DETAILED ANALYSIS OF THE $0^+ - 0^-$ INVERSION DOUBLET IN D_2NCN and HDNCN CYANAMIDE

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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 known astrophysical species. The rotational and vibration-rotation spectrum of the parent species has already been studied in considerable detail.[a,b] Information on the deuterated isotopologues has, hitherto, been limited to transitions measured at frequencies of less, or much less, than 60 GHz.

Presently we report a detailed analysis of pure rotational and vibration-rotation transitions in the $0^+ - 0^-$ inversion doublets for the two deuterated species. The analysis is based on a 118-650 GHz spectrum for D_2NCN and HDNCN recorded at rotational resolution, and an 8-360 cm^{-1} spectrum of D_2NCN recorded with the Bruker IFS 120HR interferometer at resolution of 0.0025 cm^{-1}. The two spectra were assigned and analysed with the modified version of the AABS package[c] for *Assignment and Analysis of Broadband Spectra* and the more extensive data set for D_2NCN contains well over 2000 lines with $J \leq 80$ and $K_a \leq 15$. The measured transition frequencies were fitted to within experimental accuracy with a unified scheme for fitting the inversion doublet transitions in H_2NCN, NHDCN and D_2NCN. The spectroscopic constants and information on the inversion potential determined from the spectra of the three isotopologues are compared and discussed.

[a] M. Birk et al., *J. Mol. Spectrosc.*, **159**, 69-78 (1993).
[b] G. Moruzzi et al. *J. Mol. Spectrosc.*, **190**, 353-364 (1998).
[c] Z. Kisiel et al., *J. Mol. Spectrosc.*, **246**, 39-56 (2007).