Nuclear Quadrupole Coupling Constants of 4-Aminobenzonitrile measured with Broadband Rotational Spectroscopy

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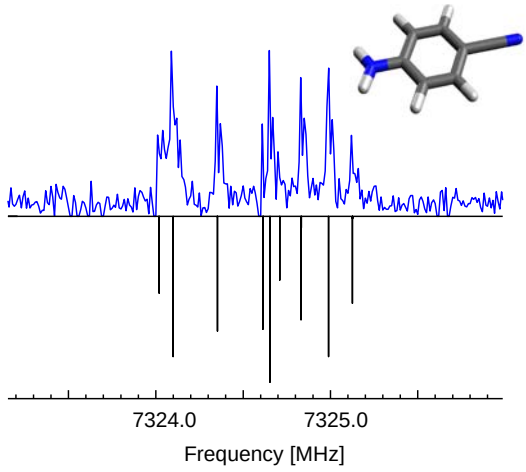
The high-resolution microwave spectrum of 4-aminobenzonitrile is presented in this contribution. The measurement was recorded using Chirped-Pulse Fourier-Transform Microwave spectroscopy (CP-FTMW) of translationally and rotationally cold molecules in a supersonic jet. With this new technique, a broad rotational spectrum can be measured in a very short time by using a microwave excitation chirp with frequencies from 2 - 8.3 GHz. The analysis of the rotational spectrum will give insights into the structure and the electronic configuration of this molecule.

The measured 4-aminobenzonitrile spectrum shows a-type transitions from J = 0 to J = 5 in our frequency range. It has a complicated, but clearly resolved, quadrupole splitting due to the coupling of the two ^{14}N nuclei. From the spectrum we are able to determine the rotational, the distortional and the ^{14}N-quadrupole coupling constants. The appearance of an additional splitting due to an inversion motion of the amino group still has to be confirmed. 4-aminobenzonitrile and other structurally related molecules like 4,4´-dimethylaminobenzonitrile were discussed in terms of twisted intramolecular charge transfer (TICT) effects in recent publications [1]. To learn more about these effects, a comparison of the nuclear quadrupole coupling constants of these molecules and the differences in their structure could be interesting.

In addition to that, a future project concerned with the recognition process between aromatic molecules and carbohydrates will be presented. This important and interesting process in nature will be investigated in model systems using CP-FTMW spectroscopy.



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[1] R. G. Bird, J. L. Neill, V. J. Alstadt, J. W. Young, B. H. Pate, D. W. Pratt, *J. Phys. Chem A.* **2011**, *115*, 9392-9398.