

DEUTERATION EFFECT STUDY ON THE VIBRATIONAL DYNAMICS OF PHENOL AND PHENOL-WATER COMPLEX BY PICOSECOND TIME-RESOLVED IR-UV PUMP-PROBE SPECTROSCOPY IN A SUPERSONIC MOLECULAR BEAM

YASUNORI MIYAZAKI, YOSHIYA INOKUCHI, and TAKAYUKI EBATA, *Department of Chemistry, Graduate School of Science, Hiroshima University, Japan.*

The vibrational energy relaxations of the OH and OD stretch of phenol-d₀ and phenol-d₀-(H₂O) complex and phenol-d₁ and phenol-d₁-(D₂O) complex, respectively, are investigated by picosecond IR-UV pump-probe spectroscopy. The key to understand their dynamic is well-suited to a two-step Tier model. For phenol-d₀, an energy flow is described by the intramolecularVR steps: "OH stretching level" → "doorway state" → "bath state". The intramolecularVR lifetime of phenol-d₀ is obtained to be 14 ps. On the other hand, the OD stretching vibration of phenol-d₁ exhibits quantum beats, followed by the intramolecularVR with a lifetime of 90 ps. In contrast, for the phenol-water complex, the intramolecularVR lifetime of OH(OD) stretch becomes 4.3 ps(12 ps) and an energy flow is described by the intramolecular and intermolecular processes, which lead to VP (vibrational predissociation). Although the energy difference is 1000 cm⁻¹, no remarkable change of intermolecularVR and VP lifetimes is found in the hydrogen-bonded phenol-water complexes.