PERTURBATIONS AND VIBRATIONAL ENERGIES IN ACRYLONITRILE FROM GLOBAL ANALYSIS OF ITS MM-WAVE TO THZ ROTATIONAL SPECTRUM

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The rotational spectrum of acrylonitrile has recently been studied in some detail up to THz frequencies.[a,b] The perturbation between the ground state and $v_{11} = 1$ that was initially identified in the parent[a] has also been observed in other isotopologues.[b] The considerable energy difference between these states (228.29991(2) cm^{-1} in the parent) was, in all cases, determined entirely from perturbations in rotational transitions.

Many other perturbations in rotational transitions have been identified, allowing the $v_{15} = 1$ level to be added to the analysis.[c] We have now extended the broadband coverage of the rotational spectrum even further, and have been able to add the fourth vibrational state, v_{11}=2, to the global analysis. The current coupled fit encompasses well over 12000 transition frequencies and delivers precise vibrational energy information entirely on the basis of many fitted perturbations in rotational transitions. The present work was used to further refine the features for identifying perturbations built into the AABS package for Assignment and Analysis of Broadband Spectra.[d]

[a] Z.Kisiel, L.Pszczółkowski, B.J.Drouin, C.S.Brauer, S.Yu, J.C.Pearson, *J. Mol. Spectrosc.*, **258**, 26 (2009).
[b] A. Krasnicki, Z.Kisiel, B.J.Drouin, J.C.Pearson, *J. Mol. Struct.*, **1006**, 20 (2011).
[c] Z.Kisiel *et al.*, MH09, 66th OSU International Symposium on Molecular Spectroscopy (2011)
[d] Z.Kisiel, L.Pszczółkowski, I.R.Medvedev, M.Winewisser, F.C.De Lucia, E.Herbst, *J. Mol. Spectrosc.*, **233**, 231 (2005).