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

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Malonaldehyde is an open 5-membered ring molecule which exhibits interesting quantum-mechancial 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 100-1000 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.

[a] P. 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.

[b] A. Alparone and S. Millefiori, *Chem. Phys.* **290** (2003) 15-25.