

THE CONFORMATIONAL LANDSCAPE OF TYROSOL AND ITS HYDRATES

ALBERTO MACARIO, SUSANA BLANCO, JUAN CARLOS LOPEZ, *Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Valladolid, Spain.*

2-(4-Hydroxyphenyl)ethanol, commonly known as Tyrosol, is a powerful antioxidant in the human diet, mainly found in olive oil. It also presents other biological properties such as cardiovascular drug or geroprotector agent, among others. As it widely known, these biological properties are related with its molecular structure and its conformational landscape. Here we presented the study of the molecular structure and conformational panorama of tyrosol and its mono- and dihydrated complexes, by means of gas-phase high-resolution rotational spectroscopy. From a vast number of predicted conformers, three of them have been experimentally identified for the monomer. The large amplitude motions interconverting the predicted and observed forms have been studied by means of computational methods. Five different conformers were observed for the monohydrated complex, all of them preserving the monomer structures with the water being able to interact as a proton acceptor with both hydroxy groups. In this competition between these two groups the interaction with the hydroxy group attached to the phenyl ring seems to present a higher stability. This is corroborated with the observation of two conformers of the dihydrated complex, which also preserves the structures of the two most stable monomer forms with water dimer forming a cycle only with the hydroxy group attached to the phenyl ring.