



High-resolution spectroscopy of nitrous acid HONO and its deuterated species DONO in the far-infrared

A. Dehayem (1), O. Pirali (2), I. Kleiner (1), and J. Orphal (1)

(1) Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS, Université de Paris-XII, 61, av. du Général de Gaulle, 94010 Créteil Cedex, France, (2) Laboratoire de Photophysique Moléculaire (LPPM), CNRS, Bât. 350, Université de Paris-Sud, 91405 Orsay Cedex, France

Nitrous acid (HONO) is an important source for tropospheric OH radicals. However, the chemical mechanisms for heterogeneous production of HONO are still not well established. In order to improve the spectroscopic knowledge of this molecule and its deuterated species DONO, high-resolution absorption spectra in the far-infrared ($20\text{--}650\text{ cm}^{-1}$) have been recorded in our laboratory with a resolution of 0.003 cm^{-1} , using a Bruker IFS-120 HR interferometer, equipped with a Germanium beamsplitter and a Helium-cooled bolometer.

Starting with predictions based on previously published studies in the mid-infrared spectral region^(1–4), we have assigned pure rotational transitions of both the *cis*- and *trans*- isomers of HONO up to high values of the J (>40) and K_a (>20) quantum numbers.

We also have recorded and analysed the spectra of the deuterated species of nitrous acid (DONO) in the same spectral range ($20\text{--}650\text{ cm}^{-1}$) thus completing the previous work of *Halonen et al.*⁴ ($1200\text{--}500\text{ cm}^{-1}$ and $550\text{--}300\text{ cm}^{-1}$).

For both HONO and DONO, calculations of the rotational energy levels were performed using a Watson-type reduced Hamiltonian. Using previously published microwave data⁵ (for transitions with low quantum numbers) together with the data from

the present study, improved ground state rotational constants for all four molecules (*cis*- and *trans*- HONO and DONO) were determined. Such constants are indispensable to assess the quality of high-level *ab-initio* calculations and to predict the spectra of these molecules at atmospheric conditions.

¹F. Melen and M. Herman, J. Phys. Chem. Ref. Data 21, 831-881 (1992)

²J.-M. Guilmot, M. Godefroid, and M. Herman, J. Mol. Spectrosc. 160, 387-400 (1993)

³J.-M. Guilmot, M. Godefroid, and M. Herman, J. Mol. Spectrosc. 160, 387-410 (1993)

⁴L. O. Halonen, C. M. Deeley, I. M. Mills, and V.-M. Horneman, Can. J. Phys. 62, 1300 (1984)

⁵D. J. Finnigan, A. P. Cox, A. H. Britain, and J. G. Smith. J. Chem. Soc. Faraday Trans. II, 68, 548 (1972)