CONTINUING RESEARCH INTO THE OVERTONE SPECTRA OF TRIMETHYL AMINE

BRANT BILLINGHURST, KATHLEEN GOUGH, *Department of Chemistry, University of Manitoba, Winnipeg, Manitoba, Canada*; HENRIK G. KJAERGAARD AND GEOFF LOW, *Department of Chemistry, University of Otago, Dunedin, New Zealand*.

The CH bonds in trimethylamine that lie trans to the nitrogen lone pair are known to be much longer than the gauche CH. This is the most extreme known example of the trans lone pair effect, depicted by frontier molecular orbital theory as a delocalization of the lone pair electrons into the anti-bonding orbitals of the trans CH bonds. The spectrum of trimethylamine has been the subject of much study over the years, ranging from the fundamental infra-red of trimethyl amine and selectively deuterated derivatives to the overtone spectra of trimethylamine. We have collected the overtone spectra (1st - 5th) of some deuterated derivatives in order to improve the assignment of the overtone peaks. A harmonically coupled anharmonic oscillator local mode mathematical model has been used to predict the intensity of the absorbtions in the overtone regions.