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 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 constant $F = 45.8965 \pm 0.0082$ 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), responsible to the pure rotational transitions.