

Millimeter-wave spectroscopy of hydantoin in its vibrationally excited states

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Hydantoin (Imidazolidine-2,4-dione), a precursor to the amino acid glycine, is of astrobiological interest due to its detection in meteorites. [1] In a previous study, Alonso et al. [2] used laser ablation and FT-MW spectroscopy to determine the nuclear quadrupole coupling constants of the nitrogen nuclei in the vibrational ground state, while also assigning spectra of various decomposition products. Our previous work involved heating hydantoin to $\sim 150^\circ\text{C}$ to measure its pure rotational spectrum, determining precise rotational and centrifugal distortion constants for the ground and two excited states. [3] However, the study also revealed numerous unidentified spectral lines, leaving their assignment as an open problem. The present study, therefore, aims to assign these unidentified millimeter-wave lines and clarify the interactions among the excited vibrational states with the aid of theoretical calculations.

We have so far assigned approximately 3,000 rotational transitions of hydantoin in the millimeter-wave band, 865 of which are attributed to four novel excited vibrational states. To support our analysis, we performed structural optimization and force field calculations at the B3LYP/aug-cc-pVQZ level. The calculations show that among the 27 fundamental vibrations of hydantoin, the lowest in energy are, in order: ν_{27} (55 cm^{-1} , HCNC twist), ν_{26} (147 cm^{-1} , NCO twist), ν_{25} (367 cm^{-1} , HNCO wagging), and ν_{18} (393 cm^{-1} , CNC wagging). Among the six identified excited vibrational states, two states exhibit nearly identical rotational constants. These values are also consistent with the calculated vibration-rotation interaction constant for the ν_{27} mode. Accordingly, these two states were tentatively assigned as the tunneling-splitting components of the ν_{27} mode.

