SPECTRAL ANALYSIS OF IMIDAZOLE EXTENDED INTO THE MILLIMETER-WAVE REGION.

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Heterocyclic organic compounds are assumed to play a pivotal role in Earth's prebiotic chemistry. Imidazole is a five-membered aromatic ring containing two nitrogen nuclei. It is a vital part of various fundamental biological molecules, such as the amino acid histidine and purine nucleobases. While imidazole has been previously studied in the lower frequency regime ($<$ 40 GHz) [1], the study has been extended over a larger frequency range to improve centrifugal distortion constants for astronomical searches. Recently, we have extended the frequency range up to 295 GHz. The broadband rotational spectrum of imidazole was recorded in selected frequency regions (2-8, 13-15.5, 18-26, 75-110, and 260-295 GHz) and the rotational transitions for the parent molecule in the vibrationally ground state were assigned [2]. The present work focusses on the assignment of the rotational transitions for the singly substituted 13C - 15N isotopologues in their vibrationally ground states and the parent molecule in its vibrational excited states. The transitions for all of the species in the lower frequency region showed resolvable hyperfine splitting (HFS), because of the two 14N nuclei ($I = 1$). But in the higher frequency regime (75-295 GHz), the lines did not show detectable HFS and hence were assigned without taking HFS into account. This provided us with a new set of spectroscopic constants derived from the global fit, allowing for a more accurate determination of quartic and sextic centrifugal distortion constants. The isotopic data allowed for the deduction of the exact coordinates of the atoms and the precise structural determination of imidazole in the gas phase. The extended sets of rotational parameters obtained are essential for making accurate predictions for astronomers to use for observational searches in the interstellar medium in the millimeter-wave region.

References: [1] D. Christen et al. Z. Naturforsch., 37, 1378 (1982) [2] B. M. Giuliano et al. A&A 628, A53 (2019)