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

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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 (Δv=1 to 4) and by intracavity dye laser photoacoustic spectrometry (Δv=5 and 6) at low resolution (0.5 to 2 cm^{-1}).
The different couplings likely to affect these spectra (anharmonic coupling of the νCH 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.

[a]C. Lapouge and D. Cavagnat, J.Phys. Chem., to be published
[b]D. Cavagnat and L. Lespade,J.Chem.Phys.106,7946,(1997)