

ROTOR-VIBRATOR COUPLING EFFECTS IN METHYL CH STRETCHING OVERTONE SPECTRA OF GASEOUS TOLUENE

D. CAVAGNAT, L. LESPADÉ and C. LAPOUGE, *LPCM, Université Bordeaux I, F-33405 Talence Cedex.*

The methyl CH stretching overtone spectra of toluene and of its deuterated derivatives ($C_6D_5CH_3$, $C_6D_5CH_2D$ and $C_6D_5CHD_2$) have been recorded by FTIR ($\Delta v=1$ to 4) and by intracavity dye laser photoacoustic spectrometry ($\Delta v=5$ and 6) at low resolution (0.5 to 2 cm^{-1}).

The different couplings likely to affect these spectra (anharmonic coupling of the ν_{CH} mode with the methyl group internal rotation, Fermi resonance coupling with combination states involving CH stretch/methyl bending modes) are considered. The parameters used to model these couplings are determined partly from ab-initio calculations^a, partly from fitting simultaneously the spectra of the different isotopic compounds.

A preliminary analysis of the obtained results is presented. An attempt to compare them with those determined from the study of the corresponding overtone spectra of nitromethane^b (which presents a similar hindering barrier to the methyl group rotation) is made in order to check the effect of the molecular environment of the methyl group on IVR phenomena.

^aC. Lapouge and D. Cavagnat, *J.Phys. Chem.*, to be published

^bD. Cavagnat and L. Lespade, *J.Chem.Phys.*106,7946,(1997)