ANALYSIS OF INTERACTIONS BETWEEN EXCITED VIBRATIONAL STATES IN THE $FASSST$ ROTATIONAL SPECTRUM OF $S(CN)_2$

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We present a final report on comprehensive analysis of the almost continuous 110-375 GHz FASSST rotational spectrum of the $S(CN)_2$ molecule. The previous preliminary results[a] have been considerably extended, and precise spectroscopic constants have been determined for the ground states of the parent, the ^{34}S, and the ^{13}C isotopomers. Transitions in twelve vibrationally excited states of the parent have also been assigned and analysed, including first excited states of the ν_4, ν_7, ν_8, ν_9, and ν_3 normal modes.

A triad of closely spaced vibrational levels was identified near 370 cm^{-1}, and a quartad near 500 cm^{-1}. Many different anharmonic resonances between the constituent levels were observed in the rotational spectrum. Most of those could be successfully accounted for with multistate fits, allowing determination of deperturbed spectroscopic constants and several accurate vibrational energy differences. The interesting issue of the reliability of effective single state fits for vibrational states subject to anharmonic resonances will be discussed. Analysis of this spectrum stimulated the creation of the AABS package for $Analysis\ and\ Assignment\ of\ Broadband\ Spectra$[b,c] and more advanced stages of the analysis led to further developments in the package, which will be described.

[a] Z.Kisiel, O.Dorosh, I.R.Medvedev, N.Behnke, F.C.De Lucia, E.Herbst, M.Winnewisser, FC05, 60th Ohio Symposium (2005)
[b] Z.Kisiel, L.Pszczółkowski, I.R.Medvedev, M.Winnewisser, F.C.De Lucia, E.Herbst, *J. Mol. Spectrosc.* **233**, 231 (2005)
[c] Z.Kisiel, PROSPE – Programs for Rotational Spectroscopy, `http://www.ifpan.edu.pl/~kisiel/prospe.htm`