

IR LASER INDUCED CIS ↔ TRANS ISOMERIZATION OF NAPHTHOL IN THE ELECTRONIC EXCITED STATE

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The IR laser induced cis ↔ trans isomerization reaction has been carried out for 1- and 2-naphthol and their hydrogen(H)-bonded clusters in the S_1 state in supersonic jets. A specific isomer in the jet was pumped to the CH or OH stretching vibration in S_1 by a stepwise UV-IR excitation and the dispersed emission of the final product was observed. In both molecules, the isomerization was observed only for the H-bonded clusters but not for bare molecules in the examined energy region ($E_v \leq 3510 \text{ cm}^{-1}$), indicating the reduction of the isomerization barrier height upon the H-bonding. At low energy, the yield of the isomerization was high, while the yield decreased rapidly with the increase of energy. The energetics and dynamics controlling the isomerization yield will be discussed. A DFT and time dependent DFT calculation was performed for estimating the barrier height of the isomerization for S_0 and S_1 and S_2 for bare 2-naphthol and its cluster to investigate the difference of the barrier height at different state and to investigate the effect of hydrogen-bond.