SUBMILLIMETER-WAVE ROTATIONAL SPECTRA OF DNC

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Spectroscopic investigations of DNC have been less extensive than those for HNC. See Brünken *et al*.[a] and Bechtel *et al*.[b] for relevant references. In the present investigation, rotational transitions of DNC have been observed in the submillimeter-wave region in an extended negative glow discharge in a gas mixture of CD_4 and N_2. The dissociative recombination reaction of $DCND^+$ with electrons is thought to be a dominant channel to produce DNC in highly excited vibrational states; the rotational lines in levels up to (008) are observed. The rotational and centrifugal distortion constants are determined for these states along with those for the (100) state. The measurement accuracy is high enough to determine some higher order vibration-rotation interaction constants. The least-squares fits were straightforward except for (004), (006), and (008), where very small but significant perturbations were found.

A striking isotope effect was observed on the vibrational temperature in this investigation. The vibrational temperature for the ν_3 mode for DNC is as high as 4000 K and the rotational transitions are observable in states up to (008), while the corresponding temperature is about 1500 K for HNC. The vibrational temperature for the ν_1 mode is about 1000 K for DNC and about 1300 K for HNC. The bending vibrational mode is not excited, and the vibrational temperature for the ν_2 mode is only about 400 K. The origin of this conspicuous excitation of the ν_3 mode of DNC is not obvious. However, it should be closely related to mechanism of the dissociation of HCNH and DCND. Apparently the difference in the masses of the departing H/D is a factor causing this difference, but the vibrational temperature for ν_3 of DCN is not particularly high, about 1000 K. When the D atom departs from the D-C side, apparently the C-N vibration is highly excited. On the other hand, when the D-N bond is broken, not much excitation of the C-N vibration occurs.

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[a] S. Brünken, H. S. P. Müller, S. Thorwirth, F. Lewen, and G. Winnewisser, *J. Mol. Strunct.*, **780-781**,3 (2006)

[b] H. A. Bechtel, A. H. Steeves, and R. W. Field, *Astrophys. J.*, **649**,L53 (2006)