# DETERMINATION OF THE PROTON TUNNELING SPLITTING OF MALONALDEHYDE IN THE GROUND STATE BY MILLIMETER-WAVE SPECTROSCOPY

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Due to the proton tunneling motion, the ground state of malonaldehyde is split into a doublet. The $tunneling - rotation$ transitions connecting the lower($0^+$) and upper($0^-$) components of the tunneling doublet were observed by submillimeter-wave spectroscopy employing BWO tubes. So far, more than two hundred $Q$- and $R$-branch tunneling-rotation transitions were identified in the frequency region of 642-745 GHz together with about fifty pure rotational lines for both the $0^+$ and $0^-$ sublevels.

The present submillimeter-wave data were analyzed together with the reported pure rotational lines by the millimeter-wave[a] and TuFIR[b] spectroscopy. The proton tunneling splitting in the ground state $\Delta_0$ = 647046.208 $\pm$ 0.019 MHz, and the tunneling-rotation interaction consatnt $F$ = 45.8965 $\pm$ 0.0082 MHz, were determined as well as the rotational and centrifugal distortion constants for each tunneling sublevels. ¿From the line intensities, the $a$-component of transition moment, responsible ¿to the tunneling-rotation transitions, turned out to be about one tenth of the $b$-component of dipole moment (2.58 D[a]), responsible to the pure rotational transitions.

[a] S. L. Baughcum, Z. Smith, E. B. Wilson, and R. W. Duerst, J. Am. Chem. Soc., 106,2265 (1984). [b] D. W. Firth, K. Beyer, M. A. Dvorak, S. W. Reeve, A. Grushow,and K. R. Leopold, J. Chem. Phys., 94,1812 (1991).