

P5399: A ubiquitous kinetic coupling between torsion and in- and out-of-plane XH_3 wagging vibrations for an XH_3 group attached to a planar frame.

Jason R. Gascooke and Warren D. Lawrance. Flinders University

- Analysing microwave spectra for molecules containing a methyl group usually begins with the assumption that the methyl torsion can be treated separately from the other vibrations.
- But, in toluene, UV and IR spectra reveal an interaction between torsion and vibration (see figure).
- Does this matter? Yes, if you want to understand the physical behavior of the methyl group and what the spectroscopic constants are telling us about its motion.
- So, we want to know whether toluene is a “one-off”, or if the interaction between torsion and vibration is more general.
- Watch the full talk to find out why **torsion-vibration interactions are the norm when the methyl group is attached to a planar frame**, not the exception.

