EXTENDED LABORATORY INVESTIGATION OF THE PURE ROTATIONAL SPECTRUM OF THE CH_2CN RADICAL IN THE (SUB-)MILLIMETER REGION (79-860 GHz)

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The cyanomethyl radical, CH_2CN, is considered a key reactive intermediate in the interstellar medium (ISM) since its first detection [1]. To date, the radical has been detected in several environments of the ISM using pure rotational data available in the literature, limited to frequencies below 280 GHz [2,3]. The radical is also postulated to participate to the formation of complex organic molecules, such as cyanoacetaldehyde [4]. To enable the detection of the CH_2CN radical in current high frequency astronomical surveys, laboratory re-investigation of its spectrum at submillimeter wavelengths appears essential. We have investigated the pure rotational spectrum of CH_2CN at room temperature in the 75-900 GHz domain. The radical was produced using a H-abstraction method from CH_3CN using F atoms. To record pure rotational transitions, we used two spectrometers: a commercial broadband chirped-pulse (CP) spectrometer covering the 75-110 GHz spectral region and a tunable single-frequency absorption spectrometer exploiting a frequency multiplication chain with a large spectral coverage (here, 140-900 GHz). A combined fit of the literature data and our newly measured transitions (involving N" and K_a" up to 42 and 8, respectively) yields to an improvement of the rotational parameters; in particular the A rotational constant and K-dependent parameters. This work allows for confident searches of the radical in cold to warm environments of the ISM, over a wide frequency range. In addition, the broadband capacities of the CP spectrometer has also revealed very efficient in the study of discharge products (synthesized by the reaction between CH_3CN and F atoms in this work). I will present both aspects of this work: the improvement of the spectroscopy of CH_2CN and the analysis of the chemical composition of the discharge by CP spectroscopy.

[1] W. M. Irvine et al., The Astrophysical Journal Letters (1988) 334, L107 [2] S. Saito et al., The Journal of Chemical Physics (1997) 107, 1732 [3] H. Ozeki et al., American Astronomical Society (2004) 617, 680 [4] B. Ballotta et al., ACS Earth and Space Chemistry (2021) 5, 1071