

MILLIMETER/SUBMILLIMETER SPECTRUM AND PRECISE EQUILIBRIUM STRUCTURE OF 1H-1,2,4-TRIAZOLE

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1H-1,2,4-Triazole is a five membered aromatic heterocycle with 3 inequivalent nitrogen atoms. This molecule exists as an equilibrium of two tautomers; 1H-1,2,4-Triazole (C_s) and 4H-1,2,4-triazole (C_{2v}), with the 1H tautomer being dominant. 1,2,4-Triazole is predicted to exist in the atmosphere of Titan, forming in aerosols containing known constituents HNC and NH_3 , where identification relies on accurate spectral information. The rotational spectrum of 1H-1,2,4-triazole was reported by Bolton et al.^a, but only the ground state rotational constants were determined. Here we present the 70-700 GHz spectrum of 1H-1,2,4-triazole with spectral frequencies comparable to telescopes such as ALMA. Analysis of this spectrum resulted in improved rotational constants and an accurate determination of the sextic and quartic centrifugal constants. We also obtained tentative least-squares fits of transitions for all vibrationally excited states below 1200 cm^{-1} , where the majority appear to be perturbed by Coriolis interactions. A partial structure determination of 1H-1,2,4-triazole, derived from three isotopologues, has been reported previously. Recent work on other heteroatomic compounds has achieved impressive accuracy and precision in the determination of semi-experimental (r_e^{SE}) equilibrium structures. Using deuterium-enriched triazole samples, we have determined rotational constants for 27 isotopologues of 1H-1,2,4-triazole including multiple isotopic substitutions of all atoms. As a result, we have obtained a complete r_e^{SE} structure that is in full agreement with an r_e structure determined with high-level quantum chemistry. Here we will report on the spectroscopic and structural analysis of 1H-1,2,4-triazole.

^aBolton, K.; Brown, R. D.; Burden, F. R.; Mishra, A. The microwave spectrum and structure of 1,2,4 triazole. *J. Mol. Struct.* 1975, 27 (2), 261–266