

## MICROWAVE SPECTROSCOPIC STUDY OF THE ATMOSPHERIC OXIDATION PRODUCT *m*-TOLUIC ACID AND ITS MONOHYDRATE

MOHAMAD AL-JABIRI, ELIJAH G SCHNITZLER, NATHAN A SEIFERT, WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada.*

*m*-Toluic acid is a photo-oxidation product of *m*-xylene, a chemical byproduct of the oil and gas industry, and is a common component of secondary atmospheric aerosol. Organic acids, such as *m*-toluic acid, are also thought to play an important role in the initial steps of aerosol formation, which involves formation of hydrogen bonded clusters with molecular species, such as water, ammonia, and sulfuric acid.

Somewhat surprisingly, the rotational spectrum of the *m*-toluic acid monomer has not been studied before. We have identified four stable conformers using ab initio calculations at the MP2/6-311++G(2df,2pd) level of theory. The two lowest energy conformers are rather close in energy and their rotational spectra were measured using a Balle-Flygare type microwave spectrometer. The structures and barriers to methyl internal rotation were determined.

We have identified four isomers of the monohydrate of *m*-toluic acid using ab initio calculations. Measurements of the microwave spectra of the two lowest energy isomers are underway with a newly constructed chirped pulse microwave Fourier transform spectrometer in the frequency range from 2 to 6 GHz. The spectra and analyses will be presented.