THE MILLIMETERWAVE SPECTRUM OF n-BUTYL CYANIDE

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The rotational spectrum of n-butyl cyanide (C_4H_9CN) 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 n-butyl cyanide is likely to be found in interstellar hot core environments. This is indicated by the discovery of n-propyl cyanide (C_3H_7CN), the next smaller alkyl cyanide, in the ISM[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 astronomic line surveys.

Furthermore, there are two less abundant conformers, *cis*-gauche-gauche and *trans*-gauche-gauche, which have not yet been detected in the rotational spectrum[b]. Due to the increased sensitivity of the new spectrometer, it seems possible now for the first time to identify their sectroscopic fingerprints in the recorded data.

[a] A. Belloche, R. T. Garrod, H. S. P.Müller, K. M. Menten, C. Comito, and P. Schilke, Astronomy & Astrophysics **499**, 215 (2009)

[b] R. K. Bohn, J. L. Pardus, J. August, T. Brupbacher, W. Jäger, J. Mol. Struct. **413–414**, 293 (1997)