

## TRANSIENT CHIRALITY AND MICROSOLVATION IN p-ETHYLPHENOL

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p-Ethylphenol (PEP) and other volatile phenols appear in wines contaminated with *Brettanomyces* yeast giving undesirable off-aromas (“Brett” or phenolic character) which spoil wines even at very low concentrations. These phenols are produced by an enzymatic transformation of the hydroxycinnamic acids present in wines. In this work, we have analyzed the rotational spectrum of PEP and its microsolvated complexes using CP-FTMW spectroscopy in the 2-8 GHz region. The equilibrium configuration of PEP has the ethyl group carbon plane perpendicular to the phenyl ring while the OH group lies in the ring plane. The two possible orientations of the OH group originate two non-superposable enantiomeric forms, energetically equivalent, but with opposite signs for the  $\mu_b$  electric dipole component. The interconversion of both enantiomers by the OH internal rotation leads to a situation of transient chirality. This motion is expected to have a two-fold periodic potential energy function with the torsional states appearing as doublets as happen in phenol. The rotational spectrum reflects this behavior. The  $\mu_a$  spectrum consists of single lines resulting from the collapse of the individual torsional  $0^+$  and  $0^-$  spectra. The  $\mu_b$  transitions, forbidden within each torsional state, are allowed as chiral  $0^+ \leftrightarrow 0^-$  transitions. Therefore, the  $\mu_b$ -type spectrum consists of doublets spaced twice the energy difference between the  $0^+$  and  $0^-$  torsional states. We have observed the  $^{13}\text{C}$  and OD isotopologues and have determined the molecular structure of PEP along with the internal rotation potential energy profile. In addition, we have measured the spectra of the PEP- $\text{H}_2\text{O}$ , PEP-Ne- $\text{H}_2\text{O}$ , and PEP-( $\text{H}_2\text{O}$ ) $_2$  complexes. The PEP- $\text{H}_2\text{O}$  and PEP-Ne- $\text{H}_2\text{O}$  spectra show doublets with 1:3 intensities revealing the water rotation dynamics exchanging the H atoms. For these species the spectra of different isotopologues  $^{13}\text{C}$ , D,  $^{18}\text{O}$ , and  $^{22}\text{Ne}$  have been also measured to determine their structures.