IDENTIFICATION AND ASSIGNMENT OF THE FIRST EXCITED TORSIONAL STATE OF CH_2DOH WITHIN THE o_2, e_2, AND o_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_2DOH 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 o_2, e_2, and o_3 torsional levels to $K = 9$. All the torsional levels in the first excited torsional state have been connected with microwave accuracy transitions except o_3 $K = 2$. Strong rotational interactions between the o_2 $K = 0$ and $K = 2$ states and the e_2 $K = 4$, o_2 $K = 1$, o_3 $K = 2$ and o_3 $K = 3$ levels are observed. A week avoided crossing between e_1 $K = 12$ and e_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.

[a] El Hilali, Coudert, Konov, and Klee, *J. Chem. Phys.* **135** (2011) 194309.

[b] Pearson, Yu, and Drouin, *J. Mol. Spectrosc.* **280** (2012) 119.