ROTATIONAL TRANSITIONS IN THE ν_9 AND ν_7 VIBRATIONAL STATES OF cis-HCOOH

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The energy difference between cis-HCOOH and $trans$-HCOOH in the gas phase, ca. 1365 cm^{-1}, was determined from a handful of MW transitions detected in formic acid at room temperature and reported in 1976[a]. A full analysis of the ground state spectrum of the cis rotamer based on FIR date was not provided until 2002[b]. For over 20 years unsuccessful efforts have been made to find vibrational bands of the cis rotamer in the gas phase IR spectrum. In the meantime, ab initio calculations and matrix spectra have yielded substantial information about the vibrational modes of this molecule[c]. We report here the first quantitative gas phase information about the excited vibrational states ν_9 and ν_7 of cis-HCOOH, obtained from FASSST measurements between 115 and 375 GHz, in a 6 m cell heated to 443 K. To date 427 transitions have been assigned for ν_9, and 336 for ν_7. The rotational and centrifugal distortion constants for these two states will be presented, together with a new set of ground state constants.

[a] W. H. Hocking, *Z. Naturforsch. A* bf 31, 1113–1121 (1976).
[b] M. Winnnewisser et al.,*J. Mol. Spectrosc.* **216**, 259–265 (2002).
[c] E. M. S. Maçôas et al., *J. Mol. Spectrosc.* **219**, 70–80 (2003).