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Photophysics of protonated vanillin in the gas phase: a laser action spectroscopy and theoretical approach

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Protonation and deprotonation processes in derivatives of aromatic systems play an important role in various areas of chemistry. The 'competition' between different centers to accept or donate a proton depends on a number of parameters, including electron density effects. This competition can result in the formation of different tautomers, each one having a different photophysical behavior. Vanillin serves a model system with three functional groups exhibiting distinct characteristics (see Figure 1). In this work, we first set out to determine the protonated tautomers formed in vanillin from an electrospray source, using different laser action techniques (such as IRMPD room temperature and UVPD in cryogenic ion trap). The results indicate that protonation predominantly occurs at the oxygen atom of the carbonyl group (C=O). Moreover, through the analysis of the results, we were able to unambiguously determine the configuration of the observed protonated tautomer. These results are partially in agreement with the order of stability predicted by theoretical calculations with DFT and MP2 methods. We will discuss apparent deviations from theoretical predictions concerning the observed isomer. Furthermore, both theoretical calculations and experiments reveal a spectroscopic pattern similar to that of protonated benzaldehyde (benzene with HC=O group) in terms of electronic absorption, highlighting the significant influence of the HC=O group on the photophysics of the system. Finally, we will briefly address the challenges encountered in the analysis of the deprotonated species, such as the interpretation of the IRMPD spectrum.

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