THE TORSIONAL FUNDAMENTAL BAND OF METHYLFORMATE

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Methylformate ($HCOOCH_3$) is one of the most important molecules in astrophysics, first observed in 1975.[a] The rotational structure of its ground and first excited torsional states are well known from millimeter wave measurements.[b] However, some of the torsional parameters are still not precisely determined because information on the torsional vibrational frequency $v_t = 1 - 0$ is missing.
To overcome that problem, the far infrared spectrum of $HCOOCH_3$ was recorded with a 150 m optical path in a White cell and a Bruker IFS 125 HR Fourier transform spectrometer at the AILES beamline of the synchrotron SOLEIL facility. The analysis of the very weak fundamental torsional band $v_t = 1 - 0$ observed around 130 cm^{-1} was carried out. It led to the first precise determination of the torsional barrier height and the dipole moment induced by the torsional motion.

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[a] R.D. Brown, J.G. Crofts, P.D. Godfrey, F.F. Gardner, B.J. Robinson, J.B. Whiteoak, Astrophys. J. 197 (1975) L29L31.
[b] See V. Ilyushin, A. Kryvda, E. Alekseev, J. Mol. Spectrosc. 255 (2009) 32-38, and references therein.