

OVERTONE SPECTROSCOPY IN TRANS-FORMIC ACID

M. FREYTES, D. HURTMANS, S. KASSI, J. LIEVIN, J. VANDER AUWERA, M. HERMAN, *Laboratoire de Chimie Physique Moléculaire C. P. 160/09, Université Libre de Bruxelles, 50 Avenue F. D. Roosevelt, B-1050 Brussels, Belgium*; A. CAMPARGUE, *Laboratoire de spectrométrie Physique (CNRS, UMR C5588), Université Joseph Fourier de Grenoble, B.P. 87, 38042 Saint-Martin d'Hères Cédex, France*.

Vibrational assignments of fundamental, combination and overtone bands in the main isotopomer of gaseous trans-formic acid are reported from spectra either newly or previously^a recorded using high-resolution Fourier transform spectroscopy and intracavity laser absorption spectroscopy. A total of 62 bands, with 32 newly reported ones, were observed from the lowest energy band ν_7 at 626.16 cm^{-1} up to $4\nu_1$ at 13284.1 cm^{-1} . Among these bands, 43 were firmly assigned, and 16 tentatively. Effective vibrational constants were obtained. The normal modes of vibrations were further characterized using *ab initio* calculations providing fundamental band intensities and normal mode nuclear displacements. The analysis of the rotational structure in the first CH stretch overtone band ($2\nu_2$) and in the second OH stretch overtone band ($3\nu_1$) was performed. Some rotational information could also be obtained for $3\nu_2$ and two close-lying bands, extracted from strong overlapping formic acid dimer bands.

^aD. Hurtmans, F. Herregodts, M. Herman, J. Liévin, A. A. Kachanov and A. Campargue, *J. Chem. Phys.* **113**, 1535 (2000).