ROTATIONAL SPECTROSCOPY OF THE LOW ENERGY CONFORMER OF 2-METHYLBUTYRONITRILE AND SEARCH FOR IT TOWARD SAGITTARIUS B2(N2)

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Quite recently, some of us detected *iso*-propyl cyanide as the first branched alkyl molecule in space.[a] The identification was made in an ALMA Cycle 0 and 1 molecular line survey of Sagittarius B2(N) at 3 mm. The branched isomer was only slightly less abundant than its straight-chain isomer with a ratio of about 2 : 5. While initial chemical models favored the branched isomer somewhat, more recent models[b] are able to reproduce the observed ratio. Moreover, the models predicted that among the next longer butyl cyanides (BuCNs) 2-methylbutyronitrile (2-MBN) should be more abundant than both n-BuCN and 3-MBN by factors of around 2, with t-BuCN being almost negligible.

With the rotational spectra of t- and n-BuCN studied,[c] we investigated those of 2-MBN and 3-MBN betwen $\sim$40 and $\sim$400 GHz by conventional absorption spectroscopy and by chirped-pulse and resonator Fourier transform microwave (FTMW) spectroscopy. The analyses were guided by quantum-chemical calculations.

Here we report the analysis of the low-energy conformer of 2-MBN and a search for it in our current ALMA data. Two additional conformers are higher by $\sim$250 and $\sim$280 cm^{-1}. The low-energy conformer displays a very rich rotational spectrum because of its great asymmetry ($\kappa \approx 0.14$) and large a- and b-dipole moment components. Accurate ^{14}N quadrupole coupling parameters were obtained from the FTMW spectral recordings.

[a] A. Belloche, R. T. Garrod, H. S. P. Müller, and K. M. Menten, *Science* **345** 1584.

[b] R. T. Garrod, A. Belloche, H. S. P. Müller, and K. M. Menten, *Astron. Astrophys.*, in press; doi: 10.1051/0004-6361/201630254.

[c] Z. Kisiel, *Chem. Phys. Lett.* **118** 134; M. H. Ordu et al., *Astron. Astrophys.* **541** A121.