

HIGH-RESOLUTION INFRARED SPECTROSCOPY OF DC₃N IN THE STRETCHING REGION

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Interstellar deuterated cyanoacetylene (DC₃N) has been identified in a vast variety of astronomical sources thanks to the emission of its rotational transitions. To date, the rotational spectrum of DC₃N has been accurately studied in laboratory, while the high-resolution infrared spectrum is limited to the low frequency range (200–1100 cm⁻¹). In order to support the identification of DC₃N in different spectral regions, we have investigated the infrared spectrum of DC₃N in the stretching region (1500–3500 cm⁻¹). The ν_1 , ν_2 , and ν_3 fundamentals as well as their hot-bands were recorded at 0.004 cm⁻¹ resolution using a Fourier transform infrared spectrometer. Additional pure rotational spectra in the $v_3 = 1$, $v_2 = 1$, and $v_3 = v_7 = 1$ vibrational excited states were observed between 243 and 295 GHz with a frequency-modulation millimeter/submillimeter-wave spectrometer equipped with an electric furnace. The precision of the pure rotational lines, intrinsically much higher than ro-vibrational data, allowed us to improve the accuracy of the upper state spectroscopic parameters. The rotational and ro-vibrational data of DC₃N were combined into a single fit from which a consistent set of spectroscopic constants has been determined. In addition, the ro-vibrational features of its parent species (HC₃N) have been analyzed as well because HC₃N is observed as a by-product in the same spectra. The result of the combined analysis provides a highly-precise rest-frequency catalog that can be used to model the infrared spectra of DC₃N and HC₃N.

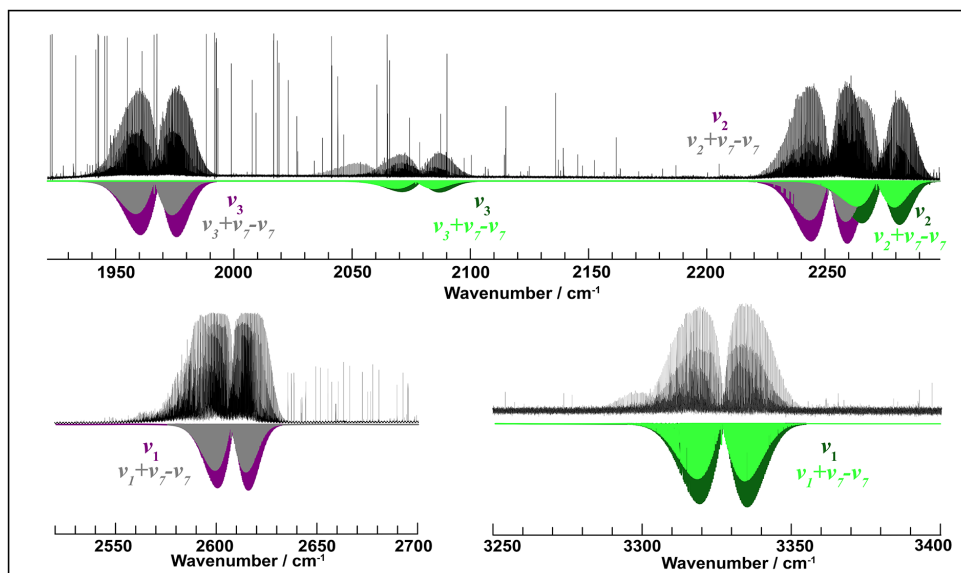


Figure 1: Portions of the recorded MIR spectra (black traces): 1930-2300 cm⁻¹, 2500-2700 cm⁻¹ and 3250-3400 cm⁻¹. Spectral simulations based on the spectroscopic constants for both DC₃N (violet traces) and HC₃N (green traces)