INTERMOLECULAR ASSOCIATION COMPLEXES OF 1,3-CYCLOHEXANEDIONE: PROBING OF KETO-ENOL TAUTOMERIC EQUILIBRIA IN COLD INERT GAS MATRIX, SOLUTION AND VAPOR PHASE BY INFRARED SPECTROSCOPY AND QUANTUM CHEMISTRY STUDY

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Cyclic β-diketo compounds are known to show markedly different physical and chemical properties compared to their linear counterparts. 1,3-cyclohexanedione, the simplest molecule among the cyclic variants was found to exist exclusively in ketoenolic form in crystal whereas appreciable amount of diketo tautomer was identified in chloroform solution. We have studied this system by means of infrared spectroscopy to elucidate its tautomeric behavior under different environmental as well as thermal conditions ranging from solid argon matrix at 8 K to carbon tetrachloride and chloroform solution at room temperature and low pressure vapor at 330 K. Besides, we have monitored its homodimeric complexes and the effect of weak CH—O hydrogen bonding on the keto-enol tautomeric equilibria. The potential energy surface of the ground electronic state has been computed by means of electronic structure calculation to corroborate the experimental findings.