

OH- $\pi$  HYDROGEN BOND IN THE COMPLEX OF STYRENE-WATER: A ROTATIONAL STUDY

YANG ZHENG, JUNCHENG LEI, GANG FENG, QIAN GOU, *School of Chemistry and Chemical Engineering, Chongqing University, Chongqing, China.*

The rotational spectra of the styrene-water complex has been investigated by using the pulsed jet Fourier transform microwave spectroscopic technique. Styrene has two  $\pi$  systems which can act as the proton acceptor and link with water through the OH- $\pi$  hydrogen bond. Ab initio calculations suggested that the vinyl  $\pi$  system is favored to form such a hydrogen bond. In contrast, the experimental evidences of four isotopologues pointed out that the water O-H group prefers to link to the benzene  $\pi$  system. The internal rotation of water around its symmetry axis splits all the rotational transitions into two component line with a relative intensity ration of 1:3.