HIGH ROVIBRATIONAL STATES OF HC_3N: ANALYSIS OF THE RESONANCE NETWORK INVOLVING THE STRONG $2\nu_5$ OVERTONE BAND

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Cyanoacetylene (HC_3N) is a major astrophysical tracer which manifests its presence in Space via strong rotational and infrared emissions. One of the most conspicuous features of its infrared (IR) spectrum is the $2\nu_5$ overtone bands located at $\sim$1300 cm^{-1} (7.7 μm), and falling near the edge of mid infrared atmospheric window. Despite extensive past investigation of the HC_3N rovibrational spectrum [1, 2], this band still lacks an accurate analysis which takes into account the complex resonance network involving the $v_5 = 2$, bending state. Here, we report on a comprehensive study of the third polyad of interacting lelvels which includes the states: $(v_4 = 1, v_7 = 2)$, $v_6 = v_7 = 2$, $(v_5 = 1, v_7 = 3)$, $v_7 = 6$, and $v_5 = 2$, located around 1300 cm^{-1}. The analysis is performed on an extensive dataset collected at SOLEIL (FAR/mid-IR) and at the University of Bologna (mid-IR and rotational data). Our objective is to retrieve a set of spectroscopic constants which have both clear physical meaning and excellent spectral predictive capability. To this aim, we adopt the ro-vibrational Hamiltonian already used for the analysis of the first and second resonance systems of HC_3N (e.g. [2]). It includes explicitly vibrational and ro-vibrational l-type resonance effects in bending overtones/combinations as well as the numerous anharmonic resonances occurring between accidentally nearly-degenerate states. The results will serve to improve the data already included in the 2020 release of the HITRAN database.

References

[1] L. Bizzocchi, F. Tamassia, M. Melosso, *et al.*, *Astrophys. J. Suppl. S.* **233**, *11* (2017).

[2] F. Tamassia, L. Bizzocchi M. Melosso, *et al.*, J. Quant. Spectrosc. Rad. Trans. **279,** *108044* (2021).