OBSERVATION OF TRANS-ETHANOL AND GAUCHE-ETHANOL COMPLEXES WITH BENZENE USING MATRIX ISOLATION INFRARED SPECTROSCOPY

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Ethanol can exist in two conformers, one in which the OH group is trans to the methyl group (trans-ethanol) and the other in which the OH group is gauche to the methyl group (gauche-ethanol). Matrix isolation infrared spectra of ethanol deposited in 20 K argon matrices display distinct infrared peaks that can be assigned to the trans-ethanol and gauche-ethanol conformers, particularly with the O-H stretching vibrations.[a] Given this, matrix isolation experiments were performed in which ethanol (C_2H_5OH) and benzene (C_6H_6) were co-deposited in argon matrices at 20 K in order to determine if conformer specific ethanol complexes with benzene could be observed in the infrared spectra. New infrared peaks that can be attributed to the trans-ethanol and gauche-ethanol complexes with benzene have been observed near the O-H stretching vibrations of ethanol. The initial identification of the new infrared peaks as being due to the ethanol-benzene complexes was established by performing a concentration study (1:200 to 1:1600 S/M ratios), by comparing the co-deposition spectra with the spectra of the individual monomers, by matrix annealing experiments (35 K), and by performing experiments using isotopically labeled ethanol (C_2D_5OD) and benzene (C_6D_6). Quantum chemical calculations were also performed for the C_2H_5OH-C_6H_6 complexes using density functional theory (B3LYP) and ab initio (MP2) methods. Stable minima were found for the both the trans-ethanol and gauche-ethanol complexes with benzene at both levels of theory and were predicted to have similar interaction energies. Both complexes can be characterized as H-π complexes, in which the ethanol is above the benzene ring with the hydroxyl hydrogen interacting with the π cloud of the ring. The theoretical O-H stretching frequencies for the complexes were predicted to be shifted from the monomer frequencies and from each other and these results were used to make the conformer specific infrared peak assignments.

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[a] Barnes, A. J.; Hallam, H. E. *Trans. Faraday Soc.*, **1970**, *66*, 1932-1940.