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

ZBIGNIEW KISIEL, LECH PSZCZÓŁKOWSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BRIAN J. DROUIN, CAROLYN S. BRAUER, SHANSHAN YU, JOHN C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA; IVAN R. MEDVEDEV, Department of Physics, Wright State University, Dayton, OH 45435, USA; SARAH FORTMAN, CHRISTOPHER NEESE, Department of Physics, The Ohio State University, Columbus, OH 43210, USA.

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.

^aZ.Kisiel, L.Pszczółkowski, B.J.Drouin, C.S.Brauer, S.Yu, J.C.Pearson, J. Mol. Spectrosc., 258, 26 (2009).

^bZ.Kisiel, L.Pszczółkowski, I.R.Medvedev, M.Winewisser, F.C.De Lucia, E.Herbst, J. Mol. Spectrosc., 233, 231 (2005).