ASSIGNMENT OF THE MM- AND SMM-WAVE ROTATIONAL SPECTRA OF RARE ISOTOPOLOGUES OF CYANAMIDE AND THE $r_m^{(1)}$ MOLECULAR GEOMETRY OF NH_2CN

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The cyanamide molecule is one of the prototype systems for the study of the large–amplitude inversion motion at the nitrogen atom, and it is also a potential astrophysical species. The mm-wave, smm-wave, and the far infrared spectra of the parent and the two principal deuterated isotopic species are now known in considerable detail.[a,b]

Presently we report an extended analysis of rotational transitions in the 0^+ and 0^- inversion states for 7 rare isotopic species of cyanamide, measured in the 118-650 GHz frequency region on a deuterated sample with natural abundance of carbon and nitrogen. The spectra of five isotopologues: $H_2N^{13}CN$, $HDN^{13}CN$, $D_2N^{13}CN$, $HD^{15}NCN$, and $HDNC^{15}N$, have been assigned for the first time. For $D_2{}^{15}NCN$ and $D_2NC^{15}N$ the knowledge of the rotational spectrum has also been considerably improved relative to preceding work.[c,d]

The availability of spectroscopic constants for 12 different isotopic species allowed determination of the complete $r_m^{(1)}$ and $r_m^{(1L)}$ geometries[e] of cyanamide, providing direct experimental information on the pyramidal nature of the NH_2 group in cyanamide and on the nonlinearity of the NCN segment. The new experimental geometry is compared with results of $ab\,initio$ calculations.

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[a] G. Moruzzi et al., *J. Mol. Spectrosc.*, **190**, 353-364 (1998).
[b] Z. Kisiel et al., *63rd OSU International Symposium on Molecular Spectroscopy*, WK08, 2008.
[c] J. K. Tyler et al., *J. Mol. Spectrosc.*, **43**, 248-261 (1972).
[d] R. D. Brown et al., *J. Mol. Spectrosc.*, **114**, 257-273 (1985).
[e] J. K. G. Watson et al., *J. Mol. Spectrosc.*, **196**, 102-119 (1999).