

## ROTATIONAL SPECTRA AND GEOMETRIES OF FOUR CONFORMERS OF ISOLATED UROCANIC ACID; AND OF A COMPLEX OF UROCANIC ACID WITH WATER

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The rotational spectra of four conformers of urocanic acid ((2E)-3-(1H-imidazol-4-yl)prop-2-enoic acid) have been measured between 6 and 18 GHz. The molecule was prepared for study through laser vaporisation of a solid target in the presence of argon gas undergoing supersonic expansion into a vacuum chamber. The solid target was composed of urocanic acid, copper powder and a small amount of polyvinyl acetate glue used as binder. Rotational constants,  $B_0$ , centrifugal distortion constants,  $D_J, D_{JK}$  and the nuclear quadrupole coupling constants of the nitrogen atoms,  $\chi_{aa}(\text{N})$  and  $\chi_{bb-cc}(\text{N})$ , have been determined through analysis of the assigned broadband rotational spectra. The geometry of each conformer was identified by comparison of the experimental results with geometries calculated *ab initio*. Isotopic substitutions at carbon and hydrogen atoms allow further insight into the molecular geometries of the two lowest energy conformers. The geometry of a complex formed between urocanic acid and water will also be described.