A SPECTROSCOPIC AND THEORETICAL STUDY OF WEAK INTRAMOLECULAR OH$\cdots\pi$ INTERACTIONS IN ALLYL CARBINOL AND METHALLYL CARBINOL

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The weak intramolecular OH$\cdots\pi$ interactions in allyl carbinol and methallyl carbinol have been studied using a combination of NIR spectroscopy and theory. The third OH-stretching overtone region of vapor phase allyl carbinol and methallyl carbinol have been recorded with intracavity laser photoacoustic spectroscopy to study the effect of an enhanced OH$\cdots\pi$ interaction in methallyl carbinol arising from the electron donating methyl group. Local mode calculations were employed to assign the observed bands. The OH-stretching transition frequency of methallyl carbinol was observed to be red shifted relative to the OH-stretching transition frequency of allyl carbinol. A red shift of the transition frequency is in this context normally interpreted as a signature of hydrogen bonding. Whether the OH$\cdots\pi$ interaction can be categorized as a hydrogen bond will be discussed in this talk.