IDENTIFICATION AND ASSIGNMENT OF THE FIRST EXCITED TORSIONAL STATE OF CH$_2$DOH WITHIN THE $\omega_2$, $\epsilon_2$, AND $\omega_3$ TORSIONAL LEVELS

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Theoretical models describing the details of asymmetric-top asymmetric-frame internal rotation remain to be fully developed and tested especially in excited torsional states. The spectrum of CH$_2$DOH offers a unique opportunity to test and develop asymmetric-top asymmetric-frame internal rotation theory. The theoretical energy levels predicted by El Hilali et al.$^a$ and combination differences of the 76 assigned torsional subbands coupled with the experimental microwave energy levels of the ground state$^b$ served as a basis for assigning the excited torsional state. The existing microwave spectra was supplemented with recordings of 1308–2010 GHz and 2450–2700 GHz. This facilitated extension of the ground state assignments to $K = 14$ and identified a number of torsional interactions. In this paper we report assignment of the $\omega_2$, $\epsilon_2$, and $\omega_3$ torsional levels to $K = 9$. All the torsional levels in the first excited torsional state have been connected with microwave accuracy transitions except $\omega_3 K = 2$. Strong rotational interactions between the $\omega_2 K = 0$ and $K = 2$ states and the $\epsilon_2 K = 4$, $\omega_2 K = 1$, $\omega_3 K = 2$ and $\omega_3 K = 3$ levels are observed. A week avoided crossing between $\epsilon_1 K = 12$ and $\epsilon_2 K = 8$ at $J = 20$ has also been identified. When the microwave results are combined with the existing infrared assignments it is now possible to predict the entire $v_t = 0$ to $v_t = 1$ torsional band to better than infrared experimental accuracy, greatly simplifying subsequent infrared assignments.