THE MILLIMETERWAVE SPECTRUM OF \textit{n}-BUTYL CYANIDE

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The rotational spectrum of \textit{n}-butyl cyanide (C$_4$H$_9$CN) was measured between 75 and 130 GHz using a novel all-solid-state spectrometer with a total absorption path of 44 m. In the course of the analysis of the spectrum, about 3000 transitions were assigned and a full set of quartic centrifugal distortion parameters with some sextic and octic terms could be determined for each of the three known conformers (anti-anti, anti-gauche(methyl end) and gauche(CN end)-anti).

The work was motivated by the fact that \textit{n}-butyl cyanide is likely to be found in interstellar hot core environments. This is indicated by the discovery of \textit{n}-propyl cyanide (C$_3$H$_7$CN), the next smaller alkyl cyanide, in the ISM\textsuperscript{a}. The increased accuracy of the model, which will be additionally extended by future laboratory measurements around 200 GHz, may now be employed for a prediction of the spectrum up to 300 GHz with a feasible uncertainty for astronomical line surveys. Furthermore, there are two less abundant conformers, \textit{cis}-gauche-gauche and \textit{trans}-gauche-gauche, which have not yet been detected in the rotational spectrum\textsuperscript{b}. Due to the increased sensitivity of the new spectrometer, it seems possible now for the first time to identify their spectroscopic fingerprints in the recorded data.