A SPECTROSCOPIC AND THEORETICAL STUDY OF WEAK INTRAMOLECULAR OH···π INTERACTIONS IN ALLYL CARBINOL AND METHALLYL CARBINOL

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The weak intramolecular OH···π 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···π 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···π interaction can be categorized as a hydrogen bond will be discussed in this talk.