VIBRATIONAL ENERGIES FOR ACRYLONITRILE FROM MM-WAVE TO THZ ROTATIONAL SPECTRA

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The THz rotational spectrum of acrylonitrile has recently been studied in detail.[a] The coverage of the ground state rotational transitions has been extended up to $J = 128$, $K_a = 29$ and it was found that at very high-J there are multiple manifestations of a perturbation between the ground state and the lowest vibrationally excited state, $v_{11} = 1$. The perturbation has been successfully fitted and the excited state energy determined at 228.29991(2) cm^{-1}, which turns out to be the largest energy difference between any two neighboring vibrational states of acrylonitrile.

Extensive broadband rotational spectra of acrylonitrile have been recorded at JPL and at OSU and provide coverage from the mm-wave region up to well into the THz. The analysis of these spectra performed with the AABS package[b] allowed identification of a ladder of pairwise perturbations extending from the ground state and connecting all successive low lying vibrational states. A global fit of all of the observed effects is expected to deliver accurate energies for the lowest vibrational states from only the rotational spectrum. The progress made towards achieving this goal is described.

[a] Z.Kisiel, L.Pszczółkowski, B.J.Drouin, C.S.Brauer, S.Yu, J.C.Pearson, *J. Mol. Spectrosc.*, **258**, 26 (2009).
[b] Z.Kisiel, L.Pszczółkowski, I.R.Medvedev, M.Winewisser, F.C.De Lucia, E.Herbst, *J. Mol. Spectrosc.*, **233**, 231 (2005).