ m region of the ethane spectrum,

Vander Auwera J., N. Moazzen-Ahmadi, and J.-M. Flaud, The Astrophysical Journal, 662:750Y757, (2007)

Pdf file of the above paper from the web:

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