

GAS PHASE SPECTROSCOPY ON HYDRATED CLUSTERS OF OXYTOCIN BY ELECTROSPRAY IONIZATION /
COLD ION TRAP TECHNIQUE

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Oxytocin (OT) is the first structure-identified peptide hormone, which has a cyclic part formed by disulfide-bridge and a C-terminal α -amidated tail. Since some studies show that oxytocin alleviates mental disorders and postpartum hemorrhage, it has been developed as pharmaceuticals, recently more focused on oral drugs. However, low membrane permeability of oxytocin impedes its oral administration. One of the important factors which affect the membrane permeability is how dehydrated structure in the membrane changes into the hydrated structure. In this work, to elucidate the effect of the hydration on oxytocin structure, infrared spectroscopy was employed on isolated hydrated oxytocin clusters ($\text{OTH}^+ \cdot (\text{D}_2\text{O})_n$, $n=1-4$), combining with theoretical calculations. The results of this study suggest that the hydration of only a single water molecule interrupts the intramolecular hydrogen bond between the cyclic moiety and the tail part. The structural deformation by the hydration will be discussed.