LABORATORY AND TENTATIVE ASTRONOMICAL DETECTION OF THIOCYANIC ACID, HSCN

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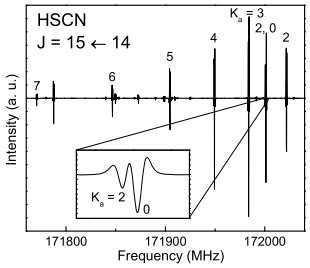

We present the first measurements of the rotational spectrum of thiocyanic acid (HSCN) in the microwave and mm-wave regions. HSCN is an isomer of the spectroscopically and astronomically well-studied molecule isothiocyanic acid (HNCS). HSCN has been calculated to lie only 4-14 kcal/mol higher in energy than the most stable isomer HNCS, yet to date HSCN had only been characterised experimentally by matrix-IR spectroscopy. We now succeeded to produce HSCN in a discharge of H_2S and either $(CN)_2$ or CH_3CN in sufficient amounts for its spectroscopic investigation in the gas phase. Three *a*-type rotational transitions in the $K_a = 0$ ladder and four in the $K_a = 1$ ladder were measured in the frequency range $10 - 35$ GHz with our Fourier Transform Microwave Spectrometer (FTM) in a molecular beam. The identification was confirmed by the observation of 6 singly and doubly substituted isotopic species at predicted isotopic shifts. Furthermore, we were able to resolve and analyse the distinctive hyperfine structure due to ^{14}N and D in all species containing these nuclei, providing additional evidence for the identification. An experimental structure derived from the isotopic measurements will be presented. For the main isotopic species additional $\Delta K_a = 0$ transitions were observed in selected frequency regions up to 350 GHz with a free-space millimeter-wave absorption spectrometer. Lines of HSCN were surprisingly strong through a dc discharge of H_2S and $(CN)_2$, allowing to observe spectra up to $J = 30$ and $K_a = 7$, as shown in the figure.

We also report a tentative detection of HSCN towards SgrB2(M) via four $K_a = 0$ a-type transitions observed in the 3-mm band with the IRAM 30m telescope. The observations yield an abundance of HSCN only a factor 2-5 lower than that of the lowest energy isomer HNCS.