

INFRARED SPECTROSCOPY OF HYDROGEN-BONDED CLUSTERS OF PROTONATED HISTIDINE

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Histidine(His), one of the essential amino acids, is involved in active sites in many enzyme proteins, and known to play fundamental roles in human body. Thus, to gain detailed information about intermolecular interactions of His as well as its structure is very important. In the present study, we have recorded IR spectra of hydrogen-bonded clusters of protonated His (HisH^+) in the gas phase to discuss the relation between the molecular structure and intermolecular interaction of HisH^+ . Clusters of $\text{HisH}^+(\text{MeOH})_n$ ($n = 1, 2$) were generated by an electrospray ionization of the MeOH solution of L-His hydrochloride monohydrate. IR photodissociation spectra of $\text{HisH}^+(\text{MeOH})_{1,2}$ were recorded. By comparing with the results of the DFT calculations, we determined the structures of these clusters. In the case of $n = 1$ cluster, MeOH is bonded to the imidazole ring as a proton acceptor. The most of vibrational bands observed were well explained by this isomer. However, a free NH stretch band of the imidazole ring was also observed in the spectrum. This indicates an existence of an isomer in which MeOH is bounded to the carboxyl group of HisH^+ . Furthermore, it is found that a protonated position of His is influenced by a hydrogen bonding position of MeOH. In the case of $n = 2$ cluster, one MeOH molecule is bonded to the amino group, while the other MeOH molecule is separately bonded to the carboxyl group in the most stable isomer. However, there is a possibility that other conformers also exist in our experimental condition. The details of the experimental and theoretical results will be presented in the paper.