OBSERVATION OF THE VAN DER WAALS BENDING BANDS OF THE Ar-DCN CLUSTER BY MILLIMETER-WAVE SPECTROSCOPY IN SUPERSONIC JET EXPANSION

STEPHANE BAILLEUX, K. HARADA, A. MIZOGUCHI and K. TANAKA, *Institute for Molecular Science (IMS), Okazaki, 444-8585 Japan*.

In order to understand the potential energy surface of the very floppy Ar-HCN cluster[a], it is essential to observe the van der Waals vibrational bands of the deuterated species, Ar-DCN[b]. We have applied the millimeter-wave absorption spectroscopy combined with the pulsed-jet expansion technique to the measurement of ro-vibrational transitions of the $\Sigma_1 \leftarrow \Sigma_0$ and $\Pi_1 \leftarrow \Sigma_0$ subbands of Ar-DCN between 182 and 294 GHz.

We found that diluting DCN (2%) in a mixture of Ar and Ne (up to 50%) lead to a 5 times greater signal-to-noise ratio compared to DCN diluted in pure Ar. Moreover, Ne also contributes to reducing the line width (250 kHz FWHM). In total, 53 rovibrational transitions split into hyperfine components due to the Nitrogen nucleus were observed, leading to an accurate determination of the molecular parameters. The subband origins are determined to be 189017.3969(98) and 195550.745(18), and the rotational constants are $B = 1926.8792(24)$ and $B = 1967.8744(20)$ in the Σ_1 and Π_1 bands, respectively (all constants in MHz). Other parameters also include the quadrupole coupling constants, the Coriolis coupling constants between the Σ_1 and Π_1 bending bands. The intensities of the P- and R-branch of these two bands are strongly affected by the Coriolis interaction.

[a] K. Uemura, A. Hara, and K. Tanaka, J. Chem. Phys., 104, 9747 (1996). [b] M. Shirasaka, and K. Tanaka, J. Mol. Spec., 185, 189 (1997).