

CHARACTERISATION OF THE MOLECULAR GEOMETRY OF 2-ETHYLFURAN...H₂O BY MICROWAVE SPECTROSCOPY

CHARLOTTE CUMMINGS, *School of Chemistry, Newcastle University, Newcastle-upon-Tyne, United Kingdom*; NICK WALKER, *School of Natural and Environmental Sciences, Newcastle University, Newcastle-upon-Tyne, United Kingdom*.

Microwave spectroscopy is a powerful technique for the study of weakly bound complexes formed between aromatic/heteroaromatic rings and other small molecules. However, there has been limited studies of binary complexes formed between alkyl-substituted heteroaromatic rings and water. The rotational spectrum of 2-ethylfuran...H₂O was recorded while probing a gaseous mixture of 2-ethylfuran, water and an inert carrier gas (argon or neon) using Chirped Pulse Fourier Transform Microwave (CP-FTMW) spectroscopy. Microwave spectra of five isotopologues of this complex have been assigned and analysed to determine rotational constants (A_0 , B_0 , C_0) and centrifugal distortion constants (D_J , D_{JK} , d_1). A previous microwave spectroscopy study^a identified two conformations (C_s and C_1) of 2-ethylfuran in a helium supersonic expansion. The C_s conformation is planar, with the ethyl group lying coplanar with the ring, while the ethyl group in the C_1 conformation is tilted out of the plane of the ring. The analysis of the molecular geometry of the monohydrate complex has revealed that the binary complex is formed with the C_1 conformation of 2-ethylfuran only and is stabilised by a primary O_W-H...O hydrogen bond. Additionally, non-covalent interaction (NCI) and natural bond orbital (NBO) analysis have revealed the presence of additional weak interactions between the oxygen atom of the water molecule and the ethyl group. Preliminary results of 2-ethylimidazole...H₂O and 2-ethylthiazole...H₂O will also be discussed.

^aH. V. L. Nguyen, *Journal of Molecular Structure*, 2020, **1208**, 127909.