LOWEST VIBRATIONAL STATES OF ACRYLONITRILE

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Recent studies of the broadband rotational spectrum of acrylonitrile, $H_2C{=}CHC{\equiv}N$, revealed the presence of multiple resonances between rotational levels in different vibrational states. The resonances affect even the ground state transitions and their analysis allowed determination of vibrational term values for the first three excited states above the ground state[a] and of vibrational energy differences in several polyads above these states.[b] At that time there was no infrared data of sufficient resolution to assess the reliability of the resonance based vibrational energy determinations.

We presently report results based on a 40-700 cm^{-1} high-resolution spectrum of acrylonitrile recorded at the AILES beamline of the SOLEIL synchrotron. This spectrum was reduced by using the AABS package[a,c] and allowed assignment of vibration-rotation transitions in four fundamentals, five hot bands, and one overtone band. The infrared data and previous measurements made with microwave techniques have been combined into a single global fit encompassing over 31000 measured transitions. Precise vibrational term values have been determined for the eight lowest excited vibrational states. The new results validate the previous estimates from rotational perturbations and are also compared with results of *ab initio* anharmonic force field calculations.

[a] Z. Kisiel, et al., *J. Mol. Spectrosc.* **280** 134 (2012).
[b] A. López, et al., *Astron. & Astrophys.* **572**, A44 (2014).
[c] Z. Kisiel, et al., *J. Mol. Spectrosc.* **233** 231 (2005).