CHARACTERISATION OF THE STRUCTURE OF THE HYDROGEN-BONDED COMPLEX, THIAZOLE...$(H_2O)_2$, BY FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY

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The microsolvation of aromatic and heteroaromatic rings has been the subject of many microwave spectroscopy studies in recent years. In 2020, Li et al. reported the geometry of the monohydrate complex of thiazole.[a] Since thiazole contains multiple sites at which intermolecular bonds can form, a complex of thiazole with two water molecules was subsequently searched for. The rotational spectrum of thiazole...$(H_2O)_2$ was recorded over the frequency range 6.5-18.5 GHz while analysing a gaseous sample containing thiazole, water and argon by Chirped-Pulse, Fourier-Transform Microwave (CP-FTMW) spectroscopy at Newcastle University and by COBRA (coaxially oriented beam-resonator arrangement)-FTMW spectroscopy at Chongqing University. Aided by density functional theory (DFT) calculations, the spectrum of thiazole...$(H_2O)_2$ was assigned and rotational constants (A_0, B_0 and C_0), centrifugal distortion constants (D_J, D_{JK}, d_1 and d_2) and nuclear quadrupole coupling constants (χ_{aa} and χ_{bb-cc}) of nitrogen atoms were determined. The microwave spectra of four isotopologues of thiazole...$(H_2O)_2$ have been assigned allowing the determination of structural parameters which include intermolecular bond lengths and angles.

[a] W. Li, J. Chen, Y. Xu, T. Lu, Q. Gou and G. Feng, *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, 2020, **242**, 118720