

A NEW LOOK AT A CHIRAL PROTOTYPE: ROTATIONALLY RESOLVED MW AND UV SPECTRA OF JET-COOLED 1,1'-BI-2-HYDROXYNAPHTHALENE

S. DAVIS, D. F. PLUSQUELLIC and R. D. SUENRAM, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899.*

Recent efforts towards characterization of biologically relevant molecules exploiting rotationally resolved gas phase spectra will be reported. The experimental techniques for i) generating sufficient densities of supersonically cooled molecules with high melting points ( $T > 200\text{C}$ ) and ii) obtaining rotational resolution of large aromatic system having  $> 20$  heavy atoms will be presented. The low resolution ( $\sim 1\text{cm}^{-1}$ ) UV spectrum of structurally chiral 1,1'-bi-2-hydroxynaphthalene has been obtained. The LIF spectrum near 342 nm reveals the presence of two prominent features separated by  $50\text{ cm}^{-1}$ . This splitting is tentatively interpreted in terms of an exciton interaction arising from the proximity of the two naphthol subunits. The results of ongoing efforts to obtain the rotationally resolved spectra, which are expected to further validate this interpretation, will be discussed. Furthermore, the rotational constants obtained from both MW and UV studies will provide detailed structural information. In particular, the dihedral angle defining the out-of-plane orientation between the two naphthol ring systems, which gives rise to the chiral nature and therefore the degree of optical activity, will be accurately determined. Additionally, relationships between the experimental results and theoretical predictions will also be discussed.