BARRIERS TO INTERNAL ROTATION AND MOLECULAR GEOMETRIES OF COMPLEXES FORMED BETWEEN ISOMERS OF METHYLTHIAZOLE AND WATER STUDIED BY MICROWAVE SPECTROSCOPY

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The (V_3) barriers to internal rotation of many five-membered heteroaromatic rings have been investigated using microwave spectroscopy. The rotational spectra of 2-methylthiazole···H_2O, 4-methylthiazole···H_2O and 5-methylthiazole···H_2O were recorded over the frequency range 7.0-18.5 GHz using Chirped Pulse Fourier Transform Microwave (CP-FTMW) spectroscopy. The complexes were generated in a supersonic expansion containing low concentrations of a methylthiazole isomer and water in an argon buffer gas. In total spectra of five isotopologues of each complex have been assigned and analysed. The fitting of observed *A*-species transition frequencies to Watson's S-reduced Hamiltonian within PGOPHER gave "effective" fits of each complex. Global fits (simultaneous fitting of both *A*- and *E*- species transitions) have been performed using XIAM allowing the determination of rotational constants (A_0, B_0, C_0), centrifugal distortion constants (D_J, D_{JK}, d_1, d_2) and nuclear quadrupole coupling constants (χ_{aa}(N) and χ_{bb}(N) - χ_{cc}(N)) as well as the V_3 barrier to internal rotation. The monohydrate complexes are formed by a non-linear hydrogen bond between H_2O acting as the hydrogen bond donor and the nitrogen atom of the methylthiazole ring which is the hydrogen bond acceptor. The influence formation of the monohydrate complex on the V_3 barrier will be discussed.