

ROTATION-VIBRATION SPECTRA OF MALONALDEHYDE OBTAINED WITH FAR-INFRARED SYNCHROTRON RADIATION

D. W. TOKARYK, S. C. ROSS, D. FORTHOMME, J. E. PRESCOTT, *Department of Physics and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3*; K. M. T. YAMADA, F. ITO, *EMTech, AIST, Tsukuba-West, Tsukuba, Ibaraki, Japan*.

Malonaldehyde is an open 5-membered ring molecule which exhibits interesting quantum-mechanical effects due to tunnelling of one of its protons. This results in a 21 cm^{-1} tunnelling-splitting in the ground vibrational state, which has been well-studied by microwave spectroscopy^a. We have taken far-infrared Fourier transform spectra of malonaldehyde at the Canadian Light Source synchrotron, and have recorded a number of rotation-vibration fundamental bands between $100\text{-}1000\text{ cm}^{-1}$ at 0.00096 cm^{-1} resolution. The data permit us to determine with high precision the changes in the tunnelling-splitting induced by vibrational excitation. We have also observed spectra at 240 and 219 cm^{-1} that appear to be transitions from the two components of the ground vibrational state to a common upper state that is not mentioned in conventional vibrational analyses of malonaldehyde^b. We will offer suggestions as to the nature of the newly-observed state.

^aP. Turner, S. L. Baughcum, S. L. Coy and Z. Smith, *J. Am. Chem. Soc.* **106** (1984) 2265-2267; T. Baba, T. Tanaka, I. Morino, K. M. T. Yamada and K. Tanaka, *J. Chem. Phys.* **110** (1999) 4131-4133.

^bA. Alparone and S. Millefiori, *Chem. Phys.* **290** (2003) 15-25.