Millimetre-wave spectroscopy of N-cyano metilamine

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N-cyano metilamine (CH_3NHCN) is a structural isomer of amino acetonitrile (NH_2CH_2CN), an important astrophysical molecule thought to be chemically related to (possibly a direct precursor of) the simples amino acid, glycine. Amino acetonitrile has been detected towards the galactic centre in Sgr B2(N). Its fractional abundance was estimated to be 2×10^{-9}, with an excitation temperature, T_{exc} ~100 K. Observational evidences point to a chemical pathway based on grain-surface chemistry, and the detection of its isomer with the –CN moiety on the amine group would provide useful hints to constrain the formation pathway of more complex nitrogen bearing species.

The rotational spectrum of CH_3NHCN is rather complex due to the presence of two quadrupolar ^{14}N nuclei, and two large amplitude motions: the methyl internal rotation and the amine –H inversion through the *ab* principal axis plane. While the hyperfine structure is not resolvable in the millimetre regime, the internal dynamics of the molecule produces a significant complexity. Tunnelling between both torsional and inversion potential minima splits each J_{KaKc} rotational levels into fours substates labelled A^+, E^+, A^-, and E^-. The magnitude of the two effects is similar, thus no simple factorisation of the Hamiltonian into two “simple” internal rotation subproblems (one each inversion species) holds strictly.

N-cyano metilamine is unstable in ordinary laboratory conditions thus the isolation of a pure sample prepared by ordinary organic chemistry is not feasible. In our study, we adopted a pyrolysis methods which starts from stable precursors (e.g., dimethyl cyanamide, $(CH_3)_2NCN$). A steady, slow flow of fresh pyrolysis product was then kept into the absorption cell while the spectrum is recorded; this provided the strongest absorption signals, even if the spectral contamination from side products turned out to be a serious issue.

We carried out a preliminary study of the rotational spectrum of CH_3NHCN in selected frequency regions spanning the 80-350 GHz interval. To date, lines belonging to all four substates were identified and analysed through an “effective-fit” or “band-by-band” approach, i.e., employing a different Watson-type Hamiltonian for each rotation-inversion state. This method turned out to moderately successful for the ‘+’ states, but to a much lesser extent for the ‘–’ states.