

## FAR-INFRARED SYNCHROTRON-BASED SPECTROSCOPY OF PROTON TUNNELLING IN MALONALDEHYDE

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Malonaldehyde ( $C_3O_2H_4$ ) is a prototype molecule for the study of intramolecular tunnelling proton transfer. In the case of malonaldehyde, this transfer occurs between the two terminal oxygen atoms in its open-ring structure. Although the ground state tunnelling splitting of  $21\text{ cm}^{-1}$  has been accurately determined from microwave studies<sup>a</sup>, the splitting has never been obtained with high resolution in any excited vibrational state. The  $\nu_6$  vibrational band was investigated in a diode laser jet experiment<sup>b</sup> in 2004, but the researchers were not able to identify the (-) parity tunnelling component and so could not determine the splitting. We have collected high-resolution far-IR Fourier transform spectra from a number of fundamental vibrational bands of malonaldehyde at the CLS (Canadian Light Source) synchrotron in Saskatoon, Saskatchewan, exploiting the considerable gain in signal-to-noise ratio at the highest resolution available afforded by the intense and well-collimated beam. We will report on our tunnelling-rotation analysis of the anti-symmetric out-of-plane bend near  $384\text{ cm}^{-1}$  and present its tunnelling splitting value.

<sup>a</sup>T. Baba, T. Tanaka, I. Morino, K. M. T. Yamada, K. Tanaka. *Detection of the tunneling-rotation transitions of malonaldehyde in the submillimeter-wave region.* J. Chem. Phys., **110**, 4131-4133 (1999)

<sup>b</sup>C. Duan, D. Luckhaus. *High resolution IR-diode laser jet spectroscopy of malonaldehyde.* Chem. Phys. Lett., **391**, 129-133 (2004)

